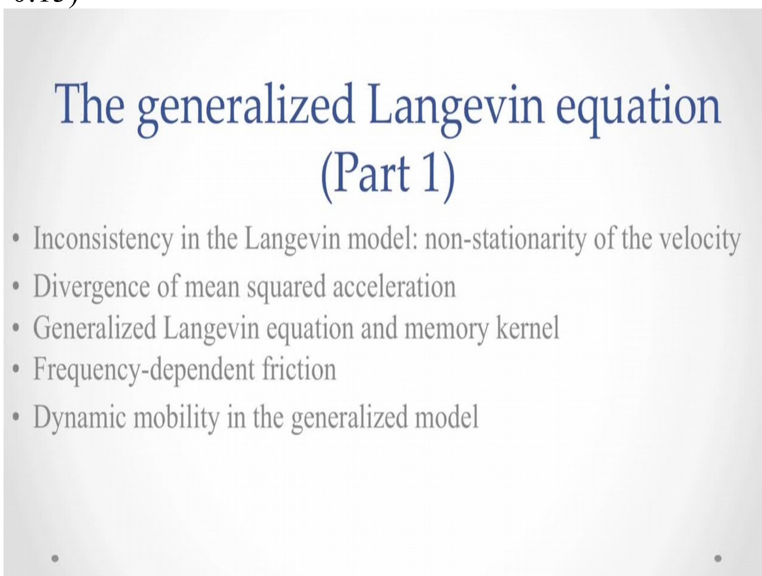
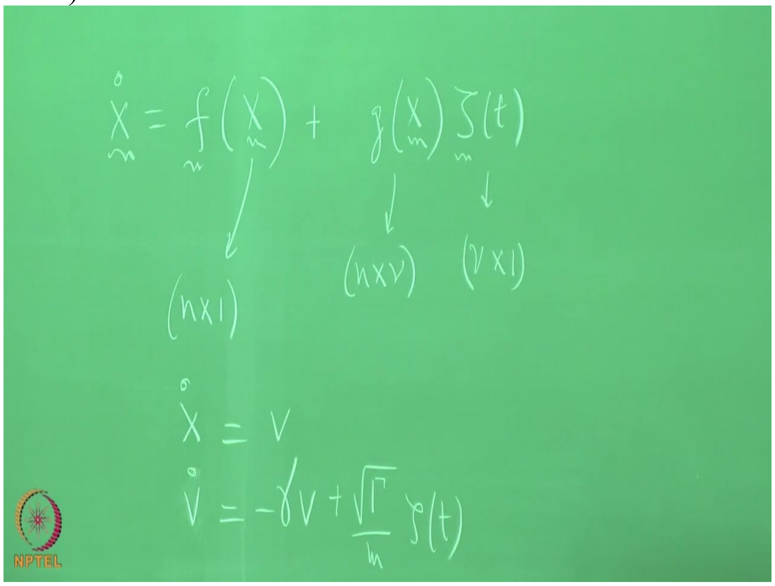
Non-equilibrium Statistical Mechanics
Professor V. Balakrishnan
Department of Physics
Indian Institute of Technology Madras
Module No 01
Lecture 20: The generalized Langevin equation (Part 1)

(Refer Slide Time: 0:15)



So let us take a look at another aspect of the langevin model. We have seen that there is a connection between the general diffusion type of stochastic equation for a diffusion process and the Fokker Planck equation, corresponding Fokker Planck equation. Before I go on, let us take care of one of the questions that was raised. The question is as follows.

(Refer Slide Time: 0:43)



In a multidimensional proffers, if you have an equation of the form, X dot equal to some vector valued function of all the Xs + a multiplicative noise, so this was G of X times zeta of T where this is set of noises independent noises, and the dimensionality of this was nyu. So remember that this was nyu times 1 column vector where as this was an N times nyu matrix rectangular matrix and the idea was that if X is this quantity, is an N dimensional noise represented by an N dimensional column vector, then the question being asked is these components are independent of each other, they are different noise components, want a nyu but because of the presence of this, does it not mix up the various noise components?

Yes. In general, that is the most general possibility because even in the most trivial of instances when nyu was 1 and N was equal to 2, remember you had an equation of the form X dot equal to V and V dot equal to - gamma V, the drift term on this side + a noise which was square root of gamma over M times the white noise, Gaussian white noise. Now the question is, is it not true that this noise affects the X itself? Sure it does. So there is already a coupling. It is a coupled set of equations in any case.

So what this is saying is that the most general possibility is that the strength of each of these noises is dependent on the current values of all the random variables which are anyway coupled to each other dynamically. So there is nothing inconsistent about it. It is perfectly reasonable. What is true is that these noise components are specified independently. So the statistics of this noise is taken to be quite independent of what is happening to the output variables, the driven variable X. You have to prescribe for me all the statistical properties of this multidimensional noise before I can tell you what the dynamics of the driven variables is. That is certainly true.

And the whole assumption in this kind of modelling is that the driven variables do not affect that noise. So there is no feedback onto the noise from the driven variables. We take this in the simplest langevin cases. We took the noise to come from the heat bath and I said that the effect of the motion of a single Brownian particle on the heat bath is negligible. It does not throw it out of equilibrium or anything like that. So it is in that philosophy.

This is a very general philosophy that you prescribed for me an external noise of some kind, statistics of this noise is prescribed independent of what is happening and then the statistics of the driven variable X is dependent on solving these set of equations, couple of equations. So that is the philosophy behind this stochastic differential equation approach with a driving noise. Okay. The different components of this are uncorrelated with each other in the simplest case, we take them to be Cartesian components for instance.

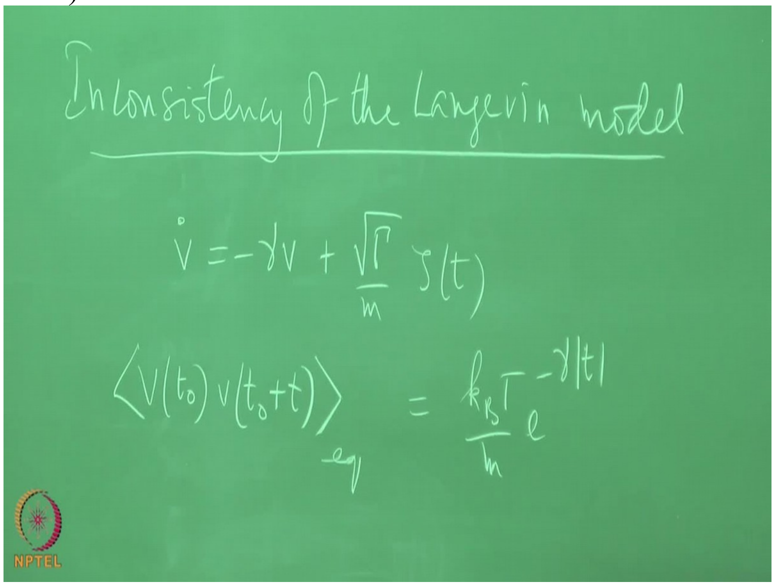
They are uncorrelated with each other. But there is no reason why the coupling should not be such that the instantaneous strength of this noise as it acts on anyone of the variables depends on all the other variables and that is where this G comes in. So is this clear?

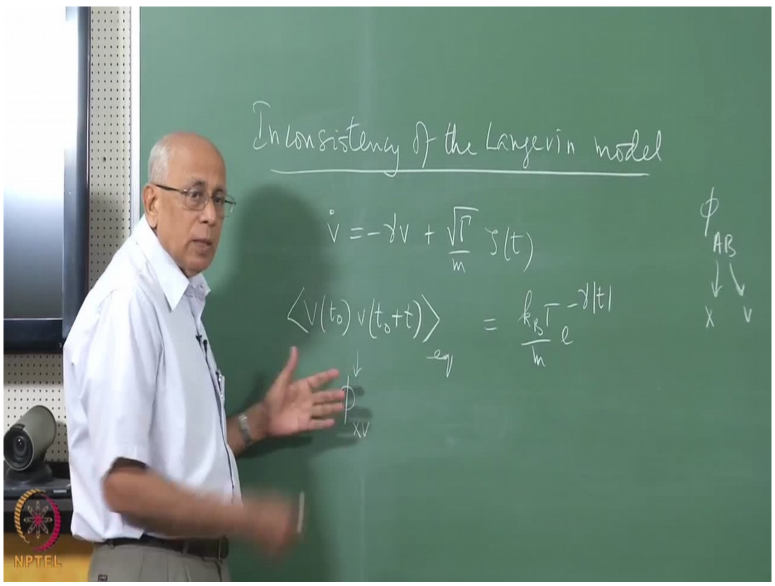
Student: Yes sir.

Professor: okay.

Now let us go back and let me point out what is wrong with the langevin model. We will see where some serious problems come. And we will do in the simplest context which is that of a tag particle, a Brownian particle moving in a fluid and again the essential physics is already contained in one dimensional, in the one dimensional case. So let us go back to that.

(Refer Slide Time: 5:12)





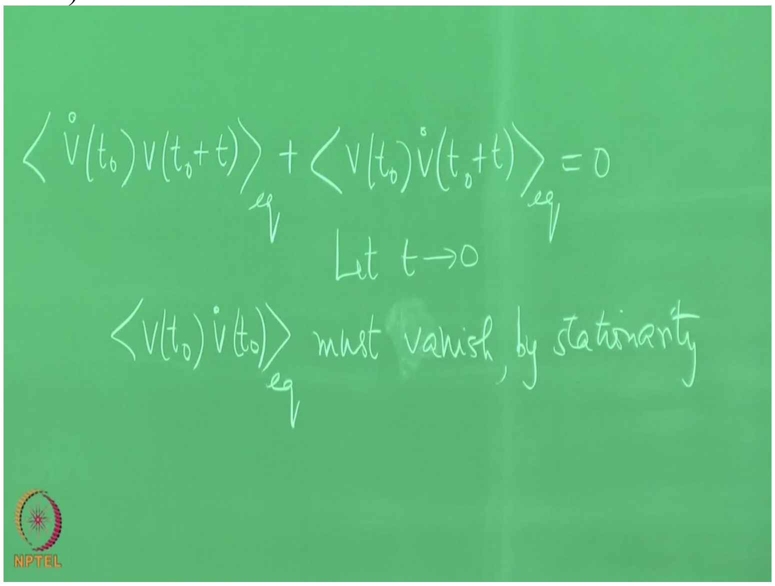
Let me call this inconsistencies of langevin. So 1st I will point out the inconsistency and later on we will fix it on physical grounds. We will so to speak derive or deduce an improved langevin model which will take care of this immediate problem of what main problems are, flaws are in this model. So recall once again that for the velocity process, velocity of a Brownian particle, we had an equation of the form V dot is equal to - gamma V + square root of gamma over M zeta of T where this was Gaussian white noise. 0, mean and a Delta correlation.

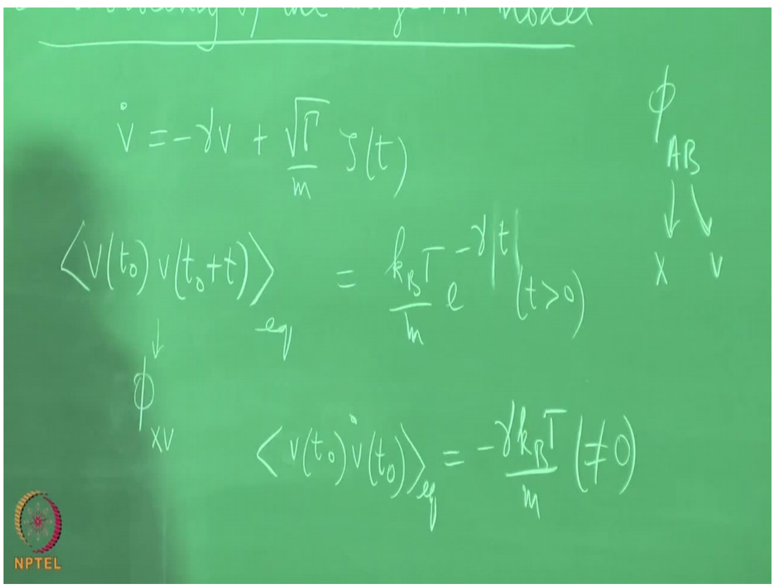
And this was taken to be Gaussian, stationary, Markov and Delta correlated and what was the output process? It was the Ornstein–Uhlenbeck process. It was also Markov, it was also Gaussian, it was also stationary but did not have a Delta correlation. But we certainly prove that it was stationary. In particular, we prove this relation. We prove the fact that V of T not + T in equilibrium, this quantity, we calculated what it was from this using the consistency condition that asymptotically, this correlation will factor the product of averages and that the main square value remain in thermal equilibrium at the Maximillian value.

So this was found to be independent of T not and was KT over M E to the - gamma modulus T. It is a stationary correlation. Now if you go back to the general linear response theory that we whose formalism we worked out this is actually a response function and in the language of the response function, what we have is phi AB in this problem, A was equal to X and B was equal to V because we perturbed this system by applying a mechanical force, - X times is F of X F of T and then we measured the velocity, the average velocity.

So the observed variable is the velocity and the variable which is cause a coupling to the force is X, dynamical variable. And this came about as a response function. So in a sense, this quantity is in fact phi XV. Recall that in classical apart from some factor of KT or something like that, recall that in classical physics, in the classical case, we showed that this response function is beta times the equilibrium average value of A dot at 0 with B at time T and A dot at 0 is V of T not. So this was what we derived here and this is independent of T not by stationarity but look at its consequence. If you took that seriously, if you took this seriously, it immediately follows that if I differentiate this function, this quantity with respect to T not, the answer should be 0 because it is dependent of T not right. But what happens if you differentiate it?

(Refer Slide Time: 9:00)





You end up with V dot of T not V of T not + T average + V of T not V dot of T not + T equilibrium should be equal to 0 because there is no T not dependence on the right-hand side by stationarity. Now set T equal to 0 from above or T equal to going to 0, approaching 0 from above right? Then it immediately says that at any instant of time, V of T not V dot of T not equilibrium must be 0, must vanish by stationarity. So what we have to do is to let T tends to 0. Let T tend to 0 and immediately you get this.

And they are classical variables. So it does not matter in which order they appear. What it says is that the velocity at any instant of time is not correlated with with the acceleration at the same instant of time. That is consistent certainly with our assumption that the force drives the acceleration and not the velocity. So it is sort of reasonable that the velocity is not correlated with the acceleration at the same instant of time okay. And in any case, it is demanded by stationarity.

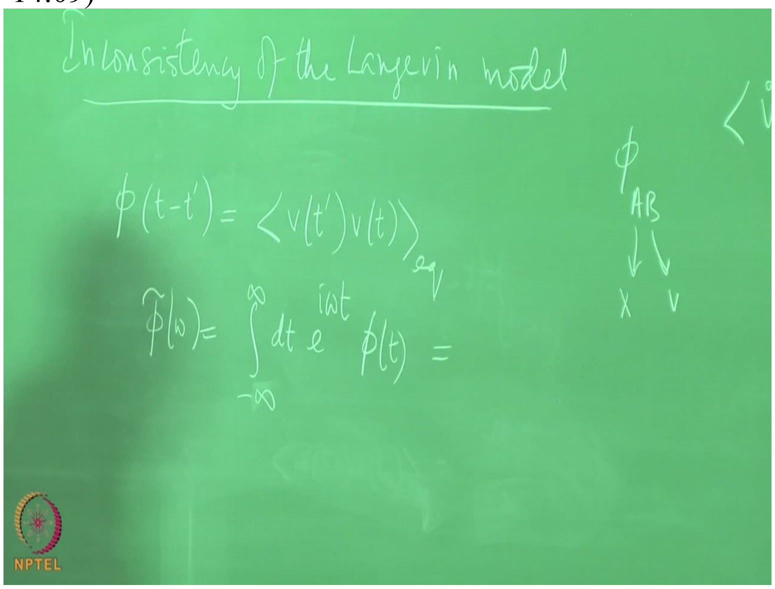
But if I do that here, if I differentiate with respect to T and then set T equal to 0, it is like differentiating this guy here. So let us take T to be positive. If T is positive, this goes away. I differentiate both sides with respect to T and then set T equal to 0. Now that is going to give you V of T not V of T not V dot of T not in equilibrium equal to - gamma K Boltzmann T over M which is not equal to 0. All I do is to differentiate this with respect to T and put T equal to 0 from above. And you get a nonzero answer.

So it says the velocity at any instant of time, T not in equilibrium is correlated to the acceleration by this number here. The equal time correlation is not 0 identically but some finite number. Okay? And yet, V stationary which we have which we showed explicitly, this must vanish, V stationarity. So there is obviously an inconsistency somewhere in this model. So one or the other must be wrong. Either this or that must be wrong okay. Now the stationarity this thing by the way we derived this by making an assumption.

When we computed this correlation function, we assume that the velocity is uncorrelated with the force at later instants of time including that particular instant of time itself. So we made that assumption and that now leads to a result which is inconsistent with that assumption out here. So there is something wrong somewhere. Stationarity on the other hand we proved under very general considerations from linear response theory, we showed the stationary tea of this correlation, or the response function and yet this is happening. Let us see there are any other problems.

So you agree that there is a serious problem here. The equal time correlation between a variable and its derivative should be 0 if the variable is a stationary random variable but according to this model, it is not. All right. Any other problem? Well, let us again look at this response function. It is phi XV. So let me drop the subscripts for a moment and argue in the following way. I would like to find out what is the mean square, the mean square velocity is KT over M in thermal equilibrium. What is the mean square acceleration? That should be some finite number. It is a physical quantity. It should be a finite number. So if I compute V dot on both sides, it should get a finite answer.

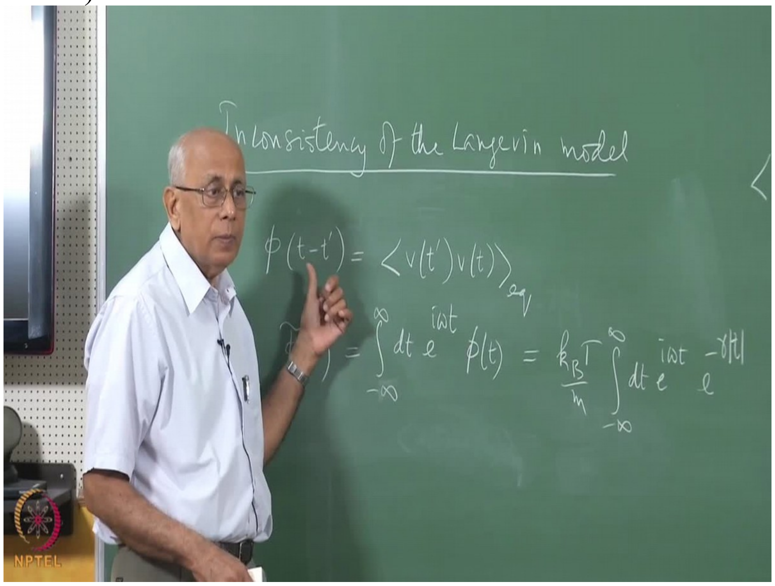
(Refer Slide Time: 14:09)

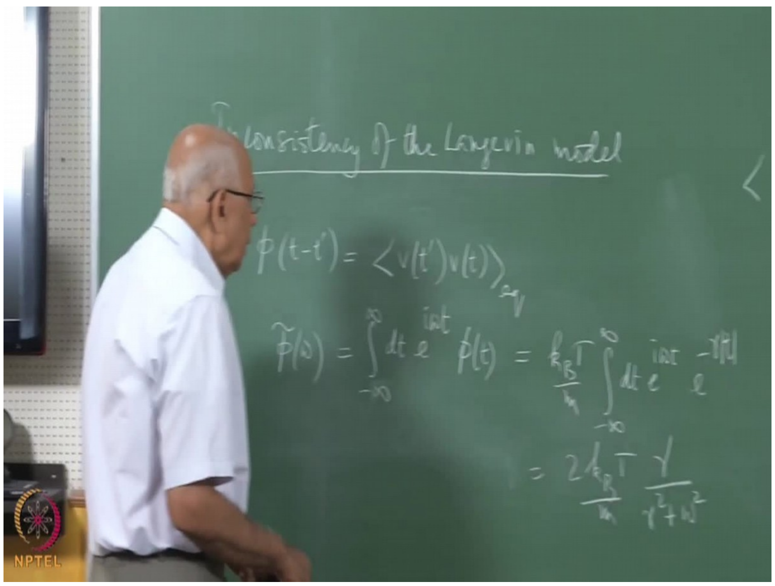


Now let us call this correlation phi of T - T prime equal to V of T prime V of T in equilibrium. That was our response function which is E to the - gamma mod T - T prime in this model. Now the Fourier transform of this is the spectral function and the moments of the spectral function cannot be computed because we have the spectral function explicitly. So what is that equal to? What is the spectral function equal to? Phi tilda of omega equal to integral 0 to infinity DT E to the I omega T times the phi of T.

That is the definition of the spectral function right. In this model, in the langevin model, we know what it is, we know explicitly what this thing is. So this is equal to, well let us compute, let us compute the power spectral density of this process, the V process which means we take its autocorrelation and we find its Fourier transform okay. So what we need is the Fourier transform which is - infinity to infinity, this is the power spectral density. And what is this equal to?

(Refer Slide Time: 15:43)





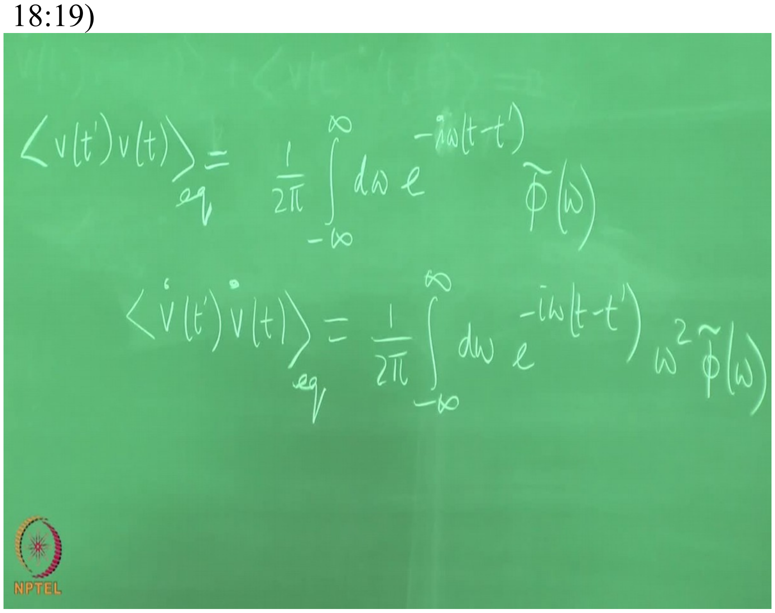
Well, we need a slightly different symbol for this whole thing. I call this the spectral function. It was, how did we define the spectral function? It was the Fourier transform of the response function. Right, so it was this. I am just trying to get my factors right. This is in fact equal to phi tilda of omega. The susceptibility was the one-sided Fourier transform, respective function is just this guy here. Now in engineering, the power spectral density is defined in various ways apart from some factor of 2 or something like that. Sometimes 2 pi, sometimes 2 times the Fourier transform of the autocorrelation function.

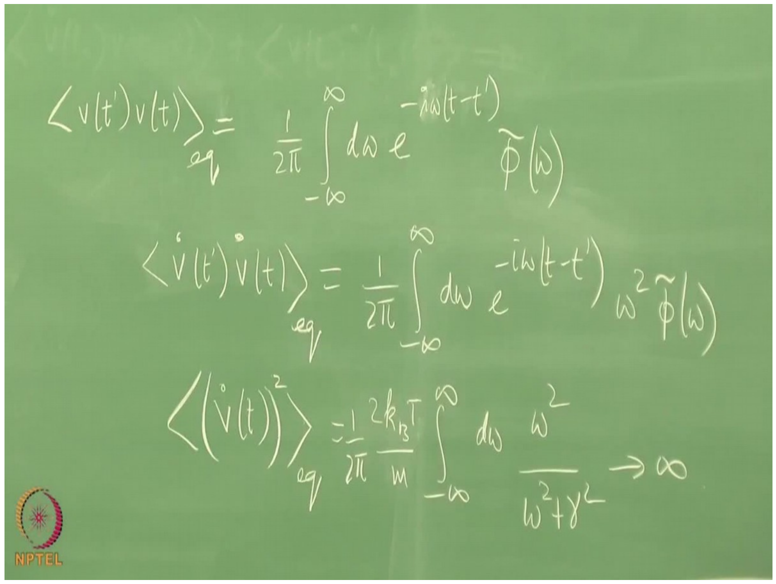
So modulo that let us just define it to be the Fourier transform itself and let us compute what this number is in the case of the velocity process. So this is equal to K Boltzmann T over M integral - infinity to infinity DT E to the I omega T E to the - gamma modulus T because recall that for T negative, this is E to the - modulus T. It is a symmetric function of T, E to the - gamma modulus T. And why should it be symmetric? Why should this quantity be symmetric? Because under time reversal, V goes to - V.

Both these fellows change signs. So this fellow does not change sign at all. Or yet another way of looking at it is, it is that time parity of A dot times the time parity of B and A dot this X dot. So it is completely consistent. But this is a trivial integral to do. This is twice the integral from 0 to infinity because it is a symmetric function and the sign part of it vanishes clearly. So you have got 0 to infinity with a 2 factor K Boltzmann T over M, 0 to infinity E to the - gamma T cos Omega T which is of course gamma over gamma square + Omega square.

It is a Lawrency. The Fourier transform of the E to the - X is a Lawrencianian K. So that is all that we are saying here. But this has a physical meaning, this quantity here because you can differentiate this on this side. Each time you differentiate with respect to T, you pull out an I omega from this. So let us do that, let us write this.

(Refer Slide Time: 18:19)





So you have V of T prime V of T, this is the correlation function. This is equal to 1 over 2 pi integral - infinity to infinity D omega E to the - I omega T - T prime phi tilda of omega by definition. That is the inverse Fourier transform right? And we know what phi tilda of omega is. So now what I do is, V dot of T prime V of T in equilibrium, again in equilibrium is with a I omega pulled down. And if I differentiate with respect to T as well, it is with a - I omega pulled down right. So immediately you get this. 1 over 2 pi integral - infinity to infinity D omega E to the - I omega T - T prime Omega square times phi tilda of omega. The 2nd moment apart from this time-dependent factor.

Now I said T prime equal to T. So that tells me V dot of T squared in equilibrium is stationary, it has got therefore be independent of time. The time dependence disappears from this thing and this is equal to1 over 2 pi integral - infinity to infinity D omega omega square phi tilda but that is equal to this fellow here. So if I put it in, it is Omega square over Omega square (())(20:16) Omega square apart from constants.

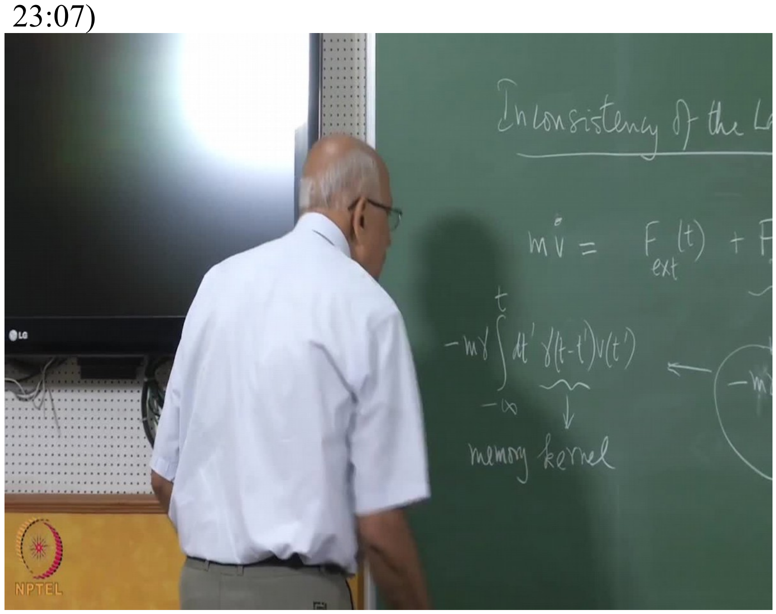
So it is equal to 1 over 2 pi 2 K Boltzmann T over M and this is. But this is a finite physical quantity. It is a mean square value of the acceleration but that is infinite. That has turned out to be infinite because this is not dying down fast enough. So it infinity, goes like 1 over Omega square and therefore goes to a constant as omega tends to infinity on the other side. So this is it tends to infinity which is clearly wrong which is clearly wrong. So again we are faced with this serious problem.

And of course, once the 2nd moment goes to infinity, the higher moments will all go to infinity. Omega 4, omega 6, etc will all go up. So the velocity process therefore will not have, its derivatives will not have finite mean square values which is clearly unphysical. Now what is the origin of this disease? Where could we have gone wrong in this business? Means I follow a very very simple model, so where could this have been wrong? There was one assumption made in deriving this model and the assumption was that the model is valid as long as you are looking out time scales which is not at the level of the molecular timescales, the collision time between molecules, but maybe 5 orders of magnitude higher. So timescales of the order of gamma inverse and greater.

If it becomes very much greater than gamma inverse, it goes to the diffusion regime but certainly, it is not valid on timescales going towards 0 on the other side. So right there we made an assumption which is not valid and now noticed that all these diseases arose when you took the time difference to go to 0. And in this case when you took the frequency to go to infinity. So infinite frequency is like 0 time, you know very small-time in the Fourier language, high frequency is like small-time and vice versa. So that is where the problem was.

Now how do we fix it? In the context of this model itself, how would we fix it? We would still like to have retarded response, we would still like to have causal response and we would like to stay within the regime of linear response right.

(Refer Slide Time: 23:07)



So clearly the one place where we made an assumption was that the acceleration of this particle, we wrote MV dot is equal to the force on the particle. So there could be possibly some external force on the particle which could be time-dependent, we do not care. And then there was a random force on the particle but this random force. So let us write it as F random of T and we said this random force has 2 components to it, 2 parts to it. One part was the systematic part and the other part was the truly random part coming from molecular collisions.

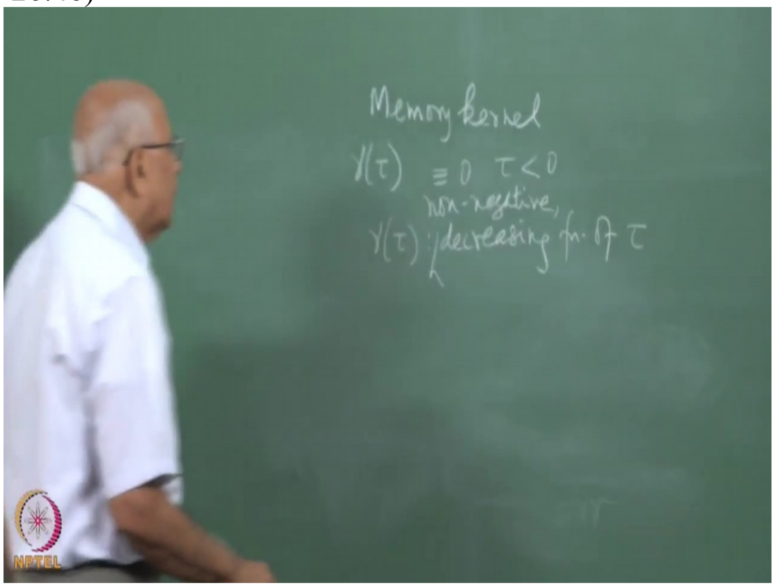
So this thing we took to be square root of gamma times zeta of T with this to be white noise and this part we took to be - gamma M gamma V of T itself. Now this friction arose saying that the friction is proportional to, the frictional force is proportional to the instantaneous velocity, assumes that this frictional force acts instantaneously, the reaction of the medium acts instantaneously on the particle. That is not true, that is not tenable, not mathematically instantaneously because the medium itself has some timescale in it, the molecules.

They cannot act instantaneously on this. So this model does not go all the way to T equal to 0 to instantaneous response. So this is the point that had to be fixed. This model is untenable at a very very short time intervals. How will we fix it? Staying within causal, retarded and linear response, how can we fix it? Well we will do the following.

We will say look, it must depend on the velocity but not on the instantaneous velocity but on the previous, the history of the velocity, earlier velocity right. So the way to fix that model is to replace this by - M gamma an integral from wherever from the infinite past okay. - infinity up to T because the certainly would not want this part to go beyond T. We are looking at the acceleration at time T. That is not going to depend on what happens to the velocity at later times right. So times the integral DT prime and it must be a linear function, so V of T prime must be there.

It must be causal, it must be retard so that means, it must only depend on the time elapsed since T prime happened. So this must be some function gamma of T - T prime. So this thing there is a function. It is a kind of memory kernel. Oh, there is no gamma here. So I make this gamma a function of time, defined only for positive values of its arguments, nonnegative values of its argument. And what other property would you like of this gamma? Well, we would certainly expect the following.

(Refer Slide Time: 26:46)

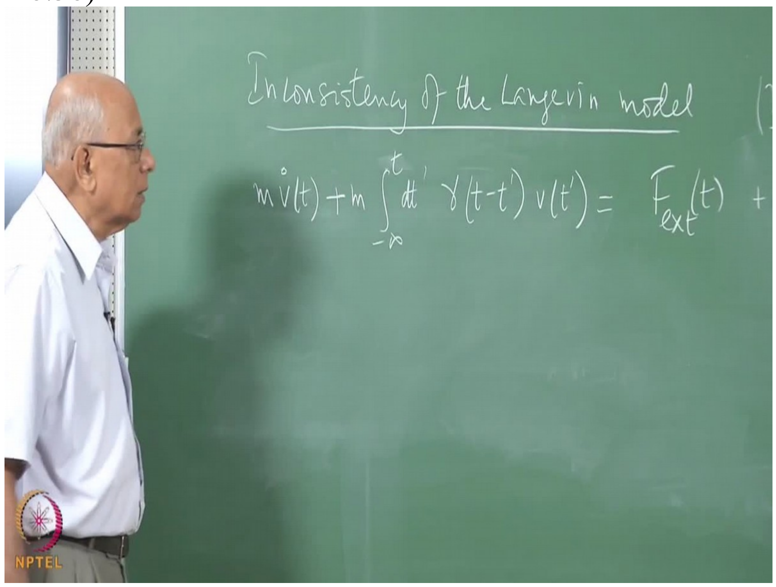


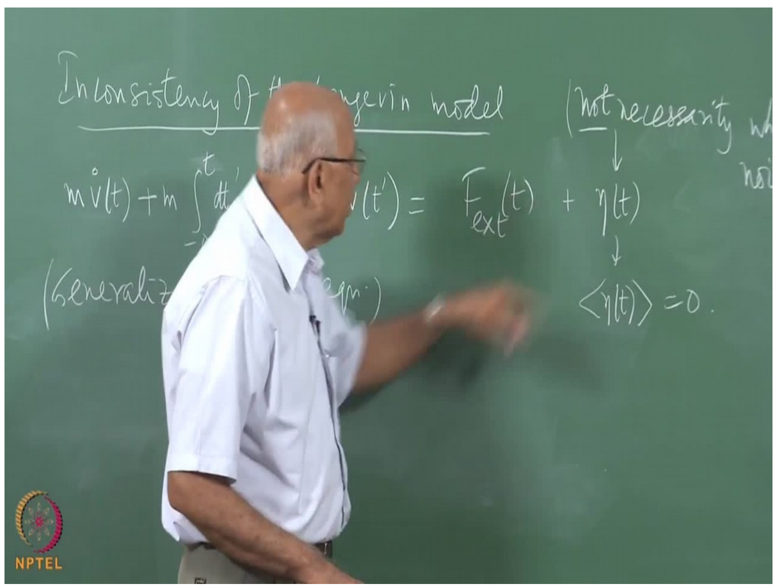
We would like gamma, let us call it gamma of tao to be neutral. Gamma of Tao memory kernel we just want to write some general properties of it. We do not want to make specific modelling of gamma but some general properties. Gamma of tao we should take it to be identically 0 for tao less than 0. Does not make sense to go. That is fixed by causality in any case but by the fact that I cut this off here but formally say that this gamma is defined only for positive values of its argument okay.

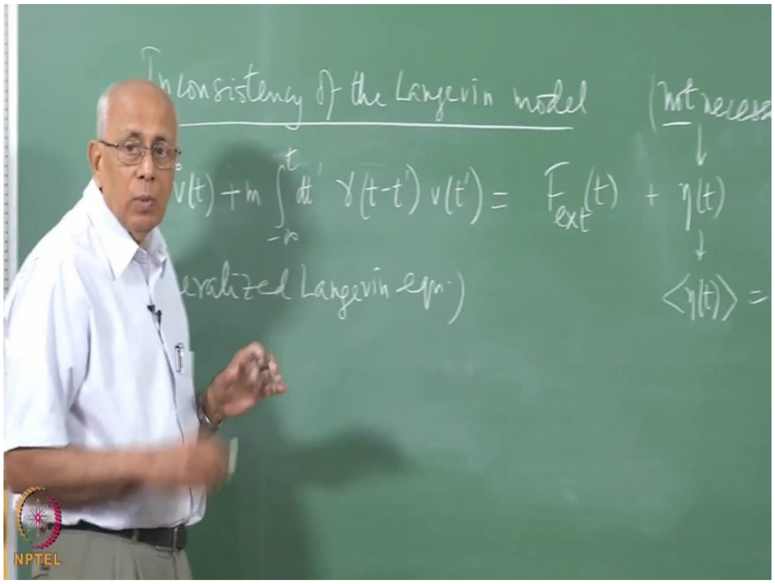
Then I expect the effect to keep going down as the elapsed time increases. So I would certainly expect that gamma of Tao decreasing function of tao. So as tao increase, I want this effect to go down. Anything else you want of gamma? Well, we would like it to go to 0 at infinity, sufficiently fast. If it does not, we are in trouble. Then we have to fix it. It will be bad. And right now I am not saying how fast it should go to 0 as Tao tends to infinity. But what else do you require? There is one more very important criterion we need, one more condition.

It represents frictional force right? So you want its sign to be positive. We do not want it to be negative. So nonnegative decreasing function. Let us put that in and see what happens.

(Refer Slide Time: 28:38)







So my langevin equation now reads M V dot of T + M, I put this M here purely for dimensional reasons so that this gamma whatever it is, still has the dimensionality of 1 over time. So - infinity to infinity DT prime oh sorry, no no no, this there is an extra time factor. We will fix that in a minute. I want to put this N here so that this N cancels out on this side completely. This we will see what dimensionality this gamma has the from this equation itself. T - T prime V of T prime equal to any force you exert on the system, some applied force deterministic force + the random part which is the eta of, the force we denoted by eta of T earlier.

So let us leave that as it is. But important, not necessarily white noise. In fact, I am going to show, it cannot be white noise okay. It is noise. It is random but we we cannot assume. We cannot, we have to prove that it is consistent to assume that is Delta correlated. We will have to see. We do not know at the moment. Pardon me.

Student: (())(30:09)

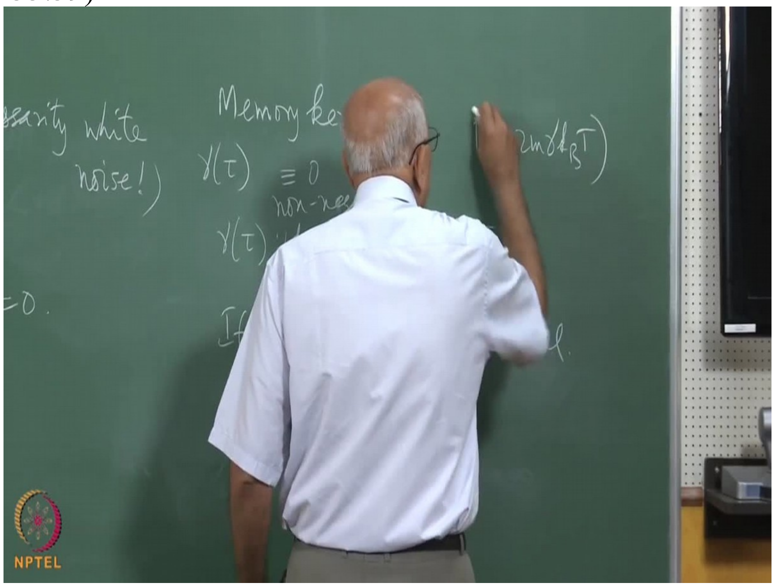
Professor: Oh, I am sorry. Because I I said already it is 0, so it cuts off but okay. By the way, you can recover the original version by saying if gamma of tao equal to gamma delta of Tao where this is a constant, implies the langevin equation langevin model. So the physical dimensionality of this kernel is gamma divided by time. There is an extra 1 over T. So it is 1 over T squared is the dimensionality because there is an extra T here and when you hit this, you get a 1 over time and then it has the same dimensions as this.

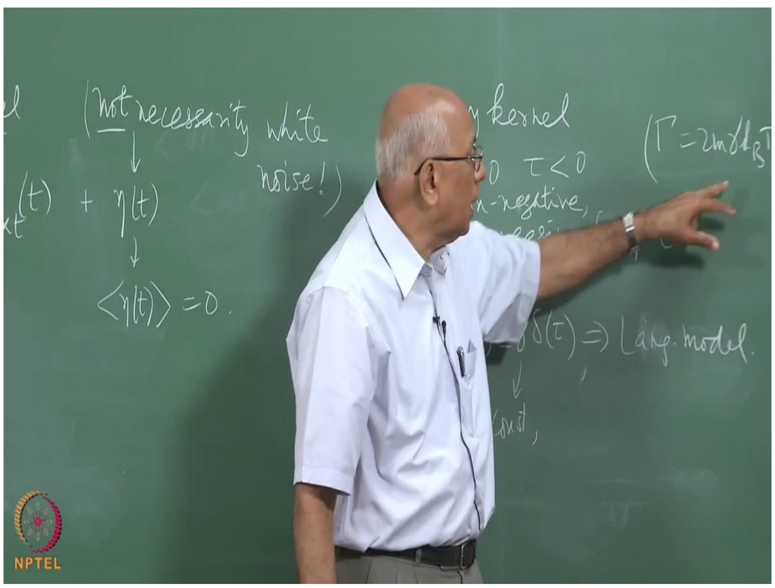
So this eta of T at the moment is just noise but not the systematic part of it. The noise from the medium. And what are the assumptions we are permitted to make of this eta of T? Well, exactly the same physical assumptions. Namely that on the average, it is 0 with or without the external force because again the assumption is you are in a heat bath and the fact that you applied an external force does not change anything, does not change thermal equilibrium, remains as it is and it certainly does not get affected by what is happening here. So we think. We do not know for sure as yet but this is a harmless assumption.

So we have no clue at the moment what sort of noise is consistent. The whole idea is to make this model consistent with causality because it looks like we are violating causality and to make it consistent with stationarity, it looked like that too was getting violated. Okay. So this is this thing here is called the generalised langevin equation and we need to fix this model in such a way that will give us the result that we know are already true. Namely this velocity should finally the probability density should turn to Maximilian, should remain in equilibrium, that it should have a stationary autocorrelation function and that the mobility of the system is governed by the by the velocity correlation.

That was a very general theorem that we deduced and that cannot be violated. So that result has to be checked through this. So the whole idea will be to fix this model in such a way of precise way that that is the only way we can fix it such that it will be consistent with stationarity causality and lead to the correct coober formulas for the mobility. In the process, we will discover the fluctuation dissipation theorems. Now remember, always keep this at the back of your mind. When this eta of T was Gaussian white noise with a strength square root of gamma, that capital gamma and this little gamma here were related to each other by this relation.

(Refer Slide Time: 33:39)





So we had this consistency condition, gamma was equal to 2M gamma K Boltzmann T. We call this the fluctuation dissipation theorem because this measured the strength of the fluctuations and that measured the dissipation in the system. We need to find out what is the new fluctuation dissipation.

Student: Will that also tell us something about (())(33:58)?

Professor: Yes, yes. So that that is going to tell us something about the correlation of X because ultimately if this fact the system is in equilibrium is happening because thermal fluctuations throw you out of equilibrium, the dissipation brings you back.

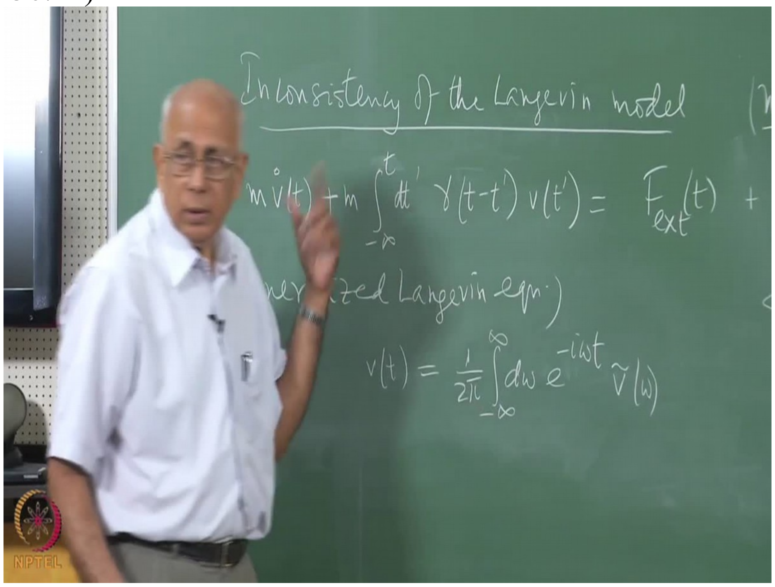
The noise itself has to play a role to bring you back to equilibrium. So there has got to be a consistency condition between these 2. Precisely what it is, we do not know at the moment. But what we do know what what I can assert and we will have to prove this is the following. That it will be inconsistent to assume this to be white noise. We will we will show that it cannot be white noise. It has got to have a finite correlation time. Not surprisingly, that correlation time will be related to this memory function.

They have to be related to each other. So there will be a relation between them. That will be the replacement of this here. Here, that will change okay. So let us see if this is going to work. By the way, this kind of business is used in understanding movement of particles and liquid but it is a much more intricate formalism than this simple stochastic equation formalism. But this is a standard model. Next step to improving the launch model before you go to the full glory or something like the BBJKY hierarchy or something like that.

But this thing here will already tell you a great deal of give you a great deal of information. Okay. So now, let us do the usual game. We are going to find average quantities. So let us find the mobility for instance and we will do this by the standard trick of saying well, the average value is 0 and what we need for the mobility is for the unit applied force, what is the average velocity? And so the average velocity per unit force applied force is called the mobility of the system.

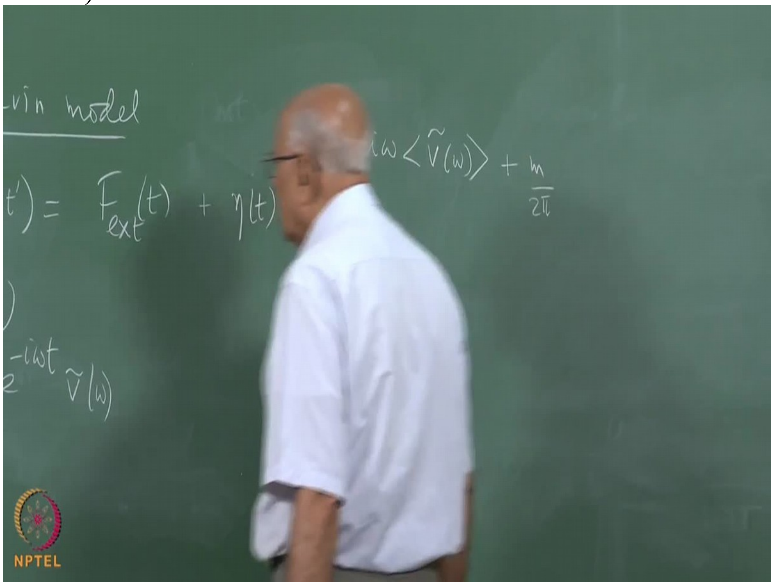
And we also define the dynamic mobility, V of omega by saying suppose I supply a sinusoidal force with frequency omega, what is the response look like, average look like? So a short way of doing that, I am not going to start from the beginning like we did for the langevin equation, is to simply say all right, let us take this thing, apply fourier transforms on both sides and see what happens.

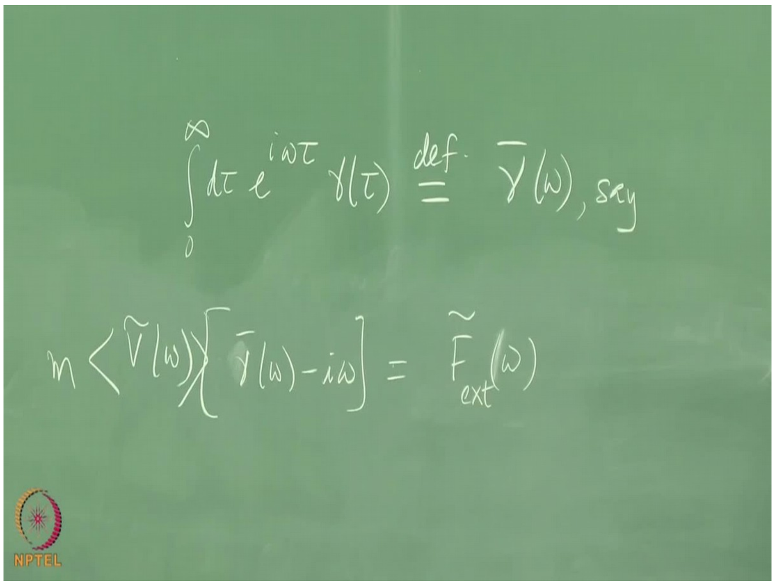
(Refer Slide Time: 36:21)



So we are going to define V of T equal to as usual our convention was 1 over 2 pi - infinity to infinity D omega E to the - I omega T V tilda of omega. And the same for eta, the same for F, et cetera et cetera. Any function of T is written in Fourier language in this fashion and then let us see what happens to this equation, what does it give and we will also take averages so that the average value of this goes to 0 anyway (())(36:56) get us. Well, if I substitute that, let us write down the equation for the average value of V of T directly or rather the average value of Fourier transform of V of T directly. So I apply this, I put this N on both sides. So the 1st gives me M times - I omega because there is a dot. And I am going to equate Fourier coefficients on both sides.

(Refer Slide Time: 37:25)





So - I omega the average value of V of omega, this term here + something or the other. + and let us do this properly. M divided by 2 pi. Yes but I am going to read out Fourier coefficient, so let us do this slowly. Pardon me.

Student: (())(37:51).

Professor: Yes, it is a convolution.

I am not, okay since here has forestalled me, this is a convolution integral, it stops at T and we can write down what this is going to be. It is going to be the one-sided Fourier transform of this V of, of this gamma because the integral gets cut off and then you equate Fourier coefficients. So I hope you see that directly and the 2 pis cancel out everywhere, here, here, here et cetera and you end up with this. V tilda of omega times - I omega + I need a symbol for this quantity, integral 0 to infinity D Tao E to the I omega Tao times gamma of Tao. That is going to be the integral over DT prime.

When I change variables from T - T prime to Tao, this integral will run from 0 up to infinity. It will get inverted and the - sign will go away. I replace T prime by Tao which is T - T prime. Then this becomes gamma of Tao and the E to the I omega - I omega T which came in the Fourier transform, is going to give you E to the - I omega T times E to the I omega Tao okay. So let us give this a name. It is not gamma tilda because this is a one-sided Fourier transform.

Student: (())(39:21)

Professor: Yes but right now I to keep the rotations straight so that you do not want to be confused that sometimes I define it that way and sometimes I do not.

We have said gamma of Tao is defined for positive values of its, nonnegative values of its argument. So only this thing, so this is definition, let us call it gamma bar of omega. So the response function I use ki, I just said that is the susceptibility because that is the standard symbol. For this, I know there is no standard symbol. Let us just call it gamma bar. I have used star for complex conjugation, not not a bar. So it is gamma bar of omega - I omega in this fashion clear, is equal to F tilda external of omega M times.

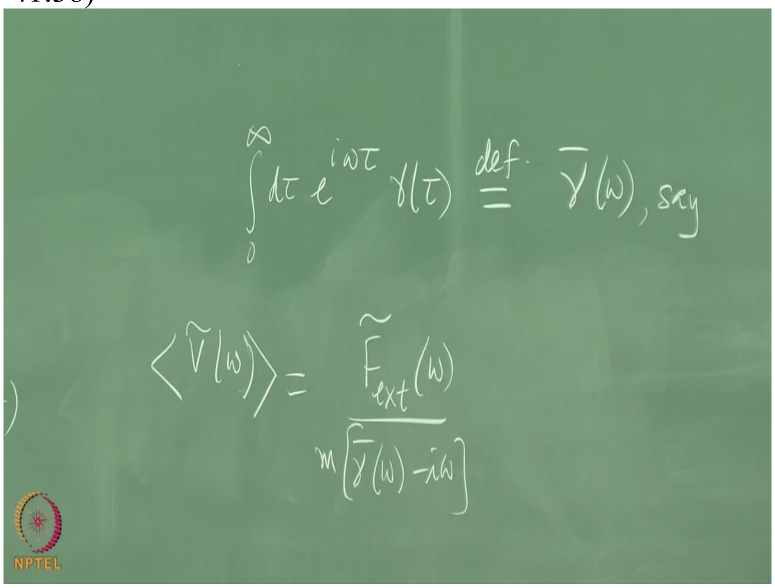
There is nothing to average in the deterministic applied force. So that is just F tilda and the eta tilda goes away because the average is 0. So if I divide this by V tilda of Omega, so therefore pardon me?

Student: (())(40:51)

Professor: Yes, I have done that. I have done that sorry. Ah, thank you. Yes, of course.

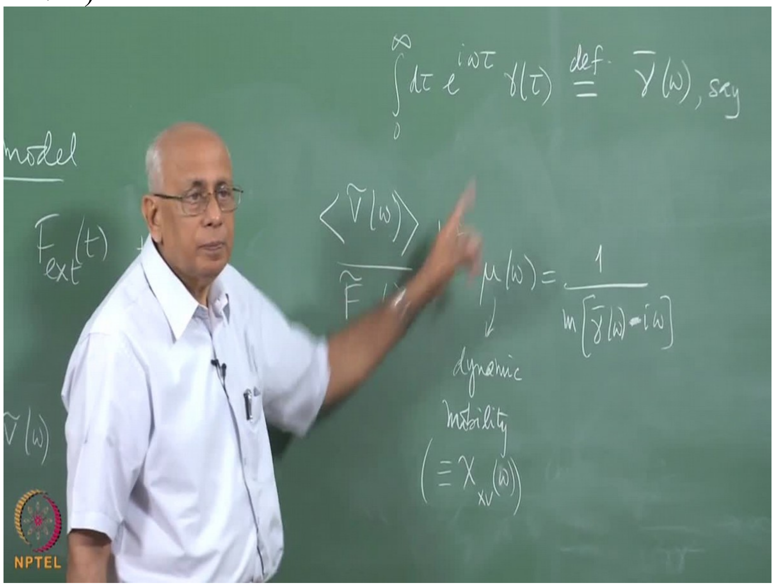
It is the average. It is the average. Why do not I write equilibrium outside? Why have not I put a subscript equilibrium? I am not in equilibrium. I have applied an external force. So this is the perturbed system and that is why the system is, the average velocity is not 0 because it is moving. In the absence of this external force, the average velocity is 0. It does not go anywhere.

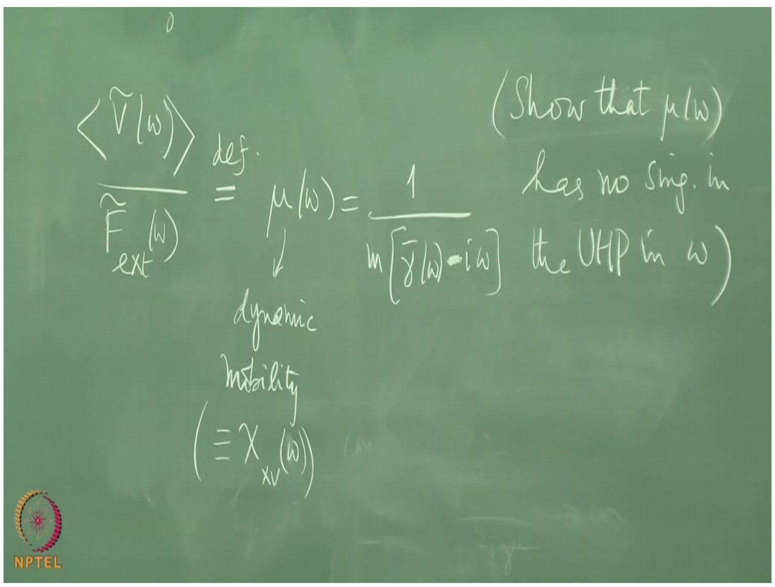
(Refer Slide Time: 41:38)



But I will still retain this notation. I will still retain the notation this bracket here because I am doing a full average. There is an average over the initial condition V not and then there is an average over V not, all possible V nots okay. So I do not care. I am not even going to specify what that ensemble is. This is and the average is 0, and that immediately gives me this.

(Refer Slide Time: 42:14)





But we know that this fellow divided by this F tilda external of Omega, we know this is by definition the dynamic mobility which in this model is 1 over M gamma bar of omega - I omega. This is the dynamic mobility. It is a susceptibility. And what kind of generalised susceptibility is it? It is ki XV of omega because I am applying a force which is purely mechanical. - X times F external is change in the Hamiltonian of the system and therefore, you get this. So but there is no difference to Hamiltonians or anything like that. Once I put in friction, it is not a Hamiltonian system anyway but I do not care.

The model still works. So in the sense of generalised susceptibility, this is what the mobility is but in simple physical terms, it is the average velocity per-unit applied force and when you apply a force which is sinusoidal, you do this division for each frequency component and you call it the dynamic susceptibility or mobility here. We know there is a general property of this guy which says that the singularities in the omega plane cannot be in the upper half plane, not with this Fourier transform convention.

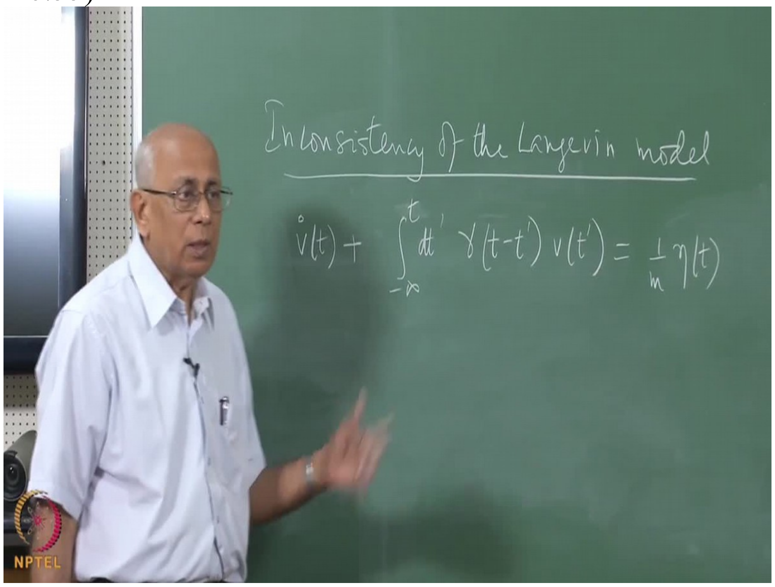
So I am going to leave it as an exercise for you to show that this, the singularities of this function, by the way this is not the constant. If it were a constant, the matter is trivial because then you know that the pole is in - I gamma. But now you have to show that the singularities of this are in the lower half plane or better still, there is no singularity in the upper half plane. So any root of this omega equal to I times gamma bar omega must be in the lower half plane okay. That follows from this representation.

So that is the susceptibility the general, in this form, in this model. We still have to see what it does in terms of the velocity autocorrelation function. We still have to compute that explicitly and we have before that this quantity is in fact the velocity autocorrelation function apart from some KT factor and then a E to the I Omega T integrated over T. We still have to show this.

So show that mew of omega has no singularities in the upper half plane. Okay. And of course you know that in the case when it is this this fellow is constant, when the memory kernel is just gamma times Delta of Tao, this thing becomes gamma, it comes out and then this is the gamma - I omega was already the dynamic susceptibility in the langevin equation. We had already found that. So it goes to that correctly but now we have to know, now we have to see what is going to happen when you put in this memory kernel.

So now we set this aside and let us go back and compute the velocity autocorrelation from this equation in the absence of the external force because the whole point of linear response theory is that the response in the presence of the perturbation to 1^{st} order in the perturbation is given by some physical quantity which is a response function dependent entirely on equilibrium fluctuations or co-relations in equilibrium with no reference to the external force at all. So that is the crux of linear response theory and we now need to show that. So now in the absence of this quantity of this external force, this is the quantity that we have.

(Refer Slide Time: 46:55)



So let us put this as 1 over M A dot T. We can remove this M. Okay. I want to find the autocorrelation function. So instead of trying to solve this integral differential equation which is by the way a mess because one way to do this is to do what we did, namely do Fourier transforms and compute formally a solution. That is not going to help us find out a correlation function very easily. So we will cut a long story short and anticipate the fact that V is a stationary process and directly calculate the autocorrelation function in equilibrium, in other words, in the absence of the external force and we will check if this assumption of stationarity was right or not post facto.

So let us write this equation down with an arbitrary time, one point I wanted to make was yes, as an equation, as an equation, mathematical equation, it is an integral differential equation. And as you know, when you have an integral differential equation of this kind, in principle, you can convert it to a differential equation but it will be an infinite order differential equation in general. So as it stands, there is no guarantee that, there is absolutely no guarantee that you have a Markov process as the output because for a Markov process, I would expect a Fokker Planck equation which has only the 2nd derivative and the velocity et cetera but this looks like there is a infinite memory in the problem.

So yes, it is indeed true that this does not lead to a Markov process. This output process V is not Markov even if this were Markovian, which we do not know right now. So it is not, it goes beyond the usual Markov process. Then next question, if it is not a Markov process, will its conditional density satisfy some kind of Fokker Planck equation? In general, you do not expect it at all but in this case, it turns out that it does. It satisfies a Fokker planck like equation, very similar to it okay. And what is needed for that? I am just trying to motivate sort of heuristically what the answers would be.

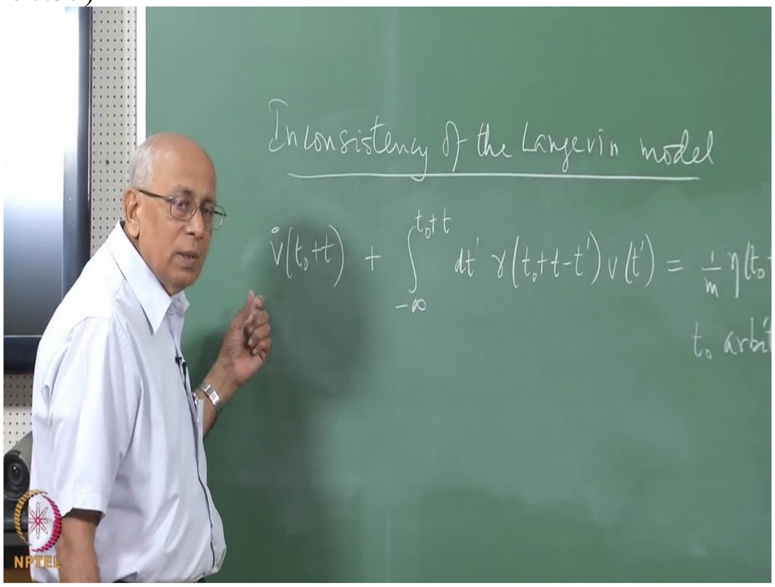
Student: Eta should do something.

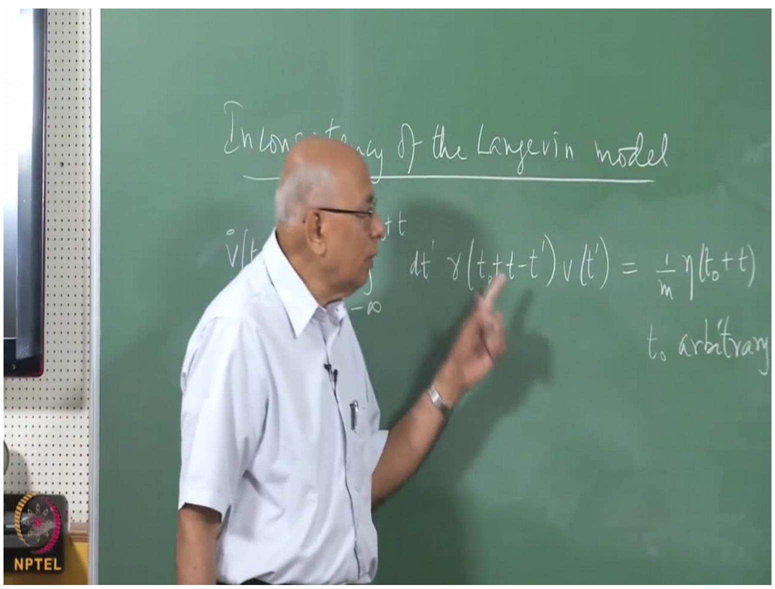
Professor: Eta should do something, yes.

Now if you are familiar with Markov processes, you know that when you have a driving force of this kind in general, if this were a white noise, then you have that langevin type equation and sure enough, you have the Fokker Planck equation. That is a rigourous mathematical equivalence. Otherwise, the partial derivative order on the right-hand side and the variable goes to infinite order. It is called the Kramers–Moyal expansion in general. It gets cut down to 2^{nd} order very crudely and roughly when higher-order cumulants vanish.

Now what sort of random variable has all cumulants beyond the 2^{nd} equal to 0? Gaussian random variable. So if this is a Gaussian noise, then it turns out that this output process in spite of this infinite memory here, still satisfies a Fokker Planck like equation. Okay. It is not Markov but it still satisfies such an equation, a great simplification. We are not going to do that. We want a more physical aspect of this. Namely we want to fix the problem with stationarity, causality, and to find the mobility, we would like to find it.

(Refer Slide Time: 50:35)





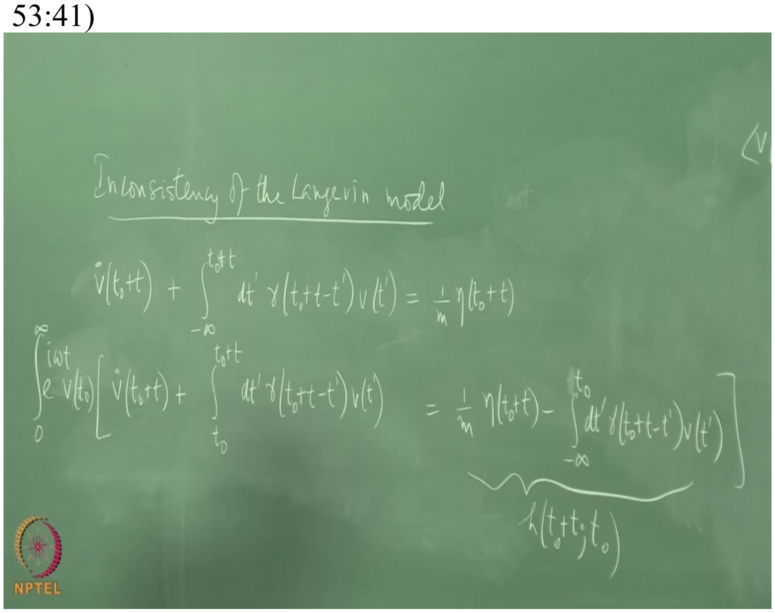
So let us do that. So let us write this equation at T not + where T not is an arbitrary number and T is any positive number. This + integral from - infinity to T not + T DT prime gamma of T not + T. T not is an arbitrary point and I am writing this equation at T not + T where T is any positive number. And now what would be the way to find out the correlation function in equilibrium? It would be to multiply this by T not on this side and then do an integral from 0 to infinity after multiplying by E to the I omega T.

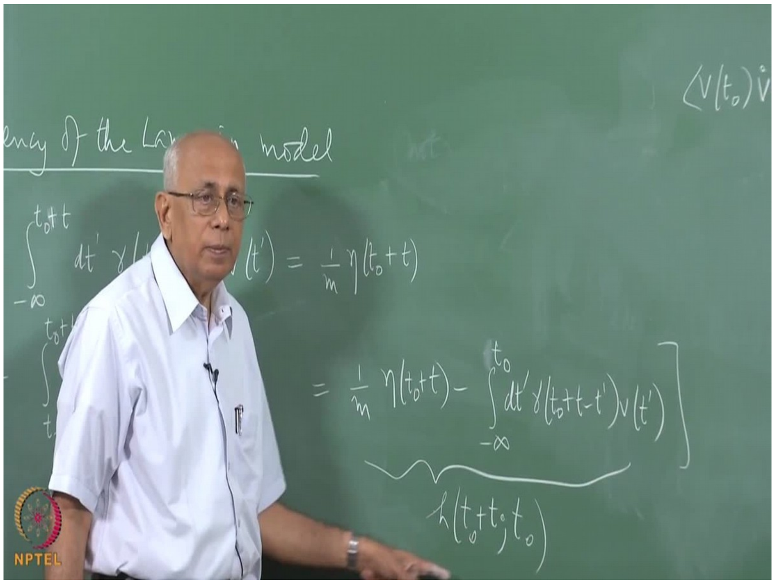
That will give me what the left hand side of the Coober formula has right? So I do that. I do not do this here but in the normal derivation for the ordinary langevin equation, we could have done that and we did do that. We found the co-relation function directly by multiplying by V of T not taking averages and arguing that V of T not is uncorrelated to eta of T not + T. We put that side equal to 0 on the average by saying that the force at a later time cannot govern the velocity at the present time.

And then we ran into this problem with stationarity, Gaussian and with causality and so on. We certainly want this property, we certainly want v of T not V dot of T not in equilibrium to be equal to 0 because we would like this thing to be stationary. It turns out that the only way to do this with this equation here, with this model, is to argue that V of T not the correlation between V of T not and the random force is not V of T not with eta of T not + T correlation equal to 0 but rather, a portion of this memory should be taken out on the right-hand side and call that is the effective force on the particle.

Now the question is, what portion? That is left arbitrary at the moment. But we know the result that we are aiming for and we want consistency here. So the argument is the following.

(Refer Slide Time: 53:41)





Look at what happens if I bring this integral up. V dot of T not + T + integral T not to T not + DT prime gamma of T not + T - T prime V of T prime is equal to 1 over M eta of T not + T - this fellow here. Now - infinity to T T not DT prime V of T not + - T prime sorry gamma. Gamma of T not + T - T prime (())(54:31). There are many ways of motivating this but the simplest is going to be the following.

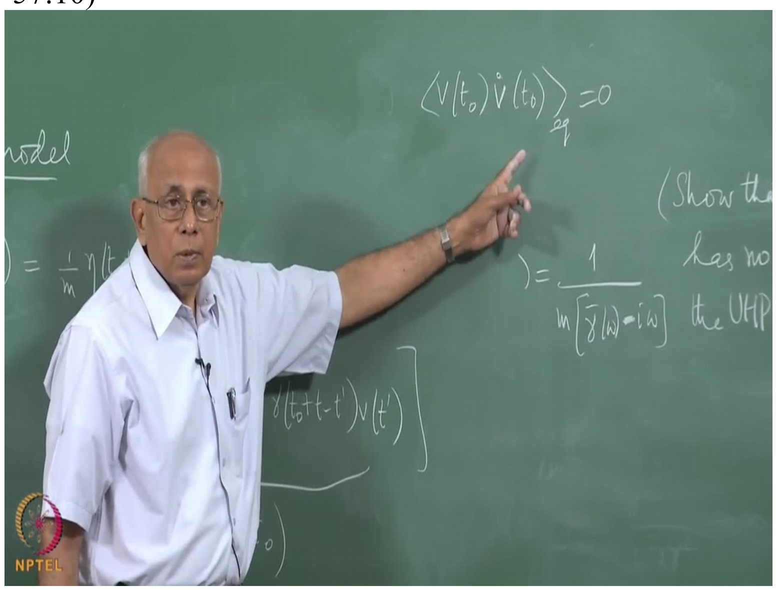
I am going to multiply both sides of this equation with V of T not E to the I omega T and do an integral on both sides of the equation after I average. So if I average this guy here, that is going to be the average that exists in the coober formula for the dynamic mobility. If this is stationary if I put T equal to 0, this part of it here should become independent right it will be equal time and should vanish. This fellow should vanish. When will that happen?

If I put T equal to 0, this integral vanishes and I am going to get this correlation equal to 0 provided the V of T not is uncorrelated with this guy. Not with eta of T not + T but this portion of the velocity history subtracted out okay. And that is the only way you can split this to achieve this point. Okay. We will see as we go along that how it becomes consistent and then we will justify it. And let us call this something else. Let us call this noise some H of its a function of T not + T but it is also a function of T not because there is a T not sitting here. And there is a T not + T sitting here.

So it is dependent on both the starting point T not and the current time T not + T and it is not stationary. This fellow is not stationary by any means. It is a function of T not + T and T not separately so therefore it is a function of T and T not separately. Now we will assume and we have to say this is consistent or not that V of T not is not correlated with H, this for any positive T okay. So that will be the next step. I have to stop here today since we have run out of time but we will take it from this point next time.

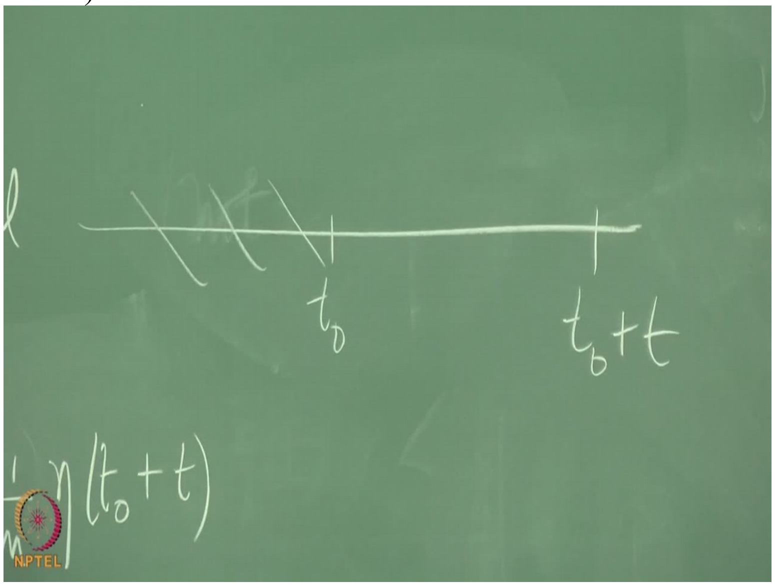
Student: V of T not (())(57:03).

(Refer Slide Time: 57:10)



Professor: We would like this to be true. We would like this to be true so that we do not have the problem which we had in the langevin model where on the one hand stationary said it should be true but the exact computation of the velocity correlation said it is not true. It is we will definitely like it to be 0. And that is achieved by saying look, let this thing trivially vanishes if T is equal to 0. So I split that portion and the rest of it. But it has got a physical meaning.

(Refer Slide Time: 57:35)



There is, on the time axis, there is some arbitrary instant T not and this is T not + T and we are writing the velocity or acceleration at this instant of time by saying that this is affected by the friction which operated all the way from infinite past up to here but that has broken up into 2 pieces, part of the velocity history which operated till here and the rest of it. And this portion of it, I am subtracting from the noise at this instant of time and arguing that the effective force, random force with which the velocity here is uncorrelated is in fact this portion, the subtracted portion.

That is the only way in which I can ensure that if T goes to 0, this correlation here is going to vanish identically. So it preserves stationarity. But now, that is fine as a kind of fixed but we need to see if it gives you the correct coober formula and it gives you the correct fluctuation dissipation theorem. By the way, there are 2 fluctuation dissipation theorems here. One of them is the statement that when you apply an external force, the response to first-order depends on equilibrium fluctuations. So it is a kind of coober formula for the susceptibility.

The formula for the susceptibility itself in terms of the response function is called the 2^{nd} fluctuation dissipation theorem because historically, the fluctuation dissipation theorem was written in the context of the langevin model where you have a specific stochastic model, langevin equation or model and then there was a connection between the dissipation constant and the strength of this random noise which you put in by hand. And that was called the 1^{st} fluctuation dissipation theorem.

So the 2^{nd} one is in fact the consequence of linear response theory directly, the 1^{st} one is specific to a stochastic model. But the 2^{nd} one must be valid as well clearly. Otherwise linear response theory does not make sense okay. So since our langevin model is a linear model, we expect that the linear response theory formulas will also be true. It is linear, causal, retarded and therefore, it satisfies the conditions required for the linear response theory formalism okay. So I hope this is clear that there are 2 of these theorems and we will write them both down explicitly and see. Okay.