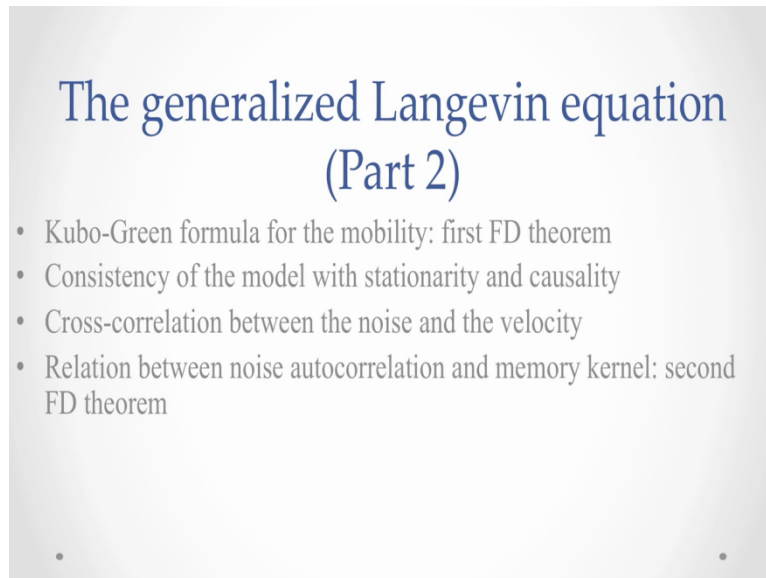


**Nonequilibrium Statistical Mechanics.**  
**Professor V. Balakrishnan.**  
**Department of Physics.**  
**Indian Institute of Technology, Madras.**  
**Lecture-21.**  
**The Generalised Langevin Equation (part 2)).**

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**The generalized Langevin equation**  
**(Part 2)**

- Kubo-Green formula for the mobility: first FD theorem
- Consistency of the model with stationarity and causality
- Cross-correlation between the noise and the velocity
- Relation between noise autocorrelation and memory kernel: second FD theorem

And if you recall problems with the original Langevin equation where that it was inconsistent with stationarity of the output process and moreover the white noise assumption probably led to this inconsistency, we have to check this out. And we also found that the power spectrum did not go to 0 fast enough when you ended up with the fact that physical quantities like mean square acceleration were infinite. So we also had some issue with causality, which were rather subtle, we make this assumption that the velocity was not correlated to the noise at later times. But what happens at equal times, we are not, we are rather vague about this.

So we need to fix all these problems and for that we imposed, we introduced this generalised Langevin equation and what I am going to show today is that it solve these problems. It is completely consistent, it is a consistent way of describing the velocity of a Brownian particle in terms of some memory or frequency dependent friction. And it also provides answers, correct consistent answers to these problems with stationarity, with causality and so on and so forth. Let us see now systematically how this goes.

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GLE:

$$m\dot{v}(t) + m \int_{-\infty}^t dt' \gamma(t-t')v(t') = \eta(t) + F_{ext}(t)$$

stationary noise,  $\langle \eta(t) \rangle = 0$

$\frac{\langle v(t) \rangle}{F_{ext}} \rightarrow \mu(0)$  (static mobility)

$\frac{\langle \tilde{v}(\omega) \rangle}{\tilde{F}(\omega)} = \tilde{\mu}(\omega) = \frac{1}{m[\gamma(\omega) - i\omega]}$  (dyn. mobility)

$\gamma(\omega) = \int_0^{\infty} dt e^{i\omega t} \gamma(t)$

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So generalised Langevin equation, and we looked at it in the case of a single velocity component of a Brownian particle. This equation said  $m\dot{v}$  of  $t + m$  times integral from  $-\infty$  to  $t$  of  $\gamma(t-t')$   $v(t')$  was equal to the noise on the right-hand side, whatever that was. And that now I am just going to say it is the noise and that is it, we are not going to specify anything about it except to say it is a stationary noise, so some  $\eta$  of  $t$ , stationary noise with the average value equal to 0. That is it, that is the only assumption.

We have to see in a consistent way what kind of statistic is attainable for this kind of noise. When we took averages, we computed the mobility of the particle, so they said that the average value of the velocity, per-unit applied force, when I apply the external force, this thing becomes  $+ F_{ext}$  of  $t$ , so this is a generalised Langevin equation and we said that the average velocity to first-order and the external forces, in this case it is a linear equation, so it is actually an exact relation. This quantity diverted by  $F_{ext}$  for constant external force, the limit in which  $t$  tends to infinity, this quantity tends to what was called the mobility of the particle, the static mobility of the particle at 0 frequency.

The dynamic mobility is the steady-state response that you get when the force is sinusoidal with some frequency, some given frequency  $\Omega$ . So in that case we discovered that  $\tilde{v}$  of  $\Omega$  average, namely the Fourier component of the velocity at that frequency, whichever is pushing the system, divided by per-unit force, so this was  $\tilde{F}$  of  $\Omega$ , that is the component of the external force corresponding to frequency  $\Omega$ . This quantity here

was equal to the dynamic mobility. And we had in our model, we computed this quantity simply by taking Fourier transforms on both sides.

There are some niceties about taking Fourier transforms of a random function, I slur over those niceties but one can make this rigorous, the result is perfectly correct. And this turns out to be  $1/\beta$  times, if you recall  $\bar{\chi}(\omega) = \int_0^\infty dt e^{-i\omega t} \phi_{xv}(t)$  but this is a one-sided Fourier transform of the memory kernel which is defined for nonnegative values of its argument. So that is the place which we have got,  $\bar{\chi}(\omega)$  is equal to integral from 0 to infinity  $dt e^{-i\omega t} \phi_{xv}(t)$ . The assumption is the memory kernel is such that it dies down as  $t$  tends to infinity in such a way that this integral converges.

If it does not then you will have to take Laplace transforms and analytically continue to  $-i\omega$  or something like that in the Laplace transform basically. So this is the place up to which we have come. Now the question is, in linear response here we know we have a formula for the mobility, we are applying the perturbation which essentially couples by the variable  $x$  and we are measuring the average velocity  $v$ . But in the formalism of linear response theory, this quantity  $A$  is  $x$  and the quantity  $B$  is  $v$ , the velocity. So we should have compatibility with a formula which we get from linear response theory.

And the question is, is that consistent with this model or not. So we need to make sure that the model correctly reproduces that expression, the other formula. Then we can assert that these 2 are consistent with each other.

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From LRT:

$$\mu(\omega) = \chi_{xv}(\omega) = \int_0^\infty dt e^{i\omega t} \phi_{xv}(t) = \frac{1}{k_B T} \int_0^\infty dt e^{i\omega t} \langle v(t_0) v(t_0+t) \rangle_{cl}$$

$$\phi_{xv}(t) = \beta \langle \dot{x}(0) v(t) \rangle_{cl}$$

(classical)

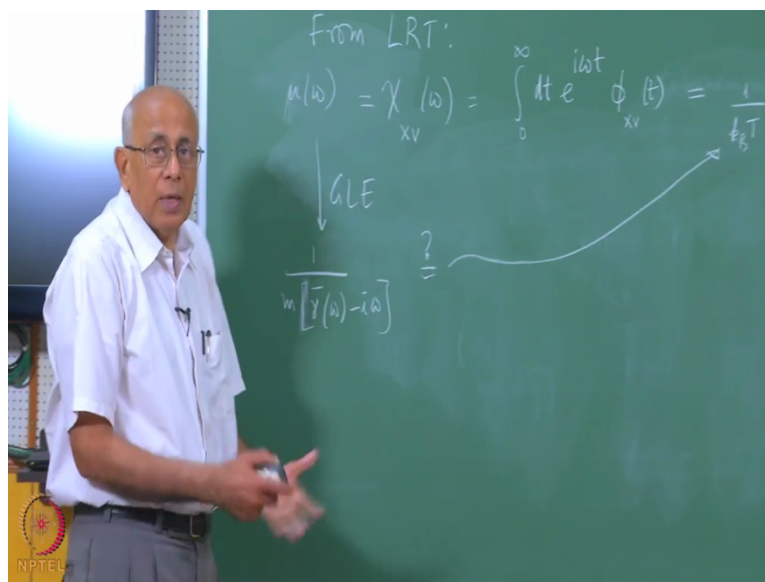
$v(0)$

NPTL

So I want to emphasise again that the general formula we have for the mobility from linear response theory is that  $\mu$  of  $\omega$ , so from linear response theory  $\mu$  of  $\omega$  is just the same as  $\chi$  of  $xv$  of  $\omega$  and we are looking at a classical particle. So this quantity is equal to the Fourier transform, this is equal to  $\int_0^\infty dt e^{i\Omega t} \Phi_{xv}(t)$ , so it is a generalised susceptibility. And the question is what is  $\Phi_{xv}(t)$  equal to and this is classical. If you recall it is equal to  $\beta$  times the expectation value, the equilibrium expectation value of  $A \cdot B$ . So this is  $x \cdot v$  of  $t$  in equilibrium. Okay.

But of course this is  $v$  of  $0$ , so linear response theory says that on general counts, that this fellow had better be equal to  $1 / (k_B T)$   $\int_0^\infty dt e^{i\Omega t} v(0) v(t)$  but  $v$  is supposed to be a stationary random variable in thermal equilibrium. So this will be some  $v(t_0)$ ,  $v(t_0 + t)$  in equilibrium.  $T_0$  is arbitrary completely because if we is the stationary random variable, then this correlation function is a function only of the time difference of the 2 arguments and the rest are function of  $t$ . So this much, the general response theory says, independent of any Langevin model, okay, that is what we found in general, in the classical case.

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Now the question is, is the generalised Langevin given equation compatible with this or not, can we derive this or not. So what we have to show is the expression you get for the mobility here in the generalised Langevin equation. So this is, this is equal to  $1 / (m \bar{\gamma}(\omega - i\omega))$  and the question is, is this equal to this quantity here in the same model. If it is then I assert that these 2 are compatible with each other, okay. So you see the logic, in the generalised Langevin equation model we explicitly found the mobility which is computing



the response straightaway and we discovered by taking Fourier transform for whatever, we discovered that it is equal to this.

On the other hand general response theory says it should be equal to that. So we need to go back to the Langevin equation, compute this quantity and see if it is integral from 0 to infinity multiplied by this gives you this. And if it does, we are done, okay. So let us see if this is true.

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From LRT:  $\chi_{xv}(\omega) = \int_0^\infty dt e^{i\omega t} \phi_{xv}(t) = \frac{1}{k_B T} \int_0^\infty dt e^{i\omega t} \langle v(t_0) v(t_0+t) \rangle$

$m \dot{v}(t_0+t) + m \int_{t_0}^{t_0+t} dt' \gamma(t_0+t-t') v(t') = \gamma(t_0+t) - m \int_{-\infty}^{t_0} dt' \gamma(t_0+t-t') v(t') \equiv h(t_0+t; t_0)$

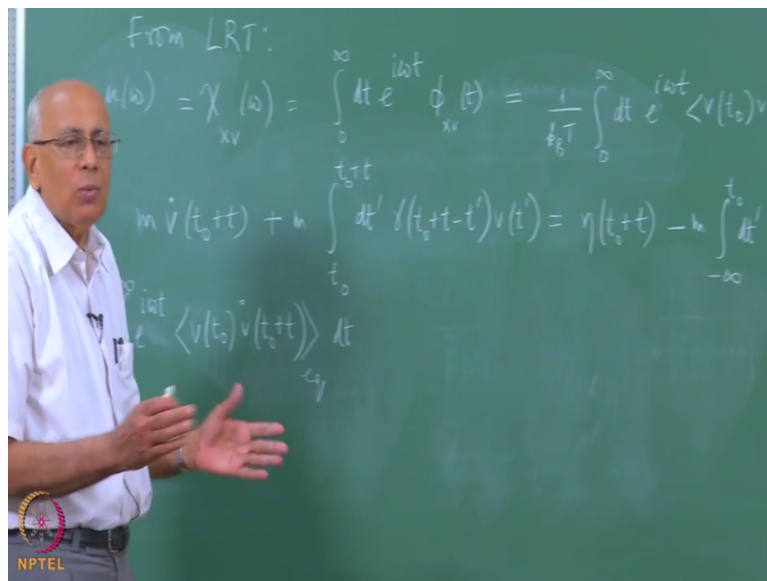
Now the way to do this is as follows. 1<sup>st</sup> of all the B must turn out to be stationary process, we must be able to show that quite rigorously and we will see that it consistently turns out to be 1, okay. And let us start, since I am anticipating myself, says it will turn out that this v is a stationary process, namely this correlation only function of t, let us start, let us take the shortcut, let us start with a Langevin equation at time t<sub>0</sub> + t whatever be t<sub>0</sub>. So I have m v dot of t<sub>0</sub> + t + m integral from - infinity to t<sub>0</sub> + t and let us break that into 2 pieces for a reason which will become clear, let us break it up into t<sub>0</sub>, t<sub>0</sub> + t, dt prime gamma of t<sub>0</sub> + t - t prime v of the prime equal to on the right-hand side the noise at that time t<sub>0</sub> + t because that is the instance at which I am writing my equation down.

- the which I took away from there, so this - m integral - infinity to t<sub>0</sub> dt prime gamma of t<sub>0</sub> + t - t prime d of t prime. Okay. So I have split the force into, the frictional force into 2 pieces, one depends on the velocity history after my initial time t<sub>0</sub> whatever it is and the other is the past history from way back when whenever. And let us do this a name, so let us call this thing by definition some h, it is a kind of noise, because this is a random variable, this is a random

variable which is imposed from outside, so let us call it some  $h$ . And what is it a function of, it has got to be a function of  $t_0$  as well as  $t$  separately.

So since  $t_0 + t$  appears here and  $t_0$  appears here separately, just write it down in that form, let me call it  $t_0 + t$ ,  $t_0$ , it is a function of both. And I define this  $h$  in this fashion. Now there is a reason why I did this. Because you see I want the velocity autocorrelation, I want the velocity to be stationary process, right. So in particular I want the correlator  $v$  of  $t_0$   $v$  of  $t_0 + t$  equilibrium average to be independent of  $t_0$ . So in particular if I take dot, if I take derivatives on both sides,  $v$  of  $t_0$ ,  $v$  dot of  $t_0$  must be 0 at the same instant.

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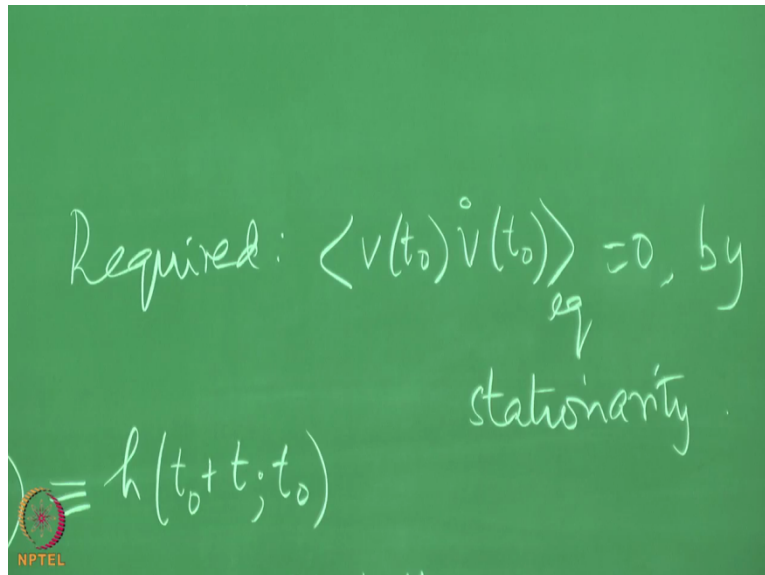


So if I left multiply by  $v$  of  $t_0$  here, I get  $m v$  of  $t_0$ ,  $v$  dot of  $t_0 + t$  and let us left multiply on both sides and take full averages. There is no external force, so everything is in equilibrium. And let us multiply this by  $e$  to the  $i \Omega t$  and integrate from 0 to infinity with respect to  $t$ . I have to do the same thing everywhere but the reason for my splitting it up till  $t_0$  is that if I set equal to 0, this integral vanishes. And then I am guaranteed that  $v$  of  $t_0$ ,  $v$  dot of  $t_0$  is actually 0 provided  $v$  of  $t_0$  is not related with this, provided. So let us impose that. Impose causality by the condition  $v$  of  $t_0$ ,  $h$  of  $t_0 + t_0$  equilibrium equal to 0 for all  $t$  greater than 0, imposes, I am going to impose it from outside.

Naïvely you would have said  $v$  of  $t_0 + \eta$  of  $t_0 + t$ , this should be 0, that is causality, this is the force at a later time cannot affect the velocity at an earlier time. But that is not consistent, that is the important thing, it turns out it is not consistent and you will see why. On the other and we do not know this condition is going to work but it has one marriage, if I do that, then

straightaway if I multiply by  $v$  of  $t_0$  here and set  $t$  equal to 0, then this integral vanishes, this becomes  $v$  of  $t_0$  with  $v$  dot of  $t_0$  and that is equal to 0, it constructs automatically. So stationarity is imposed, it is automatically satisfied, provided I can get away with this condition. Okay.

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At the moment it is an artefact, we have to see what its consequences are. Okay, is this clear, the reason why I am doing this? You could have split it anywhere, you could have split it - infinity up to this point, you could have split the integral anywhere but I can only split at one point in order to maintain the fact that I want this, I require my stationarity, it is required. And this condition, this imposition is going to achieve it, once I break the integral at  $t_0$ . By the way I should say right from the beginning, in this equation itself they give positive,  $t$  is positive.

So when I say  $t_0 + t$ , I mean instead later than  $t_0$  on this.  $T$  greater than equal to 0, I can take the limit  $t$  going to 0 but from above, always.

1<sup>st</sup> on the right-hand side, if we take the correlation with  $v$   $t_0$  and the 2<sup>nd</sup> term is related because...

Yes.

Because the 2<sup>nd</sup> term contains the whole memory and the 1<sup>st</sup> term is instantaneous because it is (( ))(17:37)

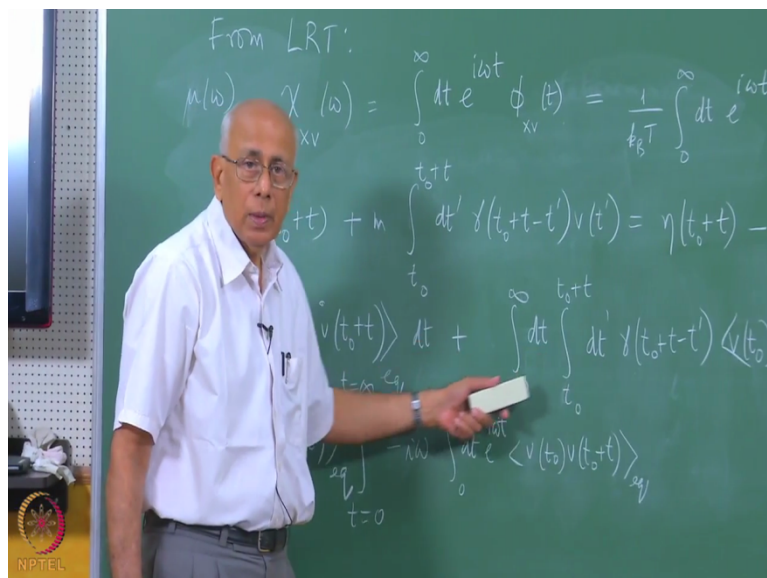
Yes. We will see, we will see. So it looks like the noise and the velocity have mixed up in some complicated way.

It does not contain any memory in the noise?

We will see, we will see what happens. It should not, it should not contain any memory, okay. We will see what happens as we go along. But right now the motivation is why I am doing this a very simple. I want that stationary and that is achieved automatically if this integral runs from  $t_0$  to  $t_0 + t$  because if I set  $t$  equal to 0 this integral vanishes, Okay. But it looks like I am paying a stiff price for it because I am going to impose this which as he rightly points out means that, if I multiply, if I take this term and multiply by  $v$  of  $t_0$  and multiply by  $v$  of  $t_0$  and take averages, these were related to each other. Okay, we will see.

So meanwhile what happens here. If I take this average here, by construction this condition has been imposed, so left multiplying by  $v$  of  $t_0$ , taking averages and integrating with respect to  $t$  with this weight factor says this term  $+ m$  times integral from 0 to infinity  $dt$  integral  $t_0$  to  $t_0 + t$   $dt'$   $\gamma$  of  $t_0 + t - t'$ , this is a lot of algebra but it is worth looking at it carefully to see what happens. So you have  $v$  of  $t_0$ ,  $v$  of  $t'$ , average, equilibrium, multiplied by  $e$  to the  $i \Omega t$  and that must be equal to 0, because by construction  $v$  of  $t_0$  multiplying by  $h$  of  $t_0 + t$  the average is 0 by assumption. So this term  $+ that term was B equal to 0, okay.$

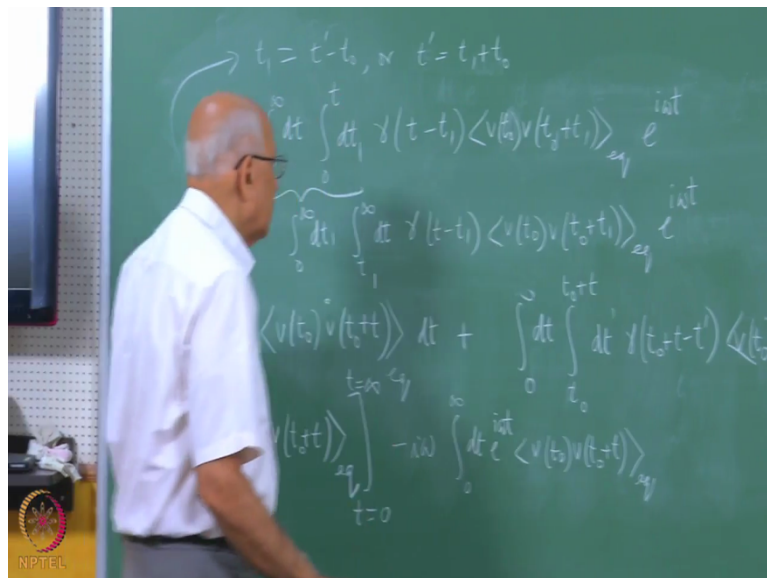
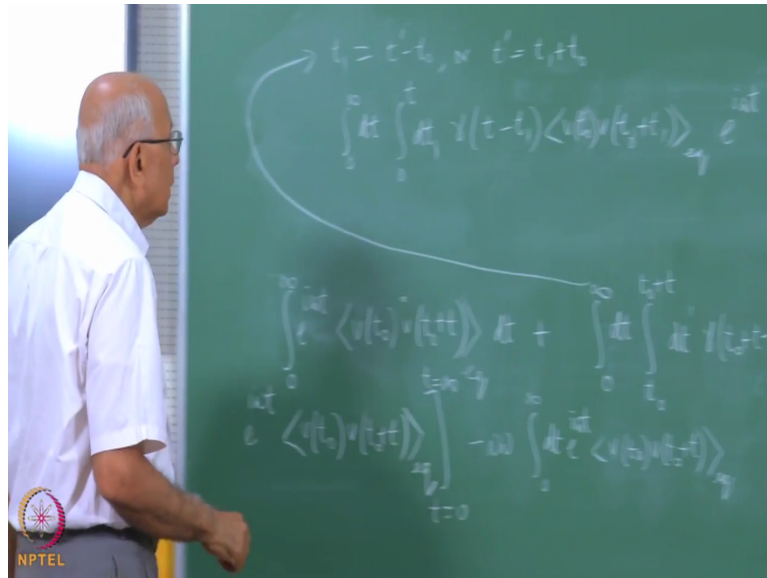
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Now let us do this integral. By the way this equal to 0 means  $m$  is removed, it is gone and this  $+ that is 0. Now what does this give us? Well this is  $t$  over  $dt$  here because this dot I can take$

to act on  $t$ , so derivative with respect to  $t$  and so I do integration by parts, right. The 1<sup>st</sup> term give me  $v$  of  $t_0$ ,  $v$  of  $t_0 + t$  average equilibrium times  $e$  to the  $i$   $\Omega$   $t$  at  $t$  equal to 0 and  $t$  equal to infinity, that is the 1<sup>st</sup> term. And then - since it is integration by parts, derivative with respect to  $t$  of this  $\chi$  which is  $-i \Omega$  times that. So  $-i \Omega$  integral 0 to infinity  $dt$   $e$  to the  $i \Omega$   $t$   $v$  of  $t_0$ ,  $v$  of  $t_0 + t$ , equilibrium, so that is this portion gone.

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Plus this double integral and I now need to simplify this double integral, so let me erase the board here and like we do it up here. And I will just retain this term, this integral, we will see what it does. 1<sup>st</sup> step of course, the obvious thing to do is to change variables from  $t$  prime to  $t$  prime -  $t_0$ , clearly that is a sensible thing to do because this thing here will then become 0. So let us put  $t_1$  equal to  $t_0$ ,  $t - t$  prime -  $t_0$ , is that okay. The several ways of doing this,  $t$  prime is,

all right, let us see where it gets us. So this integral becomes integral 0 to infinity dt, integral from where to where, 0 and then t prime is t0 + t, so t, 0 to t. And then is the dt prime is dt 1, more + signs, gamma of what, t, t - t1, that is this portion and then v of 0, v of t prime, t prime is t1 + t0, sorry, t0 + t1, equilibrium, e to the i Omega t, that still remains as it is, that is integral.

I need to somehow get this integral e to the i Omega t to act here some more, right. So thing to do is to interchange the order of integration, and what does this become if I interchange the order of integration? 0 to infinity t and for each value of t, t1 will go up to t. So if I interchange, right now t1 is less than t, so t is greater than t1, so this will become integral 0 to infinity dt 1, integral t1 to infinity dt, gamma of t - t1, v of t0, v of t0 + t1, equilibrium e to the i Omega t. Now let us put t - t1 equal to tao because that is the obvious thing to do. Right.

(Refer Slide Time: 25:21)

The image shows a green chalkboard with handwritten mathematical derivations. At the top, it states  $t_1 = t' - t_0$  or  $t' = t_1 + t_0$ . Below this, there are several integrals involving  $\delta(t-t_1)$ ,  $\langle v(t_0)v(t_0+t_1) \rangle_{eq}$ , and  $e^{i\omega t}$ . The derivation shows the interchange of integration order from  $\int_0^\infty dt \int_0^t dt_1$  to  $\int_0^\infty dt_1 \int_{t_1}^\infty dt$ . A substitution  $t - t_1 = \tau$  and  $dt = d\tau$  is used to simplify the expression. The final result shows the integral  $\int_0^\infty dt e^{i\omega t} \langle v(t_0)v(t_0+t) \rangle_{eq}$  with  $t = t_1 + \tau$  and  $t_1 = 0$ . An NPTEL logo is visible in the bottom left corner of the chalkboard image.

So can we get rid of this? The 1<sup>st</sup> 2 terms gave us this, so we must keep this, let us keep the last part of it, just this integral is being simplified. And let us put t - t1 equal to tao. So dt equal to d tao for a fixed t1. So there is integral 0 to infinity dt 1, integral 0 to infinity again d tao gamma of tao, so you see finally you ended up with the memory kernel integral and then this will remain as it is, v of t0, v of t0 + t1 equilibrium and then e to the i Omega t, t is t1 + tao.

So there is e to the i Omega t1, e to the i Omega tao, right. So let us bring the e to the i Omega tao here and this integral was just e to the i Omega t1, let me bring that there, then this completely factors this integral 0 to infinity d tao, e to the i Omega tao, gamma of tao, it



totally factors out. And what do we call this? We call this gamma bar of Omega, the one-sided Fourier transform of this weighted with e to the i Omega tao, this integral was gamma bar of Omega, so function of Omega alone.

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The image shows a green chalkboard with handwritten mathematical derivations. At the top, there is an integral expression:  $\int_0^\infty dt_1 \int_0^\infty dt \delta(t-t_1) \langle v(t_0)v(t_0+t_1) \rangle_{eq} e^{i\omega t}$ . Below this, a substitution is made:  $t-t_1 = \tau$  and  $dt = d\tau$ . The integral is then rewritten as  $\int_0^\infty dt_1 e^{i\omega t_1} \langle v(t_0)v(t_0+t_1) \rangle_{eq}$ . Further down, it is shown as  $= \frac{1}{k_B T} \int_0^\infty dt e^{i\omega t} \langle v(t_0)v(t_0+t) \rangle_{eq}$ . At the bottom left, the final result is given as  $\mu(\omega) = \frac{1}{m[\gamma(\omega) - i\omega]}$ . An NPTEL logo is visible in the bottom left corner of the chalkboard image.

So this becomes gamma bar of Omega, and there is already a - i Omega times the same integral, dt 1 e to the i Omega t1, v of t0, v of t0 + t1, this v of t0, V of t0 + t e to the i Omega t , instead of t1 the integration variable is t but it is the same integral. So it says this, so it says this times gamma bar of Omega - i Omega of this times this integral with a + sign is equal to 0. But what is this integral, this, this term here? If you put t equal to infinity, this becomes v of t0 v of infinity. That of course decorrelates. Your equilibrium, this t going to infinity, then this becomes a product of averages and the average velocity is 0.

So the upper limit is 0, so this therefore goes away, - whatever happens at the lower limit, that is equal to 0, right. At the lower limit e to the i Omega t is 1 as t is 0, this becomes v of t0 because t is 0, therefore you get a square, v squared of t0 in equilibrium and there was a - sign, so I move to the other side and this is equal to that, so this fellow divided by gamma bar of omega - i omega is equal to this integral. But v square in equilibrium is Kt over m, that is the maxwell indistribution. So this is K Boltzmann t over m and that is written, it is written m here and I put 1 here and remove the Kt to this side, 1 over K Boltzmann. Okay.

But this is what we call mu of omega, okay. So we have actually established directly from the Langevin equation that the mobility on the one hand is given by this, on the other hand it is the same equation says, it is also equal to this integral, weighted, this correlation function



weighted with  $e$  to the  $i\Omega t$  integrated from 0 to infinity which is with  $1$  over  $Kt$  which is exactly the linear response theory formula. Okay. So the model is consistent with linear response theory. This is sometimes called the 1<sup>st</sup> fluctuation dissipation theorem. It is different from the equation capital gammas,  $2$  little  $m$ ,  $L$  gamma  $m$   $K t$  that we got, that is the 2<sup>nd</sup> fluctuation dissipation theorem, we will come back to that.

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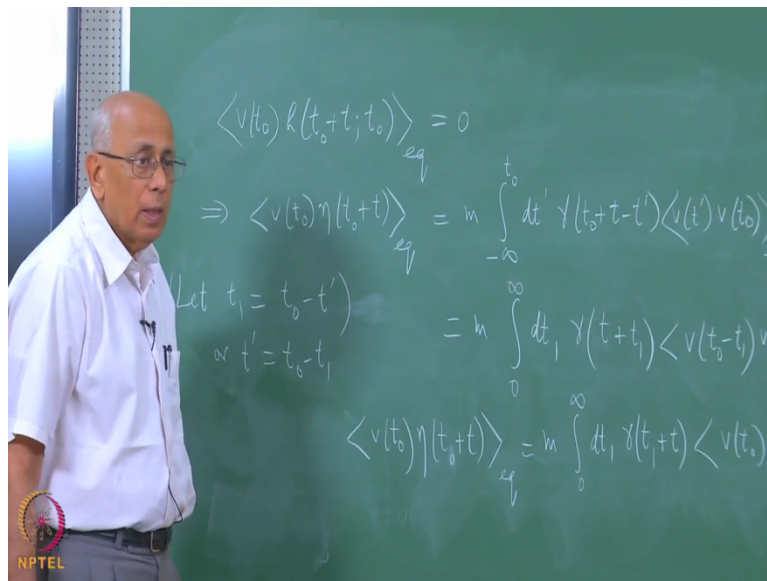
$$\chi_{AB}(\omega) = \int_0^\infty dt e^{i\omega t} \beta \langle \dot{A}(0); B(t) \rangle_{eq}$$

(I) Fluctuation-dissipation theorem

So this is just, in that sense, the formula for generalised susceptibility in terms of the correlation function which comes inside the response function is in fact the 1<sup>st</sup> fluctuation dissipation theory. So this is one way of saying it is to say that  $\chi_{AB}$  of  $\omega$  equal to integral 0 to infinity  $dt e$  to the  $i\Omega t$   $\Phi_{AB}$  but remember that  $\Phi_{AB}$  in general was equal to  $\beta$  times  $\dot{A}(0); B(t)$ , in equilibrium. This is sometimes called the 1<sup>st</sup>, in a sense it is just the desolation but this is more than that. It says the actual response function is given by this equilibrium expectation value. Okay. That is the consequence of all the dynamics you went through, both classical and quantum mechanically.

Recall what this fellow was, it was just a product of these 2 operators, these 2 quantities in the classical case, in the quantum case it stood for integral  $1$  over  $\beta$ ,  $b$  lambda, etc., etc. That is exact formula. But whatever it is, it is some correlation function and this is completely consistent with that. So the assumption be made that  $v$  of  $t_0$  is uncorrelated with  $h$  of  $t_0 + t$ ,  $t_0$ , that has led to stationarity being recovered, being maintained and the fact that the 1<sup>st</sup> fluctuation dissipation theorem which comes out of linear response theory is satisfied. What we need to do now is to go back and say all right, we made this assumption about  $v$  and  $h$ , some correlation was equal to 0, what happens then, what does that lead to?

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So let us see where it gets us. Finally it leads us to a little bit of surprise, not too surprising. It will turn out that it is no longer consistent to make  $\eta$  of  $t$  White noise, it will not be delta correlated noise at all. But it has some finite correlation time and we will see what happens. So let us go back and examine the consequence of saying that  $v$  of  $t_0$ ,  $\eta$  of  $t_0 + t$ ,  $t_0$  equilibrium is equal to 0 implies that  $v$  of  $t_0$ ,  $\eta$  of  $t_0 + t$ , equilibrium, this is the 1<sup>st</sup> term in this  $\eta$ . And then there was a  $\gamma$  - something, so we are saying this equal to 0, so that is equal to  $m$  times an integral from  $-\infty$  to time  $t_0$ ,  $dt'$   $\gamma$  of  $t_0 + t - t'$ ,  $v$  of  $t'$ ,  $v$  of  $t_0$  equilibrium.

So making this assumption is equivalent to saying this. Now what is the 1<sup>st</sup> thing we can do here? It is clear that you can immediately change variables here, so that I get rid of  $t_0$  here. So let us do that, let us put  $t_1$  equal to  $t_0 - t'$ , okay. So this implies that this quantity here is equal to  $m$  times integral, so pardon,  $t'$  equal to  $t_0 - t_1$ . So if  $t'$  is  $t_0$ ,  $t_1$  is 0 and if  $t'$  is  $-\infty$ ,  $t_1$  is infinity and then there is a  $-$  sign and the Jacobian. So this is 0 to infinity  $dt_1 \gamma$  of  $t_0 + t - t_1$ , what do we get,  $\gamma$  of  $t_0 + t - t_1$ , so it is  $-\infty$  to  $t_0 + t$ , so it is  $t_0 + t$ ,  $\gamma$  of  $t_0 + t - t_1$ , okay.

Correlation  $v$  of  $t'$ , but  $t'$  is  $t_0 - t_1$ ,  $v$  of  $t_0$ . We can simplify this little bit, okay, because we do this is stationary, this process is stationary, we have explicitly checked it out and offers of I can shift time arguments in this. What should I do, add  $t_1$  so both sides, so this is equal to, therefore  $v$  of  $t_0$ , for whatever  $t_0$  you like,  $\eta$  of  $t_0 + t$  for positive values of  $t$ , nonnegative, we can take the limit as  $t$  goes to 0 from above, equilibrium, must be equal to  $m$  times an integral 0 to infinity  $dt_1 \gamma$  of  $t_1 + t$  times correlation,  $v$  of  $t_0$ ,  $v$  of  $t_0 + t_1$

equilibrium. We could choose  $t_0$  to be 0, it does not matter, okay, just as this is independent of  $t_0$  too.

So you can put  $t_0$  equal to 0 and then you get  $v_0$ ,  $B$  of  $t_1$ , that is the correlator,  $\gamma$  of  $t_1 + t$  integrated over  $t_1$  must be equal to this. In particular, in particular we can ask, so it says for consistency you have no choice but to say that this  $v$  will be correlated with the noise, whereas this formula, so this is true for all  $t$  greater than 0. Okay. And the coupling is happening because of the memory kernel, so if you let  $t$  go to 0 from above, so let  $t_0$  from above, then it says that  $v$  of  $t_0$  at anytime  $\eta$  of  $t_0$ , namely the velocity at anytime, the output process at anytime multiplied by the input noise at the same time when you take the average value, this quantity is not 0.

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Let  $t \rightarrow 0^+$   $\lim$

$$\langle v(t_0) \eta(t_0) \rangle_{eq} = m \int_0^\infty dt_1 \gamma(t_1) \langle v(0) v(t_1) \rangle_{eq}$$

NPTEL

But there is a correlation between the 2 which is precisely given by the integral of the memory kernel, so this is  $m$  times integral from 0 to infinity  $dt_1$   $\gamma$  of  $t_1$ , and then velocity here is  $v$  of  $t_0$ ,  $t_0 + t_1$ , so you could as well write it as  $v$  of 0,  $v$  of  $t_1$  in equilibrium. And you can in fact remove this integration variable and call it  $t$ . Yah?

Why do not we express the velocity  $\langle v(t) \eta(t) \rangle_{eq}$  (39:06).

It has to be so. So it says that the random force is not all that random, you specify whatever random force you like, stationary, stationary random force, whatever you like, then the only consistent way to describe the motion of this particle is to say that there is this correlation, otherwise you violate the stationarity principle. So this...

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At instants, equal instants of time, there is a correlation. So this maintains causality, that is the whole point, this is the way causality is imposed in this model for consistency.

Is not this kind of saying that the separation we did taking gamma and eta is artificial?

Yes, exactly, so it is integrating, look, what is it you are doing, it is not any random force, to the random force on this particle, okay. So there is a characteristic of the particle that has come in, okay. And it is not surprising, it is not surprising at all for the following reason. Go back to the original Langevin equation, I have not yet come to the 2<sup>nd</sup> fluctuation dissipation theorem which I will in a second but it is not surprising because after all when you say  $m \dot{v}$ , this was the original Langevin equation, so  $m \dot{v} + m \gamma v = \eta(t)$  which was white noise, right.

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Let  $t \rightarrow 0^+$  in  $m$

$$\langle v(t_0) \eta(t_0) \rangle_{eq} = m \int_0^\infty dt \gamma(t) \langle v(0) v(t) \rangle_{eq}$$

LE

$$m \dot{v} + m \gamma v = \sqrt{\Gamma} \zeta(t)$$
$$\Gamma = 2m \gamma k_B T$$

We wrote this as square root of gamma times Zeta of t, where this was unit delta, you need correlation, delta function as the correlation, then one would think, look, this is completely arbitrarily specified, this is a property of the medium but the 2 are related. You know the not independent of each other, you know gamma must be equal to 2m gamma K Boltzmann t, okay. And we also discovered that even though you started by saying when we took averages that v was uncorrelated with Eta at the same instead of time, after you computed things, you discovered that was not really true, that v of t0, Eta of t0 was not 0 identically. I

Even this is a coupling, right, between gamma and... (0)(41:44)

Exactly, so there is the coupling back here, so this is the consistency condition, there is a reaction on the medium.

This is true for same time (0)(41:56) but it is going for all  $t$  greater than 0.

Yes yes but that is because this one is also sitting here all the way up. So this is the only way in which you can have this consistency.

This is backward correlation, it is not forward...


It is a backward correlation because this  $t$  is increasing out here.

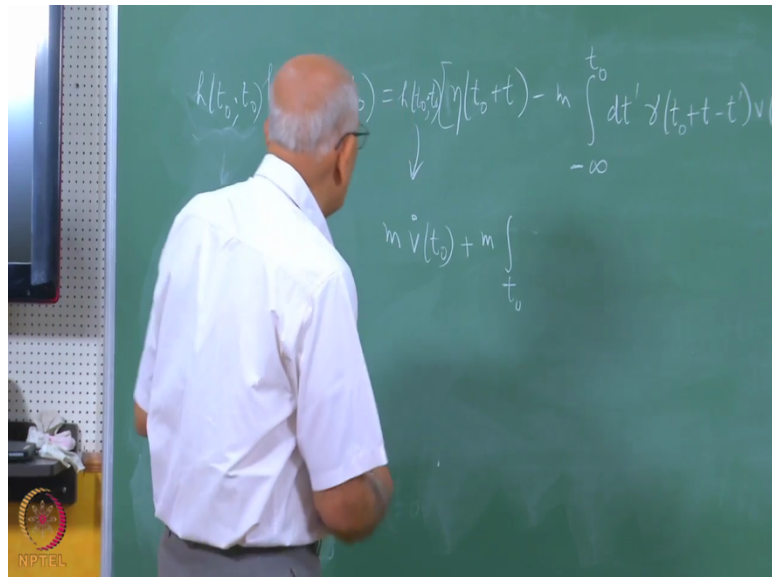

(0)(42:17)


No. No it looks counterintuitive but it is not, it is completely consistent, okay. So the separation we had in our mind that this random force is  $K$  I said that very glibly that random force due to molecules, it will not get affected by the motion of this particle and so on but it is affected. It is the random force on this particle and it has to be self consistent and determined, okay. We will see this more dramatically in a second, there is a coupling, this is indeed a coupling but we are trying to make this coupling consistent with causality, stationarity and so on, okay.

So this is, this is a relation which says that the velocity and the force, so-called random force at the same instant of time but not uncorrelated with each other, the equal times correlation is some integral. This is a number by the way, this is a pure number out here because it has got no dependence or anything, it is a pure number and that is the value that the value of this guy. In a sense it is measuring the strength of this but let us see it more dramatically. You could do the following now, you could say all right, let us start with, let us turn this around and start with... So let us keep that aside. So we know that there is a correlation between the  $V$  and  $\eta$ , keep that in mind.

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$$h(t_0; t_0)h(t_0+t; t_0) = \eta(t_0+t) - m \int_{-\infty}^{t_0} dt' \delta(t_0+t-t')v(t')$$



$$h(t_0; t_0)h(t_0+t; t_0) = h(t_0; t_0) \left[ \eta(t_0+t) - m \int_{-\infty}^{t_0} dt' \delta(t_0+t-t')v(t') \right]$$
$$m \dot{v}(t_0) + m \int_{t_0}^{\dots}$$


$$\int_0^{\infty} dt e^{i\omega t} \langle h(t_0; t_0)h(t_0+t; t_0) \rangle = \langle h(t_0; t_0) \left[ \eta(t_0+t) - m \int_{-\infty}^{t_0} dt' \delta(t_0+t-t')v(t') \right] \rangle$$
$$m \dot{v}(t_0) \rangle$$


And now let us turn this around and say what was the definition of this  $h$  of  $t_0 + t$ ,  $h$  of  $t_0 + t$  was equal to  $\int_{-\infty}^{t_0+t} dt' \gamma(t_0+t-t') v(t')$ , okay that was my definition here. Now let us multiply this by  $h$  of  $t_0$  with  $t_0$ . Just as I premultiplied by  $v$  of  $t_0$   $\gamma$  multiply with  $h$  of  $t_0$ . When I found the velocity autocorrelation, I took the  $V$  of  $t_0 + t$ ,  $V$  dot, that does not matter from the Langevin equation, pre-multiplied by  $v$  of  $t_0$  and took averages. Now I want to find the correlation of noise with itself. So I have  $h$  of  $t_0 + t$  and  $h$  of  $t_0$ , we multiply this side.

That is equal to this term here but out here for this term, this fellow here, I can substitute from the Langevin equation. I have done so for this quantity, so it must be multiplied by  $h$  of  $t_0$ ,  $t_0$  on this side but what is this fellow, this guy here? I go back to the Langevin equation and it is equal to  $m$  times  $v$  of  $t_0$   $V$  dot,  $-$ ,  $+ m$  times an integral from  $t_0$  to what?  $T_0$ , that portion went away, right, so it is  $m$  times  $v_0$ ,  $m$  times  $v$  of  $t_0$  dot. I play the same trick as before, I take this, so I take averages like that over this whole thing, substituting this for that in here, multiplied by  $e$  to the  $i \omega t$ , and integrate over  $t$  from  $0$  to infinity, over  $dt$ .

But all the quantities on the right-hand side I do the same manipulation as before, integration by parts, use this relation between  $v$  and  $\eta$  because that is going to be important, right and simplify. This is a slightly messier calculation than the previous one. There are going to be terms proportional to  $m$  square, etc., simplify the whole thing. We use the fact that we already know what  $\mu$  of  $\omega$  is. We know the integral over the velocity correlation is  $\mu$  of  $\Omega$  and that is  $1$  over  $\gamma$  bar of  $\Omega - i \omega$  with an  $m$ .

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$$\bar{J}(\omega) = \frac{1}{m k_B T} \int_0^{\infty} dt e^{i\omega t} \langle \eta(t_0) \eta(t_0+t) \rangle$$

(II FD Theorem)

NPTEL



$$\bar{\gamma}(\omega) = \frac{1}{mk_B T} \int_0^{\infty} dt e^{i\omega t} \langle \eta(t_0) \eta(t_0+t) \rangle_{eq}$$

$$\mu(\omega) = \frac{1}{k_B T} \int_0^{\infty} dt e^{i\omega t} \langle v(t_0) v(t_0+t) \rangle_{eq}$$

(I-F) theorem  
(I-F)

So use that and finally after simplification, after, which I am going to leave to you, you get the following result. You get  $m$  times  $\bar{\gamma}$  of  $\omega$  equal to  $1$  over  $k_B T$  integral  $0$  to infinity  $dt$  of  $\langle \eta(t_0) \eta(t_0+t) \rangle$ .

That is the 2<sup>nd</sup> fluctuation.

That looks like a fluctuation, it looks like one of these theorems, which says that one-sided Fourier transform of some correlation is some, this  $m$  is not the mobility but the memory kernel itself on this side. But you can say now look that is not simple enough because this still involves the velocity, it does not involve the noise  $\eta$  alone. This  $h$  is not the stationary noise, that is why you need both arguments here. But if you use the properties of this correlator which we derived from this equation, then one can show that this quantity is exactly equal to  $\langle \eta(t_0) \eta(t_0+t) \rangle$ . Now, it is equal to it, it is equal, period. This portion is exactly equal to this.

So you end up with this relation which says  $\bar{\gamma}$  of  $\omega$  equal to  $1$  over  $m k_B T$  integral  $0$  to infinity  $dt$   $e^{i\omega t} \langle \eta(t_0) \eta(t_0+t) \rangle$ . This is the 2<sup>nd</sup> fluctuation theorem, just for comparison let us write the 1<sup>st</sup> one down, the 1<sup>st</sup> one was  $\mu$  of  $\omega$  equal to  $1$  over  $m$ , sorry  $1$  over  $k_B T$  integral  $0$  to infinity  $dt$   $e^{i\omega t}$  the output process  $v$  of  $t_0$ ,  $v$  of  $t_0+t$ . So the dynamic mobility which measures the response of the system to an external force in linear response theory is this one-sided Fourier transform of this correlator of the output process.

On the other hand this is specific with the Langevin model, this more general in linear response theory because in the Langevin model we explicitly find the model for the velocity

is all the equation of motion, random equation. It says that the correlation of the force, stationary force is not arbitrary for it must be related to the friction kernel, memory kernel in this fashion. This is equivalent of the fluctuation dissipation theorem, the capital gamma etc. Because how do you recover that? By saying that this memory kernel is just a delta function, then this gamma bar, this gamma of  $t - t'$  is just delta of  $t - t'$  times the constant gamma.

This fellow would become gamma out here, this would be delta function but half a delta function because you are integrating 0 to infinity, so you will get half here and capital gamma on top and you get capital gamma is  $2 m \gamma$  little K, little K Boltzmann  $t$  we should give you the original theorem back again, okay. But this is the general version of it. And what is the big lesson it is telling us, it is saying that nice in the generalised model, this Eta here is stationary, fine, but it cannot be delta correlated because if it is delta correlated omega dependence. And then this side is omega dependent, so it is not consistent.

So this is immediately telling you that the moment you introduce a memory kernel, the noise cannot consistently be white noise, it has got to be coloured noise, and there is a correlation time. And what is that correlation time? You define the correlation time by putting omega equal to 0 here, right and then dividing by the mean square value. So it gives you a quantity of dimensions time and that in this case is just the memory kernel. So little gamma of  $t$ , little gamma of  $t dt$  from 0 to infinity is going to specify for your correlation time.

Correlation in the force somehow describes the memory and velocity (( ))(53:56).

Yes, exactly, then it says in the generalised model you cannot independently, just as in the original model you cannot independently specify little gamma, the friction constant and the strength of the white noise, you can independently do it, in exactly the same way the more general statement is you cannot specify the memory kernel and the random forces correlation independently, they are related in this fashion, it is a consistency check on the model. And when that is satisfied, you now in model buildings you do what you like, you sell a random force which is stationary, and then say it is consistent with a Langevin equation with the specific memory kernel, not any old memory kernel.

On the other hand in modelling, empirically, if you discover that this friction in model by a memory kernel which is maybe an exponential of some function of time decreasing functions, that fixes for you so correlation of the noise. The manner in which this correlation behaves, it

fixes for you through these relationships here. And that is what is more generally done, it depends on the model building that you have in mind. So you could say all right, this thing here is exponentially correlated with some correlation time  $\tau$ , single exponentially correlated.

That is the 1<sup>st</sup> thing you do, it is a markov process, we will assume it is Gaussian, we will assume it is stationary, I mean to say is not delta correlated what exponentially correlated, maybe a non- (( ))(55:29) process. Then it has a correlation which is exponential in time, that fixes for users memory kernel. It fixes  $\gamma$  bar of  $\omega$  from which you can find what sort of  $\gamma$  of  $t$  you should have had in order to have this. So that is an interesting exercise, simple exercise. Take this to be an exponentially correlated,  $e^{-t/\tau}$ , then figure out what is this guy going to be.

And therefore what is  $\gamma$  of the going to be memory kernel, that would be the simplest model in this instance, okay. So this kind of brings us to an end of this part of the program, we will, there are some loose ends to be tied up, I will mention them to the extent and I can remember. We will talk about them tomorrow and then go on from there.