

Physical Applications of Stochastic Processes
Prof. V. Balakrishnan
Department of Physics
Indian Institute of Technology-Madras

Lecture - 12
Langevin Dynamics (Part 1)

So let us continue with our study of the Fokker-Planck equation and for the next lecture or two we are going to talk about physical model of particle in a fluid undergoing random kicks due to the molecular collisions and at the same time possibly be subject to some external force but let us look at the case first where you just have free diffusion of a particle in a fluid. I would not specify at the moment how big this particle has to be.

We will come a little later and distinguish between different time scales and we will see under what conditions this whole thing applies but right now we take a very naïve approach and say alright suppose I have a small particle in a fluid and this is undergoing collisions, random collisions due to the agitation, thermal agitation of the molecules of the fluid. What kind of equation of motion can we write for this system here?

Recall that we made a correspondence. We said we stated that there was a correspondence between certain kinds of stochastic differential equations describing diffusion processes and the corresponding Fokker-Planck equation. So what I am about to do now is a physical example of that in a very simple case in which the drift term will be a linear, linear in the variable. So let us look at this in little bit of detail.

Again, you refresh your memory. I said that if you had a stochastic equation in some random variable x , I use the symbol x but now for this application I am going to use x for the Cartesian coordinate of the particle. So let us be neutral and call it ψ or something like that.

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$$\dot{\xi} = f(\xi) + g(\xi)\eta(t)$$

Gaussian
white noise

$$\frac{\partial}{\partial t} p(\xi, t | \xi_0)$$

$$= -\frac{\partial}{\partial \xi} [f(\xi)p] + \frac{1}{2} \frac{\partial^2}{\partial \xi^2} [g^2(\xi)p]$$

$\langle \eta \rangle = 0$
 $\langle \eta(t)\eta(t') \rangle = \delta(t-t')$

So if you have a stochastic equation of the form $\dot{\xi} = f(\xi) + g(\xi)\eta(t)$ and this was white noise, Gaussian white noise in fact satisfying $\langle \eta \rangle = 0$ and the autocorrelation $\langle \eta(t)\eta(t') \rangle = \delta(t-t')$. Under those conditions, this was equivalent to a Fokker-Planck equation for the conditional density of this ξ with some initial condition of the form $\delta(\xi - \xi_0)$ at $t = 0$.

Say this is equal to $-\frac{\partial}{\partial \xi} [f(\xi)p] + \frac{1}{2} \frac{\partial^2}{\partial \xi^2} [g^2(\xi)p]$. This was the Fokker-Planck equation whereas that was the stochastic differential equation for this random variable ξ . Now let us look at some the simplest example. We even wrote this down.

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$$\dot{x} = \sqrt{2D} \eta(t) \Leftrightarrow p(x, t | x_0) \text{ satisfies}$$

$$\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2}$$
~~$$\dot{v} = \frac{\sqrt{\Gamma}}{m} \eta(t) \Rightarrow v(t) = v_0 + \frac{\sqrt{\Gamma}}{m} \int_0^t dt' \eta(t')$$~~

$$\overline{v(t)} = v_0 + \frac{\sqrt{\Gamma}}{m} \int_0^t dt' \overline{\eta(t')} = v_0$$

$$\overline{v^2(t)} = v_0^2 + \frac{\Gamma}{m^2} \int_0^t dt_1 \int_0^t dt_2 \overline{\eta(t_1) \eta(t_2)}$$

I said if the position of a particle undergoing diffusion on a line satisfies \dot{x} equal to square root of $2D$ times η of t . This immediately implied that $p(x, t)$ with some initial point x not satisfies the diffusion equation $\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2}$. That was the correspondence we had made. But now let us be a little more detailed and ask look whatever force the particle is subject to is going to cause an acceleration.

So let us say that the equation of motion that you should write down for this particle moving in one dimension or one Cartesian coordinate of it. Let us call the velocity v and we should really say well $m \dot{v}$ that is the acceleration should be equal to whatever force it is subject to and in the simplest instance you would say this force is a completely random force. It is due to all these molecular collisions. I do not know anything about it.

So in the simplest instance you would say this is equal to η of t itself in this fashion but of course dimensional reasons and as well as the fact that this η of t need not have unit delta function strength but some arbitrary number. So let us call it equal to square root of some γ times η of t where this is some constant which we may or may not be able to determine in a self-consistent way to start with okay. Now what does this imply.

This immediately implies a Fokker-Planck equation for the for the quantity of interest namely the velocity distribution function density function but instead of writing this down let us take this

stochastic equation seriously and ask whether it makes any physical sense or not before we do this. Now, this will of course mean \dot{v} is this and you can formally solve this equation. This is a stochastic differential equation but it is very simple and we can formally in principle we can solve it.

So this will of course immediately imply that v of t equal to some initial condition whatever it be some initial value $v_{\text{not}} + \text{square root of } \gamma \text{ over } m \int_0^t dt' \eta$ of t' prime okay. Now remember our physical context. We have a fluid. We imagine a fluid in which we are looking at one Cartesian component of the velocity of some tagged particle and this fluid is taken to be a thermal equilibrium at some temperature t okay.

Then it says the velocity is equal to this, the instantaneous velocity but what we are interested in is averages always. So what is the average value of v of t . Now when we say averages I got to be a little careful. Average over what ensemble? We have already specified an initial condition. So it is an average over all those particles whose initial value of the velocity is given to be some number v_0 right. It is not an average over all possible initial velocities as well.

That will come a little later. So we have 2 pluses of averages. One is over a sub collection of particles whose initial velocity is v_{not} and then we say look let us average over v_{not} as well over some initial distribution or since I said already that the fluid is in thermal equilibrium at temperature t over say the Maxwellian distribution at temperature t . That is what I should do really.

So to distinguish between these 2 things, these 2 kinds of averages let me put an overhead bar to denote averages over a given initial condition v_{not} and then a subsequent average over these v_{not} s will give me a final average for which I will use angular brackets. So this will immediately imply that \bar{v} of t bar is equal to well average of v_{not} but v_{not} is a deterministic given number of course v_{not} plus the average of this integral but the integral is essentially a summation over different values of η of t' prime.

So since 2 different sums commute in either order this overhead bar is the same as putting it inside the integral right. So this becomes plus square root of gamma over m integral 0 to t dt prime eta of t prime an average over all realizations of this eta of t prime. Now the physical assumption is that you are looking at one particle that is with a small number of degrees of freedom inside a huge collection of particles in thermal equilibrium.

And the heat bath which is providing the fluctuations on the of the velocity of this particle that is not going to be affected by what this particle does. So whether I fix the initial velocity of the particle or not is not going to affect the average value of the random force at all. So as far as eta is concerned whether I put a bar or take a full average it does not matter at all. We have already assumed that it is got 0 average. It is a Gaussian white noise.

So this quantity is actually 0, this integral and this becomes equal to V not since the average value of this random force is 0 in any case okay. So, so far so good. It just says the average value remains this which is physically expected. You are saying that the force can be as much as much to the right as to the left and the average velocity component is 0, the average is 0. It remains whatever it was initially. But what does this tell you? What is v square of t?

If you compute the square of the velocity then I have to find the square of this guy and find the average. So it is evident that there is a term which is v not square and then there is twice v not times this and then I want to take an average. So let us put that average in there. There is nothing to average here and then I have v not times eta of t prime averaged but v not comes out of the averaging and it is just the average of eta of t prime again.

So the cross terms average again goes to 0 but then I have a term which is plus gamma over m square when I square this term here and then I have to take 0 to t dt let us call it dt 1 so that I do not mess around with primes and then again 0 to t dt 2 eta of t 1, eta of t 2 with an average out there. But that quantity is not the product of averages because eta is a random variable with a delta correlation, this guy.

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$$\overline{v^2(t)} = v_0^2 + \frac{\gamma}{m^2} \int_0^t dt_1$$

$$= v_0^2 + \frac{\gamma t}{m^2}$$

So I have to put that delta correlation there and then it says that v square of t average is v not square plus γ over m square. An integral over this with delta function, did I put the, yes a delta of $t_1 - t_2$ in here okay and that contributes as long as $t_1 = t_2$ and that always contributes for all values of t_1 between 0 and t and that is easy to see because if you draw a little picture, here is t_1 , here is t_2 and in each case you are going to integrate from 0 to t in this fashion and the delta function constraint tells you t_1 equal to t_2 out there.

So it says if you do the t_2 integration first which is the way I have written it here then it is clear that no matter what t_1 I have between 0 and t there is a value of t_2 as you scan this at which the delta function fires. So I can therefore remove the t_2 integral and replace wherever t_2 appears I replace it with t_1 okay and that gives you 0 to t dt_1 and this integral is gone, the t_2 integration is gone which therefore gives v not square + γt over n square.

So it gives us this rather unphysical result which says that the square of the average value of the square of the velocity increases without bound as t increases okay. If you identify the temperature with $\frac{1}{2} m v^2$ average this means that if you leave this particle untouched, you keep a beaker of fluid then the average kinetic energy of any particle in there increases without bound okay and the effective temperature increases without bound.

So it is completely unphysical, complete. So this cannot be right. This model cannot be right. This equation cannot be right because there is nothing else that can go wrong here okay. You might say oh this perhaps this is unphysical perhaps this is not correct. I should not use a delta correlation. I should use an exponentially decaying correlation with some finite correlation time but even if you did that you would still get an unphysical answer and I leave you to check this out.

Even if I took this quantity to be some $e^{-t/\tau}$ for some very small value of τ and computed what this number is explicitly you would still get an unpleasant answer here. It would still be unphysical and this is not right. So the only thing that can possibly be incorrect would be the initial model itself. This model cannot be right okay. And whatever I left out of it, I have left out the fact that there is a systematic component in the random force.

This force η is completely random uncorrelated and so on. That is fine, but however if this tagged particle starts moving in one direction at a velocity higher than the average velocity it gets hit back by the friction in the problem, by the viscosity. The very same molecules that cause fluctuations in its velocity will also damp out these fluctuations by having more collisions from the front than from the back if you are moving in this direction okay. So this means that I have to modify this model and this is not correct and let us see what the correct model is.

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Handwritten mathematical derivations on a chalkboard:

$$\dot{x} = \sqrt{2D} \eta(t) \Leftrightarrow p(x,t|x_0) \text{ satisfies}$$

$$\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2}$$

$$\dot{v} = -\gamma v + \frac{\sqrt{\Gamma}}{m} \eta(t) \quad (\text{Langevin eqn.})$$

$$v(t) = v_0 e^{-\gamma t} + \frac{\sqrt{\Gamma}}{m} \int_0^t dt' e^{-\gamma(t-t')} \eta(t')$$

$$\overline{v(t)} = v_0 e^{-\gamma t}$$

The correct model would be $m \dot{v}$ equal to there is an η of t so there is a square root of γ times η of t that part certainly exists that was the original model but there is a portion which says there is a viscous damping and for small velocities Newton's law viscosity tells you the viscous drag is proportional to the force but with an opposite sign right. So this is equal to minus $m \gamma v$ plus this but γ is a quantity which has dimensions of 1 over time so that it matches this on this side. It is a friction coefficient.

I took out the m explicitly because it is easier that way right. So this is my model. This is by the way the simplest example of what is called a Langevin equation where this is again Gaussian white noise but there is a systematic component to the random force. A model, again it is a model and we have to see whether it makes any physical sense or not. Now look at what is going to happen. We repeat exactly what we did before and I divide through by m .

Then average $v(t)$ equal to the solution now, by the way we can write down the solution first, let us do that. So the solution is $v(t) = v$ not but that is multiplied by e to the $-\gamma t$ because there is this term here $+$ square root of γ over n integral from 0 to t dt' prime e to the $-\gamma t - t'$ prime η of t' prime; because this is of the form dy over $dx + p$ of x times $y = q(x)$.

And you have the standard formula for solving a first order differential equation of that kind, an inhomogeneous equation and this gives you the explicit solution. That is already telling us we are on the right track because it immediately tells us that v of t average is v not e to the $-\gamma t$ because whether this factor is present or not when you take the average of η it is again 0 so you have this feature here.

Already getting us on the right track because it says that if t becomes very large compared to γ inverse this says the average velocity goes to 0 which is exactly what you would expect. There is no reason why the memory of the initial condition should remain forever when you have viscosity in the system it is going to be damped out. So this is a good feature that it exponentially vanishes as t increases okay and what does the square do. It does exactly what happened earlier except for that extra factor.

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$$\begin{aligned}
\overline{v^2(t)} &= v_0^2 e^{-2\gamma t} + \frac{\Gamma}{m^2} \int_0^t dt_1 \int_0^t dt_2 e^{-\gamma(t-t_1)} e^{-\gamma(t-t_2)} \delta(t_1-t_2) \\
&= v_0^2 e^{-2\gamma t} + \frac{\Gamma}{m^2} \int_0^t dt_1 e^{-2\gamma t} e^{2\gamma t_1} \\
&= v_0^2 e^{-2\gamma t} + \frac{\Gamma}{2m^2\gamma} (1 - e^{-2\gamma t}) \\
&= \frac{\Gamma}{2m^2\gamma} + \left(v_0^2 - \frac{\Gamma}{2m^2\gamma} \right) e^{-2\gamma t} \xrightarrow{t \rightarrow \infty} \frac{\Gamma}{2m^2\gamma}
\end{aligned}$$

So this is now v not square e to the $-2\gamma t$ because that factor remains $+\gamma$ over m^2 once again $\int_0^t dt_1 \int_0^t dt_2 e^{-\gamma(t-t_1)} e^{-\gamma(t-t_2)}$ and then an $\delta(t_1-t_2)$ whose correlation average value is $\delta(t_1-t_2)$. Exactly the same way as before we can now do the t_2 integration and replace t_2 with t_1 everywhere.

So this integral is easy to do. It is v not square e to the $-2\gamma t + \gamma$ over m^2 $\int_0^t dt_1$ and then there was already an e to the $-2\gamma t$ sitting here and then you had e to the $\gamma t_1 e$ to the γt_2 but now t_2 is equal to t_1 right. So e to the $2\gamma t_1$ and that is the integral; e to the $2\gamma t$ comes out of the integration and then you have to do this fellow here.

So this is v not square e to the $-2\gamma t + \gamma$ over $2m^2\gamma$ because when I do this integration that factor comes out downstairs and then e to the $2\gamma t_1$ from 0 to t here. The first term will cancel out and give you a 1 and the second one gives you e to the $-2\gamma t$ because this integration is e to the $2\gamma t_1 - \gamma t - 1$. So that is the result out here and this has no exponential blowup, this linear blowup.

This does not increase unboundedly as t goes along because these exponential factors cancel and go to 0 and it looks like it is going to some constant which is what you should expect because if you are in thermal equilibrium it should remain fixed in thermal equilibrium right. You could

also rewrite this as equal to $\frac{\gamma}{2m} \frac{d}{dt} \langle v^2 \rangle - \frac{\gamma}{2m} \langle v^2 \rangle$.

This is for a given v_0 for some over the sub ensemble of particles with a given v_0 this is what you get and now what happens to it as t tends to infinity. Well, $\langle v^2 \rangle$ tends to infinity. This becomes $\frac{\gamma}{2m} \langle v^2 \rangle$, independent of the initial condition. It is forgotten the initial condition and it tends to some fixed limit out there. So remember that this average is being taken over a conditional density. The condition being that the initial condition is v_0 .

So it is being taken really that average is being taken over this $p(v, t)$ given a v_0 . This thing is given to you. We have not yet found this. We have not yet even written down the Fokker-Planck equation for this process but already it is telling us that the mean square value has this structure better have this structure from the Langevin equation itself and now if you insist that in equilibrium this whole thing is independent of time as t tends to infinity.

Now if you insist that this should be true at all instance of time because this fellow here is in thermal equilibrium. Another way of saying it is let us compute what $\langle v^2 \rangle$ average is over a full average. So I compute $\langle v^2 \rangle$ of t and what can that be. How do I compute it from $\langle v^2 \rangle$ bar of t . I should now average over all v 's right. Over what ensemble should I average this? It is in thermal equilibrium; so over the Maxwell distribution right.

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$$\langle v^2(t) \rangle = \int_{-\infty}^{\infty} v^2(t) p(v_0) dv_0$$

$$\left(\frac{m}{2\pi k_B T} \right)^{1/2} e^{-mv_0^2/2k_B T}$$

$$= \frac{\Gamma}{2m^2\gamma} + \left(\frac{k_B T}{m} - \frac{\Gamma}{2m^2\gamma} \right) e^{-2\gamma t}$$

So I need to compute, I need to compute v square of t equal to integral v square of t bar over p of v not dv not where this thing here is the equilibrium or stationary distribution and that is of course m over $2\pi k$ Boltzmann T to the power half e to the $-mv$ square over $2k$ Boltzmann T in v not. So I have to do the average over this distribution right and then I get v square average here. Let us do that and look at what happens.

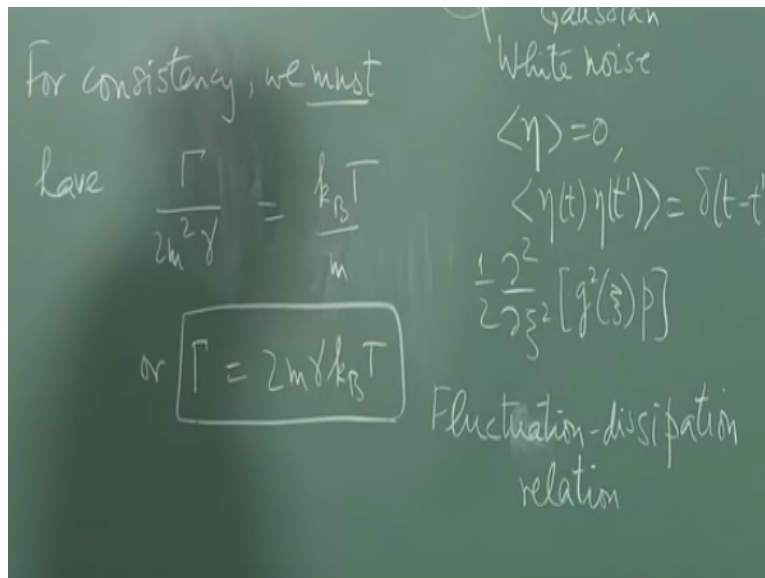
This is equal to, well this fellow is a number, there is nothing to average and p of v not is a normalized distribution so you are back with this, this is got to be as it is. So this is equal to γ over $2m$ square γ plus this quantity is averaged over. You need to average over this definitely but what is the value of v not square average over the Maxwell distribution where the average kinetic energy is half kt . It is only one degree of freedom. That is just a Gaussian.

When once you put that in and do a Gaussian integral you discover that the half mv not square average is equal to half kt right. So v not square average is kt over m . So this immediately tells us this is k Boltzmann t over m - γ over $2m$ square γ e to the -2γ . But this cannot depend on time. The system is in thermal equilibrium right. It cannot depend on time and the only way that can happen is if this is equal to that right.

So if this is equal to that if γ is such that this quantity is equal to that the time dependence goes away because the system is in equilibrium. At no time does half mv square average change.

It remains kT over m because the system is in thermal equilibrium and that is completely consistent with the fact that if this goes away you get exactly kT over m here once again. You need that because if this constant had been different from that constant you are in trouble. The fact that you insist that this should be equal to that automatically gives the right value here also.

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So it says that consistency requires we must have Γ over $2m$ square $\gamma = k$ Boltzmann T over m or capital Γ equal to $2m$ little γ k Boltzmann T . This is required by consistency. Now what does it physically? Well if you go back to the Langevin equation, that equation was \dot{v} equal to $-\gamma v$ with a minus sign equal to $-\gamma v + \text{square root of } \gamma/m \eta$ of t .

Now this measured the viscous damping in the medium, the viscosity in the medium which damped out fluctuations. This measured the strength of these fluctuations how far does it get pushed out in some sense, how strongly does it get kicked and now we are saying that the two are not independent parameters. The larger the viscosity the larger the fluctuations here or conversely the larger the fluctuations the larger the viscosity must be to damp out those fluctuations and maintain thermal equilibrium.

There is therefore a connection between the source of fluctuations and the dissipation in the system okay and this is the first example of it, the simplest example of it. It is called the

fluctuation dissipation relation or theorem if you like in some case. We will come across more further examples of this but this is the simplest of the lot okay. You are already familiar with this in the context of thermal noise in the register, electrical register.

You know if you have an electrical register due to the Brownian motion of the electrons in it voltages are set up at the 2 ends and there is a current which fluctuates and flows in this register and this current you can ask this fluctuating current what is the power spectrum of this fluctuating current. How much is the power carried by it in some given frequency window okay. We will talk about power spectra of noise a little later.

But we know that there is a relationship which connects the dissipation in the register measured by the resistance to this the temperature on the right hand side. So we know that the power spectrum of the fluctuations in the response of the system is related to the resistance multiplied by the temperature and is called the Nyquist relation. This is the Nyquist relation in this context. It is exactly the Nyquist relation for thermal noise or Johnson noise whatever okay.

But physically what it means is the same the same fluctuations that give rise to white oscillations or which give rise to randomness in the velocity are the ones also responsible for the dissipation in the system and there is a consistency condition between the two. You cannot have one unboundedly growing independent of the other in this context. It is required for thermal equilibrium. This is required to maintain thermal equilibrium.

So we will put that in henceforth and now notice that once you put it in this thing here becomes equal to $k_B T$ over m independent of T . So it is already starting to tell us that perhaps this v of T is really going to be a stationary Markov process. We started with that assumption. We already put that in.

I have not explicitly shown it here but we already when we wrote this Langevin equation, to cut a long story short, once you have a Langevin equation of this kind then what it means is if this is a Gaussian white noise, in other words it is a stationary Gaussian delta correlated Markov process then you are guaranteed that this v the output or driven variable is going to be a

stationary Gaussian Markov process but not delta correlated. It will have a finite correlation time. What do you think will be the correlation time in this velocity?

Or what time scale is this thing losing its or what time scale is this average value going to 0. It is going e to the $-\gamma t$. So there is only one such time scale in the problem which is $1/\gamma$. So indeed it will turn out $1/\gamma$ is the velocity correlation time. With that information there which you got there we can actually write down the solution completely to the Fokker-Planck equation fully but we would not quite do that as yet.

We will just see what the Fokker-Planck equation is before we do this. But we are going to use this connection henceforth. Now let us write that Fokker-Planck equation down immediately using this correspondence between the Langevin equation and the Fokker-Planck equation. We will write it down then look at what its solution is. In the meantime we will compute the velocity autocorrelation function.

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The image shows a chalkboard with the following handwritten equations:

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

$$\frac{\partial}{\partial t} p(v, t | v_0) = \gamma \frac{\partial}{\partial v} (v p) + \frac{\gamma k_B T}{m} \frac{\partial^2 p}{\partial v^2}$$

$$p(v, t | v_0) = \delta(v - v_0) \text{ (I.c.)}$$

$$\frac{d}{dv} \left[\frac{k_B T}{m} \frac{dp_{eq}}{dv} + v p_{eq} \right] = 0$$

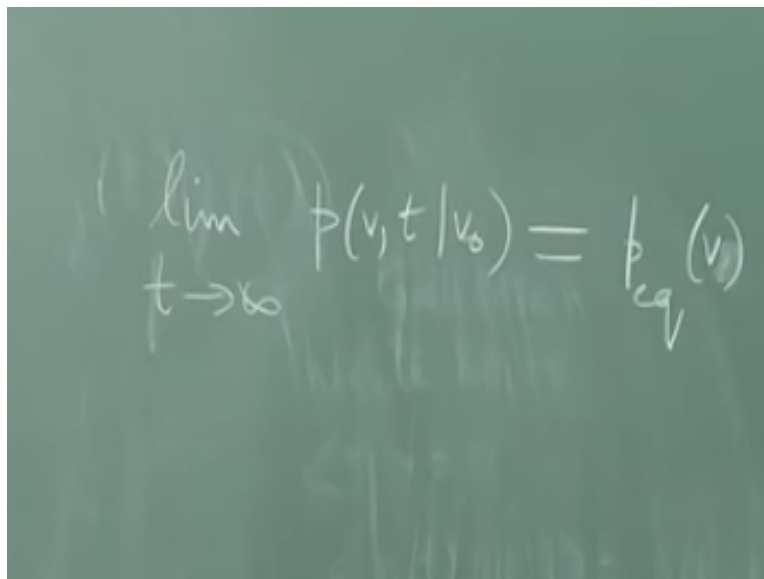
So now that we know what this little γ is this is equal to $-\gamma v$ plus this fellow is $2m \gamma k_B T$ with a square root over m so let us take that over m . That is the Langevin equation where we put in this consistency condition okay and what does that imply at once. It at once implies that $\frac{\partial}{\partial t} p(v, t | v_0)$ must satisfy, the drift term is this but remember by looking at our general rule here it is minus.

So the minus cancels gamma is a constant delta over delta p v times p the same p plus one half the square of this guy and the half this kills that so you have gamma k Boltzmann T over m d 2 p over delta v 2. This was the original Fokker-Planck equation, the first one written down okay. We use the term in general for the second order master equation with up to second derivative but this was the original one with a linear drift term out here okay.

Now of course you can take this equation and ask what is its solution but we need the initial condition and that is obvious here. The initial condition is p of v, t v not equal to delta of v - v not. This is the initial condition, of course. What is the stationary distribution? Is there a stationary distribution in this problem? Unlike the diffusion equation where everything went to 0 the question is, is there a stationary distribution in this problem.

That would be found by putting this equal to 0 and then asking what happens to this stationary distribution. What should you expect as a stationary distribution, the Maxwellian. I should expect the Maxwellian once again right.

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$$\lim_{t \rightarrow \infty} p(v, t | v_0) = p_{eq}(v)$$

Because I should expect that limit t tends to infinity p of v, t v not should be equal to p equilibrium of v. The memory of the initial condition should be raised and you should have the equilibrium distribution again if this process is a stationary random process. So let us see if that

happens. Well, the stationary distribution now does not have any t dependence so I write ordinary derivatives with respect to v and it must be this quantity must be equal to 0.

Of course gamma is a constant so let us get rid of that and then it says d over dv of gamma, gamma goes away, k Boltzmann T over m dp equilibrium over dv plus v times p equilibrium equal to 0. That is the equation that I have right if it exists and it should be normalized to unity and so on. So what does it say? It says this quantity in the bracket should be a constant independent of v.

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The image shows a chalkboard with the following handwritten equations:

$$\dot{v} = -\gamma v + \frac{\sqrt{p}}{m} \eta(t) = -\gamma v + \sqrt{\frac{2\gamma k_B T}{m}} \eta(t)$$

$$\frac{\partial}{\partial t} p(v, t|v_0) = \gamma \frac{\partial}{\partial v} (v p) + \frac{\gamma k_B T}{m} \frac{\partial^2 p}{\partial v^2}$$

$$p(v, t|v_0) = \delta(v - v_0) \text{ (I.c.)}$$

$$\frac{k_B T}{m} \frac{d p_{eq}}{dv} + v p_{eq} = \text{const. (indep of } v)$$

So erase this and write this. I want this p equilibrium to be a normalizable distribution. So p equilibrium must vanish as mod v tends to infinity. That is a necessary condition. Otherwise it is not normalizable. We are going to integrate minus infinity to infinity so the function had better vanish at the end point sufficiently rapidly. I want all moments of this also to be finite. I want the mean square for example to be finite.

I want it to be equal to kt over m right. So you want this also to go to 0. You want this quantity to go to 0 at infinity faster than any power of v because you want all these moments to be finite. Therefore it is derivative also will go to 0 faster than any power of v. The value of the constant therefore is 0 because it is independent of v and when v is plus tends towards infinity the value is 0. Therefore it is the value everywhere okay. Is that is that clear? Okay. So this constant is 0.

Well there is another way to write this down to look at it. You know if you write this Fokker-Planck equation down you can also write it like a continuity equation.

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$$\frac{\partial}{\partial t} p(v, t | v_0) = \gamma \frac{\partial}{\partial v} (v p) + \frac{\gamma k_B T}{m} \frac{\partial^2 p}{\partial v^2}$$

$$\frac{\partial p}{\partial t} + \frac{\partial j}{\partial v} = 0$$

$$p(v, t | v_0) = \delta(v - v_0) \text{ (I.C.)}$$

$$\frac{k_B T}{m} \frac{\partial p}{\partial v} + v p = 0$$

$\xrightarrow{v \rightarrow \infty} 0$

You can write $\frac{\partial p}{\partial t} + \frac{\partial j}{\partial v} = 0$. This is $\text{div } j$ in one dimension with v being the independent variable and what is j it is just this fellow but without the equilibrium, without the equilibrium, time dependent with the time dependent density.

That is the current. This j is the probability current. You do not want this current to be finite at infinity. You do not want any flux at infinity of probability. So this guy must be 0 at infinity but in the case of the stationary distribution it is 0 everywhere for all values of v because it is got to be a constant.

“Professor - student conversation starts” Sir, in that case will it always be 0. Pardon me. In that case scenario at infinity, yes the boundary condition at infinity will be such that this quantity $\frac{k_B T}{m} \frac{\partial p}{\partial v} + v p$ where this is time dependent the conditional density, this will tend to 0 as v tends to infinity mod v tends to infinity. It appears that in every problem it will become 0? Not necessarily. We are going to do finite problems where this may not be 0 okay. **“Professor - student conversation ends”**.

For instance, if I had not a velocity but it is a diffusing particle say and on one side I have a barrier where if it hits that barrier it bounces back and forth and on the other side I have a barrier where it absorbs like a sponge for instance then this boundary condition on the right hand side is not true if it is an absorbing barrier. It is only saying the flux is 0. So it is equivalent to saying that there is a reflecting boundary condition.

But here it is at infinity. So this is a natural boundary condition that this whole thing vanishes at infinity otherwise you do not even have a normalizable density okay. So I used a physical argument to say that I want this equilibrium distribution to have finite moments, in particular I want the finite variance so that I can relate it to the average kinetic energy and so on okay. So this thing immediately tells me if I solve this equation, it is an ordinary first order differential equation.

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$$\frac{\partial}{\partial t} p(v, t | v_0) = \gamma \frac{\partial}{\partial v} (v p) + \frac{\gamma k_B T}{m} \frac{\partial^2 p}{\partial v^2}$$

$$p(v, t | v_0) = \delta(v - v_0) \text{ (I.C.)}$$

$$\frac{dp_{eq}}{dv} + \frac{mv}{k_B T} p_{eq} = 0$$

$$\Rightarrow p_{eq} \propto e^{-\frac{mv^2}{2k_B T}}$$

Of course it immediately says mv over k Boltzmann T times this is 0 and that of course automatically implies that p equilibrium apart from a normalization constant is e to the $-mv^2$ over $2k$ Boltzmann T . All I have to do is to integrate this, move it to the right hand side separate variables and that is it and that is your Maxwellian distribution back again. So we now know that this equation, this Fokker-Planck equation is consistent with the equilibrium distribution. The Maxwellian distribution.

Can we write a solution of this equation down, a time dependent solution which satisfies this initial condition? What key input would you need for that? We should be able to solve this equation, that is one thing, but it is a hard equation to solve. At least it is not a trivial equation to solve and you have to integrate this second order partial distribution equation. It is first order in time, second order in space and so on and so forth. We could do the following.

We could ask what is the mean square value, mean value etc. for a given initial condition which we derived from the Langevin equation but the question is can we do it directly from the Fokker-Planck equation. Yes we can, yes we indeed can. Suppose I multiply both sides by v and integrate. Then this is the rate of change of the mean value of v and that satisfies an ordinary differential equation because if I integrate, I multiply by v all I have to do is to integrate by parts to bring these derivatives out of this p and write it as some averages.

So you can get an equation for \bar{v} and $\overline{v^2}$ by multiplying the v^2 and ask can those be and do they form a closed set of equations or not and in this case they do and you can solve them. So you would have the variance and the mean, the conditional variance and the mean. And then what else would be needed. What assumption would you need to say that that is sufficient?

What kind of process, continuous process are you familiar with in which a knowledge of the variance and the mean is sufficient to write, a Gaussian ρ . If this were Gaussian, that would be it. All higher cumulants are gone and then we could write this solution down explicitly. **“Professor - student conversation starts”** Ya. Sir, isn't it just the fact that there is a correspondence between the Langevin equation and the Fokker-Planck equation and you already use the fact that v is not Maxwellian in the Langevin equation. So isn't this the reflection of that coming back in the. Yes, absolutely. **“Professor - student conversation ends”**.

So this should be consistent. Otherwise, I will be very surprised. But we have not yet said that this is the solution of this we have not said is a Gaussian. That is not so obvious as yet. If it were then this would be immediately true. I could write the solution down explicitly. All I need to know is what does the variance do and what does the mean do and I can write this down

immediately provided it were a Gaussian because I know how to write a Gaussian down once you give me the mean and the variance.

In fact, let us go back there and ask what is the variance of this guy? What does the variance look like? So we need to compute. We go right back at this stage and say we have an expression for v square we got an expression for v average and let us see what the conditional variance looks like. So that is a good exercise to do.

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$$\overline{v(t)} = v_0 e^{-\gamma t}$$

$$\overline{v^2(t)} = v_0^2 e^{-2\gamma t} + \frac{\Gamma}{2m^2\gamma} (1 - e^{-2\gamma t})$$

$$\text{Var}[v(t)] \Big|_{\text{given } v_0} = \frac{\Gamma}{2m^2\gamma} (1 - e^{-2\gamma t})$$

$$= \frac{k_B T}{m} (1 - e^{-2\gamma t})$$

We have v of t bar is v not e to the $-\gamma t$ and we have v square of t average equal to v not square e to the $-2\gamma t + \frac{\gamma}{2m^2\gamma} (1 - e^{-2\gamma t})$ in this fashion. That was what v square is. So the variance v of t so let us say for given v not we should always remember that this is with a conditional ensemble then in a given v not this is equal to this fellow minus this square.

So this cancels out and you end up with $\frac{\gamma}{2m^2\gamma} (1 - e^{-2\gamma t})$. Notice that v not gets rid, is gone. There is no dependence on v not at all. Whatever be the initial v not some given v not the variance of the velocity does not reflect it at all and it is gone. And now if you put in the fluctuation dissipation relation which just says the system remains in equilibrium then this fellow here is $k_B T$ over $m (1 - e^{-2\gamma t})$.

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$$\frac{\partial}{\partial t} p(v, t | v_0) = \gamma \frac{\partial}{\partial v} (vp) + \frac{\gamma k_B T}{m} \frac{\partial^2 p}{\partial v^2}$$

$$p(v, t | v_0) = \delta(v - v_0) \text{ (I.c.)}$$

If $p(v, t | v_0)$ is a Gaussian, then

$$p(v, t | v_0) = \text{Normalization} e^{-\frac{(v - \bar{v}(t))^2}{2 \text{Var}(v(t))}}$$

If I now assert without proof at the moment that the solution to this with this initial condition is a Gaussian, if the solution is a Gaussian is a Gaussian then we can write it down p of v t v not must be equal to e to the power $-v - v$ of t bar square over twice the variance whatever it is divided by times a normalization factor, times this guy right. We can explicitly write it down. Well let us put those factors in and see what it is. So it looks big but it is actually very straightforward.

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$$p(v, t | v_0) = \left\{ \frac{m}{2\pi k_B T (1 - e^{-2\gamma t})} \right\}^{1/2} \exp \left\{ -\frac{m(v - v_0 e^{-\gamma t})^2}{2k_B T (1 - e^{-2\gamma t})} \right\}$$

P of v , t v not equal to now the variance is given to you. It is this guy here. So it is 1 over root 2 pi sigma square and sigma square is here. So it is equal to m over 2 pi k Boltzmann T , $1 - e$ to the -2 gamma t and this guy here and the whole thing is to the power of half one over square root of

$2\pi\sigma^2$ and then e to the power exponent $-\frac{1}{2}\frac{v^2}{\sigma^2}$ not e to the $-\frac{1}{2}\frac{v^2}{\sigma^2}$ that is the mean square σ^2 and that is $\frac{1}{2}m$ and then there is a $2\sigma^2$ is $2kT$ $1 - e^{-\frac{1}{2}\frac{v^2}{\sigma^2}}$.

Looks complicated but it is actually very simple in structure okay. Again you have to check that as t tends to infinity it goes to the Maxwellian the right Maxwellian and indeed it does because as t tends to infinity this goes away the exponent. That goes away, this goes away and you have mv^2 over $2kT$ which is precisely the Maxwellian as it should be. What happens as t goes to 0. It becomes singular. It becomes you got to be very careful taking limits.

It becomes singular because this becomes this t goes to 0 this factor goes away. You have e to the $-\frac{1}{2}\frac{v^2}{\sigma^2}$ not whole square and then this fellow here vanishes. So intuitively it is clear that the only contribution will come from $v = v_0$ so that the numerator also vanishes and it should in fact go to the delta function. So it starts as a singular not square integrable and thinks a singular delta function distribution and then smooth becomes smooth, becomes a Gaussian.

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So in pictures what it does is the following. If I plot v here then initially it is a spike at v equal to v_0 not a delta function spike and asymptotically it is a Gaussian the equilibrium distribution in

velocity and as time increases the mean value which is also the peak in this case shifts gradually to the left like v not e to the $-\gamma t$. So after a little bit of time it looks like this and then the peak shifts it comes down so that the area under the curve remains 1 always.

And it finally settles at the Maxwellian distribution which is just what you would expect this thing would do. And we need to prove of course that the solution is a Gaussian. That takes a little bit of doing but it is not very hard in this context. We can actually compute the other cumulants and discover that they are all 0 and then it is exactly this. There are other ways of solving this and we will not do that right now. We will come back and if time permits we will talk about other ways of solving this equation okay.

Because I want to also introduce another stochastic equation and for the position of a harmonically bound particle which would look exactly like this and you know all about the harmonic oscillator so we can use that knowledge to solve this equation. But you can see physically this is happening. What is remaining in this context is to ask what does the velocity correlation itself do?

What does the correlation of the velocity do and then there are several questions that arise which we will all answer successively namely what about the position of the particle. We made this model, we have solved the equation of motion, we found v of t , we found its average distribution and so on. What about the position and then a much deeper question should we not really look at this particle in phase space namely both x and v together.

And then should we not write down a stochastic differential equation for this quantity and then find this distribution or conditional density in phase space for both position and velocity together. That is really what we should do because then we could put external forces on the particle and write the correct Langevin equation down and solve it in phase space because dynamics happens in phase space so we will do that. We will write.

That will mean a multidimensional, 2 dimensional Fokker-Planck equation but we can do that without much difficulty and we will see how the physics goes in. Just one remark here and that is to find the following quantity. We found already v square of t .

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$$v(t)v(t') = v_0^2 e^{-\gamma(t+t')}$$

$$+ \frac{\gamma}{h^2} \int_0^t dt_1 \int_0^{t'} dt_2 e^{-\gamma(t-t_1)-\gamma(t'-t_2)} \delta(t_1-t_2)$$

Let us do v of t v of t prime and find the average here where t and t prime are both positive numbers but different numbers. I leave this as an exercise to you because you would have exactly the same thing as before. Again, each of these is v not e to the $-\gamma t$ etc., so there is going to be a v not square e to the $-2 - \gamma t + t$ prime. Those will be the first terms.

Then there would be one term where you have a v not term multiplying an η an η of t^2 say and then a v not multiplying η of t^1 . Those averages go away and then you are left with plus γ over m square integral 0 to t $d t_1$ 0 to t prime $d t_2$ in this fashion e to the $-\gamma t - \gamma t$ prime $- t_2$ in this case times η of t_1 , η of t_2 average and that is a delta function. So you have a delta function. Now you got to be careful okay.

So this much is straightforward. But now in removing this delta function to do the integral you have to be a little careful. So let us for example see in pictures what happens. Here is t_1 , here is t_2 . This fellow is integrated up to t . The other guy is integrated up to t prime. Let us suppose t prime is smaller than t . We also have to look at the case where it is larger. But this whole thing is completely symmetrical in t_1 and t_2 .

So we could actually interchange after we find the result. So let us suppose this is t prime and what is the constraint on the integration, the delta function and where does that fire? On a line which is at 45 degrees. So it clearly fires on this line. This is the line $t_1 = t_2$. This is the case t_1 greater than t prime. Otherwise, the rectangle is upwards. Now what does that tell you? It says that you are going to fix the t_1 and scan t_2 .

So you fix the t_1 and you are scanning t_2 in this fashion and of course you hit this delta function. You fix the next t_1 and scan you hit the delta function. And you can do this till a t_1 hits t prime and after that you get 0 as the answer. So the integration gets cut off at this point here. So this thing reduces to integral 0 to t prime $dt_1 e^{-\gamma(t - t_1) - \gamma(t' - t_1)}$, one second.

You can set $t_1 = t_2$ inside the integrand by using the delta function constraint but the t_1 integration is constrained to stop at t prime okay and then you have to do this integral etc., etc. If t were greater than t prime do the t_2 integration later, do the t_1 first. Not surprisingly what answer would you expect finally of this. What kind of function of t and t prime would you expect?

I would expect it to be symmetric under t and t prime getting exchanged with each other right. But we also know that if it is a stationary process I would expect this to be a function of the time difference and I want it to be symmetric. So what would you expect? We will expect $\exp(-\gamma|t - t'|)$. I would expect the answer to be $\exp(-\gamma|t - t'|)$. So show that this fellow reduces to $\exp(-\gamma|t - t'|)$.

It suffices to do it for t greater than t prime and then use this symmetry out here and you will see therefore that the velocity is exponentially correlated okay. Then there is a very powerful theorem which says there is only one process which is Gaussian which is continuous process which is one-dimensional process which is Gaussian, stationary, and Markov and exponentially correlated and that is this process and nothing else.

And various other processes can be reduced to it by changes of variables, reparametrization and so on. So that is the reason why this is worth studying in such great detail in addition to this particular example here okay. So we will take it up from this point and I will point out how we can extend this to phase space and see what exactly where the diffusion approximation comes in and so on. We have got to understand the role of this gamma a little harder, a little better. We will do that. Okay, so we take that up on Monday.