

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

Lecture - 13
Langevin Dynamics (Part 2)

Right, so let us get started. Just to recap where we ended last time, we ended with the statement that if you looked at the velocity of a particle satisfying the Langevin equation, the stochastic differential equation

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The image shows a chalkboard with handwritten mathematical equations. On the left, the Langevin equation is written as $\dot{v} = -\gamma v + \frac{\sqrt{\gamma}}{m} \eta(t)$. Above the noise term $\eta(t)$, there is a note "GWN Noise" with a downward arrow. An equivalence symbol \Leftrightarrow is in the center. On the right, the Fokker-Planck equation is written as $\frac{\partial}{\partial t} p(v,t) = \gamma \frac{\partial}{\partial v} (v p) + \frac{\gamma kT}{m} \frac{\partial^2 p}{\partial v^2}$, with "(FPE)" written at the end.

Which recall was \dot{v} is $-\gamma v + \sqrt{\gamma/m} \eta(t)$ and this was a Gaussian white noise, a Gaussian white noise which was delta correlated and had mean 0. Then we discovered this was entirely equivalent to and this was the statement made, it was entirely equivalent to the Fokker-Planck equation for the conditional probability density of the velocity which was $\frac{\partial}{\partial t} p(v,t)$ given some initial condition v not.

This was equal to $\gamma \frac{\partial}{\partial v} (v p) + \frac{\gamma kT}{m} \frac{\partial^2 p}{\partial v^2}$. This is the Fokker-Planck equation and this was the Langevin equation. This was a stochastic differential equation of the first order with a white noise term here and it said that the corresponding probability density for some specified initial condition satisfied this Fokker-Planck equation, second order partial differential equation. I have put in the fact that the

consistency requires that the system if it is in thermal equilibrium, consistency requires that this quantity be related to little gamma according to gamma = 2 m gamma k Boltzmann T.

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Langevin eqn $\dot{v} = -\gamma v + \frac{\sqrt{\Gamma}}{m} \eta(t)$ $\Leftrightarrow \frac{\partial}{\partial t} p(v, t|v_0)$
 GW Noise $\eta(t)$
 $\Gamma = 2 m \gamma k_B T$
 Soln. to the FPE. The O-U process,

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

We will put that consistency condition in all the time because it implies that the system is in thermal equilibrium. So in a sense what this probability density describes is the approach of some arbitrary initial condition to the equilibrium distribution, the Maxwellian distribution. So it is really telling you something about the manner in which equilibrium is approached and how does it equilibrate. It equilibrates due to collisions, due to thermal collisions right, alright.

So given these 2, they form a pair out here one can also ask what is the correlation of the velocity itself like what is the solution to this Fokker-Planck equation like and so on and I mentioned that the solution itself is a Gaussian once again just as the noise is. So this was the driving force and is Gaussian and so is the output variable v, it is a Gaussian.

And the solution to the Fokker-Planck equation was the Ornstein-Uhlenbeck process which read p of v, t v not equal to there is a normalization factor and then it was a Gaussian which is the exponential of - v - v not e to the - gamma t whole square. That is the mean v not e to the - gamma t the conditional mean/2k Boltzmann T - m times that into 1 - e to the - 2 gamma t and then there is a normalization factor which was m over 2 pi k Boltzmann T 1 - e to the - 2 gamma t.

This to the power half times that exponential. It is a Gaussian, okay in which the mean slowly drifts from v not to 0 and the variance slowly broadens till it hits the value at equilibrium, the thermal equilibrium value of kt over n okay. So we know everything about the velocity from this. Now the question is what is the correlation time of the velocity and this requires, you can do this in many ways.

We could start by the Langevin equation here and ab initio compute the correlation time correlation function autocorrelation by asking what is v of t_1 , v of t_2 averaged over all realizations of this noise and I left that as an exercise to you. We found the mean square and I said now find what the correlation looks like.

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$$\gamma \frac{\partial}{\partial v}(vP) + \frac{\gamma k_B T}{m} \frac{\partial^2 P}{\partial v^2} \text{ (FPE)}$$

$$\langle v(t_1)v(t_2) \rangle = \frac{k_B T}{m} e^{-\gamma|t_1-t_2|}$$

Doob's Theorem: The only ^{continuous,} stationary, Gaussian, exponentially correlated process is the OU-process.

And if you have done that then you know that the expectation value of $v(t_1)v(t_2) = k_B T / m e^{-\gamma|t_1-t_2|}$. So it is exponentially correlated okay. Now there is a little theorem which says and this theorem is due to Doob, it is called Doob's theorem and it says the following. In effect it says that the only continuous, this is a continuous process, this v is a continuous random process.

The only continuous stationary Gaussian process is the Ornstein-Uhlenbeck process. It is a Markov process and it is a the Ornstein-Uhlenbeck process in particular. So note, note the

conditions. The only, the only stationary Gaussian exponentially correlated process, I forgot to say that earlier. So all the conditions are important. You want stationarity. This process is certainly stationary, v is a stationary random process as is the noise here. It is Gaussian.

We see that the distribution function is a Gaussian, this guy here, they are density function. It is exponentially correlated out here. And the only such process is Markov and moreover on top of it the Ornstein-Uhlenbeck process okay. All the conditions are needed. If you drop for instance Gaussian and said what about a stationary Markov process which is exponentially correlated.

The only continuous and this should be continuous because otherwise we have directly before as we have already seen an example of a process which is stationary, which is Markov, which is exponentially correlated and that is the dichotomic Markov process. The dichotomous Markov process had all these conditions but it was a discontinuous process. It jumped from one value to another and certainly not Gaussian or anything like that.

You could ask are they continuous, stationary, non-Gaussian processes which are exponentially correlated and which are Markov also? Yes, this is a whole family of such processes. They are many such processes but they can be classified into 5 families in all just as a matter of curiosity let me mention that these are examples of processes which are continuous, stationary, Markov, and exponentially correlated but which are different from the Ornstein-Uhlenbeck process because they are not Gaussian okay.

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$$p(x, t | x_0) \xrightarrow{t \rightarrow \infty} p(x)$$

If $p(x)$ satisfies $\frac{dp}{dx} = \frac{A(x)}{B(x)} p(x)$

$a_0 + a_1 x$

$b_0 + b_1 x + b_2 x^2$

And such processes are those for which this quantity p of ψ t ψ not this asymptotically as t tends to infinity tends to the stationary probability density p of ψ where this p of ψ satisfies satisfies the equation $\frac{dp}{dx} = \frac{A(x)}{B(x)} p(x)$ and this fellow is at best linear of the form $a_0 + a_1 x$ $p(x)$ we will just use the symbol x for this whole thing and this guy is quadratic.

So consider those processes for which the stationary distribution satisfies this differential equation. These are called Fischer processes where A is at best a linear function of x and B is at best a quadratic function and of course these are constants whose values can be adjusted. So for instance you could have a situation where these 2 go away and this is a constant here and so on. You can easily see the conditions under which this p of x is going to become a Gaussian.

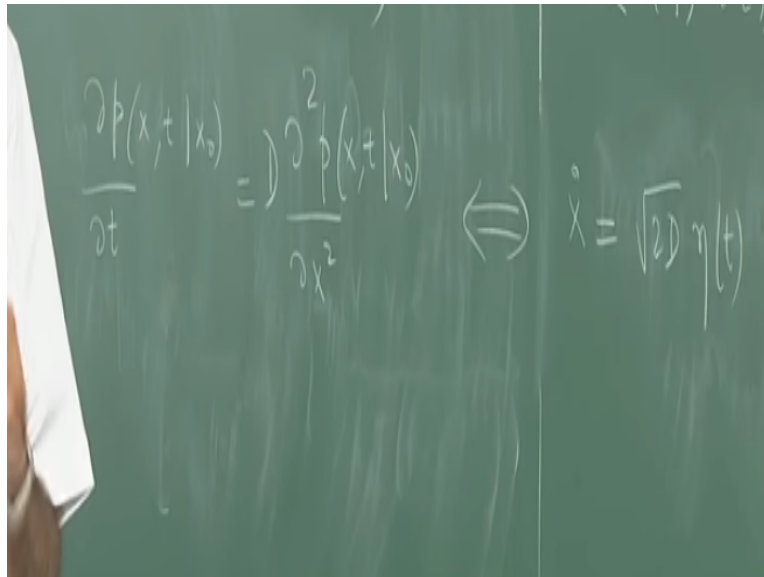
You want to basically have an x there and nothing more and then it becomes a Gaussian. But if you have any of these possibilities you have other kinds of processes, random processes which are continuous, stationary, exponentially correlated, and Markov but not Gaussian and Doob's theorem does not apply in those cases. So there are such processes and they are useful in certain context but we are focusing here on this theorem here.

There are other processes which are discontinuous like the dichotomous Markov process. There is another process called the Kubo-Anderson process and yet another called the kangaroo

process. I will talk about these a little later when we come to some applications and they too will be exponentially correlated in certain special cases but you will see they are not Gaussian and they are Markov but they are not Gaussian. So this is a very useful theorem this guy here. The velocity is exponentially correlated in the Langevin equation okay. Now where does that get us?

What we need to see is what happens to the other piece of information that we know and we will find that out by taking the continuum limit of a random walk itself. So let us look at the position variable of this diffusing particle and we know that the position variable in some limit satisfies its probability density, satisfies the diffusion equation.

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So we have a statement which says delta p, I will use the same symbol p, it should not be confusing for the probability density of the position of x, t given some starting point say x not over delta t = D times d 2 p. This is the ordinary diffusion equation and we know this x of t is also a Markov process continuous. This should imply a stochastic differential equation of what kind. This implies immediately by the rule that we had earlier this should be the corresponding “Langevin equation” in this case should be x dot equal to there is no drift term.

This term is missing and we just have a diffusion term and by this correspondence I talked about it is square root of 2D times eta of t where this again is Gaussian white noise which is unit delta correlated. How does this link up with that. After all x is a position variable corresponding to the

integral of the velocity. So the question is how does this connect up with this result here, in what limit is this result going to go over into whatever this says.

Mind you this says that the velocity this guy here, \dot{x} is the velocity is delta correlated. On the other hand we know from this Langevin equation that the velocity is exponentially correlated right. Under what conditions is that exponent going to become a delta function if γ tends to infinity, if γ tends to infinity or if you like if γt is much bigger than 1 right. So we keep that in the back of our minds that on time scales on which t is much bigger than γ^{-1} it is as if the velocity is delta correlated.

After all what is the graph of this function look like if I plot this correlation function as a function of t and say $c(t) = \frac{k_B T}{m} e^{-\gamma |t|}$. This guy looks like this. It is an $e^{-\gamma |t|}$, looks like that. It is a symmetric function and you can see that when γ becomes very large this function is going to be 0 everywhere unless t is 0. So it is going to become like a delta function spike.

Well, that gives us the hint that says this must be the limit of either γ going to infinity or more physically the situation where t is much bigger than γ^{-1} . Therefore γ^{-1} can be neglected, essentially set to ≈ 0 . So let us see how that comes about, where this comes about from. For that let us go back and compute what is the exact mean square displacement because what is the thing that this implies.

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$$\frac{\partial p(x,t|x_0)}{\partial t} = D \frac{\partial^2 p(x,t|x_0)}{\partial x^2} \quad \Leftrightarrow$$

$$\langle (x(t) - x(0))^2 \rangle = 2Dt$$

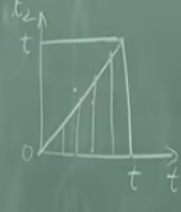
This diffusion equation immediately implies that the variance that the expectation value of x of $t - x$ of 0 whole square this quantity this guy equal to $2Dt$ and that trivial to do because we know the solution of this the free solution of this. It is the Gaussian e to the $-x - x$ not square over $4Dt$. You put that in integrate over x square and you get this result right. This is diffusive behaviour. It says the mean square displacement goes like linearly in the time.

That is pure diffusive behaviour right. Now let us see if that is exact or it is an approximation from what did you talk about so far it is clearly an approximation. So the question is what is the “exact result” in this case and that is easily found because all we have to do is to go back and say **(Refer Slide Time: 16:29)**

$$\langle (x(t) - x(0))^2 \rangle = \int_0^t dt_1 \int_0^{t_1} dt_2 \langle v(t_1)v(t_2) \rangle$$

$$= 2 \frac{k_B T}{m \gamma} \int_0^t dt_1 \int_0^{t_1} dt_2 e^{-\gamma(t_1+t_2)}$$

$$\dot{x} = \sqrt{2D} \eta(t) = \frac{2k_B T}{m \gamma} \int_0^t dt_1 (1 - e^{-\gamma t_1})$$

$$= \frac{2k_B T}{m \gamma^2} \left[\gamma t - 1 + e^{-\gamma t} \right]$$


$X(t) - x(0)$ square this guy equal to $x(t) - x(0)$ is the integral of the velocity 0 to t dt $v(t)$ and I want to square it and then take the average. So it is clear this is equal to 0 to t dt 0 to t dt average value v or t v of t . Full average over the initial condition as well because I have put these bars here okay and we need to compute this number, this quantity okay.

But now we have the explicit expression for this correlation function and this is by definition true. This thing is equal to that by definition, by the very definition of velocity this is true. So this is equal to $k_B T$ over m integral 0 to t dt integral 0 to t dt $e^{-\gamma |t_1 - t_2|}$. Now what is the region of integration? In the variables t_1 and t_2 the region of integration is 0 to t in each case 0 to t in each of these cases right.

This is a symmetric function of $t_1 - t_2$. So if you reverse the sign of $t_1 - t_2$ the function does not change and you are going to integrate over this unit square over this square from 0 to t . In this range the value at any point is equal to the value of the function at this point. It is completely symmetric. So the integral can be written as equal to twice 0 to t dt 0 to t_1 dt_2 right.

So I integrate in t_2 only up to t_1 which means in this function I integrate like this up to that point and that is way I scan it. I fix the t_1 between 0 and t , I integrate in t_2 up to t_1 and I go on to the next value of t_1 and integrate and it gives me this. And now since t_1 is always bigger than t_2 I can get rid of this and write it as $t_1 - t_2$ and I put the factor 2 outside which is equal to twice $k_B T$ over m integral 0 to t dt $e^{-\gamma t_1}$.

And then I integrate $e^{-\gamma t_2}$ from 0 to t_1 . So that is trivial. This is equal to $e^{-\gamma t_1} (1 - e^{-\gamma t_1}) / \gamma$. But this I can write as $1 - e^{-\gamma t_1}$, so which is equal to twice $k_B T$ over $m \gamma$ and then I have to do this integral which of course is equal to t the first term is t and then this minus cancels against that so it is a $1 - e^{-\gamma t}$. That is the integral right.

So let us pull out this γ square here. I will write this as $\gamma t - 1 + e^{-\gamma t}$. That is the exact expression for the mean square displacement for a particle obeying the

Langevin whose velocity obeys the Langevin equation. What does it do for very small gamma, for small t? This is really not a very good model for t much less than gamma inverse.

But is a good model for t of the order of and bigger than gamma inverse certainly it is a good model. What does it do? Just for fun, what does it do for t much less than gamma inverse. So gamma t tending to 0 say. What is the leading term? Well, I have to expand this; the 1 cancels, the gamma t cancels. So you are left with gamma square t square over 2! right.

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The image shows a chalkboard with the following handwritten derivation:

$$\langle (x(t) - x(0))^2 \rangle \xrightarrow{\gamma t \rightarrow 0} \frac{k_B T}{m} t^2$$

$$= \langle v^2 \rangle t^2$$

$$\xrightarrow{\gamma t \gg 1} \frac{2 k_B T}{m \gamma} t$$

$$\Rightarrow D = \frac{k_B T}{m \gamma}$$

So this becomes $x(t) - x(0)$ whole square is equal to this whole thing and this tends as gamma t tends to 0 the leading behaviour is $k_B T$ over m the 2 cancels with the 2!, the gamma square cancels and then t square right which is of course equal to v square in thermal equilibrium t square because the mean square velocity is in a fluid in thermal equilibrium at temperature t this is equal to precisely $k_B T$ over m because half $m v$ square must be half $k_B T$ by the equipartition theorem.

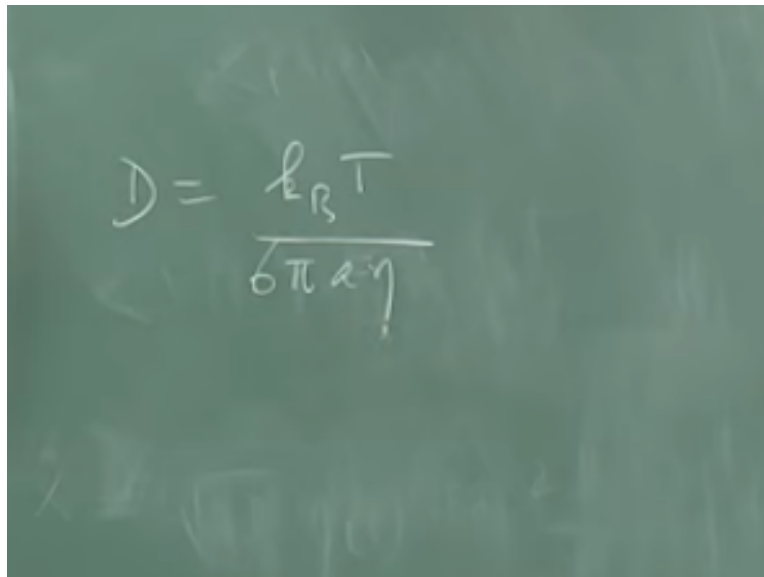
So this is certainly true from the Gaussian. So v square average is found by averaging over the Maxwellian distribution and it gives you this. In other words the root mean square displacement is the root mean square velocity multiplied by the time. It is almost ballistic but with this effective velocity which is a root mean square velocity as you would physically expect right but what is interesting here is a long time limit.

So what happens to this as γt tends to infinity, much greater than 1. What happens in that limit? Well, this term is certainly negligible, that is negligible. This guy is becoming extremely large. So you end up with and one of the γ cancels so it is twice $k_B T$ over $m \gamma$ times t but that is precisely the result we got from the diffusion equation which said that the mean square displacement goes like twice the diffusion constant times t .

You get exactly the same thing and now as a bonus you get a formula for the diffusion constant. Earlier, the diffusion constant and the diffusion equation was an input. It was just a parameter you put in. But now you have related it to a microscopic parameter. So this implies, this thing implies D is $k_B T$ over $m \gamma$. That is a fundamental result.

This is the result that was used by Einstein to determine Avogadro's number in his early work on Brownian motion because what he did was to argue that if you looked at these particles, spherical particles of radius a or something like that then $m \gamma$ times v is a retarding force that must be by Stoke's law equal to $6 \pi a \eta v$ right.

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A photograph of a chalkboard with the equation $D = \frac{k_B T}{6 \pi a \eta}$ written in white chalk. The chalkboard is dark green and has some faint, illegible markings in the background.

So that comparison immediately tells you that D is $k_B T$ over $6 \pi a \eta$. Of course this quantity here is the gas constant divided by Avogadro's number. So it gives you a formula for Avogadro's number if you know all the other parameters in the system. Does this mean by the

way that the diffusion constant in a fluid is directly proportional to the temperature? You would expect things would diffuse faster at higher temperatures right.

Would it go linearly? What would it do? The viscosity is very strongly dependent on the temperature, by the Arrhenius formula. So it increases much more rapidly than that. So there is a huge dependence due to this. This is in fact irrelevant practically compared to this activation form that is the Arrhenius form that is sitting here in eta okay. But anyway it gives us a formula for the diffusion constant. In fact you can go further.

We used the fact that in the Langevin model the velocity was exponentially correlated. We do not have to do that. We do not really have to do that. What we need is the following.

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The image shows a chalkboard with the following handwritten equations and text:

$$\langle v(t_1)v(t_2) \rangle$$

$$\langle (x(t) - x(0))^2 \rangle = \int_0^t dt_1 \int_0^{t_1} dt_2 C(|t_1 - t_2|)$$

$$= 2 \int_0^t dt_1 \int_0^{t_1} dt_2 C(t_1 - t_2) = 2 \int_0^t dt_1 \int_0^{t_1} dt' C(t')$$

Let $t_1, t_2 = t'$

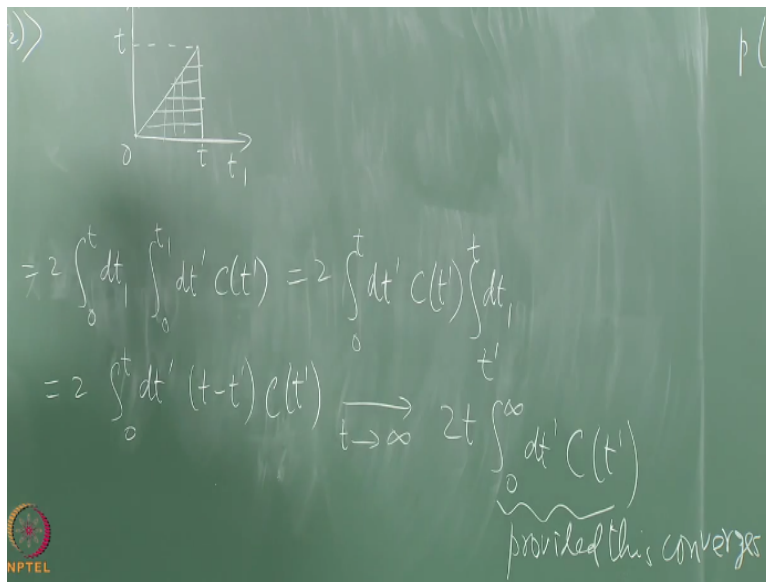
We need to recognize that this guy is equal to integral 0 to t dt 1 integral 0 to t dt 2 times the velocity correlation function right. So let me call that c of modulus t 1 - t 2 and this fellow here stands for v of t 1, v of t 2 okay. All we need is the statement that this v is a stationary process so that that c of t 1 - t 2 the velocity correlation is a function of the modulus, the time difference and the modulus of the difference okay.

So all we need is that piece of information and then we are done actually from here because now we will immediately get a formula for the differential constant in general even outside the

Langevin model because as soon as you have this this function here out here which is a symmetric function you can write this as twice the usual thing. So write this as twice $\int_0^{t_1} dt_2 c(t_1 - t_2)$ okay. Now let us put $t_1 - t_2$ equal to t' say.

I want to change from t_2 to t' okay. So this becomes equal to twice $\int_0^{t_1} dt_1 \int_0^{t_1} dt_2 c(t_1 - t_2)$ and then what do I get? When t_2 equal to t_1 the limit is 0 and when $t_2 = 0$ the limit is t_1 but there is a minus sign between dt_2 and dt' . So it again gives you $\int_0^{t_1} dt' c(t')$. Again gives you exactly the same thing okay. But what does this look like now?

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The region of integration, here is t_1 and here is t' and it says integrate up to this point. So it says this is t , this is 0, this is also t and when integrating over this triangle. For each t_1 you are integrating up to t_1 in t' . Instead of doing that way we could as well flip the integration and integrate in this direction in this fashion okay. So what does that become? This is equal to twice integral again t' must run from 0 to t that is clear from this figure $\int_0^{t_1} dt'$ and since this guy does not depend on t_1 I can bring it out.

So c of t' and then a integral over dt_1 and what should that run over? t' ran from 0 to t_1 . t_1 was always bigger than t' right. So if you are going to scan it this way then it is clearly running from t' up to t . So this integral is from t' up to t . One way to

remember it is that t_1 is bigger than t' therefore t' is smaller than t_1 okay. So instead of raster going vertically you go horizontally. But that is a trivial integral to do right.

So it says this quantity is twice $\int_0^t dt' t - t' c$ of t' right. That is exact. We have not made any assumption except that the velocity is a stationary random process and that the velocity autocorrelation function is a symmetric function of its argument, an even function of its argument. That actually follows from the time reversal property of the velocity. I have not proved that here explicitly but we have seen that in our specific example that this is true.

So this is it. This is the general thing. Now we ask what does this guy do as t becomes very large. There is no guarantee that c of t' is such that this integral converges when t becomes infinite. No guarantee as of now. But if it converges then what does it mean? This means that as t tends to infinity the large t limit this factor in general is going to die down as the upper limit increases. It is a correlation. It is going to die down as the argument increases.

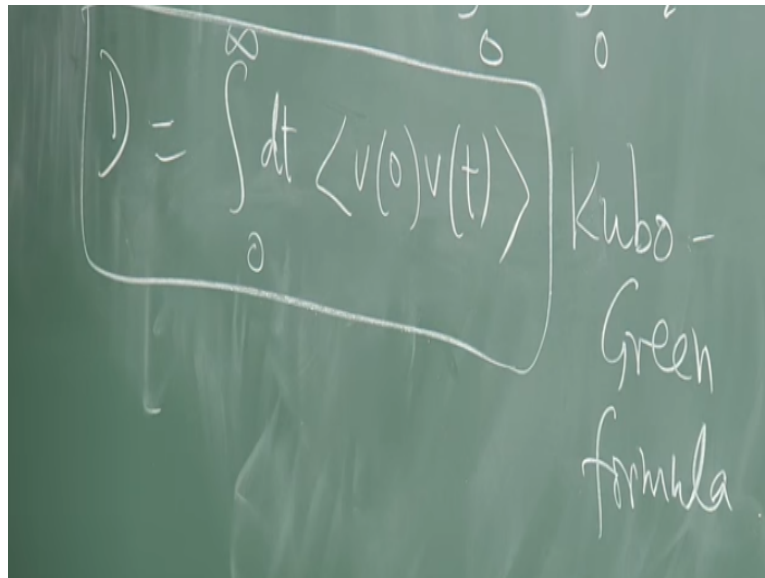
So in this factor if t becomes very large this is negligible compared to this. So you can pull it out of the integral but you might argue oh that may not be correct because what about the contribution from those regions of integration where t' is comparable to t . Then you cannot throw out t' relative to t . But those are large values of t' and for those this takes care of the convergence. It goes down.

You can say this much more rigorously using this dominated convergence theorem but the fact is that as long as this integral over c of t' is finite this is guaranteed to be twice $t \int_0^\infty dt' c$ of t' provided this converges. If this integral of the velocity correlation function over 0 to infinity does not converge that is a symptom that this behaviour is not going to be proportional to t asymptotically.

But if it converges there is no doubt that it is equal to this guy here. But we know that asymptotically the diffusion constant is defined as the limit of the mean square displacement/ $2t$

as t tends to infinity. That is the definition of the diffusion constant. So what does it tell us finally?

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$$D = \int_0^{\infty} dt \langle v(0)v(t) \rangle$$

Kubo -
Green
formula

It says in general I might as well write it as v of 0 v of t drop the primes and write it in this fashion okay. So I shift the origin to 0 . This is a stationary autocorrelation function and the integral of it from 0 to infinity gives me the diffusion constant. This is called a Kubo-Green formula. It is an example of what is called a Kubo-Green formula where various response functions susceptibilities and so on and so forth are given as autocorrelations integrals over autocorrelations in equilibrium okay.

It is part of a more general definition where you subject this particle to a sinusoidal force and ask what is its steady state response going to be depends on the frequency dependent mobility and that will have fourier Laplace transform here e to the i ω t and at $\omega = 0$ the static susceptibility is called the related to the diffusion constant okay. Well that takes us into non-equilibrium statistical mechanics. I do not want to get into that here.

But just to tell you that the specific case of the Langevin model where this guy was kt over m e to the minus γt is going to immediately give you D is kt over m γ but this is the more general formula okay. Okay so now we understand where this diffusion thing came from. It

came in the limit when gamma became very large or in the regime in which gamma t was much bigger than unity okay.

Then the diffusion equation is a good approximation to the position of this variable. The next question that arises is can I not look at the position and velocity together in phase space and try to write down a formula or function expression for an equation for the distribution not of x and v independently but for the conditional distribution in x and v together, the joint distribution. Yes, indeed we can.

But we need to write down now the corresponding Langevin equation for this and what does that look like?

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The image shows a chalkboard with the following handwritten equations:

$$\dot{x} = v$$

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

$$\vec{\psi} = \begin{pmatrix} x \\ v \end{pmatrix}$$

$$\dot{\vec{\psi}} + R \vec{\psi} = \frac{\sqrt{\Gamma}}{m} \eta(t) \begin{pmatrix} 0 \\ \eta(t) \end{pmatrix}$$

$$R = \begin{pmatrix} 0 & -1 \\ 0 & \gamma \end{pmatrix} \Rightarrow R^2 = \gamma R$$

Well, let us write it down and see what happens. So you have x dot and that is of course equal to v by definition and v dot equal to - gamma v in our model + square root of gamma over m eta of t. That was the Langevin equation of this guy here. So let us regard these 2 together as a vector Langevin equation. I should worry about dimensions but let us assume these are all in dimensionless units and let us introduce a psi vector which is equal to x v in this fashion okay.

Then we have a vector Langevin equation for a two component vector which looks like this. It says psi dot equal to and let us bring this v to this side, so plus some matrix times psi because

these 2 guys are linear in the coordinate position. In fact x does not appear here at all. So let us say there is some matrix R which takes care of the dissipation, this guy here equal to square root of γ over m , a vector value η of t and this fellow stands for 0 the usual η of t .

Remember that capital γ is little $2 m \gamma k t$. We are going to put that in always as a consistency condition. What is this vector, this matrix R ? ya, it is going to be $0 - 1 0 \gamma$ to take care of these 2 guys, bring them to this side and then γ becomes positive this becomes negative out here. Acting on x , v is going to give you precisely these equations okay.

Now just as we solve the ordinary Langevin equation by using this integrating factor e to the minus γt I need to now use the integrating factor e to the $- R t$ and it is a 2 by 2 matrix. So I need to exponentiate this matrix to find that Green function right. Now that is not very difficult to do because you notice that R square, this implies that R square if I multiply twice together is going to give me a $-\gamma$ on that side and a γ square in the denominator.

So this is equal to γ times R . So once you have that the exponential is trivial because then R cubed is γR square which is γ square R and so on. So R to the power n is just γ to the $n - 1$ times R and therefore you can compute the exponential. So in principle you can write the solution down and take averages and so on as we did earlier. So in principle you can find all the correlations.

You can find v of 0 , v of t , x of 0 , v of t we can do all these things. But you must remember that x is not a stationary random variable. It is the integral of the velocity and the velocity is a stationary random variable. When you integrate, this stationarity property is lost. But it does not matter. You can specify initial conditions, x not v not etc., and compute this whole thing.

But you would now ask just as I have a Langevin equation here with white noise is this not equal to a Fokker-Planck equation equivalent to some Fokker-Planck equation, a matrix Fokker-Planck equation this time, will involve some matrixes etc. But for the joint distribution of x and v and indeed that is so. This implies the following equation.

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the following FPE for $\rho(x, v, t | x_0, v_0, 0)$

$$\frac{\partial \rho}{\partial t} = R_{ij} \frac{\partial}{\partial \xi_i} (\xi_j \rho) + \left(D_{ij} \right) \frac{\partial^2 \rho}{\partial \xi_i \partial \xi_j}$$

$\xi_1 = x, \xi_2 = v$

$$D_{ij} = \begin{pmatrix} 0 & 0 \\ 0 & \frac{\gamma k_B T}{m} \end{pmatrix}$$

So this guy implies the following, implies the following Fokker-Planck equation for the density of x and v together. So let us not use the symbol p for it. Let us use the symbol ρ of x v t given x not and v not at $t = 0$ okay. So let us specify that at the initial instant of time you had some initial position, some initial velocity and this is the one particle density phase space density or conditional probability density in this case okay.

It implies the following equation $\Delta \rho / \Delta t$ equal to and then because this thing is a drift term is linear in this case it is $R_{ij} \Delta \rho / \Delta \xi_i \xi_j$ times ρ it is got to be scalar so it just contracted plus $D_{ij} \Delta^2 \rho / \Delta \xi_i \Delta \xi_j$ where I have to explain what these matrixes are. This guy here this D_{ij} is just $0, 0, 0, \gamma k_B T / m$ because the noise is only in the second equation.

In principle we could have had a noise here too separately but then \dot{x} is v by definition in this example, there is no voice there and the noise is in the velocity because it is the force that is random. So it appears in the equation for the acceleration okay and a summation over repeated indices is implied ξ_1 by definition equal to x ξ_2 by definition is v . So it implies this equation. Again by this equivalence between the stochastic differential and Langevin equation and the Fokker-Planck equation for a two-dimensional diffusion process in this case and what does that look like. What does this equation look like now?

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$$\frac{\partial \rho}{\partial t} = -\frac{\partial (v\rho)}{\partial x} + \gamma \frac{\partial (v\rho)}{\partial v} + \frac{\gamma k_B T}{m} \frac{\partial^2 \rho}{\partial v^2}$$

$$\frac{\partial \rho}{\partial t} + v \frac{\partial \rho}{\partial x} = \gamma \frac{\partial (v\rho)}{\partial v} + \frac{\gamma k_B T}{m} \frac{\partial^2 \rho}{\partial v^2}$$

$$\rho(x, v, 0 | x_0, v_0, 0) = \delta(v - v_0) \delta(x - x_0)$$

$$P(v, t | v_0) = \int_{-\infty}^{\infty} dx \rho(x, v, t | \dots) = \text{OU distrib. in } v$$

If we simplify it this is delta rho over delta t equal to R i j. Now R 1 1 is 0 and R 1 2 has got a minus 1 out here. So it is R 1 2 delta over delta x and then you have v times rho and what is R 1 2 minus, minus delta over delta x 0. Is there any other term? R 2 2 is not 0 right? So plus gamma times delta over delta v 0 because psi 2 was equal to v and i and j are both equal to 2 and then the only term that survives in this thing here is plus gamma k Boltzmann T over m d 2 rho over delta v2. In this case all the other terms are 0.

This is the equation satisfied by the phase space conditional density in position and velocity together. But what does this tell us? This says delta rho over delta t plus I bring it to this side and since v index are independent variables in phase space this says v delta over delta x rho equal to gamma the usual thing that appear on the right hand side. What does this remind you of? It is a v dot del. So the left hand side is like a convective derivative.

This term is like a convective derivative. You have partial delta over delta t + v dot del and that is the total derivative. So it is just very physical thing. It tells you as soon as have a flow which goes like this, this will automatically emerge. It will emerge automatically that there will be this term delta over delta t + v dot del will appear automatically and then that acts on rho to give the total time derivative and that will have the dynamics on the right hand side okay.

So this is the Fokker-Planck equation in the case when you have a phase space when you look at the Langevin equation as an equation in phase space in both x and v . The question is what sort of solutions does this have. Again, the initial condition is obvious in this case. Our initial condition is $\rho(x, v, 0) = \delta(x - x_0) \delta(v - v_0)$ and you can do this in several ways. You get a bivariate Gaussian in x and v .

So it will have terms like $e^{-\text{something}}$ or the other times v^2 and then there is an xv term and then the minus x^2 term okay. You can get some Gaussian numbers form which can be written down we can actually write the solution down. I am not going to do that here. But what is of interest was is what does this solution become what does this solution become if you reduce this to one of the two variables.

If you reduce to the v variable for which we already have a relation. So I want $p(v, t)$. This should be found by actually integrating over all x . So I integrate $\int_{-\infty}^{\infty} dx \rho(x, v, t)$ whatever and it turns out this gives you the Ornstein-Uhlenbeck distribution as it should okay which is exactly what you expect. What would you what would happen if I integrated over v instead? I would get an expression for x right.

I would get an expression for x but it will not be the solution to the diffusion equation. It would not be that Gaussian because that is only true when γt is much bigger than 1. So it is some complicated expression which will in fact involve v not as well not just x not but v not as well showing that x is not a stationary random variable okay. That is not of much interest. We can compute it. It is not of much interest. But we can ask what does this guy do when t becomes very large, what would you expect it to do.

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$$\rho(x, v, t | x_0, v_0, 0) \xrightarrow{\gamma t \gg 1}$$

$$\left(\frac{m}{2\pi k_B T} \right)^{\frac{1}{2}} e^{-\frac{mv^2}{2k_B T}} \cdot \frac{e^{-(x-x_0)/4Dt}}{\sqrt{4\pi Dt}}$$

So I take this solution, take this guy here with this initial condition and ask what is rho of x, v, t x not v not 0 as t tends to infinity or gamma t is much bigger than 1. What would it tend to? What would you expect now? I would expect the velocity to have thermalized completely and then what would be the distribution of the velocity? The Maxwellian, I would expect the Maxwellian in velocity. It would multiply a distribution in x and what would that distributions be.

The solution of the diffusion equation because this limit is a diffusion limit right. So this also is true that this becomes in this limit to Maxwellian in v times e to the - x - x not square over 4 D t over square root 4 pi D t. So let us write the Maxwellian as well. It would be equal to m over 2 pi k Boltzmann T to the power half e to the - m v square over 2 k T. So the memory of v not is gone is lost because this tends to the equilibrium distribution.

This guy there is no equilibrium distribution position. We saw in the diffusion equation everything goes to 0 at all points in an infinite media okay. Again, exactly what you would expect on physical grounds okay. So we would not go further into this. But we could ask for one more generalization which is physically very relevant. Throughout I have assumed there is no external force on this particle. I have said there is an internal random force and there is a friction for consistency. What if I impose an external force on it from some potential v of x.

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$$\dot{X} = v$$

$$\dot{v} = -\frac{V'(x)}{m} - \gamma v + \frac{\sqrt{\gamma}}{m} \eta(t)$$

$$\dot{\begin{pmatrix} X \\ v \end{pmatrix}} = \begin{pmatrix} v \\ -\frac{V'(x)}{m} - \gamma v + \frac{\sqrt{\gamma}}{m} \eta(t) \end{pmatrix}$$

Then this equation here is going to get modified because I am going to have minus out here. The potential v prime of x over m that term is going to be there m gamma v plus root gamma over m eta of t . So I have got an extra term here in this case and that is a complicated function of x depending on the potential. When it is linear function of x then I argue that the whole thing is a linear drift and I could extend this formalism.

But when this is a nonlinear function of x then I am in trouble. So we will look at what happens next time tomorrow. We will look at what happens in the general case here. We will first look at a linear problem, see what happens. A very drastic change is going to happen depending on what kind of force this is. For instance what is physically happening is that without this force this particle is diffusing clearly.

The variance of the position is becoming unbounded with time linearly. Now the question is suppose we put this in a potential such that it does not let it go too far, cost too much energy. I expect the diffusion may be curtailed. It may not be able to fluctuate that far. In other words asymptotically it is possible the variance of the displacement is going to be bounded. It is not going to diverge and we will see explicitly how this happens. So we will do that tomorrow.