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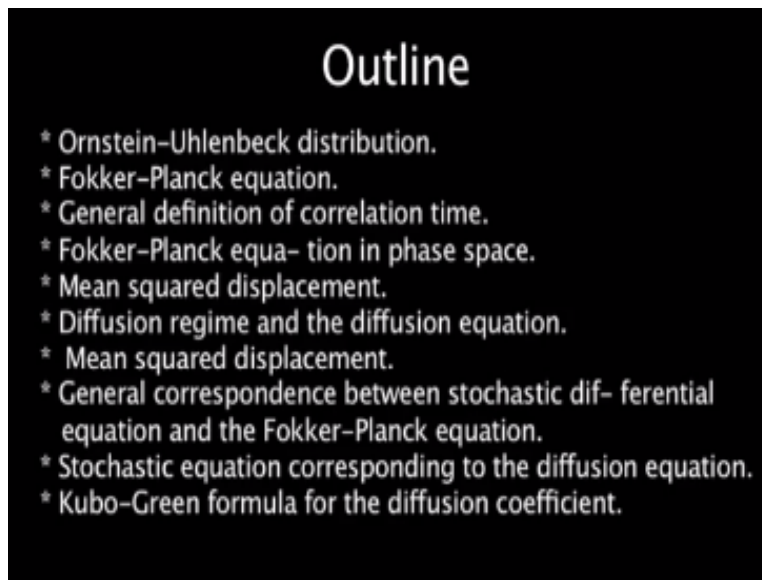
TOPICS IN NONLINEAR DYNAMICS

**Lecture 29
Stochastic dynamics (Part VI)**

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So we saw yesterday that in the simple large box model for diffusion of particles in a fluid the equation is.

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$$\frac{1}{\sqrt{1 - e^{-2\gamma t}}} \exp\left[-\frac{(v - v_0 e^{-\gamma t})^2}{2k_B T (1 - e^{-2\gamma t})}\right]$$

$$+ \frac{\partial}{\partial t} p + \frac{\partial}{\partial v} \left[\frac{\gamma v}{m} p \right] = \frac{\partial^2}{\partial v^2} \left[\frac{k_B T}{m} p \right] \quad (\text{Fokker-Planck equation})$$

$$p(v, t) \rightarrow 0 \text{ as } v \rightarrow \pm\infty$$

$m \dot{V} + m \gamma V = n(t)$ if this is a Gaussian white noise a random process with the δ correlation a Markov process which is stationary and has a δ correlation then the velocity V also turns out to be a Markov process and its conditional density turns out to be the Ornstein uhlenbeck distribution so we saw that this implied and you can show that this \Rightarrow and is implied by the fact that the conditional density

The velocity is V at time T given that it was V_0 at some instant of time $t = 0$ this quantity this was given the normalized distribution was given by $\frac{1}{\sqrt{2\pi k_B T (1 - e^{-2\gamma t})}} \exp\left[-\frac{(v - v_0 e^{-\gamma t})^2}{2k_B T (1 - e^{-2\gamma t})}\right]$ by a time dependent normalization factor multiplied by a Gaussian function which is $(v - v_0 e^{-\gamma t})^2$ by the variance which is $2k_B T (1 - e^{-2\gamma t})$ to guarantee this was the distribution which starts as a δ function at $v = V_0$ at $T = 0$ and as in Tata CLE approaches the maxwellian distribution the usual Gaussian distribution corresponding to thermal equilibrium as T tends to ∞ .

Now of course once you are given this and the fact that we is a Markov process which we have not proved but I am asserting that it is so then all probability distributions connected with v unknown n time distributions are completely known because everything could be written for a Markov process in terms of this conditional density alone but the interesting thing is this density also obeys a differential equation which looks like the diffusion equation but how another extra term and we will discuss that little bit.

Today and that equation and this stochastic differential equation are equivalent to each other the equation obeyed by this P is $\frac{\delta P}{\delta t} + \frac{\delta P}{\delta v} \left[\frac{\gamma v}{m} \right] = \frac{\delta^2 P}{\delta v^2} \left[\frac{k_B T}{m} \right]$ and it is called the master equation for the probability

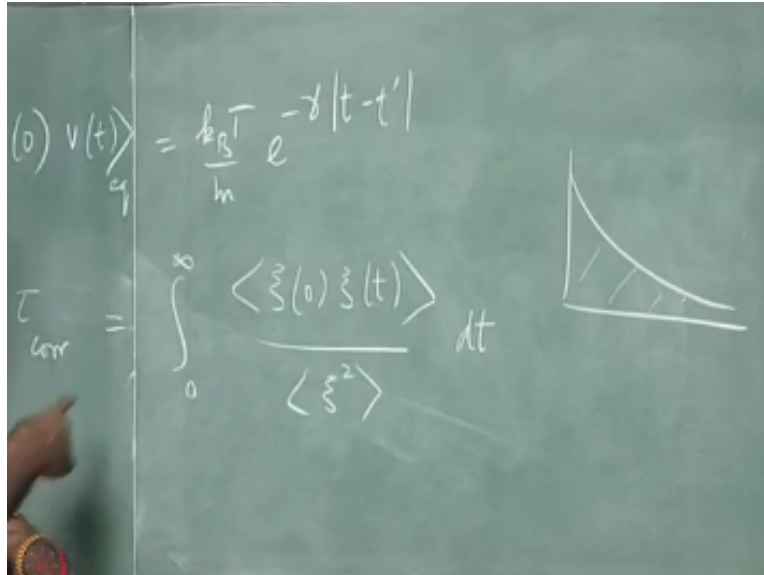
conditional density of a Markov process in this case this master equation is a second order partial differential equation and it happens to read $\frac{\partial p}{\partial t} + \gamma \frac{\partial p}{\partial v} + \frac{\gamma^2}{2} \frac{\partial^2 p}{\partial v^2} = 0$ so this equation together with the initial condition so the which is a function of V and T so P of V and T with the initial condition $p(V, 0) = \delta(V - V_0)$ and a certain set of boundary conditions.

Because its second order in space we need boundary conditions and natural boundary conditions namely $p(V, T) \rightarrow 0$ as $V \rightarrow \pm \infty$ specifies a unique solution and that is this distribution so the unique solution of this second order partial differential equation with this initial condition and this set of natural boundary conditions happens to be the honest no land by distribution one can prove this rigorously you can solve this equation explicitly by a variety of methods but we are not interested in that at the moment

But this is where the answer in the distribution appears from this particular equation the master equation for the conditional density this equation is the first example of what is called a fokker-planck equation this is a class of equations for a specific kind of Markov process which I'll mention in a minute and it is perhaps the first example or one of the first examples of a Fokker Planck equation this equation for the velocity was actually written down by Lord Rayleigh and it is sometimes called the Rayleigh equation.

But it is common parlance it is become known as the fokker-planck equation because it is an example of a class of equations to be Jackal labeled as the fokker-planck equations now we found also from this that the velocity was correlated exponentially so we found that the velocity.

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$\langle v(0)v(t) \rangle$ average $\langle v(t_1)v(t_2) \rangle$ was a function only of mod $t_1 - t_2$ I can shift the origin called zero one of the arguments here in equilibrium this turned out to be KBT over m to the $-\gamma$ mod $t - T$ try this is the way you define for a Markova process a correlation time what you do is to take this process if you have a stationary Markova process and let me denote for general stationary Markova process you take this quantity is $\langle I(0)I(t) \rangle$ take its average value that is the correlation function provided the mean is 0 at all times.

The mean is not 0 you should subtract the mean at every instant of time so let us even do that let us write the most general formula down the actual correlation function $C(t)$ we define as $\langle (I(t) - \langle I \rangle)^2 \rangle$ - average side which is time independent if it is a stationary process the average of back x this deviation from the average this quantity here would actually be the correlation function but you can easily see it is easy to check that is the same as the average value of $\langle I(t) - \langle I \rangle \rangle^2$ - mod average high whole squared.

So this thing here is in fact as $\langle I(0)I(t) \rangle$ is $\langle I \rangle^2$ so it is a generalization of the variance of the process that is all that the correlation does let us for the time being for the case of V this was 0 so let us simply drop it and then you can define a correlation time in the following way so you take this quantity is $\langle I(0)I(t) \rangle$ you normalize it by $\langle I \rangle^2$ that is the value of $T=0$ this function is guaranteed to start at one at $T=0$ and then in general it would drop off to 0 as T tends to ∞ could drop off very slowly but here it drops off exponentially fast not always guarantee but in this problem.

It drops off exponentially fast so if you took this quantity and you integrated over all T you get a quantity of dimensions time so 0 to ∞ of this if this integral converges you get a certain characteristic time in the problem and this is what you would call the correlation time of the process so that is the way pardon me so if this is a random process if there is a stationary random process then this is a way of acquiring of extracting a time scale in the problem the time scale on which the system loses memory some observable.

Yes that is a good question this question is if I look at this problem and I look at the velocity correlation time is that the same as a correlation time for say the position or anything else will see it is an interesting question we will see what happens to the position in a minute for the velocity it is so this is certainly going to give you a correlation time pardon me is this quantity this is I squared average so that this is normalized to unity otherwise.

It this quantity has a physical dimension of the square of whatever it be I want to extract time from it so I remove this quantity gets rid of the physical dimensions of and it is something which would typically look like this function here would start at one and die off and I am saying this quantity here this area under the curve is actually got the physical dimensions of a characteristic time scale is no easy it is not hard to prove.

That if you took this in the present instance this would imply at how correlation time $= \gamma$ inverse trivially follows that you simply get one over γ is the correlation time of the velocity now the next question is very nice we have something for the velocity what about the position what happens to the position something very complicated happens to the position the fact is it turns out that I was really look at the motion and phase space as we know in dynamics you must look at things in phase space.

So since I am looking at one component of the velocity the x component say I should really look at the pair X, V and then I should not even be talking about p of VT I should be talking about the joint density in phase space of xvt given say some initial position we not at T equal to zero so it is this quantity that I should look at and I should ask how does that evolved as a function of time it turns out you can write a Fokker Planck equation for that quantity.

That would correspond to writing an equation for the probability density corresponding to the pair of variables here so I write $\dot{x} = V$ and $\dot{V} =$ this look like a dynamical system except

that it is got random components here and then I could write a probability density of that kind and then ask what is the equation of it by it also satisfies the fokker-planck equation it is somewhat more complicated but we could actually write it down quite simply but me yeah the statement is dynamics happens in phase space as we know from our experience with dynamical systems.

So we are talking now about a random velocity of an individual particle the X component of the velocity say I should really talk about the position and the velocity together because that is what constitutes a point in phase space right so I should really write down a couple set of equations and here is the couple set of equations \dot{X} is V and \dot{V} satisfies this equation which is random this η is random corresponding to this stochastic differential equation I have a probability density in phase space which is given by ρ of X, V, T .

This is the probability density or when $\int dx \int dv$ this gives you the probability that if a particle starts at X_0 with velocity V_0 at time 0 it is found in the range V to $V + DV$ in velocity and X to $X + DX$ in position at time T this quantity satisfies the fokker-planck equation also which is more complicated than this equation in fact we could write this equation down let me do so that is the fokker-planck equation in phase space and it is actually not much more complicated than this yeah I should write it down really I should write down not this but I should write down our I should write down v and I should write down our not v not.

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$$\dot{x} = v$$

$$m\dot{v} + \eta v = \gamma(t)$$

$$\frac{\partial \rho}{\partial t} + \vec{v} \cdot \nabla_{\vec{r}} \rho = \gamma \nabla_{\vec{v}} \cdot (\vec{v} \rho) + \frac{\gamma k_B T}{m} \nabla_{\vec{v}}^2 \rho$$

So let us do this in several steps I should really finally aim at writing row of our V T given are not find me the motion occurs. I look at particles in this room they are moving in three-dimensional space but the move each of them is moving in a six dimensional phase space one particle phase space six-dimensional it is not a Hamiltonian system at all this thing is not a Hamiltonian system is right over gone from that there is no way you can produce this friction in a Hamiltonian system.

I put this $m\dot{v}$ in phenomenological and I put in a random component here so we move to a stochastic dynamical system now which is in fact dissipative but now I am not saying anything like that I am saying that every particle has the particle motion occurs in phase space that is all I am saying ,I need to have equations of motion which are right down should be for all the dynamical variables and the position and the velocity of the position and the momentum they determine the state of the particle at any time so it is not Hamiltonian does not have to be Hamiltonian at all not writing any Hamiltonian down at all.

But the idea of phase space is more general than that of Hamiltonians as you know if this particle had other internal degrees of freedom then the dimensionality of the corresponding phase space would change but it is a point particle so its position and momentum you mean why do not I have what else could I have here what is the K let us call it is got to be a physical observable pertaining to the point particle what are the physical observables pertaining to a point particle at any instant of time.

They be its position and momentum that is about it is true that if i have this particle in if it turns out that there are velocity dependent forces it turns out there are other degrees of freedom interacting with it turns out for example that its basic equation of motion is six dimensional or seven dimensional. I would have to include those extra pounds but as long as I have forces conventional kinds of forces we know that the position and momentum are sufficient or in this case the position and velocity so this is the sort of quantity.

I would look at but let us first do this for one dimension and then I write it down immediately in arbitrary in three dimensions the equation turns out to be $\delta \rho$ over $\delta T + V \delta P$ over δX =whatever we wrote on the right hand side $\gamma \delta$ over $\delta V V (P)$ this time $+ \gamma k$ but over $mt^2 \rho$ over TV to this is the fokker-planck equation in phase space nothing much has happened nothing much has happened you have added this term here in fact you can intuitively guess where this term comes from what does this remind you of yes in fluid dynamics yeah $V \cdot \nabla$ it reminds you exactly of that it is a convective derivative.

So the left-hand side is really the total time derivative of row in that sense so that is all that happens and this is a very complicated solution if I write this down with initial conditions p of x v_0 is $\delta V - V_0 \delta$ of $X - X_0$ and I use natural boundary condition saying that row vanishes as X tends to $+\infty$ V tends to $+\infty$ then the solution turns out to be a fairly complicated distribution turns out to be a Gaussian jointly in X and V so it is a multivariate Gaussian distribution I am NOT going to write that down right.

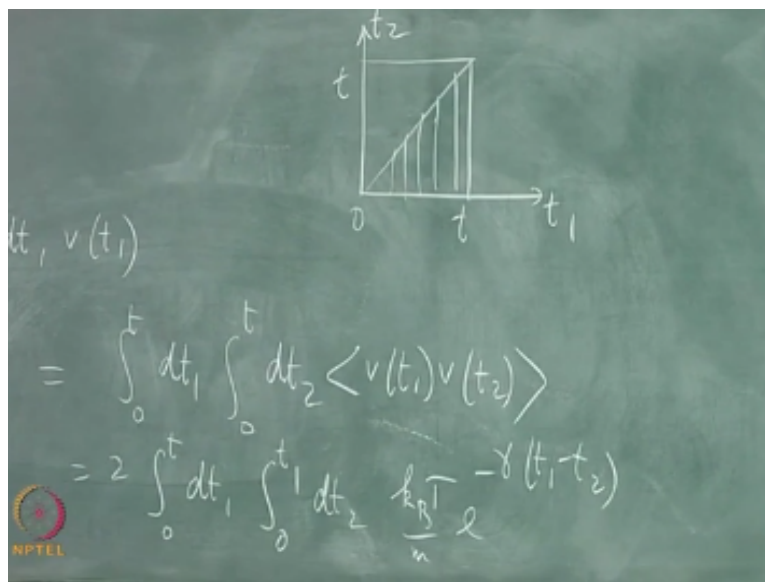
Now hopefully generalize this to ρ of R, V, T that is also obvious almost obvious let us say so what would the general equation be in six dimensional phase space how would it change this remains the same and not surprisingly this becomes $+ V \cdot \nabla$ the gradient of P gradient with respect to R of ρ and on the right hand side out here you actually have γ times the gradient with respect to V dotted with v ρ is the divergence of this required this means the components of this are the partial derivatives with respect to the three velocity components.

And this term here becomes ∇ with respect to $V^2 \rho$ that is the full 4k Planck equation for free particles in the absence of an external force in phase space and the solution is a generalized Gaussian in all these variables you can use a matrix method to solve this equation but it is a little intricate and we would not do that here so you cannot generalize these two actual motion

in a number of dimensions but our purpose now is not to do that we go back we go back to this set of equations.

The Langevin equation and ask what can we say about the position of the particle we know all we need to know about the velocity because it sets conditional density is given by the honesty Nolan by distribution what can we say about the position of the particle how far does it move in a given time so let us see what happens so we could start with the particle moving from the origin at $T = 0$ or at any point X_0 and then let us find out what it does.

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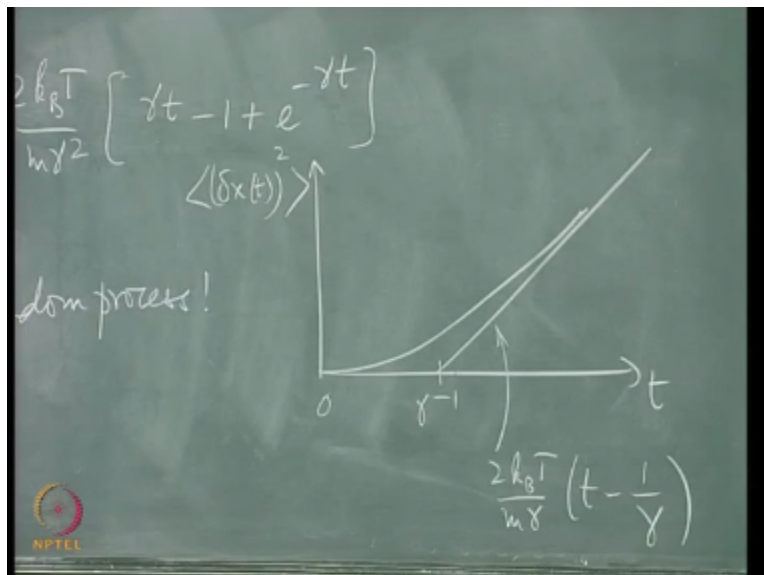
So I know that $x(t) - x(0) = \int_0^t dt_1 v(t_1)$ this is a definition of the displacement let us call this $\delta X(t)$ now I would like to find out what is the mean square displacement so all I have to do is to take the square of this and take the average in equilibrium so what is that gives us that gives us $\int_0^t dt_1 \int_0^t dt_2$ and then you have a $V(t_1)V(t_2)$ in equilibrium no external force but we already know what this is this is the exponential that I wrote down there for you can compute this number right.

You can actually calculate this number fairly straightforwardly because all you have to do is to put in that exponential there and compute it so let us do that a little trick involved here because remember that this quantity was $k_B T / m e^{-\gamma |t_1 - t_2|}$ there in other words in the $t_1 - t_2$ plane you have to integrate $\int_0^t dt_2 \int_0^{t_2} dt_1$ here this is the line $t_1 = t_2$

and you have to integrate over this whole square here but the function here is symmetric with respect to the function layer.

Because it is a function of the modulus the value at any point here is =the value reflected on this line so we could as well write this as =2 the value in one of the triangles so I could write this as 2 the value from 0 to t dt 1 and this goes from 0 to t 1 dt 2 k Boltzmann t / m e to the - γ since t1 is bigger than t2 i could just write this as the t1 - t2 without the modulus and which triangle. I am integrating / t1 from 0 to T and each time t2 is restricted it goes from 0 up to this quantity so it just goes up till there that is the integral .I am doing as a trivial integral to do is very simple and the result is the following so you end up with.

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$\langle \delta X \rangle^2$ =it turns out to k Boltzmann t / m γ and γ^2 because ,I am going to do two integrals here and the k Boltzmann t / m comes from here and then it is an integral which gives you $\gamma t - 1 + e$ to the - γ that is the result what can we say about the displacement now right away from

this result this quantity is the mean square displacement and it is a function of the time what sort of process is the displacement now if the mean square value depends on time what can you say about this process is it stationary or it is non-stationary exactly.

So that is the first problem it is not even a stationary process unlike the velocity whose statistical properties were independent of time and therefore the mean the mean square and so on were all independent of time this process is not even a stationary random process so its correlation function is going to depend on both time arguments and is not a function of the difference of the two alone so if I compute $\delta X(t_1) \delta X(t_2)$ it is a function of both t_1 and t_2 and how does this function look as a function of T if I plot $\delta X(t)^2$ exactly so it is clear that asymptotically this term and this term are going to dominate over this and this is a straight line which intersects at $t = 1/\gamma$.

So it is clear there is a straight line of this kind with some slope and this function look at what happens for very small $\gamma T < 1$ this goes like $1 - \gamma T$ which cancels both these things and then you got a $\gamma^2 t^2$ so it starts off like a parabola and then it hasn't Article II it is this value here eventually so it is clear that this function looks like this and this line here its ordinate is $k_B T$ to whatever it is to $k_B T$ $t/m - 1/\gamma$ straight line and that is the asymptote so it behaves linearly for sufficiently long times.

But at short times its quadratic and then in between it has both the exponential as well as the linear term and it is not a stationary process $X(t)$ is not a stationary turns out it is not even Markoff but there is one case where things simplify where have we come across the statement that the mean square displacement of a diffusing particle increases linearly with the time this is the famous diffusion equation prediction so if you write the diffusion equation down for the positional probability density function.

Then we can prove directly from that that the mean square displacement increases linearly with time but this is saying something else saying it is not linear it is only linear for sufficiently long times this thing here is γ inverse and if T is much bigger than γ inverse which is the velocity correlation time then the mean square displacement increases linearly with time so it is giving us a very important input it says the diffusion equation which I would normally naively write down from fixed laws of diffusion is valid only at sufficiently long times.

How long times much longer than the velocity is memory time correlation time so that is telling you something beyond the diffusion equation so now let us back and write down the diffusion equation and see what that \Rightarrow and what sort of stochastic equation that \Rightarrow again so let us go back to our logical the usual phenomenological description of diffusion is in terms of two conditional densities so let me call.

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The image shows a chalkboard with the following equations written on it:

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

$$\frac{\partial C(\vec{r},t)}{\partial t} = -\nabla \cdot \vec{j}(\vec{r},t)$$

$$\vec{j}(\vec{r},t) = -D \nabla C(\vec{r},t)$$

$$\frac{\partial C}{\partial t} = D \nabla^2 C$$

In the bottom left corner of the chalkboard, there is a small logo for NPTEL.

I need to use another symbol for it so let me use the symbol P little script there for the position of a particle at time T this is the positional probability density and what do you say about this it is like if I take a diffusing species and I write the concentration as a function of position and time I'd write the two laws of physics the fixed laws for diffusion the first one is just conservation of matter and the second law tells you how things move so the equations if you recall for the concentration of a species at time.

The equations fixed laws are δC over δT = on the right hand side this quantity is = it is = - the divergence of a diffusion current that is the continuity equation that is fixed first law it is just the conservation of matter continuity equation but the second law says something dynamic it says under suitable conditions the current $J(\vec{r},t)$ is proportional to the negative gradient of the

concentration so the current moves from the region of higher concentration to the region of lower concentration.

So it is \propto the gradient of the concentration and the coefficient here is called the diffusion coefficient D and when you put both these guys together of course you end up with the diffusion equation which says $\frac{\delta C}{\delta T} = D \nabla^2 C$ that is the famous diffusion equation the positional probability density of a single particle in one dimension now moving in one dimension satisfies the same equation this is almost by definition and therefore it \Rightarrow that we have the diffusion equation $\frac{\delta P}{\delta T} = D \frac{d^2 p}{DX^2}$.

That is the diffusion equation so we set aside the lingerie $m \nabla$ we are not going to think about it for the moment we come to this we look at this diffusion equation and ask can we say something about the motion of the particle from here well I need to specify initial conditions and boundary conditions before. I am through.

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Handwritten notes on a chalkboard:

$$p(x,0) = \delta(x), \text{ natural b.c. } p(x,t) \rightarrow 0 \text{ as } |x| \rightarrow \infty$$

$$\int_{-\infty}^{\infty} dx p(x,t) = 1, \forall t \geq 0.$$

$$p(x,t) = \frac{1}{\sqrt{4Dt}} \exp\left(-\frac{x^2}{4Dt}\right)$$

So let us start with the simplest initial condition let us assume that on the x axis the initial concentration is at $X = 0$ so the δ function at the origin so let us say that $P(x,0) = \Delta(x)$. So $T = 0$ it starts at $X = 0$ I could shift the origin as I please but let us choose the origin to be at $X = 0$ be at the initial position of the particle what are the boundary conditions you would like to put but I certainly like to have this I did certainly like to have the total concentration to be finite and the equivalent of that here is $-\infty$ to ∞ $DX p(x,t) =$ a finite quantity.

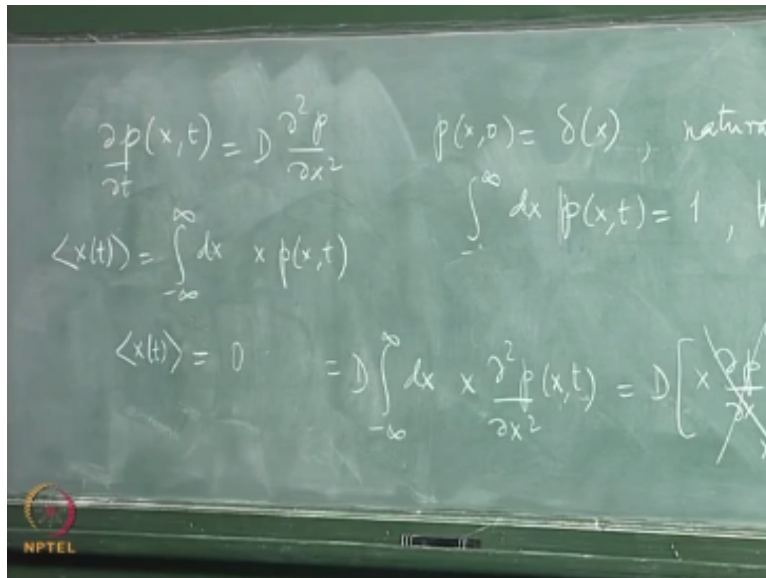
If it is a probability density function then $\int_{-\infty}^{\infty} p(x,t) dx = 1$ for $t > 0$. I certainly like to normalize this probability so it should be some non-negative function whose total area under the curve is unity and which starts as a δ function at $T = 0$. What is a necessary condition for this integral to exist? It is an integral which runs from $-\infty$ to ∞ the entire x-axis so when would that exist well this function must be integral of course but it must vanish at the endpoints otherwise this integral does not exist it must vanish sufficiently rapidly at the endpoints.

But certainly it must vanish so the natural boundary conditions natural BC $P(x,t) \rightarrow 0$ as $|x| \rightarrow \infty$ on both ends. I did like it to vanish given this initial condition and those boundary conditions this equation has a unique solution and we know the solution the famous diffusion equation solution is in fact $p(x,t)$ is the exponential of $-x^2$ over $4Dt$ and there is a normalization constant which is square root of this is the famous Gaussian solution.

It simply says that as time goes on this becomes a Gaussian then it widens out and eventually dissipates now completely the area under the curve remains one at all times but this curve broadens finally p vanishes at every point but the total area is one that is the fundamental Gaussian solution to the diffusion equation or the heat conduction equation these are all identical equations well for one thing we can find the value of the mean value of x or the mean square of x etcetera you can in fact do that without solving this equation.

But once you have it you can write it down how do you find the mean value of x how do you find $\langle X(t) \rangle$ average from this equation without solving the equation.

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What would you do well I would like to compute $\langle x(t) \rangle = \int_{-\infty}^{\infty} dx x p(x,t)$ if this is normalized to unity then this is the definition of the mean value so let us do that let us multiply both sides of this equation by x and integrate over x overall x so what happens. I multiply this by x on both sides and integrate from $-\infty$ to ∞ I have integral $-\infty$ to ∞ $dx x \frac{\partial}{\partial t} p(x,t)$ this quantity is $= D$ times an integral $-\infty$ to ∞ $dx x \frac{\partial^2}{\partial x^2} p(x,t)$ but remember the T dependence comes entirely from here.

So I can actually pull this out once it is integrated over x this is just a function of T alone and I can pull that out and since its function of T alone again simply write it as d over DT but what is this quantity $=$ by definition it is the mean value $\langle x \rangle$ so it says $d \langle x \rangle / dt$ of T $=$ this and the obvious thing to do is to integrate by parts so if I integrate this by parts this gives me d times $\int_{-\infty}^{\infty} dx x \frac{\partial p}{\partial x}$ at $x = -\infty + \infty - d$ times an integral $-\infty$ to ∞ dx times the derivative of this function with respect to x .

Which is one and the integral of this which is $\int_{-\infty}^{\infty} dx \frac{\partial p}{\partial x}$ so it just gives me $\frac{\partial p}{\partial x}$ over δx this fashion but this is zero because we would like all moments of this quantity of x I like the mean value the mean square value and so on to be finite which means that p of x T must not only go to zero as $|x|$ goes to ∞ but must go to 0 faster than a near as negative power of x otherwise that moment would diverge therefore since this goes to zero faster than any negative power of x as x goes to $+\infty$ this quantity goes to zero so this is gone and what does this do this gives you just the surface terms $p @ +\infty$ and PS mind at $-\infty$ which are 0.

So that is gone and therefore you find this is which \Rightarrow that this quantity is a constant but if I start at the origin at $t=0$ this is 0 at $T = \text{zero}$ and since it must remain constant it is 0 at all times so just telling you physically the fact that if we start with a symmetric initial distribution and let diffusion occur without bias the dis a still the distribution would remain symmetric at all times the average would remain 0 at all times so this is identically 0 what happens to the mean square displacement that is not 0 of course this is non-trivial.

So I would like to find $x^2(t)$ which is this and I start by finding x^2 on the side I multiply by x^2 so I have d/dt of x^2 of T on the right hand side this is what we are going to get I am going to put an x^2 here and integrate over X the first term the surface term will have an $X^2 DP/DX$ which goes to 0 and the next term will be a $-D$ times an integral $-\infty$ to ∞ the derivative of x^2 which is $2x$ so there is a 2 and then there is a DX and then an $X \delta P$ over δX the derivative of x^2 the integral of dy over DX .

Which is this and now I integrate by parts once again so that gives me $-2 dx$ times p at $-\infty$ to $+\infty$ that vanishes once again and then a $+ \text{sign}$ to D times the derivative of this which is unity and the integral of this which is P itself integrated but the integral of P is one because it is normalized so it is just this it finally leaves you with just $2D$ which \Rightarrow at once that x^2 of $T = 2 dt + \text{a constant}$ but at $t=0$ this is 0 and so the constant drops out and you end up with this famous result that the mean square displacement in diffusion is linearly proportional to time and the coefficient of proportionality is $2d$.

In each dimension of motion in three dimensions by computed r^2 it would be average x^2 + average y^2 + average z^2 which will give me $6DT$ now how does that tell you with the result there this thing here is certainly not a linear function of T except in the limit γT much bigger than one and these two must match therefore in the diffusion regime so we could call this the diffusion regime t much better than inverse in that regime x^2 average of $t = 2 dt$ we got something even more interesting if that is the case I must then equate this phenomenological coefficient D .

We just got put in by hand with what we got from the microscope $\pi c \text{ mo} \nabla$ here and that \Rightarrow but to dt here must be to dt there and that immediately tells you it is to sitting here and the γ cancels and you end up with $d = \text{the diffusion coefficient}$ is not arbitrary it is related to the dissipation in the system and it is related in this particular fashion this is another expression of

the fluctuation-dissipation relationship that I talked about the last time so a diffusion actually tells you how things spread out of fluctuations act on the system and γ tells

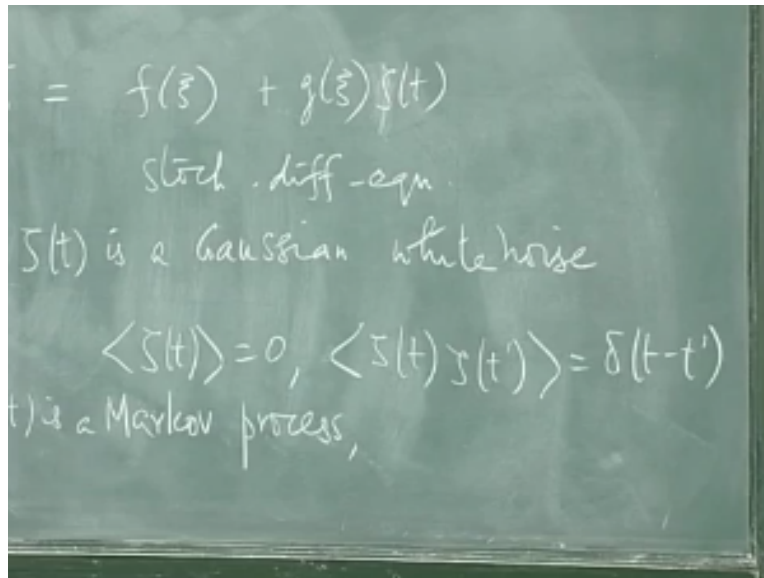
You how the dissipation in the system α and there is a connection between them this is also related to the viscosity of the fluid so now you could go back and ask what does this mean what sort of stochastic equation does X satisfy in order for this to happen and for this we need to know a little bit about the connection between stochastic differential equations and the corresponding master equations the Fokker-Planck equations. I write that relationship down without proof and it is as follows the relationship only yes that is what happened.

I mean that particular microscopic model no not at all that is only a model as it stands so we have no guarantee of this at all finally you have to test against experiment whether the model is successful or not so the statement made is the following and now by hindsight we can mention what in this particular problem what the resolution of this whole business is the time between collisions the time of interaction between two molecules is of the order of 10^{-15} seconds that is the sort of electromagnetic interaction time.

The time between collisions is of the order of a second or less the next time scale is the velocity correlation time which under normal circumstances for the kind of loads we are talking about would be of the order of microseconds so diffusion the diffusion equation would be a good approximation to the transport phenomenon on timescales much greater than microseconds that is it so there are lots and lots of time scales in the problem they are well separated from each other which is why this trick works finally and of course in a dense fluid under different conditions and so on things can get much more complicated the velocity is not given by the simple launch of my equation the point.

I want to make here from the point of view of dynamical systems is that for a given stochastic differential equation you can write down a Fokker-Planck equation for the conditional density and it is as follows?

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So if you have a random variables I and it is given by a first-order stochastic differential equation of the kind \dot{z} is some function of z we do not care what some function which gives you the drift of this thing + a white noise of this kind. Let me call it Z of T x perhaps a function of t where F and G are given functions and Z of T is a Gaussian δ correlated stationary Markov process with zero mean so we will make that assumption Z of T is a Gaussian white noise with zero mean $\langle \xi(t) \rangle = 0$ $\langle \xi(t)\xi(t') \rangle = \delta(t-t')$ I have absorbed.

Whatever constant sits here in this G if this is the stochastic differential equation obeyed by the random variable as I then this \Rightarrow of T is a Markov process whose conditional density satisfies a Fokker-Planck.

(Refer Slide Time: 45:58)

$p(\xi, t)$ satisfies

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

$$\frac{\partial p(x, t)}{\partial t} = \frac{\partial^2 p(x, t)}{\partial x^2}$$

$$x = \sqrt{2} \xi(t) \quad (f=0, g=\sqrt{2})$$

Equation of the following kind P of Z satisfies δP over $\delta T = -\delta$ over δ S I f of Z P of Z T + one-half G^2 this is the Fokker-Planck equation satisfied by P this is rigorously provable so the moment you have a random variable driven in this fashion by white noise stationary Gaussian δ correlated Markov process with zero mean then you are guaranteed that the output process P is a Markov process whose conditional density satisfies this equation this is generally given the name the Fokker-Planck equation and what we had is a special case in that case the equation we had for v if you recall was $v \dot{=} -\gamma V +$ what a white noise is of P over 1 over m times this so was essentially a constant in that problem so once we have this let us go back and ask what about the diffusion equation.

What kind of process was that well the diffusion equation said δP of X T over δT was $=d^2 P$ of X T over δx^2 so it corresponding to a situation but F was 0 this term did not appear at all and this term here was a constant which is given by g so it is quite clear that the stochastic differential equation $x \dot{=}$ is given by a white noise on the right-hand side and it is just square root of two $d x$ 0 so if you put $G = \sqrt{2} D$ $1/2 g^2$ is in fact d that is what we have so $f=0$ g was just a constant and this tallies with what we already know if this is a white noise its 0 correlation time is zero.

And we already saw that the displacement behaves this mean square displacement behaves linearly in the diffusion regime when T is much bigger than γ inverse in other words when the time scale is much larger than the correlation time of the velocity or another way of saying it is

on time scales compared to which the velocity correlation time is zero and acts like a white noise so really these two things are not contradictory at all but there is a consistency condition which connects one to the other here in fact that can be generalized.

It does not have to be and this is not the final thing I want to mention it does not have to be the launch of our model at all you could in fact start from very general considerations and ask what is the diffusion equation what does the diffusion constant do and that is not hard to see there is a final thing I am going to talk about.

(Refer Slide Time: 49:41)

Handwritten mathematical derivation on a chalkboard:

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

$$= 2 \int_0^t dt_2 \int_{t_2}^t dt_1$$

$$= 2t \int_0^t dt' \langle v(0)v(t') \rangle$$

The diagram shows a square in the t_1 - t_2 plane with axes labeled t_1 and t_2 . The square is divided into a grid, and a diagonal line is drawn from the origin to the top-right corner. The region below the diagonal is shaded, representing the integration region for the double integral.

So all we have to do is to start with this statement that the displacement in a time T is in fact the integral of the velocity over that time and then if I compute the square of this and I have rich this gives me this quantity $\int_0^t \int_0^{t_1} dt_2 dt_1$ and then I have $\langle v(t_1)v(t_2) \rangle$ from you t_1 to average and if the velocity is stationary in equilibrium that is all I want in other words the energy does not change at all everything is in thermal equilibrium then independent of what the form of this quantity is I could in fact simplify this whole thing

So the first step is to write this as this is a symmetric function so it is a function of $|t_1 - t_2|$ so the first step is to write it as $2 \int_0^t dt_1 \int_0^{t_1} dt_2 f(t_1 - t_2)$ now what have we done well here is t_1 here is t_2 and this is 0 to t 0 to t and I am integrating in this fashion but I could equally well integrate by interchanging orders of integration in this

fashion so if you interchange orders of integration here this becomes $\int_0^t dt' \int_{t'}^{\infty} dt$ on this side and this integral $\int_0^t dt'$ is always bigger than $\int_t^{\infty} dt$.

So it runs from t' to up to t sorry up to t' that is right $\int_{t'}^{\infty} dt$ and then this function of t' and now I change variables to $t_1 - t_2$ inside to $t_1 - t_2$ what happens to the lower limit of integration this becomes a zero and then this integral is trivial to do one of the integrations is trivial to do and to end up with a result which is $2 \int_0^t dt' \int_{t'}^{\infty} dt$ if you like or let me call it $\int_0^t dt' \int_{t'}^{\infty} dt$ in this fashion and then inside is $\langle v(0) v(t) \rangle$ of T this quantity is expected to start at one and decrease to 0 and the integral runs up to t what is the asymptotic $t \rightarrow \infty$ behavior of this well this term is going to dominate and this limit will go up to ∞ the parts where t' becomes comparable to t would be damped.

Because they go down here so it is clear that the $T \rightarrow \infty$ limit of this the asymptotic behavior of that is in fact this quantity for sufficiently long x goes to $2 D t$ times.

(Refer Slide Time: 53:56)

$$D = \int_0^{\infty} dt' \langle v(0) v(t') \rangle_{eq}$$

(Kubo-Green formula)

And integral from 0 to $\infty dt' \langle v(0) v(t') \rangle$ but if you insist that this should be $= 2 D T$ by definition it gives you a basic formula for the diffusion coefficient so it \Rightarrow that eventually the diffusion coefficient is intimately connected to the velocity correlation and independent of the

$\langle v^2 \rangle$ is $\int_0^t \int_0^\infty dt' \dots$ I might as well drop the prime here v of $\langle v^2 \rangle$ in equilibrium so it says the transport is determined by equilibrium fluctuations and thermal equilibrium the fluctuations of the velocity.

This has a name it is an example of what is called a Kubo-Green formula in the launch of a model this was $k/m e^{-\gamma t}$ and of course that give you D is $k/m \gamma$ but that was specific to the model but this is much more general all you need is that in this integral converges actually does not even have to converge you can show that the D if the process is diffusive and not super diffusive or anything like that then this D is actually the analytic continuation of the Laplace transform of this to $s=0$.

So you can put in an e^{-st} then it is the Laplace transform of the velocity correlation and if you after doing the integral go to $s=0$ that is the diffusion constant so this is in fact the beginning of the subject of non-equilibrium statistical mechanics but our interest here was from the point of view of dynamical systems and what I wanted to show you was that even if you include noise then the formalism changes a little bit it is more convenient to talk about phase space densities or densities now like the invariant measures.

We talked about earlier to talk about time-dependent probability density functions right equations for them and solve them and you get all the averages that you need and of course you could ask more complicated questions like what happens if you have a combination of deterministic and random components to the dynamics things get harder and harder but the formalism is well laid out so the model of the story is eventually you have to use statistical methods you have to write down equations for from either from or from other.

Inputs either from the dynamical equations or otherwise you have to write down equations for distribution functions the probability densities are the measures and then after that finds statistical averages of the quantities that you want and then there may be internal consistency conditions like the one we found $\langle v^2 \rangle$ here which you have to impose general they are not if the things of the random is the noise is totally different.

It is an external source they may not be such consistency conditions so very few general lessons but there are some pointers as to what one should do in such cases with that maybe I should stop here today you.

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