

Physical Applications of Stochastic Processes
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Lecture - 14
Langevin Dynamics (Part 3)

So today what we will do is to look at this in a more general context and write down multidimensional Fokker-Planck equations and apply to the case of particles moving in phase space itself.

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The image shows handwritten notes on a chalkboard. At the top, it says "Gaussian white noise". Below that, the equations are written as follows:

$$\dot{x} - v = 0$$

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

where $\langle \eta(t) \rangle = 0$ and $\langle \eta(t) \eta(t') \rangle = \delta(t - t')$. The probability density function is given as $p(x, v, t | x_0, v_0, 0)$. The Fokker-Planck equation is written as $\frac{\partial}{\partial t} p + R \frac{\partial}{\partial \mathbf{s}} p = \frac{\sqrt{\Gamma}}{m} \eta(t) \cdot \begin{pmatrix} 0 \\ \eta(t) \end{pmatrix}$, where $\mathbf{s} = \begin{pmatrix} x \\ v \end{pmatrix}$ and $R = \begin{pmatrix} 0 & -1 \\ 0 & \gamma \end{pmatrix}$. A note on the right says $(\Gamma = 2m\gamma k_B T)$.

So to recall to you what the equations were you had an equation which said $\dot{x} - v$ was equal to 0 that just says the velocity is the derivative of the position and then $\dot{v} + \gamma v$, this is the friction part, the systematic part of the random force on it. This was equal to square root of gamma over m eta of t where this was Gaussian white noise. In other words it is a delta correlated Gaussian process stationary Markov process which is delta correlated with unit strength.

So $\eta(t) = 0$ and $\eta(t) \eta(t')$ equal to delta function of $t - t'$ okay. And now the question is what is the corresponding Fokker-Planck equation satisfied by the probability, conditional probability density in both x and v jointly. So we are asking for the equation satisfied by p of x, v, t given that it started from x not and v not at time 0. It is important to remember that

earlier we had equations only in v and of course the equation satisfied by v was the Fokker-Planck by v was the Langevin equation.

We got a Fokker-Planck equation for it and the solution turned out to be the Ornstein-Uhlenbeck distribution and we discovered also that the velocity process was exponentially correlated and that it was a stationary random process okay. So that much we have already seen. Well now the question is what does this look like. What equation is satisfied by this quantity here corresponding to the set of equations here?

Now it turns out that if you have a general process a multidimensional process of this kind if we put them together in some vector form and you call that vector ψ say ψ dot plus if you got a linear drift $R \psi$ this is some constant matrix here acting on this column vector here. If this is equal to on the right hand side you have the usual noise of some kind. So we have γ over m and then η is a vector or η of t and this stands this this quantity ψ stands for x and v and this η of t stands for 0 η of t .

There is no noise here in this equation but there is a noise driving noise on this side due to the collisions with the other particles in the fluid. If you have a Langevin equation, a stochastic differential equation of this kind corresponding to it this quantity ψ its conditional probability density satisfies a certain Fokker-Planck equation and that Fokker-Planck equation is given by the following.

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

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

It is given by $\Delta \rho / \Delta t$ and let me call it ρ , let me call this ρ so that you know that it is a phase space density. This is equal to on the right hand side you have $R_{ij} \Delta \rho / \Delta \psi_j$ that is the drift term, the first term plus a $D_{ij} \Delta^2 \rho / \Delta \psi_i \Delta \psi_j$ where this matrix D_{ij} is in this case a 2 by 2 matrix which is 0, 0, 0 and then whatever was the matrix which came out from one half the square of this guy here.

But remember that consistency required that γ was equal to $2 m \gamma k_B T$. That was the fluctuation dissipation theorem. This is what kept the velocity in equilibrium and the Maxwellian was retained in time. Then one half the square of this guy the 2 goes away there is an m on top it comes and that m cancels out here with this m square give you a factor in the denominator. So you are going to get $\gamma k_B T$ over m .

That is what this guy is and that is the Fokker-Planck equation okay. All we have to do and there is a summation over repeated indices; i and j run over 1 and 2 okay. Now in this problem what is R ? Well from these 2 equations it follows that R in our problem here is equal to 0, -1, 0, and γ . So R_{12} is -1 R_{21} is 0. There is no x here and then R_{22} is γ out here and that is it. So that is the Fokker-Planck equation.

All we have to do is to write it out explicitly and you immediately see that $\Delta \rho$ this thing here is equal to in this particular problem are 1, 2 with a minus sign so there is a - Δ over

δ_i is equal to 1. So there is an δ over $\delta \psi_i$ $R^{-1/2}$ is what we need. So this is equal to 1. That gives me a minus δ over δx and this is 2. So that is a v times ρ out here and that is it.

There is one more term which is $R^{-2/2}$ which is δ over δv $\gamma v \rho$ that is the $2/2$ part plus the only term that survives in this term here is $D^{-2/2}$. That is the only non-zero element here and then it becomes δv^2 . So plus $\gamma k \text{ Boltzmann } T$ over $m d^2 \rho$ over δv^2 . That is it okay. Now of course v is independent of x because it is a dynamical variable which is independent of x .

So this is equal to $-v \delta$ over $\delta x \rho + \gamma$ times δ over $\delta v v \rho + \gamma k \text{ Boltzmann } T$ over m . This is the Fokker-Planck equation satisfied by a fairly complicated partial differential equation. This portion was already there in the Fokker-Planck equation satisfied by the conditional density of the velocity itself. So was this. But there is an extra term here out here and this is like a convective derivative because it is $v \delta$ it is like $v \cdot \text{del}$ in free dimension.

Just a one dimensional analog of that. So if you bring it to the left hand side you have d by dt d over dt of ρ the full derivative equal to whatever is on the right hand side with this linear drift and this extra diffusive term here. Now the question is what is the solution? Well, depends on the initial condition and we are talking about this conditional density. So at $t = 0$ this satisfies ρ of $x, v, 0$ at x not v not is δ of x minus x not del of $v - v$ not.

So with that initial condition if you solve that partial differential equation with the boundary condition that these things vanish as x and v tend to infinity you get Gaussian's as the solution finally. We are not going to do that here but you end up with some complicated Gaussian solution okay; a bivariate Gaussian both an x and v . So it will have terms like e to the $-x^2$ - e to the $-v^2$ and e to the $-$ or $+ x v$.

The interesting question to ask is what happens to this as t tends to infinity. In this problem t tending to infinity means t much greater than the velocity correlation time γ inverse.

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$$\begin{aligned}
\frac{\partial \rho}{\partial t} &= -\frac{\partial}{\partial x}(v\rho) + \frac{\partial}{\partial v}(\gamma v\rho) + \frac{\gamma k_B T}{m} \frac{\partial^2 \rho}{\partial v^2} \\
&= -v \frac{\partial \rho}{\partial x} + \gamma \frac{\partial}{\partial v}(v\rho) + \frac{\gamma k_B T}{m} \frac{\partial^2 \rho}{\partial v^2} \\
\rho(x, v, t | x_0, v_0) &\xrightarrow{t \gg \gamma^{-1}} \left(\frac{m}{2\pi k_B T}\right)^{\frac{1}{2}} e^{-\frac{mv^2}{2k_B T}} \left(\frac{1}{4\pi Dt}\right)^{\frac{1}{2}} e^{-\frac{(x-x_0)^2}{4Dt}}
\end{aligned}$$

So it turns out that rho of x, v, t given x not v not tends as t becomes much bigger than the correlation time it tends to the Maxwellian in v and the Maxwellian in v is of course m over 2 pi k Boltzmann T to the power half e to the - v square over 2 k Boltzmann T. So the velocity thermalizes and then you have the positional part and that of course is 1 over 4 pi dt to the power half e to the - x - x not whole square over 4 Dt.

You would recognize this to be the limit of the Ornstein-Uhlenbeck distribution as t tends to infinity. That is just the equilibrium Maxwellian distribution and that is the solution to the ordinary diffusion equation. The question is what is this capital D and we saw by comparison of the Langevin equation with the diffusion equation in the longtime limit we also saw that the other consistency condition was D is k t over m gamma.

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$$\Gamma = 2m \delta k_B T$$

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

So is there an equilibrium distribution, no. Because as t tends to infinity this vanishes out here. So it says that there is no stationary distribution for ordinary diffusion at all. Everything goes to 0. The whole Gaussian goes down flattens out to 0. The velocity however thermalizes and the velocity is a stationary random process it thermalizes okay. One could ask alright this is the phase space density what happens if I integrate over one of the variables. I should get the distribution in the other variable right.

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$$v + \delta v = \frac{\sqrt{\Gamma}}{m} \eta(t)$$

$$\langle \eta(t) \rangle = 0$$

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

$$\int_{-\infty}^{\infty} dx p(x, v, t | x_0, v_0) = \left[\frac{m}{2\pi k_B T (1 - e^{-2\gamma t})} \right]^{1/2} \exp \left\{ -\frac{m(v - v_0 e^{-\gamma t})^2}{2k_B T (1 - e^{-2\gamma t})} \right\} \leftarrow 0 \text{ U}$$

$$\int_{-\infty}^{\infty} dv p(x, v, t | x_0, v_0) = ?$$

So if you did this, if you took the exact solution if you did integral over dx rho of x, v, t not over the full space what should this give you. What would you expect it to give? It should give you, well it should be still a function of time because all you have done is to take the joint

distribution in x and v and you integrate it over the position. So it should give you the conditional density in the velocity alone and what is that distribution.

It is not the Maxwellian, that the limit distribution. The Ornstein-Uhlenbeck distribution. So it will end up with exactly the Ornstein-Uhlenbeck distribution. So this thing here will become m over $2\pi k \text{ Boltzmann } T$ $e^{-\frac{v^2}{2\gamma t}}$, that is the variance to the power half exponential of $-v$ minus the mean value which is $e^{-\gamma t}$. Remember this is conditional on this initial condition always.

So it is this square divide m times that over $2k \text{ Boltzmann } t$ $1 - e^{-2\gamma t}$. This is the Ornstein-Uhlenbeck distribution. So indeed it will turn out after you integrate over the position you end up with this okay. What would you expect if you integrate over the velocity instead. What do you think you will get if you did minus infinity to infinity $d v$ rho of x, v, t x not v not. What should you get? What would you expect? Would it be this? Would it be this?

What does your intuition tell you? Would it be that distribution? I got rid of the velocity altogether. So do you think it would be that distribution? That is only valid in the diffusion limit. That is only valid for t much greater than γ inverse. We are not saying anything like that here. We are just integrating over v . So what would you expect? It is the positional distribution. No doubt about it. It is the positional conditional distribution density in the position.

It will be a Gaussian because you have got a bivariate Gaussian you are integrating over one variable you are going to get a Gaussian in the other variable no doubt but much more complicated than that simple diffusion equation solution. It is some Gaussian. You need to know the exact solution of this equation in order to be able to do that. I am not going to write it down here. I will give it to you in writing elsewhere. It is a complicated formula.

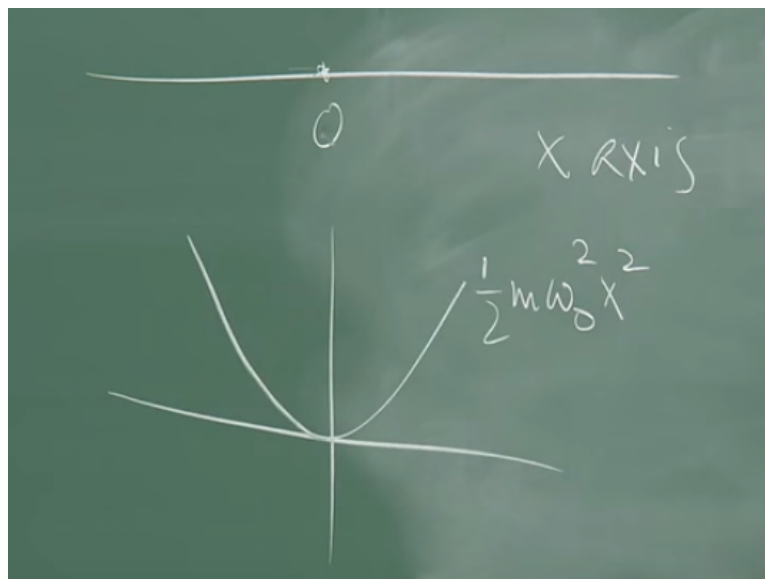
But that distribution will tend as γt tends to infinity will tend to that diffusion equation solution okay. And interestingly enough there is no simple formula here. Whatever distribution you get here that does not obey any simple master equation okay. So although the phase space density itself obeys this master equation the Fokker-Planck equation and the velocity process

itself obeys the Fokker-Planck equation the position does not obey such an equation simple equation at all except in the diffusion limit when you go to this long distance.

And if I have several ways of seeing this that the position is not a stationary random process we will talk about the Wiener process very shortly and then you will see how complicated the position actually can become okay and what Brownian motion means and so on and so forth okay. So, so much for this that this distribution has an asymptotic limit which does this and when you integrate the position you end up with the Ornstein-Uhlenbeck distribution.

Now we can generalize this a little bit go a little further. We can ask what happens if I had an external force on the problem. What would then be the effect of an external force? One way to approach this is to ask is to look at a slightly different model. Instead of a free particle, let us look at the problem of an oscillator, a simple harmonic oscillator.

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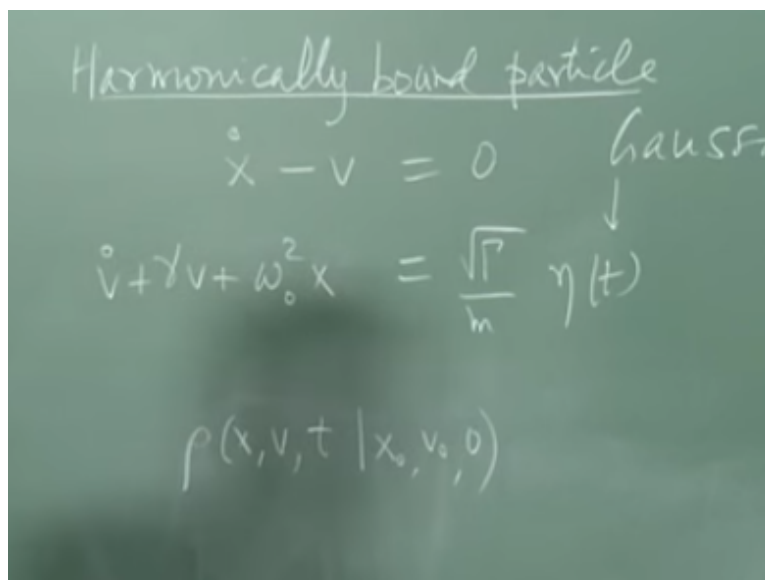
Now what we are talking about is a particle on the x axis. Here is x equal to 0 and this is a simple harmonic oscillator in the absence of any external force. But we now imagine it is in a fluid with viscosity and this particle is being hit randomly by the other particles in the fluid okay and we want a Langevin type model for its motion here. So there is a white noise exactly as in this case but there is also a systematic part of the force which corresponds to putting in the harmonically bound particle namely this thing is in a potential.

Now this potential is going to do something interesting. The actual harmonic oscillator potential is $\frac{1}{2} m \omega^2 x^2$ as you know. Now the first effect of this potential is that the translation symmetry on this x axis is lost because this point becomes a special point. There is a potential here. The other thing is you are it is as if this particle is connected by a spring, a harmonic spring to the origin and therefore there is a strong restoring force if the displacement is very far away from the origin.

So you might expect okay there is going to be 2 effects here. One of them is the random force due to the other particles which is tending to diffuse move this particle away and make its mean square displacement diverge as a function of time. The other effect is this restoring force which is always acting where the question is what is going to happen to this particle. Will it diffuse or will it not? Well the variance of the displacement diverge as t tends to infinity.

If it does so linearly you know that it is diffusive. If it goes to a finite constant then you know it is no long range diffusion at all. So the question is what is going to happen. So that is the physical question. We can answer it in the following way. I can write this down by adding to this the restoring force and that of course is $- m \omega^2 x$ and I have divided out by m .

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Handwritten equations on a chalkboard:

Harmonically bound particle

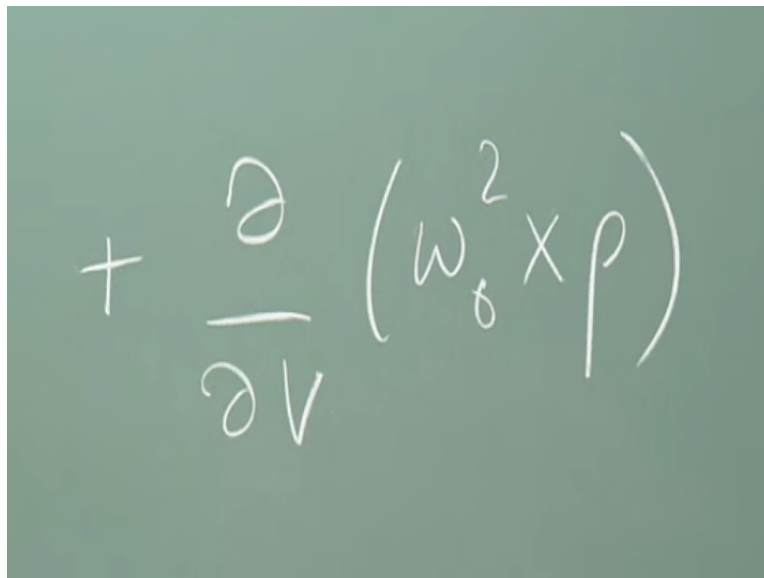
$$\dot{x} - v = 0 \quad \text{Gauss}$$
$$\dot{v} + \gamma v + \omega_0^2 x = \frac{\sqrt{\Gamma}}{m} \eta(t)$$
$$p(x, v, t | x_0, v_0, 0)$$

So there is also a term $v \cdot + \gamma v + \omega_0^2 x$. Let me call it ω_0 , the unperturbed frequency of this oscillator. So this is the case of a harmonically bound particle and that is the equation. Everything else is unchanged, exactly as it is. Now, of course the velocity once again thermalizes and there is an equilibrium velocity distribution which is again the Maxwellian distribution.

But there is also this potential energy term coming from the potential in which the particle is okay. So now what happens; exactly as before, I can write down the same problem. I have ρ of x, v, t and we could start it from 0 for example just to make sure that it is simplest condition but whatever it is given some x not given some v not at 0 the question is what does this particle do? What does the density satisfy?

Again, the same Fokker-Planck equation as before, same as this exactly but whereas in the previous case this fellow was equal to 0, R was equal to $0 - 1 \ 0 \ \gamma$. What is it now? Remember there is an extra term here $\omega_0^2 x$ and this is appearing with a coefficient x in the equation for v . So it means there is a term here which is $\omega_0^2 x$. That is the only difference between the 2. Everything else goes through exactly as before.

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$$+ \frac{\partial}{\partial v} (\omega_0^2 x \rho)$$

So there is going to be here another term which is equal to plus. There is a term which is equal to $\frac{\partial}{\partial v}$ and what would this be? It is in the v equation okay so $R \ 2 \ 1$ is what

contributes. So this is $\frac{\partial \rho}{\partial v} \omega^2 x$. It is the term of that kind. Because it is going to contribute to a $\frac{\partial \rho}{\partial v}$ because it is R^2 and this is a 1 so there is an x inside, $\omega^2 x$ okay.

That is the only change and we have an exact answer for the Fokker-Planck equation satisfied by a harmonically bound particle in phase space and of course ω^2 is constant so let us write that out.

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The image shows a chalkboard with the Fokker-Planck equation for a harmonically bound particle. The equation is written in two lines:

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

$$0 = -v \frac{\partial \rho}{\partial x} + \omega_0^2 x \frac{\partial \rho}{\partial v} + \gamma \frac{\partial}{\partial v} (v \rho) + \frac{\gamma k_B T}{m} \frac{\partial^2 \rho}{\partial v^2}$$

So let us write this as equal to $-v \frac{\partial \rho}{\partial x} + \omega^2 x \frac{\partial \rho}{\partial v} + \gamma \frac{\partial}{\partial v} (v \rho) + \frac{\gamma k_B T}{m} \frac{\partial^2 \rho}{\partial v^2}$ because this time x is independent of v so that comes out just as out here v was independent of x so it came and that the Fokker-Planck equation okay. Now the solution to this is very different from the solution in the absence of ω altogether okay. What do you think will happen, physically what do you think will happen?

Think back to equilibrium statistical mechanics. If you have a free particle free gas the position is irrelevant and the position is equally spaced distributed entirely in the container then it is only the velocity that is relevant okay. So gas and thermal equilibrium classical gas you only talk about velocity distribution at a given temperature. The position is taken to be uniform throughout but now there is a harmonically bound particle.

So it is clear that the energy of this particle, there is a contribution which is half $m\omega^2 x^2$ to the potential energy of this particle and we know that the relative probability of any value of the energy is $e^{-\epsilon/kT}$. So you would expect to get in equilibrium the distribution would be biased towards $x = 0$ obviously. Most probable value of x would be 0 in this case and what is the actual distribution? It is the Boltzmann distribution right. So what is the actual equilibrium distribution?

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$$P(x, v) = e^{-\frac{mv^2}{2kT}} e^{-\frac{m\omega_0^2 x^2}{2kT}}$$

So equilibrium of x and v or the stationary distribution from equilibrium statistical mechanics what would this be? It is $e^{-\epsilon/kT}$ and that is it normalized, appropriately normalized. So this guy would obviously be $e^{-mv^2/2kT}$ that the kinetic energy part - $m\omega_0^2 x^2/2kT$, that the potential energy part right times normalization factors; e^{-ax^2} where a is a positive constant if you integrate you end up with square root of π over a . So it is square root of a over π , a is the normalization right.

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$$P_{eq}(v) = \sqrt{\frac{m}{2\pi k_B T}} \sqrt{\frac{m\omega_0^2}{2\pi k_B T}} e^{-\frac{mv^2}{2k_B T} - \frac{m\omega_0^2 x^2}{2k_B T}}$$

So this thing here equal to square root of m over 2 pi k Boltzmann T square root of m omega not square over 2k Boltzmann T. this is the normalized distribution such that if you integrate over x and v you are going to get unity completely. So the distribution factors into something in x, a Gaussian in x and a Gaussian in v velocity. You expect this on physical grounds that this is going to happen okay and that is it.

So this exact solution will reflect that, will reflect precisely this. Now tell me does the variance of the mean displacement diverges the function of time do you think or no. We cannot, it cannot because the limit value limiting distribution in position is a Gaussian and Gaussian has finite variance completely. So there is no long range diffusion. The behaviour is not diffusive. It is tending to a Gaussian random variables.

It is going to do exactly what the velocity does except for a change of constant here and so on. Notice dimensionally everything is okay because the Maxwellian distribution in velocity must have physical dimensions one over the velocity so that p of v B v is equal to 1 when you integrate right. So there is an m here and there is an m kT which is ml square T to the - 2 and the m cancels and you got a l square T to the - 2 square root which is l T inverse.

So this whole thing the velocity is in fact one over velocity one over velocity in physical dimensions and similarly this is going to be one over length because the T to the - 2 cancels here

okay. So this is perfectly correct dimensionally and you end up with distributions which are stationary distributions in this case. So the mean square displacement will not diverge. What will it be actually, the mean square displacement. What do you think this will be?

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The image shows two equations written on a chalkboard. The first equation is $\langle v^2 \rangle_{eq} = \frac{k_B T}{m}$. The second equation is $\langle x^2 \rangle_{eq} = \frac{k_B T}{m \omega_0^2}$.

What do you think v square will be in equilibrium? What should this be? $k_B T$ over m because half $m v$ square will have half $k_B T$ so this is $k_B T$ over m . x square in equilibrium. What will this be? No long range diffusion is possible and that is reflected by the solution to this guy. Again, this is a bivariate Gaussian this fellow here is a bivariate Gaussian which will now tend in as t tends to infinity it will tend to this equilibrium distribution here.

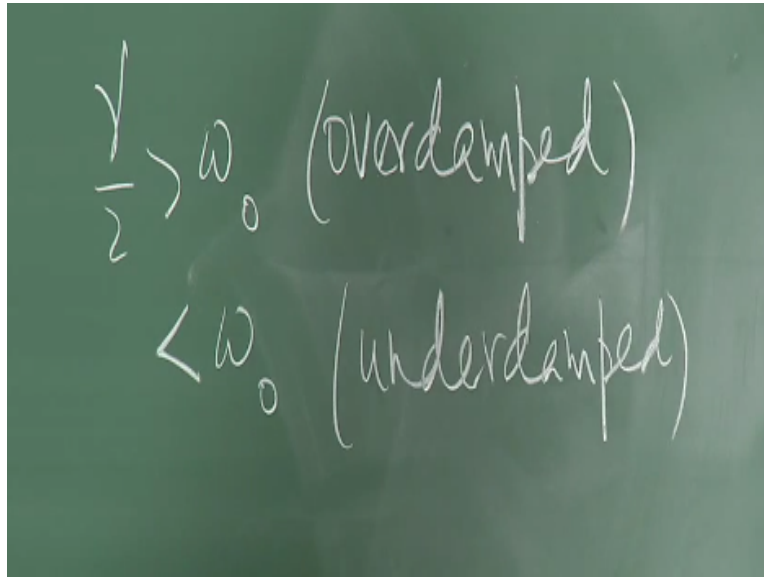
But there is an interesting wrinkle here. What do you think is the relaxation time for the position and the velocity? You can tell what this is by looking at these equations here and in a minute you will see what the difference is in a minute. You see what happens is the velocity thermalizes over a time scale γ inverse. That is the correlation time of the velocity but the position does not thermalize with that right.

For instance if it is an underdamped oscillator, it is clear that it is going to reach equilibrium values in an oscillatory fashion always. If it is overdamped it is going to go monotonically and so on. So the ω_0 and γ together will provide 2 time scales in this problem and what is

the criterion for over damping of an oscillator given this natural frequency ω_0 and a damping constant γ both of which have time dimensions of frequency.

So you know that in this general expression you end up with γ^2 , whether that is bigger than ω_0^2 or smaller than ω_0^2 etc.

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This is overdamped and of course less than ω_0 is underdamped. We do not care what it is. This equation is valid in general. Whatever the value of ω_0 and γ this equation is true in general and there is a complicated solution, a bivariate Gaussian solution but the relaxation times of the two are different from each other altogether. We will see in a minute and show you what the relaxation, effective relaxation time is for the case of the position.

Because you can also ask in this problem in which I am telling you, I am asserting even without writing the general Gaussian solution down that x does not diffuse the behaviour of there is no diffusion, long range diffusion here and that there is a stationary distribution both in x and v in this case. Both x and v are stationary Gaussian processes in this case. So here if you integrate over the velocity, you will end up with the distribution for the position whose solution is some kind of Gaussian and describes a stationary random process.

It is a distribution conditional density, is a stationary that of a stationary Markov process. Similarly for the velocity as well okay. Now, we could ask can we quickly see what the position

itself does. How do we get at it assuming that the velocity has thermalized. What would one do in this case? Well, this is what one would write down. I will start with the second equation and write it in this form.

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$$\ddot{x} + \gamma \dot{x} + \omega_0^2 x = \frac{\sqrt{\Gamma}}{m} \eta(t)$$

High friction limit

$$\dot{x} = -\frac{\omega_0^2}{\gamma} x + \frac{\sqrt{\Gamma}}{m\gamma} \eta(t) = -\frac{\omega_0^2}{\gamma} x + \sqrt{\frac{2k_B T}{m\gamma}} \eta(t)$$

$\ddot{x} + \gamma \dot{x} + \omega_0^2 x = \frac{\sqrt{\Gamma}}{m} \eta(t)$ okay and then I look at the overdamped oscillator case in other words very high friction. So this is called a high friction limit. There is a systematic way of doing this. I have divided by m but imagine putting the m here and saying this term dominates very high friction γ is very large. Then the inertia term can be neglected okay.

The effect of the mass is supposed to be light. The friction is supposed to be very high and then m can be neglected, this original term and then it becomes a Langevin equation just like the velocity Langevin equation for a free particle right. Except there is slight difference here. Now you got an equation which says $\dot{x} + \frac{\omega_0^2}{\gamma} x = \frac{\sqrt{\Gamma}}{m\gamma} \eta(t)$ let us put it on the right hand side.

So $\dot{x} = -\frac{\omega_0^2}{\gamma} x + \frac{\sqrt{\Gamma}}{m\gamma} \eta(t)$ That is the Langevin equation for the position in this limit okay. So let us simplify it a little bit and what does this give you. This is equal to $-\frac{\omega_0^2}{\gamma} x + \sqrt{\frac{2k_B T}{m\gamma}} \eta(t)$

$m \gamma$ whatever it was right and there is an $m \gamma$ out here. So this is square root of $2k$ Boltzmann T over $m \gamma \eta$ of t okay in this limit, in this high friction limit okay.

So that is a Langevin equation. Compare this with the Langevin equation for the velocity for a free particle. What did we get?

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A photograph of a chalkboard with handwritten text and an equation. On the left, the words "Compare with" are written vertically. To the right, the Langevin equation for velocity is written: $\dot{v} = -\gamma v + \sqrt{\frac{2\gamma k_B T}{m}} \eta(t)$. The square root term is written as $\sqrt{\frac{2\gamma k_B T}{m}}$ with $\eta(t)$ written to its right.

We found that \dot{v} compare with \dot{v} equal to $-\gamma v +$ square root of γ over m that was equal to square root of $2 \gamma k$ Boltzmann T over $m \eta$ of T compare with that. So apart from this thing γ here being replaced by ω not square over γ and then this constant changing to this other constant it was exactly the same in structure right. So what is the Fokker-Planck equation for this p here? So what is this going to be?

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High friction limit

$$\dot{x} = -\frac{\omega_0^2}{\gamma} x + \sqrt{\frac{F}{m\gamma}} \eta(t) = -\frac{\omega_0^2}{\gamma} x + \sqrt{\frac{2k_B T}{m\gamma}} \eta(t)$$

$p(x,t|x_0)$ satisfies

$$\frac{\partial p}{\partial t} = \frac{\omega_0^2}{\gamma} \frac{\partial}{\partial x} (xp) + \frac{k_B T}{m\gamma} \frac{\partial^2 p}{\partial x^2}$$

P of x, t assuming that you start from some origin at $t = 0$, the x not we do not care satisfies $\frac{\partial p}{\partial t}$ equal to okay and what is the first term on the right hand side. This is a simple Langevin equation for which you can write the Fokker-Planck equation immediately right. So this is equal to ω_0^2 over γ $\frac{\partial}{\partial x} (xp)$ because everything is in x xp that is the drift part + one half the square of this guy whatever this was + $k_B T$ over $m\gamma$ $\frac{\partial^2 p}{\partial x^2}$.

That is the Fokker-Planck equation for p of x, t right. Do you recognize $k_B T$ over $m\gamma$, what is that? That is the diffusion constant, that is the diffusion constant. So what we have got here is what happens in the high friction limit to a harmonically bound particle as it diffuses. So there is a correction if you lime due to the potential to the diffusion term. This is D capital D . Without this ω_0^2 not it would be $\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2}$.

That is the plain diffusion equation and you have long range diffusion but now you got this extra term here okay. As soon as you have that what does that imply? It says something very interesting.

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Stationary distribn $p_{st}(x)$.

$$\frac{d}{dx} \left[\frac{dp_{st}}{dx} + \frac{m \omega^2 x}{k_B T} p_{st} \right] = 0$$

It says immediately that a stationary distribution would exist p of x as t tends to infinity and it should satisfy an equation in which this term is 0, Δp over Δt is 0 right. It must satisfy stationary distribution p stationary of x must satisfy d over dx . So let us write it down of k Boltzmann T over $m \omega^2 x$ $d p$ stationary over $dx + \omega^2 x^2$ over $k_B T$ p stationary $= 0$.

What I have done is to save this term is a function of x alone now so this goes away and I have just put that in and this is it oh there is an x d over dx x times p stationary equal to 0 which implies of course that this comes out and then if I take this down there it says $m \omega^2 x^2$ over $k_B T$. Therefore this is a constant independent of x . That is the current and if you say the current is 0 at infinity p stationary vanishes and so on and derivatives vanish then the constant is 0 everywhere.

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$$\frac{d p_{st}}{dx} + \frac{m \omega_0^2 x}{k_B T} p_{st} = 0$$

$$\Rightarrow p_{st} = \frac{1}{\sqrt{2\pi k_B T}} e^{-\frac{m \omega_0^2 x^2}{2 k_B T}}$$

So we can get rid of this in an infinite medium and is equal to 0 implies p stationary equal to e to the power $-\frac{m \omega_0^2 x^2}{2 k_B T}$. All I have to do is to integrate x and that is x^2 over 2 with a minus sign and then a normalization constant which is $\frac{m \omega_0^2}{2 k_B T}$ square root, 2π and that is the solution which is exactly what we get from equilibrium statistical mechanics.

So we got the Gaussian, stationary Gaussian there. There is no long range diffusion etc. But the general equation is this here. This equation is the equation satisfied by a diffusing particle in the presence of an external force a potential in this case, a harmonic potential in this case. It is called a Smoluchowski equation.

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Stationary

$$\dot{x} + \omega_0^2 x = \frac{\sqrt{\Gamma}}{m} \eta(t) \quad \text{Smoluchowski eqn.}$$

high friction limit

$$\dot{x} = -\frac{\omega_0^2}{\gamma} x + \frac{\sqrt{\Gamma}}{m\gamma} \eta(t) = -\frac{\omega_0^2}{\gamma} x + \sqrt{\frac{2k_B T}{m\gamma}} \eta(t)$$

$p(x,t|x_0)$ satisfies $\frac{\partial p}{\partial t} = \frac{\omega_0^2}{\gamma} \frac{\partial}{\partial x}(xp) + \frac{k_B T}{m\gamma} \frac{\partial^2 p}{\partial x^2}$

This equation here is an example okay. And that term is generally applied to the diffusion equation in the presence of an arbitrary external force. We are going to apply it to other situations as well. For instance we put a magnetic field, this particle is charged and you put a magnetic field and moves in 3 dimensions and the question is what kind of probability density the position and velocity and the phase space density have and that is the question we are going to answer. But this is an, the simplest example of a Smoluchowski equation okay.

One can generalize this a little bit and say, it does not have to be a harmonic potential. It could be any function, any force you like. We need that because we are soon going to do the case of a magnetic field. So what do these equations look like.

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Particle in a potential $V(x)$

$$\dot{x} = v$$

$$\dot{v} = -\gamma v - \frac{1}{m} V'(x) + \frac{\sqrt{\Gamma}}{m} \eta(t)$$

So particle, and let us write in a potential let us say V of x and let us write the phase space equation down and then see what happens. So again let us do it in one dimension first and then we will generalize this to higher dimensions okay. So we have $x \text{ dot} = v$ equal to 0. But now let us put the v on the right hand side, $x \text{ dot} = v$ and $m v \text{ dot} = - m \gamma v$, that is the systematic part and then there is a term which is $- V \text{ prime of } x$.

That is the force on the particle plus whatever is the random force. Plus, so let us divide through by this guy as always $1 \text{ over } m + \text{square root of } \gamma \text{ over } m \eta \text{ of } t$ and now this $v \text{ prime of } x$ may be nonlinear in x . That makes the equation extremely hard to solve because you no longer have a linear drift. Now we got a really hard problem in our hands. So the question is what does this solution look like?

What does this thing look like in general? What does the phase space density Fokker-Planck equation look like okay. So for this we need a slight generalization of the linear drift case where the drift matrix was given by R . Now it is some complicated nonlinear function in general.

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

$(n \times 1)$ $(n \times v)$ $(v \times 1)$

$$\langle \eta_i(t)\eta_j(t') \rangle = \delta_{ij} \delta(t-t')$$

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial \xi_i} (f_i \rho) + \frac{\partial^2}{\partial \xi_i \partial \xi_j} [D_{ij}(\xi) \rho], \text{ where } D_{ij} = \frac{1}{2} (g g^T)_{ij}$$

So let us say as usual that we have an equation of the form $\dot{\xi}$ equal to some vector valued function f of ξ . I have in mind putting this ξ as the x 's and v 's depending on how many dimensions there are, all the dynamical variables plus a multiplicative noise which is let us say g of ξ on this η of t okay and let us be completely general. We do not know what the dimensionality of this ξ is.

If it is a particle moving in one dimension then there is an x and a v . If it is moving in 3 dimensions then there are 3 x 's and 3 v 's and so on and so forth and we have so far been looking at the case where the noise is just in that single component of the velocity but there could be different noises on different components. They could be completely uncorrelated noises. For instance if the particle moves in 3 dimensions you resolve it into 3 Cartesian coordinates.

There is no reason to expect that all the forces in all the directions are identical. They are completely uncorrelated. In fact what we will do end up doing is to say that this force η_i of t η_j of t' expectation where i and j are Cartesian components would be uncorrelated with each other if i is not equal to j . So I am going to say this is equal to $\delta_{ij} \delta(t - t')$. For instance we are going to do things like that. So we need to keep that in mind.

So let us be completely general and say that this is an N -dimensional object so I write it as a column vector in other words n by 1 object, column vector of this kind. So is this and this noise

could be in some of the components. It may not have any noise at all in some of the others. For example there is no noise here, no explicit noise okay. So let us say this fellow here is ν by 1. So it is ν dimensional white noise. There are ν of these guys, $\eta_1, \eta_2, \dots, \eta_{\nu}$. Then this g in general, this would be an n times ν matrix so that when it acts on the ν times 1 it is going to give you an n by 1 okay. That is the general situation okay.

Then corresponding to this equation this implies, by this correspondence we have between a Markov process the Langevin type equation for a Markov process and the corresponding Fokker-Planck equation for a diffusion process and the Fokker-Planck equation we have $\frac{\delta \rho}{\delta t}$ equal to in this case $\frac{\delta}{\delta \psi_i} \psi_i \rho$ and summed over the components i sorry $f_i \rho + \frac{\delta^2}{\delta \psi_i \delta \psi_j} D_{ij}$ which could in general be a function of this ψ because this guy is ρ where $D_{ij} = \frac{1}{2} g_i^T g_j$ okay. This is a transpose.

That is the generalization okay. Remember that g is an n by ν matrix. So g^T is a ν by n . So this whole thing turns out to have the right dimensions out here. And that is the general Fokker-Planck equation and what we need to do is to apply to this case out here. The reason I need this generalization is because this is not linear. In the oscillator case this was linear and I just identified that R matrix and the matter was over. But now this is not linear.

So the solutions in general would not be Gaussians or anything like that. They are fairly complicated things if at all. And at the moment we do not know if there is a stationary distribution or not at all. So what does this give us?

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Particle in a potential $V(x)$

$$\dot{x} = v$$

$$\dot{v} = -\gamma v - \frac{1}{m} V'(x) + \frac{\sqrt{\Gamma}}{m} \eta(t)$$

$$\xi = \begin{pmatrix} x \\ v \end{pmatrix} \quad f = \begin{pmatrix} v \\ -\frac{V'(x)}{m} - \gamma v \end{pmatrix}$$

It says in this case $\delta \rho$ over δt equal to and first we got to do this term here so exactly as before we are going to have f in this problem. So let us write down the f psi in this problem is just x and v ; f in this problem is equal to there is a v and there is a $-v$ prime of x over $m - \gamma v$. D_{ij} mercifully is easy enough. It is exactly as before because again this is just constants out here. This is 0 out here.

What is new in this problem; n is 2, little n is 2 because it is a 2-dimensional object. What is little n ? Just 1, just 1. So it is a very trivial problem in this case.

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$$\frac{\partial^2}{\partial \xi_i \partial \xi_j} \left[D_{ij}(\xi) p \right], \text{ where } D_{ij} = \frac{1}{2} (g g^T)_{ij}$$

$$\begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{m} \end{pmatrix}$$

So D_{ij} once again this matrix in this problem is again 0, 0, 0 γ $k_B T$ over m half g transpose etc okay. So we can write down what this equation is in one dimension.

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$$\frac{\partial \rho}{\partial t} = -v \frac{\partial \rho}{\partial x} + \gamma \frac{\partial}{\partial v} (v \rho) + \frac{T'(x)}{m} \frac{\partial \rho}{\partial v} + \frac{\gamma k_B T}{m} \frac{\partial^2 \rho}{\partial v^2}$$

(Kramer's equation)

$\Delta \rho$, $\rho \Delta t$ equal to $-v \Delta$ over Δx ρ . That is one portion that comes from here because there is a minus sorry minus. So I took f on the right hand side so it is a minus sign okay and then plus $\gamma \Delta$ over Δv 0 , that term will always remain and then there is a term which is Δ over Δv this thing so this is equal to plus v prime of x over $m \Delta$ over Δv ρ that is this term plus the usual plus $\gamma k_B T$ over $m d^2 \rho$ over Δv^2 .

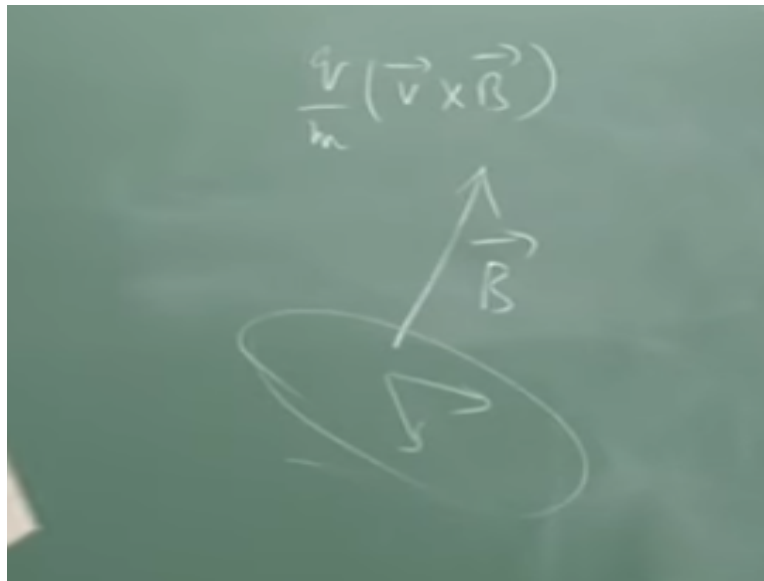
This is the one dimensional phase space density, conditional density for particles moving on the x axis alone, just one component and it is got this extra term here due to the external force okay or the potential, applied potential. Everything else is familiar as it stands. This equation is called the Kramer's equation. We will write down generalizations of this to three dimensional problems etc. It is fairly very straightforward to write it down in three dimensions.

In fact I urge you to do this as an exercise. Do this in general when you would write this as a vector and this equation too as a vector. Now this γ arises from a fluid and is related to the viscosity of the fluid which will take to be isotropic. So it is the same in all the directions, does not matter, for all the Cartesian components.

And this of course would be replaced by the gradient, minus the gradient of the potential and then for the noise take this to be η_i corresponding to a v_i and η_i is delta correlated such that different Cartesian components are not correlated to each other okay and write the general Kramer's equation down in three dimensions for the phase space density as a function of vector \mathbf{R} vector \mathbf{v} and t . So that is a fairly straightforward generalization.

What would happen if you put this particle in a magnetic field? What kind of force does it see? That is an interesting case. I mean we are going to do this problem but just to anticipate what is going to happen. What do you think will happen?

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So I put a magnetic field in some direction like this and you have this particle moving in three dimensions inside a container, a fluid and it is diffusing and there is also this magnetic field. What do you think will happen? Well, the particle will tend to do cyclotron motion around the direction of this field right. On the other hand it is also diffusing. What is the force applied by this magnetic field on the particle? It is the Lorentz force right. So there is a q times \mathbf{v} cross \mathbf{B} .

So there is going to be an extra term on the right hand side which is q over m \mathbf{v} cross \mathbf{B} . That force is not derivable from a potential, from a scalar potential which is a function of position. It is a velocity dependent force but the problem is still very tractable and solvable, why is that?

What is it about this force that makes the problem solvable completely? It is linear. It is linear in v .

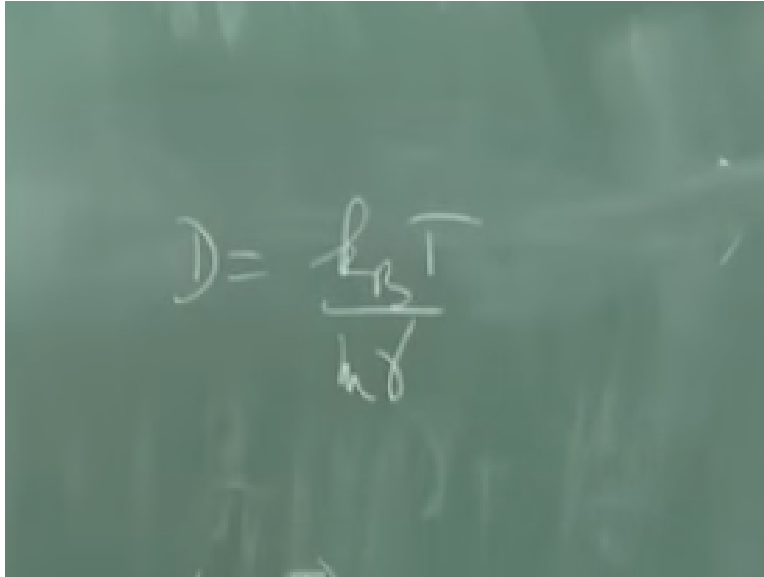
So as soon as we have a linear problem this drift matrix becomes R which is a constant matrix and then I have a problem of exponentiating this constant matrix the Green functions can be found etc., etc. Maybe complicated in principle but in practice it is doable completely. So the fact that it is linear is very crucial. So this problem can be solved. It is a velocity dependent force. Of course it is going to look like this term.

It is going to have a v but the difference of course is that $v \cdot \dot{v}$ will involve v^2 and v^3 whereas this term is just v in $v \cdot \dot{v}$ etc. So it will mix it up and secondly this γ represents the effect of dissipation. As you know if you put a particle in the magnetic field, a free particle its energy does not change, kinetic energy does not change. So there is no loss of energy at all. So that portion of the drift term will be reversible in time but this portion will not be.

This is what leads to things tending to an equilibrium etc. Now tell me suppose I have a gas of charged particles and there is overall neutrality maintained by some background and then these particles are diffusing at some finite temperature, clearly if I put a magnetic field that field does no work on these particles whatsoever. So will it change the Maxwellian distribution at all if it is in equilibrium? It should not change this Maxwellian distribution.

The temperature will remain exactly the same. Nothing is going to happen. But will the diffusion constant get affected? What will happen? What do you think is going to happen to this?

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

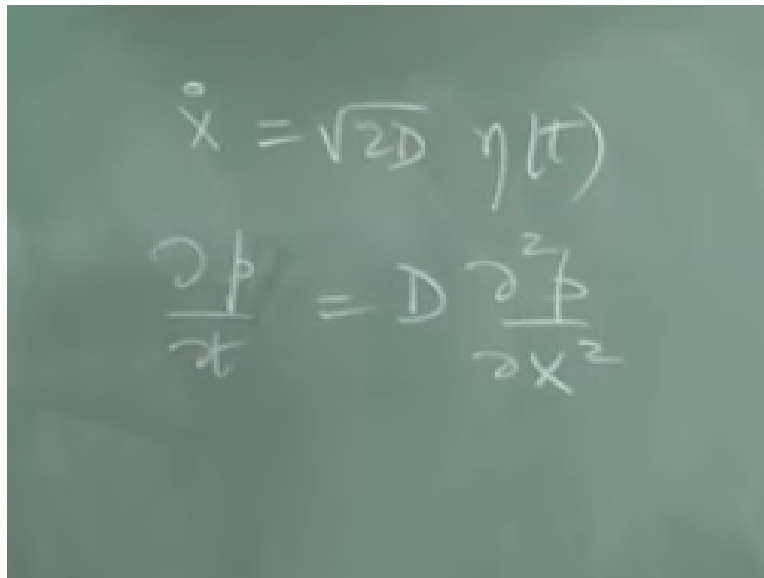
Well we know that otherwise if it is one-dimensional motion we know that this D was equal to $k_B T$ over $m \gamma$. That by the way remains true no matter how many dimensions the particle moves in because each Cartesian component, the variance goes like $2 D t$ and if you have 3 components then the R^2 goes like $6 D t$ that is all that happens. So the D is exactly the same $k_B T$ over $m \gamma$. But now I put a magnetic field. What do you think is going to happen?

This isotropy is broken. There is a specific direction, singled out by the magnetic field. Will the diffusion along this direction be affected at all? It would not be affected at all because there is no force in this direction at all. On the other hand in the perpendicular plane there are 2 other directions in this plane. The diffusion is inhibited because when it tries to diffuse there is a cyclotron motion kicking in trying to make it curve its path back again.

So we are going to discover that this diffusion tensor D_{ij} is not going to be a constant times the unit matrix. It is going to be such that the x and y components are not as large as the z component. So D_{33} if you put the magnetic field in z direction is going to be bigger and in fact we expect it to be just $k_B T$ over $m \gamma$ but in the other 2 directions the diffusion constant is going to be inhibited. We will see explicitly how that comes about. But that is just a physical argument.

We will write it down explicitly and see what happens here. So this equation here, this basic equation, the Kramer's equation is a starting point for discovering whether the system has a stationary distribution or not and so on. What we are going to do now next is to first take care of the problem of the magnetic field and after that I am going to go back and say let us look at the diffusion process itself, the simple diffusion equation itself a little more carefully.

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The image shows two equations written on a chalkboard. The first equation is $\dot{x} = \sqrt{2D} \eta(t)$, representing the Langevin equation. The second equation is $\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2}$, representing the diffusion equation.

And ask what sort of process is the process x where the density of x the probability density of x obeys a $\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2}$ the original diffusion equation in one dimension and the corresponding Langevin equation which in this case was just \dot{x} equal to square root of $2D$ times η of t in the diffusion limit. This means that you got time scales much bigger than γ inverse and then the particle is essentially as if the velocity is uncorrelated.

It is delta correlated is a noise in this case. In this approximation you have \dot{x} as just white noise on the other side and the corresponding density obeys the ordinary diffusion equation. This is called Brownian motion, mathematical Brownian motion and this process x this x process is called a Wiener process and it is the integral of white noise.

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$$\dot{x} = \sqrt{2D} \eta(t) \Rightarrow x(t) - x(0) = \sqrt{2D} \int_0^t dt' \eta(t')$$

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

Because formally what is happening this will imply that formally x of $t - x$ of 0 equal to integral 0 square root of $2D$ times integral 0 to t dt' prime η of t' prime. So what we have is a process that is the integral of white noise and is much less singular than the white noise itself which has this delta function kind of correlation and we are going to ask what is this x of p .

It is called a Wiener process and we are going to study it and its sample parts in some detail okay. So that will be the next program because this thing is what acts as a paradigm the very model for random process, as random as you can get in some sense and it has a lot of interesting properties. Once we do that I will come back and make a connection between this and the Ornstein-Uhlenbeck process which as I told you is a unique, continuous, stationary, Gaussian, Markov process.

It is a unique process and we will see that there is a theorem which will tell you that in some sense if you studied this process the Wiener process you studied all Gauss-Markov processes. We will see how this is done by mapping okay. So that will be the next start. Thank you.