

**Non-equilibrium Statistical Mechanics**  
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**Module No 01**  
**Lecture 18: Fokker-Planck equations (Part 2)**

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## Fokker-Planck equations (Part 2)

- FPE for general (nonlinear) drift and diffusion coefficients in the multi dimensional case
- Kramers' equation for phase space PDF in an applied potential
- Asymptotic form of the phase space PDF
- Diffusion regime (or high-friction limit): Smoluchowski equation for the positional PDF
- Overdamped oscillator: OU distribution for the positional PDF

Right. Let us now today look at the correspondence between a stochastic differential equation for a diffusion process and the corresponding Fokker Planck equation

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General SDE  $\leftrightarrow$  FPE correspondence

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

$\leftrightarrow$

$$\frac{\partial p(v,t)}{\partial t} = \gamma \frac{\partial (vp)}{\partial v} + \frac{\gamma k_B T}{m} \frac{\partial^2 p}{\partial v^2}$$
$$p(v,0) = \delta(v-v_0)$$

$\rightarrow p(v,t) = \text{OU distribn.}$

So let us call this the general stochastic differential equation and the Fokker Planck equation correspondence. Just to refresh your memories, let us go back and look at what we had come out with in the case of the ordinary equation. There we had  $\dot{V}$  the velocity, one component was  $-\gamma V +$  the noise. This noise after I divided by  $M$  etc etc, this turned out to be square root of  $2\gamma kT$  over  $M$  and then there was a  $\zeta$  of  $T$  here. I used the fluctuation dissipation theorem divided by  $M$  and so on and then you have, you had a  $2M\gamma kT$  divided by  $M^2$  square.

I put it inside the square root. So this becomes  $M$ . And this implied if you recall the original Fokker Planck equation for the the Ornstein–Uhlenbeck distribution like distribution. So this implied immediately that the conditional density of  $B$  satisfied this equation  $PVT$  divided by  $T$  is equal to  $\gamma$  Times  $\Delta$  over  $\Delta V$   $V$  times  $P + \gamma kT$  over  $M$ . This was  $k$  Boltzmann  $T$  over  $M$   $D^2P$  over  $DV$ . And we have to solve this with some specific initial condition,  $V$  not for instance. So the initial condition was  $P$  of  $V, 0$  equal to a delta function at  $V$  not.

And this led to  $P$  of  $VT$  equal to the Ornstein–Uhlenbeck distribution. That was the 1<sup>st</sup> Fokker Planck equation we came out with, right? We also saw what happened if we assume the velocity to be a delta correlated process. Then we were in the diffusion regime.

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for  $t \gg \tau$   
(or high friction limit)

$$\dot{x} = \sqrt{\frac{2k_B T}{m\gamma}} \zeta(t)$$

↕

$$\frac{\partial p(x,t)}{\partial t} = \left( \frac{k_B T}{m\gamma} \right) \frac{\partial^2 p}{\partial x^2}$$

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So we saw that for  $T$  much much greater than  $\gamma$  inverse which we could implement by actually going back to this equation and then throwing out the inertia term and retaining just this term here. In which case, we had a term, high friction limit or high friction limit, we had  $\dot{X}$ , that is  $V$  is equal to the same thing here but square root of  $2 K \text{ Boltzmann } T$  over  $M \gamma \zeta$  of  $T$  because this term was negligible and I took this on this side and brought the  $\gamma$  down and we ended up with that thing which then imply here, just as this automatically implied it.

So similarly back here, you have  $\Delta P$  of  $X T$  over  $\Delta T$  equal to  $K \text{ Boltzmann } T$  over  $M \gamma D^2 P$  over  $D X^2$ . This was the ordinary diffusion equation because this quantity was the diffusion coefficient.

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$$\dot{X} + K X = \begin{pmatrix} \text{const} \\ \gamma(t) \end{pmatrix}$$

$(n \times 1)$   
 $(n \times n)$  drift matrix

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$$\frac{dX}{dt} + K X = (\text{const; coeffs}) \zeta(t)$$

$(n \times n)$   
 drift matrix

$$\frac{\partial \rho}{\partial t} = K_{ij} \frac{\partial}{\partial x_i} (x_j \rho) + D_{ij} \frac{\partial^2 \rho}{\partial x_i \partial x_j}$$

on limit)  
 (t)  
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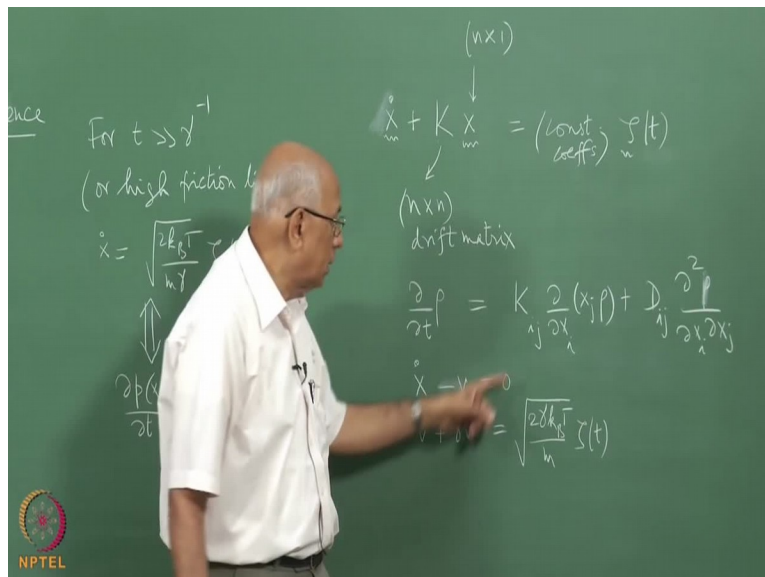
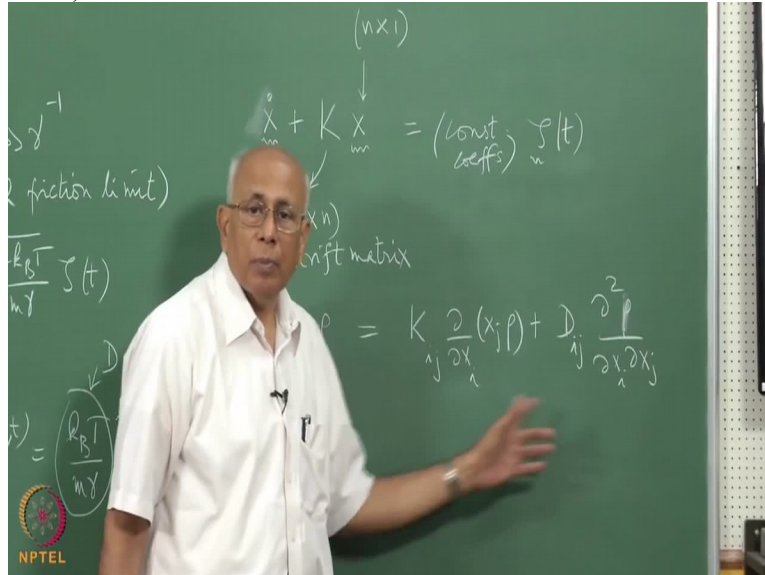
So these are special cases of a more general result which I wrote down which was that if you have an equation which says  $\dot{X} + \text{some matrix } X$ , this is a higher dimensional process and this is some, this quantity is an  $N$  by  $1$  column vector and the drift was linear in it. This here on the right-hand side was equal to some coefficients, constant coefficients, not a function or anything like that times the noise of some kind. So there was some coefficients, constant coefficients and we will make this precise in a minute.

And then there was a vector valued noise,  $\zeta$  of  $T$ . So these are all  $N$  by  $1$  quantities and this is an  $N$  by  $N$  drift matrix. So if you had a situation like this which is a special case which is a generalisation of this fellow here right? So the reason we want that is because we want to be able to write down Fokker Planck equations for the phase space density, joint density in  $X$  as well as  $V$  together. So if you had a situation like this then this immediately implied that  $\Delta$  over  $\Delta T$  and whenever there is a phase space density namely a density in more than one variable, I use the symbol  $\rho$  so that it is distinct from this little  $P$  okay.

So this quantity  $\Delta$  over this quantity here was equal to  $K_{ij} \Delta$  over  $\Delta x_i \Delta x_j \rho +$  some matrix, constant matrix formed from these coefficients here and the natural thing to call it is a diffusion matrix  $D_{ij} \Delta^2 \rho$  over  $\Delta x_i \Delta x_j$ . This diffusion matrix there is a definite prescription for finding it from these coefficients. We are going write it in a more general case. So I do not I am not bothered about writing this down in need special case or anything like that. Suffice it to say that just like in these cases, this was a constant, this was a constant, et cetera.

Essentially, it is square of this constant divided by 2. That is what it is but I will not make it a little more systematic.

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So you end up with an equation like this. This is the Fokker Planck equation right? Now we can apply this to the situation which we did earlier, namely the langevin particle in one dimension and then we did this quickly for 3 dimensions. So in one dimension, this was of the form  $X \dot{\text{dot}}$  was equal to  $V$ . So  $X \dot{\text{dot}} - V$  equal to 0 and  $V \dot{\text{dot}} + \gamma V$ , this thing here essentially we are writing this equation again, is equal to whatever is there, square root of 2 gamma  $KT$   $K$  Boltzmann  $T$  over  $M$ , in this fashion, zeta of  $T$ .

So the noise, the vector noise is 0 in the 1<sup>st</sup> row and it is equal to this fellow in the 2<sup>nd</sup> row. So the coefficient, the matrix of, the column vector of coefficients is just this and this. But you actually need a matrix here.

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The chalkboard contains the following handwritten equations:

$$\frac{\partial \rho}{\partial t} = K_{ij} \frac{\partial}{\partial x_i} (x_j \rho) + D_{ij} \frac{\partial^2 \rho}{\partial x_i \partial x_j}$$

$$\begin{pmatrix} x_1 = X \\ x_2 = V \end{pmatrix}$$

$$\dot{X} - V = 0$$

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

$$K = \begin{pmatrix} 0 & -1 \\ 0 & \gamma \end{pmatrix}$$

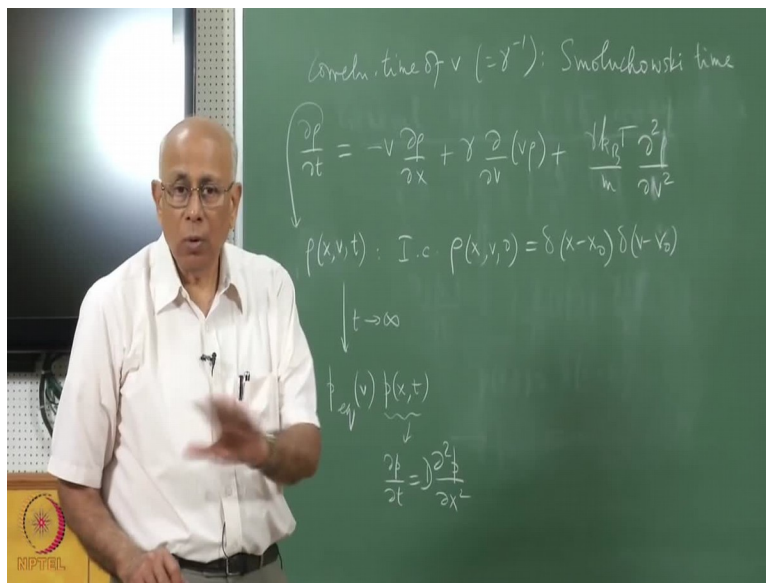
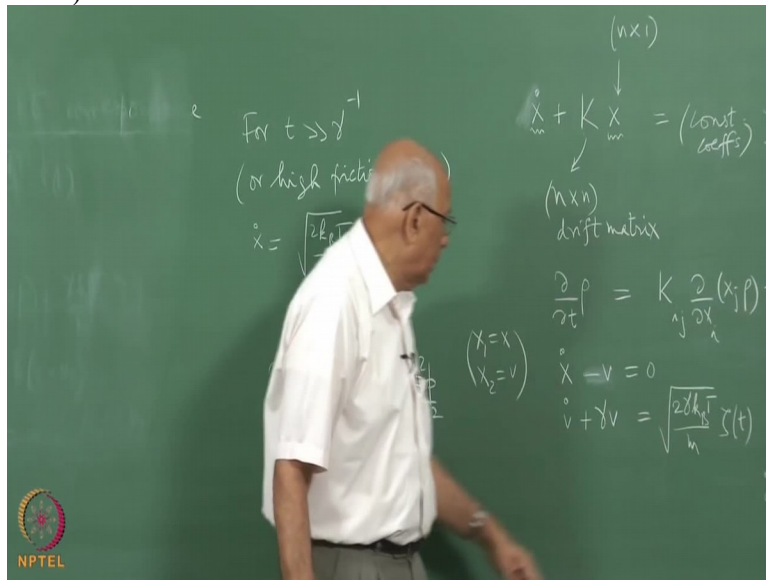
$$D = \begin{pmatrix} 0 & 0 \\ 0 & \frac{\gamma k_B T}{m} \end{pmatrix}$$

So in this particular problem, let us write what these things were. K was the matrix 0, - 1, let us then let us show this thing here. By the way the identification is X1 equal to X, X2 equal to V. That is the identification which we are making to write this down. Then it is 0, - 1 and then a 0 here and a gamma here, this gamma. So it is a linear drift matrix. In fact, it is more than that. It is even simpler than that. It is constants everywhere here and it is 0s along this which helps.

And DIJ in this case, let me call that matrix D whose elements are DIJ. I do not want to write V alone here without subscripts goes I have used that for the symbol. I have used that symbol for this quantity and we will stick to that. This thing here is a call to 0, 0, 0, K Boltzmann T over M. So that is the equation obeyed by the phase space density and we have done this already. So let us write that out and then we are going to new material.



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Now that immediately implies that the phase space density satisfies  $\Delta \rho / \Delta T$  equal to now we need to put this in KIJ, so the 1<sup>st</sup> term is with - sign as you can see and then you have a K12, that is the only element which is present here which is - 1 and therefore it is  $\Delta \rho / \Delta X$  of  $V \rho$  with a - sign. But  $V$  is independent of  $X$ ,  $X_2$  is independent of  $X_1$ . This is equal to -  $V \Delta \rho / \Delta X$  is the 1<sup>st</sup> am and then K21 is anyways 0. K22  $\Delta \rho / \Delta V$  times whatever is sitting here, whatever is sitting inside here which is  $\gamma$  okay.

So the next term is +  $\gamma \Delta \rho / \Delta V$  times  $V \rho$ .  $\Delta \rho / \Delta X_2$   $X_2 \rho$  and  $X_2$  is  $V$ . And then the only term present from the diffusion matrix is the 22 term. That is the only

term that is nonzero out here. So that gives us exactly what we had in the original Fokker Planck equation,  $\gamma K \text{ Boltzmann } T \text{ over } M V^2 \rho \text{ over } \Delta V^2$ . This is the question satisfied by the phase space density  $\rho$  of  $X$ ,  $V$  and  $T$ . And you are supposed to solve this equation with some given initial conditions.

So you are supposed to solve it the initial conditions,  $\rho$  of  $XV$  is 0 equal to  $\Delta$  of  $X - X$  not,  $\Delta$  of  $V - V$  not. It is a little harder to solve than the Fokker Planck equation for the velocity process alone which did not have this term  $K$ . And then we got the Ornstein–Uhlenbeck distribution. Now you have to use this term as well and solve it. It is not such a trivial solution but the solution is a general Gaussian in both  $X$  and  $V$ , a joint Gaussian in  $X$  and  $V$ .

And that Gaussian has the property that as  $T$  tends to infinity, this Gaussian goes to the  $P$  equilibrium in  $V$ , the Maxwellian distribution multiplied by the solution of the diffusion equation which of course vanishes as it tends to infinity strictly everywhere but we want a leading behaviour. In the asymptotic regime, this is  $P$  of  $X$ ,  $T$  and this satisfies  $\Delta P \text{ over } \Delta T \text{ equal to } \frac{D^2 P}{DX^2}$ . That is the regime in which the velocity has lost its memory,  $\gamma T$  is much much greater than  $\gamma$  inverse.

$\gamma$  inverse is called the smoluchowski time okay. The correlation time of the velocity, this is  $\gamma$  inverse is called. So it sets a timescale in the problem. There is also a length scale in this problem. There is no potential, there is no general external potential because if the particle were moving in a potential like a harmonic oscillator potential or something like that, you could get a length scale in the problem but here there is no length scale at all from the potential, no potential.


But there is still a length scale and what would that be? There is a characteristic timescale in the problem which is  $\gamma$  inverse. Well, there is a characteristic velocity in the problem and therefore there is a carrier or a speed and therefore there is a length scale. What is the characteristic speed in this problem? There is one quantity of dimension, speed. The mean square in equilibrium from this right?



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$$\text{I.c. } \rho(x, v, 0) = \delta(x - x_0) \delta(v - v_0)$$
$$\langle v^2 \rangle_{eq}^{1/2} = \sqrt{\frac{k_B T}{m}}$$

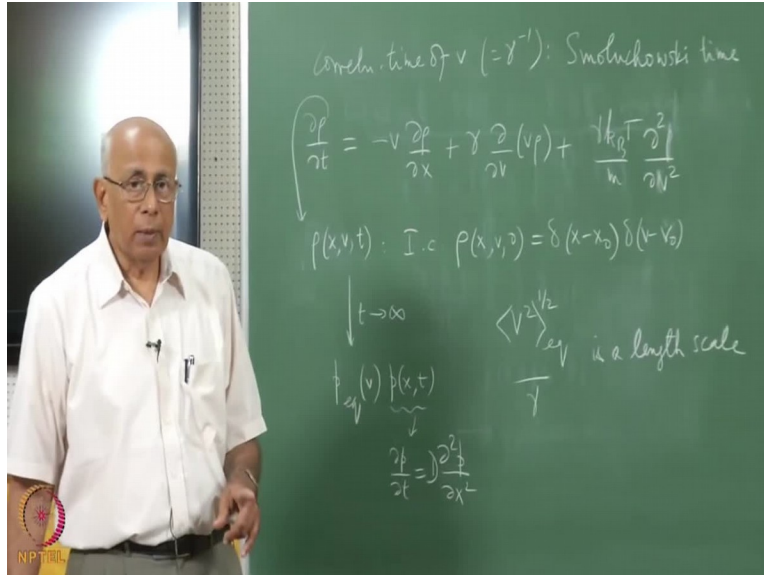
(x, t)



$$\text{I.c. } \rho(x, v, 0) = \delta(x - x_0) \delta(v - v_0)$$
$$\frac{\langle v^2 \rangle_{eq}^{1/2}}{\gamma} \text{ is a length scale}$$

(x, t)





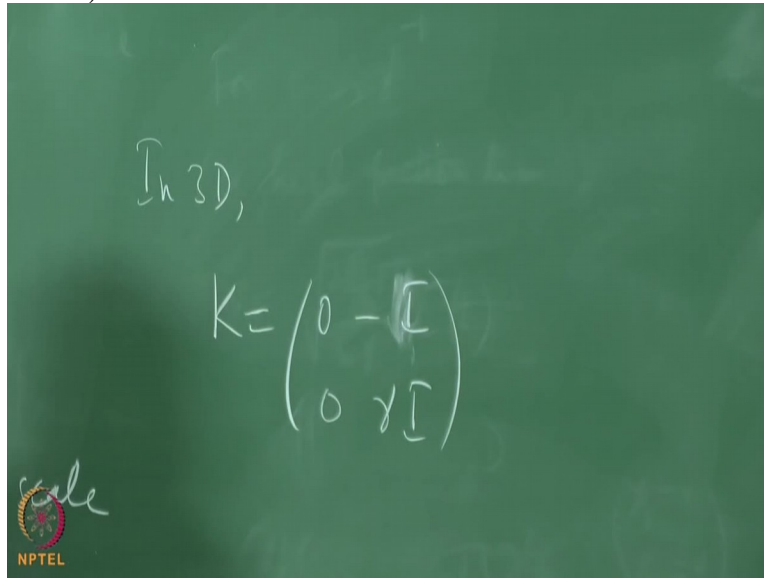
So this  $V$  square equilibrium is  $K$  Boltzmann  $T$  over  $M$ . Square root sorry. This quantity gives you a speed, characteristic speed. Therefore there is also a length scale. What would you do? You divide by  $T$  inverse  $X$ ? So you, so this fellow here, put this in is characteristic length scale in this problem. This is  $LT$  inverse, this is  $T$  inverse. So it is an  $L$ . You can compute what it is. You can compute what it is. For the Brownian particles we are talking about, we know what the masses are between  $10$  to the  $-12$  and  $10$  to the  $-15$  kilos, we know what the temperature is,  $300$  Kelvin.

So we know  $KT$ , we know what  $\gamma$  is because  $\gamma$  is related to the viscosity of a fluid, take water at room temperature for instance, then  $\gamma$  is of the order of  $10$  to the  $-6$ ,  $-7$  seconds. Therefore we know what this quantity is. We can compute what this length scale is. It is indeed very tiny. It is very very tiny. All right. But we keep at the back of our mind, that there is such a length scale even in the absence of an external potential okay. So having got this far, we would like to know what happens next.

What happens if I put the system under an external force, under an applied potential? Like the harmonic bound particle, suppose there is a potential present,  $X$  dependent potential, what would happen to these equations? Well, the 1<sup>st</sup> thing that would happen is that your Langevin equation would become different. Co-incidentally we also saw what the three-dimensional generalisation of this was. We wrote this three-dimensional generalization. This becomes  $V$  dot gradient with respect to  $R$  rho, this becomes gradient with respect to  $V$  dot, the divergence of  $V$  times rho with respect to  $V$  here.

And then this is the Del Square with respect to  $V$ . So that part is over. And in general, the solution is some kind of Gaussian which would asymptotically become something like this. Writing it down in 3 dimensions is very messy but in one dimension, one can write the explicit solution down okay.

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$$\text{In 3D,}$$
$$K = \begin{pmatrix} 0 & -I \\ 0 & \gamma I \end{pmatrix}$$

By the way one important point in the three-dimensional case, whatever we wrote here in terms of that drift matrix,  $K$  and so on is still true but in that case what would happen is in 3D for example, this matrix  $K$  would become  $0 - \text{the identity matrix}$ ,  $0, \text{gamma times the identity matrix}$  where  $I$  is a 3 by identity matrix. So this is fairly straightforward. This is 6 by 6 object. So the generalisation is kind of trivial. The reason I am emphasising this is because we would like to what did we do in the original langevin case?

We actually solved the equation of motion, the langevin equation and then started taking velocity averages and so on. Now you have a matrix equation to solve which will involve the exponentiation of this matrix. You will have to do  $\int_0^t E^{-K(t-s)} ds$ . Just as we found  $E$  to the  $\text{gamma T}$ , we have  $E$  to the  $\text{KT}$ . That would be your integrating factor if you like. But  $E$  to the  $\text{KT}$ , this matrix has interesting properties and therefore you can find immediately the eigenvalues are 0 and gamma, so you can actually find the exponential quite explicitly and write the rest of the solution. All right.

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Brownian particle in a potential  $V(x)$

$$\dot{X} = v$$
$$\dot{v} = -\gamma v - \frac{1}{m} V'(x) + \sqrt{\frac{2\gamma k_B T}{m}} \zeta(t)$$

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So now let us turn what happens when you have a potential, it is a Brownian particle in a potential. And again, let us do the one-dimensional case 1<sup>st</sup>. So you have as before  $X$  first let us do the phase space distribution and then we will come back and do the positional distribution. So it will be technically a little easier because you can see what are the approximations involved because we need to now know what is the diffusion regime, we need to know that 1<sup>st</sup>. So let us look at the phase space problem.

$X$  dot equal to  $V$  as before and  $V$  dot is  $-\gamma V$  same model as before. But now there is an external potential, some  $F$  of  $X$  and I divide it by  $M$ . So it is  $-\frac{1}{M} V'$  of  $X$ . This is some potential in a potential,  $V$  of  $X$  capital  $V$  of  $X$ , is that term present and then the last term is exactly as it was before  $+\sqrt{\frac{2\gamma k_B T}{M}} \zeta(t)$ . This consistency condition to keep the system in equilibrium is going to remain in any case. No matter what  $V$  of  $X$  does, it would still remain because what happens is that the velocity will still thermalise and there is the external potential acting on the particle.

We do not care about it but the velocity will thermalise and of course the distributions themselves will become very different. There is no reason why now if I solve, if I write down the phase space density, why the solution should be a generalised Gaussian? No reason at all. The introduction of this  $V'$  of  $X$  makes the equation of motion non-linear. Earlier in all the

cases, we looked at the equation of motion was linear in the dynamical variables, there was an external noise. But now that is gone.

Student: Unless V of X is...

Professor: Unless V of X is either a constant or a quadratic, is either a linear function or a quadratic function. If it is a linear function, then this becomes a constant like gravity for instance. If this thing is a quadratic function, it is like the oscillator problem. But in all other cases, the equation of motions themselves become non-linear in the dynamical variables and that will going to make it complicated. Okay. Now what is the way in which we write down the Fokker Planck equation? We cannot do what we did earlier because we have this fellow which is a non-linear term right? So the general correspondence goes like this. We do not care how many, what the dimensionality of our phase space variables is. It could be N dimensional in general.

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General diffusion process:

$$\dot{X}_m = f_m(x) + g_{\nu m}(x) \int_m(t) \quad (1 \leq \nu \leq n)$$

$(n \times 1)$   $(n \times 1)$   $(n \times \nu)$   $(\nu \times 1)$   
 matrix matrix

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x_i} [f_i p] + \frac{\partial^2}{\partial x_i \partial x_j} [D_{ij} p]$$

$$D = \frac{1}{2} (g g^T)$$

$$D_{ij} = \frac{1}{2} \sum_{\alpha=1}^{\nu} g_{i\alpha} g_{j\alpha}$$

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So let us write the general langevin equation. General diffusion process has a stochastic equation which is X dot equal to on the right-hand side, some possibly non-linear function of the variables and this is also vector value. So this guy here, X is N by 1 column matrix and this is an N by 1 vector force, there is a force for each of these components and thats in general a function of all the axis, all the coordinates. We have still not taken the most general case where this could be explicitly time-dependent but I said, we are not going to look at those problems at the moment.

+ a  $G$  of  $X$ , this is multiplicative noise in general. But you look at times the noise, but look at what happened? So this is some  $\zeta$  of  $T$ . In general, this is some matrix acting on this column vector but look at what happened in the earlier case? The equation  $\dot{X} = V$  did not have any noise on the right-hand side. But  $\dot{V} = \text{something}$  on the other hand a noise because we wrote an equation for a random force on the particle. So the dimensionality of this noise may be lower than the dimensionality of your phase space variable.

So we have to allow for that. So suppose this fellow is a  $n_y$  by 1 column matrix. So you have  $N$  equations for the components of this but only  $n_y$  of them have noise on the right-hand side. And what is the smallest value that  $n_y$  can have?

Student: 1.

Professor: 1. If it has 0, then everything is deterministic. We are not, we do not even have a stochastic equation.

1 less than equal to  $n_y$  less than equal to  $N$  because all  $N$  of them might have noise. We do not care. Right? Then what sort of matrix has this got to be? This is got to be an  $N$  by  $n_y$  matrix. It is got to be an  $N$  by  $n_y$  matrix. This on the other hand is an  $N$  by 1, this is  $N$  by 1 and therefore  $N$  by  $n_y$  and then a  $n_y$  by 1 gives you an  $N$  by 1. That is the most general diffusion process that we can write down. There is an  $N$  dimensional dynamic a set of dynamical variables and then there is a new dimensional noise on the other side. And the noise is multiplicative in general. And then value of the noise for each coefficient could depend on all the variables dynamical variables. You can see, this is very general out here.

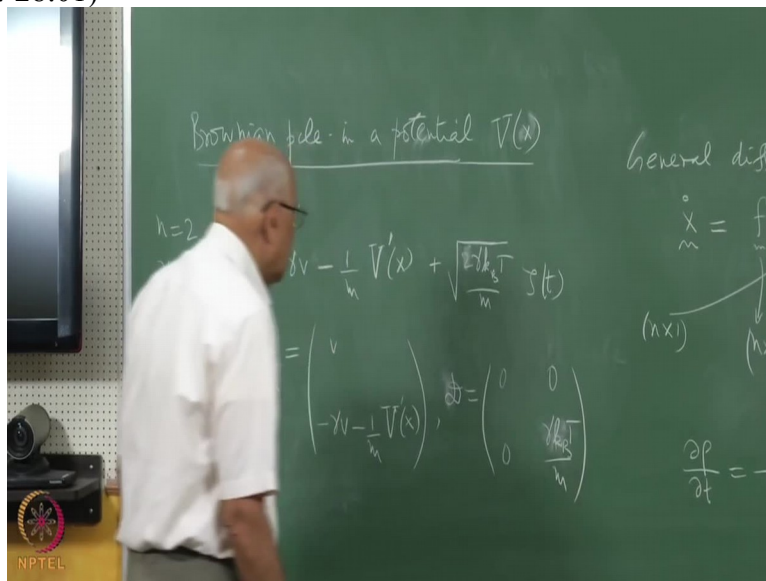
The question is, what is the Fokker Planck equation corresponding to this? I am just going to write it down. So this implies and is implied by a Fokker Planck equation which is  $\Delta \rho / \Delta T = - \Delta \cdot (F \rho)$ . It is like a generalized  $\Delta \cdot$  whatever, so it is a divergence term and then the next term is  $+ \Delta^2 \cdot (D \rho)$ . There is a diffusion matrix but is not a set of constant coefficients because you have this sitting here. So the question is what is this  $D_{ij}$  equal to? So it is clear that we have to be a little careful.

It is not just  $G^2$  as it would have been in the one-dimensional case. This matrix  $D$  is one half  $G$  matrix,  $G$  transpose matrix because this is  $N$  by  $n_y$  and that fellow is  $n_y$  by  $N$ . So the

product is N by N. D is a N by N diffusion matrix because the indices I and J run from 1 to N. And there is a summation over repeated indices. So in explicit form, this implies that  $D_{IJ}$  equal to one half the summation from Alpha equal to 1 to nyu  $G_I \text{ Alpha } G_J \text{ Alpha}$ . That is what is meant by transpose here. It is clear. So this is the general Langevin equation, the general stochastic differential equation and this is the general Fokker Planck equation.

Notice notice that this set of coefficients is not necessarily constants because it depends on this function G inside here it gets differentiated. It is inside. So this is fairly complicated here. Likewise, no matter how non-linear the force is, this drift term is, it is inside here. So given that, lets try and ask what does our equation look like here for this situation in the one-dimensional case?

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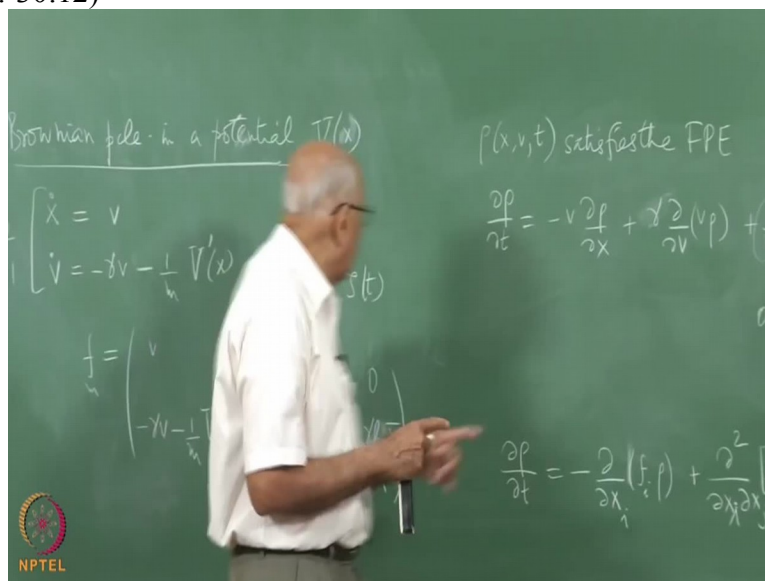


So we want an equation for  $\Delta \rho / \Delta T$  where this rho is rho of X, V and T. So this is equal to well  $X_1$  is X and  $X_2$  is V. So we want  $-\Delta / \Delta X_1$  and then F. So let us 1<sup>st</sup> write his F matrix. In this case F equal to this fellow is a column vector and the 1<sup>st</sup> one is a just V out here it is clear. And the 2<sup>nd</sup> portion is  $-\gamma V - 1 \text{ over } X V \text{ prime of } X$ . That is this column. And what is D, the matrix D? Well, it is the same as before because you can see that this thing here is acting oh in this problem, what is N equal to? 2 of course and what is nyu equal to? 1.



That is trivially true. Only one of these equations has noise, the other one does not. So this is a very trivial case but the reason I wrote this down is because I am now going to require you next to do this for the three-dimensional case when you have an external field, a potential as well as a magnetic field which will make a velocity dependent force. So that is a little intricate but it is a 6 dimensional phase space but we can write the equations down given the general expressions. Now what is this matrix equal to? It is obviously equal to 0, 0, 0 and half the square of this which is  $\gamma K \text{ Boltzmann } T \text{ over } M$  in this case. And now we are all set. All we have got to do is to copy this and write the question down for rho.

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So this is, therefore rho of XVT satisfies the Fokker Planck equation  $\Delta \rho \text{ over } \Delta T$  equal to -, there is a - here and then the V comes out because the 1<sup>st</sup> is  $\Delta \text{ over } \Delta X$  times V rho but V is independent of X as before. So this term is still present, - V  $\Delta \rho \text{ over } \Delta X$ . This is the convective derivative V dot Del with respect to the coordinate and then there is another term here and what is that? That is equal to +  $\gamma \Delta \text{ over } \Delta V$  V rho this this portion takes care of this and then there is a +  $1 \text{ over } M \Delta \text{ over } \Delta V$  of V prime of X times rho but V is independent of X. So V prime of X comes out.

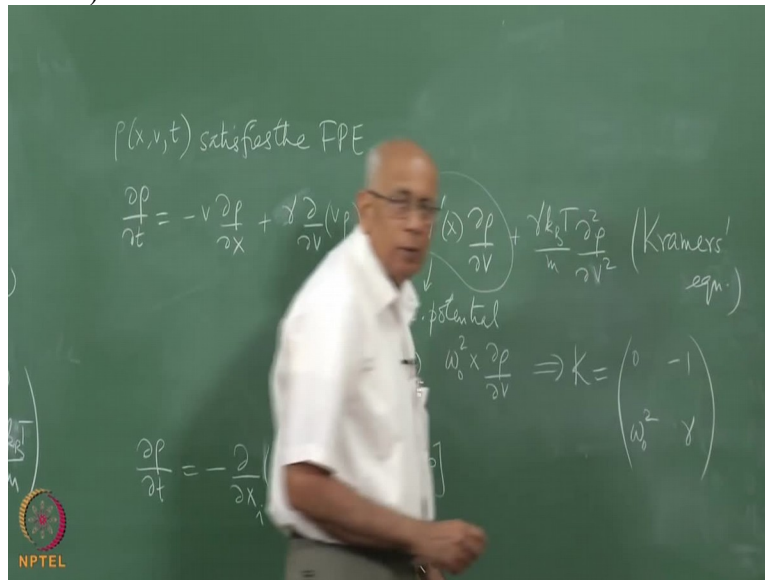
That term sits there and then finally, there is only one diffusion term here which is +  $\gamma K \text{ Boltzmann } T \text{ over } M D^2 \rho \text{ over } DV^2$ . So that is the equation for the phase space density, the one particle phase space density in the presence of an external potential, V of X for a Brownian

particle. That is the exact equation. There is no guarantee that the solution to this is a Gaussian, a joint Gaussian in  $X$  and  $V$  because this term is a mess. This term is a mess. No guarantee at all in general. It is some complicated non-linear function of  $X$  and there is no guarantee of anything here. This equation is called the Kramer's equation. Generalised to other potentials and 3 dimensions, maybe even velocity dependent forces.

So some generalisation of this, this is the simplest form of a Kramer's equation. Now of course you can recognise the oscillator case very trivially because the oscillator case goes back to the old problem. So if the oscillator case potential implies that this term is basis  $M \omega^2 X$ , so this term becomes  $\omega^2 X \Delta \rho / \Delta V$ . Sorry  $\omega^2 X \Delta \rho / \Delta V$ , this particular term. It is a linear term. So it could in fact be combined with all these fellows.

It reduces to the old case which has already been solved but this is a little harder to solve in this case because while the diffusion matrix remains the same, this will imply that this matrix  $K$  that we had written down which was  $0, -1, 0, \gamma$  in the free particle case, what would it be in this case? Remember there is an extra force here. This is  $-\omega^2 X$ . If you bring it to the left, it is  $\omega^2 X$ .  $X$  not  $V$ . Right? So the drift would have one more term. This is still  $0$ .  $X$  dot is  $-V$  but there is a term here.

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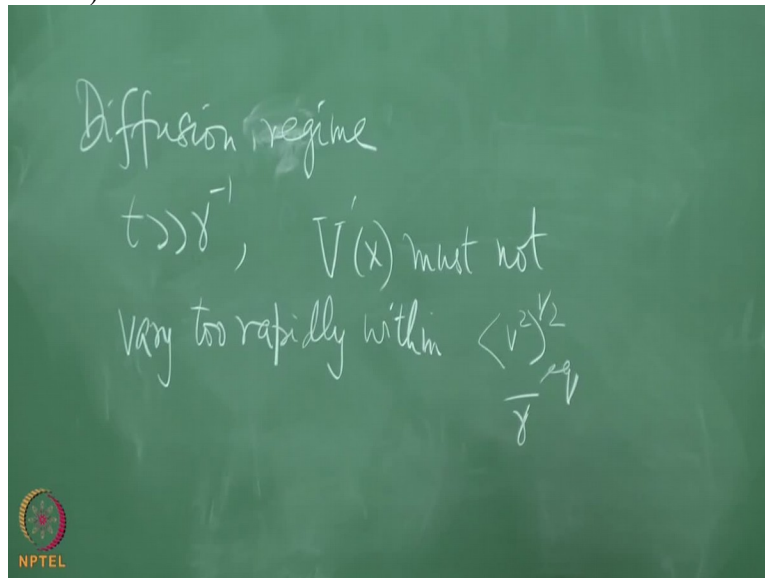


It is  $\omega$  not square in this problem. And that  $V$  would look exactly the same as before. This is not so simple to exponentiate, although it is any 2 by 2 matrix can be exponentiated. Why do I say that? Because with the 0 here, the eigenvalues are 0 and  $\gamma$  and exponentiating this matrix would have been trivial because  $K$  squared would have been proportional to  $\gamma K$  or something like that. But now that is not going to happen. There are 2 eigenvalues here which depend on both  $\gamma$  and  $\omega$  not square. Not surprisingly, they would be precisely the eigenvalues of this the 0s of the susceptibility the poles of the susceptibility.

So that depends whether they are under damped, over damped, critically damped, et cetera definitely have that. So the solution will be in terms of trigonometric functions and damped exponential in the under damped case or hyperbolic functions in the over damped case. So it is considerably more messy. Although you can exponent this. It is not hard. But this is where it would change. You can write the formal equation down. Now what do you expect the solution of such an equation to become for long times. I would still like to look at the diffusion regime and see what happens. In the free particle case when this was not there, recall that this  $\rho$  asymptotically went to a product of the equilibrium Maximillian distribution in  $V$  multiplied by the solution of the free diffusion equation in  $X$  right? Now what do you think will happen? Will that happen in this problem as well?

Well, in general you have to look at what happens when  $T$  is much more bigger than  $\gamma$  inverse, the diffusion regime or  $\gamma$  is very large, the high friction limit. So you have to ask what happens to the solution in that high friction limit. But there is also will length scale in the problem.

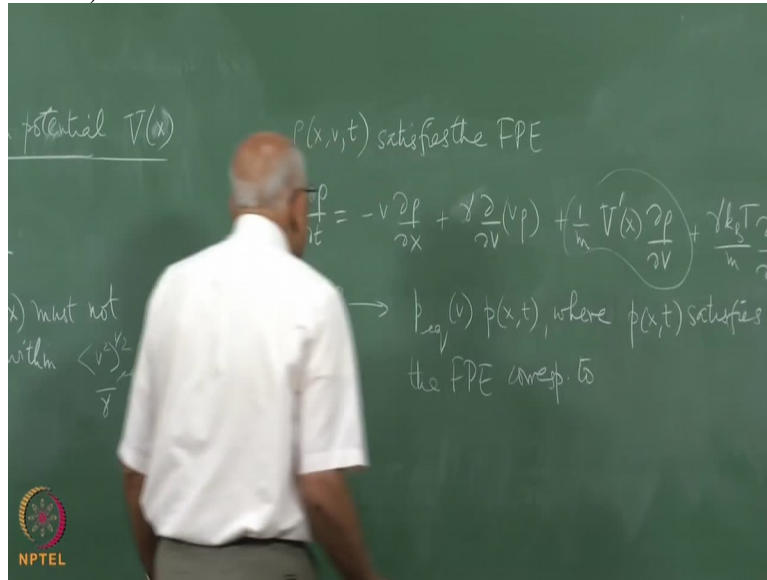
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So now the diffusion regime is defined as follows. Diffusion not only should you have  $T$  much much greater than  $\gamma$  inverse but also the force  $V$  prime of  $X$  must not vary too rapidly within the characteristic length scale. So it is as if the force did not exist at all in that length scale right or a constant or whatever. So within  $V$  square equilibrium to the half divided by  $\gamma$ . So that will be your criterion. You can compute this number and then ask, check whether  $V$  prime or the force is rapidly varying specially or not. If it is a gentle potential of some kind, it would not vary significantly.

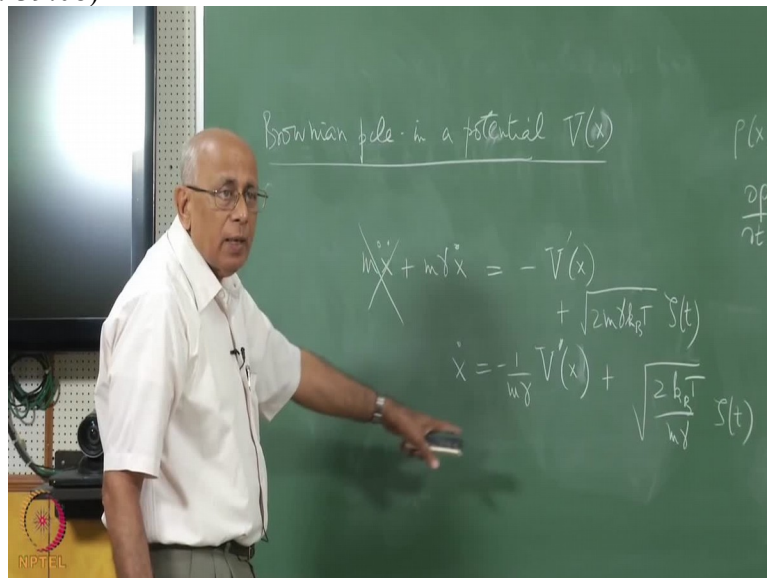
Then how would you go to this regime? What would you do? You do exactly what you did for the original free particle case. Namely you would say, I am going to throw away the inertia term, look at the high friction limit and ask what happens there right?

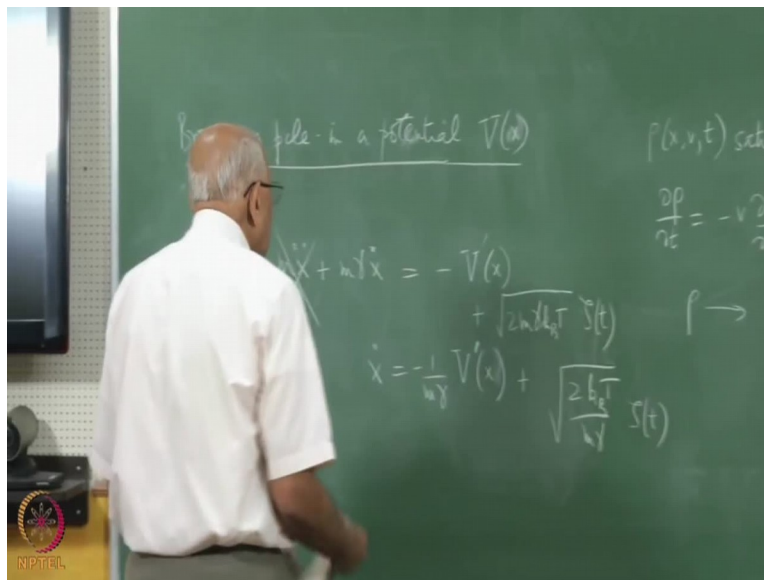
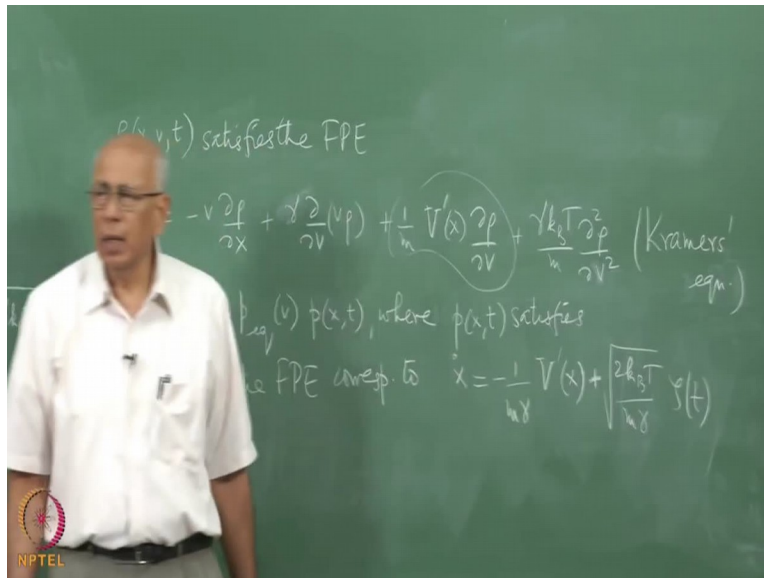
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So in that high friction limit let us write it down below this. So what happens is that this rho tends in the diffusion regime, to P equilibrium of V multiplied by an equation for P of X, T where P of X, T satisfies the Fokker Planck equation corresponding to setting the friction term, setting the inertia term to 0 right?

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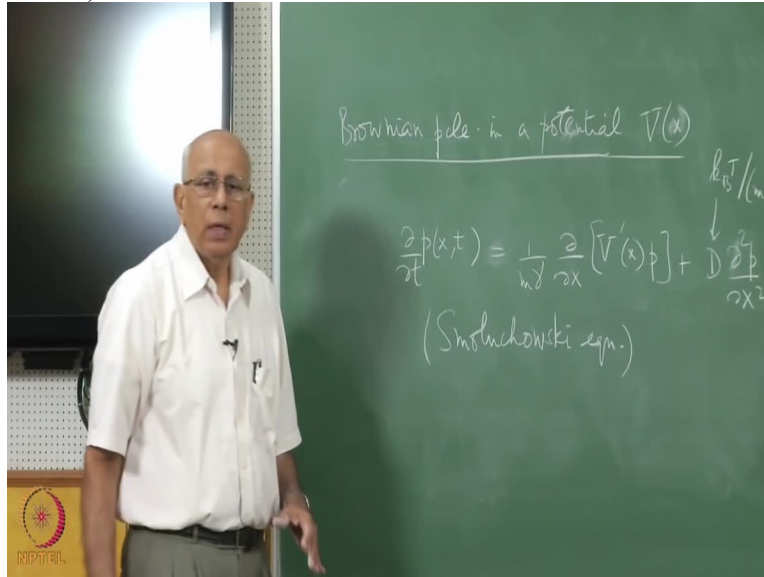


So essentially what you are doing is to take  $M \ddot{X} + M \gamma \dot{X}$  right equal to  $-V'$  prime of  $X$  + the noise. And the noise was precisely the noise that we had in the original. So  $2 M \gamma k_B T$  times  $\zeta$  of  $T$ , this term and we are dropping this term, the high friction limit. So this term dominates right? So that gives us an equation which says  $\dot{X}$  equal to  $-1$  over  $M \gamma V'$  prime of  $X$ , that is the drift term + square root of  $2 k_B T / \gamma$  times  $\zeta$  of  $T$ .

So it is  $2 k_B T / M \gamma$ . That is our old friend, square root of  $2D$  appearing again times  $\zeta$  of  $T$  corresponding to this stochastic equation right? And what is this stochastic

equation? Corresponding to  $X$  dot equal to  $-\frac{1}{M\gamma} V'(x) + \sqrt{2k_B T / M\gamma} \zeta(t)$ . That is a one-dimensional equation with non-linear term here but we know how to write the Fokker Planck equation down for it. So what would that be?

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In other words,  $\frac{\partial}{\partial t} p(x, t)$  should be equal to with a - sign so that goes away. And then you have equal to  $\frac{1}{M\gamma}$  sitting here  $D \frac{\partial}{\partial x}$  now of  $V'(x) p$  because that is inside. You cannot do anything about it. + the 2<sup>nd</sup> derivative, half of the square of this which is  $k_B T / M\gamma$  but that is just our old friend  $T$ . +  $D$  times  $D^2 p / dx^2$ . This is as before  $k_B T$ . That is a Fokker Planck equation. This equation is called the smoluchowski equation.

So it gives you the diffusion equation in the presence of a potential. But you see where it comes from. It really comes from the Fokker Planck equation in phase space. It gets reduced to this in the diffusion regime where you have to have an extra criterion now about the variation of  $V'(x)$ . We have not done the problem in the presence of a velocity dependent force. I assumed that the external force was a potential which depends only on the position. So no velocity dependent forces, no magnetic field, et cetera has been included here as yet.

Now the question is, does this have any equilibrium solution or not as  $T$  tends to infinity? We know that if it is not, this is not there, it does not. It is just the Gaussian which tends to 0, flattens out. But now this will depend on what this  $V'(x)$  is. We kind of expect that if you had in

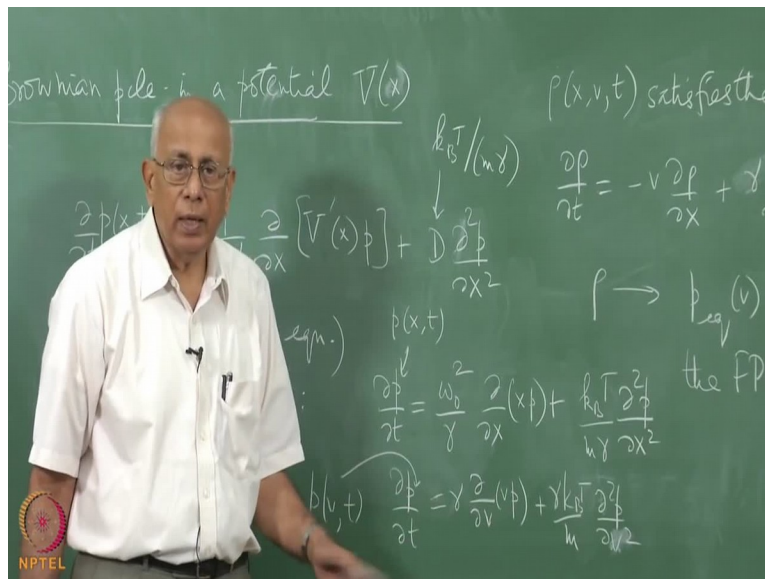


confining potential that prevents you from having long-range diffusion, then the mean square displacement will not diverge with T and therefore it might be an equilibrium case. For instance, the oscillator. Now let us look at the harmonic oscillator in the over damped, highly over damped high friction limit case.

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

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



So highly over damped, what is the smoluchowski equation for the position probability density of the highly over damped harmonic oscillator? Well, this fellow is trivial to write down. It is  $M\omega_0^2 X$  and the  $M$  cancels right? So you end up with  $\Delta p / \Delta t$  equal to

$\Omega^2 / \gamma$  times  $\Delta X$  of  $X P + D$  times, this is  $kT / M \gamma$ . That is the Fokker Planck equation. Does it remind you of any other Fokker Planck equation you have seen?

Yes, the velocity process for a free particle. What did that equation look like? That looked like  $\Delta P / \Delta T$  equal to  $\gamma \Delta V$  times  $V$  times  $P + \gamma k T / M D^2 P / DV^2$ , where this  $P$  was  $P$  of  $V, T$  whereas this  $P$  is  $P$  of  $X, T$ . It is not the same function of course. Are not these identical apart from a reinterpretation of constants? The  $\gamma$  is replaced by  $\Omega^2 / \gamma$  and same physical dimensions for both and the  $kT / M \gamma$  is replaced by  $\gamma kT / M$ .

This is the diffusion constant in the velocity space for a free particle or for a particle within the presence of a potential, it does not matter. That is the diffusion constant in position space. What was the solution to the situation? The Ornstein–Uhlenbeck distribution with a mean which went like  $E$  to the  $V$  not  $E$  to the  $-\gamma T$  and a variance which started with a Delta function with 0 and then went to the variance of the equilibrium Maxwellian. So there was an equilibrium distribution which was precisely the Maxwellian distribution.

This is exactly the same mathematically exactly the same problem. So that is why you would very often see the Ornstein–Uhlenbeck distribution process described in some books as the oscillator process. What they mean is that the conditional density of the simple harmonic oscillator, a harmonically bound particle, the Fokker Planck equation satisfying that gives you the Ornstein–Uhlenbeck distribution just as for the free particle, the velocity has this Ornstein–Uhlenbeck distribution.

In the over damped limit and the Smoluchowski this thing becomes precisely the Ornstein–Uhlenbeck distribution. Now how do you find the equilibrium distribution in this case? You would set this to equal to 0. Then you would find the current here but vanish at infinity, you would get the Gaussian.  $E$  to the  $-MV^2 / 2kT$ . What will you get here? What would be that distribution? So there is an equilibrium distribution in this case. We have to look at the general case.

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$p(x,t) \xrightarrow{t \rightarrow \infty} (\text{const}) e^{-\frac{m\omega_0^2 x^2}{2k_B T}}$

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We will subsequently or when you have an equilibrium distribution but in this case there is no doubt at all that  $P$  of  $X$   $T$  parents as  $T$  tends to infinity, there is genuinely an equilibrium distribution here because that will correspond to setting this equal to 0, then this is  $D$  over  $DX$  comes out and it becomes whatever is inside is a constant which can be set equal to 0 for normalisable distribution and then you get  $DP$  over  $DX + \omega$  square over  $\gamma$  times  $M$   $\gamma$  over  $KT$  times  $P$  equal to 0.

So what would you get? What is? And there is an  $X$ . So what kind of solution do you get? It is a Gaussian. And what would that Gaussian be? Constant times  $E$  to the power - Student:  $M$   $\omega$  not square.

Professor: Yes.  $M$   $\omega$  not squared  $X$  square over twice  $K$  Boltzmann  $T$ . Right? You expect that of course because that is the Boltzmann factor for the potential energy for oscillator. In equilibrium, you expect it to go to the Gibbs distribution, the Maxwell Boltzmann distribution. So it is  $E$  to the - the Hamiltonian and the Hamiltonian is half  $MV$  squared + half an  $\Omega$  not squared  $X$  squared divided by  $KT$  which is what is coming out. So you want that as a consistency check. Otherwise you are really off right.

So you do expect that this will go to the Maximillian that the Gaussian distribution. In the general case, no guarantee because you would have to set this equal to 0 and then ask whether

this ordinary differential equation has a solution or not. And yes, suppose it has a solution, what would that look like?

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particle in a potential  $V(x)$

$$0 = \frac{1}{n\delta} \frac{d}{dx} [V'(x) p_{eq}] + D \frac{d^2 p_{eq}}{dx^2}$$

$k_B T / (m\delta)$

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particle in a potential  $V(x)$

$$\frac{d}{dx} [V'(x) p_{eq}] + D \frac{d^2 p_{eq}}{dx^2} = 0 \Rightarrow p_{eq}(x) \propto e^{-\frac{V(x)}{k_B T}}$$

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So this becomes a DX D over DX P equilibrium, this becomes D2P over DX2 equilibrium. What would this solution look like? We want this to be equal to 0. Now of course, that simply means D over DX of this whole business, the current could be constant, it could be going to some stationary current. Then without knowledge of that stationary current, you cannot solve the problem but let us assume that at T equal to at + - infinity this thing vanishes. Then what you

have is an ordinary differential equation which says  $D \frac{dP}{dx} + \frac{1}{M\gamma} \frac{dV}{dx} P = 0$ .

But  $D$  is  $kT/M\gamma$ , there cannot be any reference to the frictional constant in the equilibrium position distribution right? So this goes away and this was a  $kT$ . So this becomes  $kT$  Boltzmann  $T$ . Now what would that tell you? Yes. This tells you, implies  $P$  equilibrium of  $X$  is proportional to  $e^{-V(X)/kT}$ . The integral of  $V'(X)$  is  $V(X)$  but that is just the Boltzmann factor which is what you expect in equilibrium. There will be  $e^{-H/kT}$  and the Hamiltonian has a kinetic part which we took care of separately and then a potential which is precisely this okay.

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The image shows a chalkboard with the following equation written in white chalk:

$$\Rightarrow p_{eq}(x) \propto e^{-\frac{V(x)}{k_B T}}$$

In the bottom left corner of the chalkboard, there is a small circular logo with the text "NPTEL" below it.

So it checks, this thing checks. There are other possibilities. We have assumed the stationary current is not there but otherwise. So this will happen whenever there is  $V(X)$  is bounded, I mean it binds the it sort of stops long-range diffusion, then the particle is bound in some sense and it cannot diffuse out to infinity and you end up with an equilibrium stationary distribution. No guarantee that it always exists but in these cases, normal cases it would exist. Okay. So magneticfield case is a little more intricate than this and we will talk about this (52:25) and then we will see that how to generalise this. Okay let us stop this.