

**Non Equilibrium Statistical Mechanics.**  
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**Lecture-22.**  
**Diffusion in a Magnetic Field.**

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## Diffusion in a magnetic field

- Langevin equations for position and velocity with a velocity-dependent force
- Smoluchowski equation for positional PDF
- Identification and calculation of the diffusion tensor
- FPE for the radial distance PDF in Brownian motion
- Corresponding LE with a drift term for the radial distance


Particle in a magnetic field      $\langle \xi_i(t) \rangle = 0$

$$\dot{\vec{r}} = \vec{v}$$

$$\dot{\vec{v}} = -\gamma \vec{v} + \frac{q}{m} (\vec{v} \times \vec{B}) + \sqrt{\frac{2\gamma k_B T}{m}} \vec{\xi}(t)$$

$$\langle \xi_i(t) \xi_j(t') \rangle = \delta_{ij} \delta(t-t')$$

$(\Gamma = 2m\gamma k_B T)$



Right, so we will tie-up one of the loose ends that was left in our discussion of the Langevin equation and Fokker-Planck equation and related matters and this had to do with the possibility that the force on the Brownian particle maybe velocity dependent. And one of the formalism is quite general, we do this in this specific case of magnetic field because that is directly accessible, experimentally accessible situation. And we have studied in the past as

well, so let us look at how to obtain the phase space density for a particle moving in a magnetic field using our correspondence between Langevin-Fokker-Planck equations.

So let us say particle in a magnetic field.

It is just a regular Langevin and not just...

This is just a regular Langevin equation and I am going to apply uniform steady magnetic field  $B$  throughout and put this particle in a thermal heat bath temperature  $t$  and ask how the Brownian motion of it is affected by the magnetic fields. So as usual all we have to do is to write down the Langevin equation, the pair of Langevin equation for the phase space variables. So we could start with  $\dot{r}$  equal to  $v$  as before. But  $\dot{v}$  is equal to the friction term, we usually friction term, so this is  $-\gamma v$  on this side.

+ this time there is a force given to the magnetic field with, which is the  $(\dot{r}) \times B$  force. So  $+\frac{q}{m} v \times B$ , that is the systematic part of this force and this is the usual noise. Now this noise term, we have been writing it as a white noise and that is the same noise we are going to assume. But now let us ask ourselves physically, you have a set of particles, Brownian particles in a magnetic field some other field does no work on these particles at all because the velocity and the magnetic field are perpendicular to each other and therefore as you know the kinetic energy of the particle does not change, only the direction of its velocity changes and it goes in a cyclotron orbit.

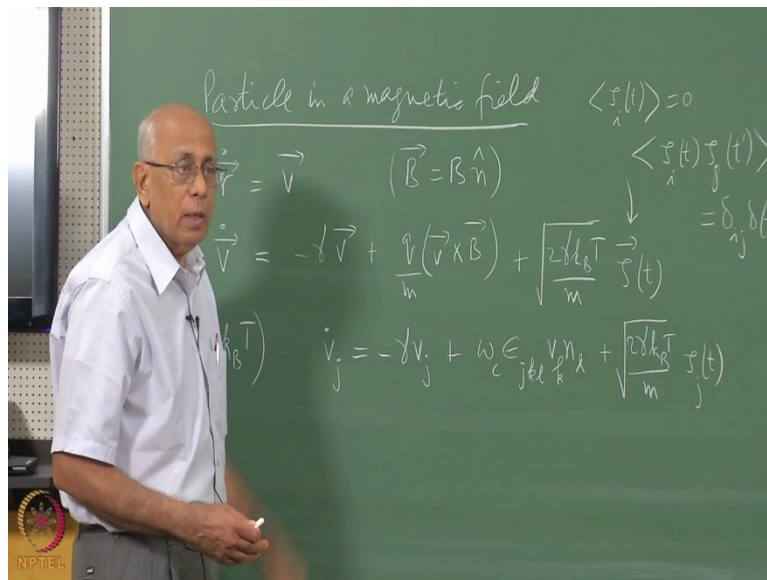
So we expect that whatever be the phase space distribution, we expect that asymptotically as  $t$  tends to infinity, the condition of probability density of the velocity for the phase space density, as far as the velocity part is concerned, it is going to be Maxwell here at the same temperature. So given that, we ask what is the condition necessary for the Maxwell distribution, again we know that the average kinetic energy must be half,  $\frac{3}{2} kT$  or whatever it is in this situation. And so we put that in right from the beginning. And how was that implemented, it was implemented by saying that the sense of this noise is related to this dissipation coefficient by this relation which we have already written down many times.  $\gamma$  is equal to  $\frac{2m\gamma}{kT}$ .


So we will put that in as we have been doing in all our examples, in which case this becomes a  $+$ , square root of, we put that in, is equal to  $\sqrt{\frac{kT}{m}}$  because it was  $m\dot{v}$  equal to whatever it was on this side and this was square root of  $\frac{kT}{m}$ , so one  $m$  cancels and we end up with this times this noise  $\sqrt{\frac{kT}{m}}$ . And this  $\sqrt{\frac{kT}{m}}$  is a

vector valued white noise is 0 mean, so its properties are  $\langle \zeta_i(t) \rangle = 0$  and of course  $\langle \zeta_i(t) \zeta_j(t') \rangle = \delta_{ij} \delta(t - t')$ . So each Cartesian component of this Zeta is Delta correlated, stationary Gaussian Markov process. Okay.

So this is a set of Langevin equations, okay. So that immediately tells us what the Fokker-Planck equation should be. The fact that you have a velocity dependence force here, means that you cannot write it like a Smoluchowski equation with the potential and derivative of the potential and so on. But of course we can still take this into account because I call this part of the drift. This whole thing is deterministic, the noises here, no one else. So I have general formalism which tells me what I should do when I have some arbitrary non-linear drifts and some arbitrary multiplicative noise. But this is a much simpler case, the noise is still additive and the drift is linear, even though it is velocity dependent, does not matter at all.

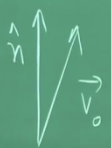
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$$M_{jk} \stackrel{\text{def.}}{=} \epsilon_{jkl} n_l$$


$$M^3 = -M$$

$$M_{jk} \stackrel{\text{def.}}{=} \epsilon_{jkl} n_l \Rightarrow (M^2)_{jk} = n_j n_k - \delta_{jk}$$

$$R(\hat{n}, \psi) = e^{M\psi}$$


$$v(t) = e^{M\omega_c t} \vec{v}_0$$


So given that we can identify all the quantities, even in the Fokker-Planck equation. Let us write it out for the velocity alone, so let us look at the velocity distribution alone. This is going to be, now this equation of motion we can simplify it a little bit, write it in components and we will not be done this earlier. So if I write any one component  $v_j$  dot equal to  $-\gamma v_j +$  and let us put the field in some given direction, so  $B$  equal to  $B$  times unit vector in some arbitrary direction  $M$ . So this becomes this  $QB$  over  $M$  which is a cyclotron frequency, that takes care of this factor here and then  $v \text{ Cross } B$ , which is  $\epsilon_{jkl} v_k B_l$ . I have just written out the components, the  $j$ th component here and the crossproduct in terms of epsilon symbol + this fellow here,  $2 \gamma K_B t$  over  $M Zeta$  at  $j$  of  $t$ , this fashion.

So that is the Langevin equation, this is the  $F$  part of it and that is the  $G$  part of it and so we can write down what the actual solution is of this equation because it is a linear equation we

can solve it explicitly or we can write the Fokker-Planck equation as the case may be. Let us see what, what this looks like a finite it out in terms of the matrix  $M$  which is a rotation matrix. So if you recall we introduced this symbol  $m_{jk}$  equal to  $\epsilon_{jkl}$ , this is the definition,  $n_l$ . It is a metric that takes care of rotations in 3 dimensions because it says that if you have this velocity vector  $v$ ,  $v_0$  in some direction and this is the unit vector  $M$ , then as you switch on the magnetic field some all that happens is the component of  $v_0$  Along  $n$  does not change and the perpendicular components presses around the direction of the field with the cyclotron frequency.

And that is given, it is stated by saying that  $v$  of  $t$  in this single deterministic problem  $v$  of  $t$  is a rotation matrix acting on this  $v_0$ , such that at time  $t$  you have gone through  $\omega C t$  as the angle. So this is equal to  $e$  to the power  $M \omega C t$   $v_0$ . And of course we know what this thing is, we can exponentially this matrix  $M$ , we have done that in the past. We know that  $M$  cubes turns out, the properties of  $M$  are very straightforward. Once you define it like this, this implies that  $M^2$   $j k$  is equal to  $n_i N_j$ , sorry  $N_j$ ,  $N_k - \Delta j k$ . So  $M^2$  is straightforward enough. And  $M^3$  equal to  $-M$ . All you have to do, so multiply once again by  $M$  and we discover that  $M^3$  is  $-M$ .

So that is the property of this matrix  $M$ . What are the eigenvalues of this  $M$  by the way? What are the eigenvalues of  $e$  to the power rotation, I mean if I define the rotation matrix about the angle  $N$ , through the angle  $\psi$  to be equal to, this turns out by the way, to be equal to  $M \psi$ , okay, we have gone through all the angular momentum generators, etc., put them all in and finally end up with the rotation matrix written in this form, that is what it represents, simplest way of remembering rotation matrix in 3 dimensions. What are the eigenvalues of this? At least one must be an eigenvalue because if you rotate around the direction  $n$ , nothing is going to happen to any vector, right which is along  $N$ .

So this means that  $n$  itself is one of the eigenvectors and those vectors along  $N$  do not change at all, so one is the eigenvalue, can you have another real eigenvalue? No because if you did, it means that you have this direction of axis of rotation, say this and then you rotate, nothing along this axis changes but all other points and vectors must change. If you have other eigenvector value which was real, then it is bad news. 1<sup>st</sup> of all know eigenvalue can have a modulus other than one because rotations is no distance is a change between particles. So it must lie on the unit circle and you cannot have any 2<sup>nd</sup> real eigenvector.

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$$\vec{v}(t) = e^{M\omega_c t} \vec{v}_0$$

$$\langle \vec{v}(t) \rangle = e^{-\gamma t} e^{M\omega_c t} \vec{v}_0$$

$$\vec{B} = B \hat{n}$$

$$m \frac{d\vec{v}}{dt} = -\gamma \vec{v} + q(\vec{v} \times \vec{B}) + \sqrt{2\gamma k_B T} \vec{\zeta}(t)$$

$$\dot{v}_j = -\gamma v_j + \omega_c M_{jk} v_k + \sqrt{2\gamma k_B T} \zeta_j(t)$$

$$\Rightarrow \frac{\partial}{\partial t} p(\vec{v}, t) = -\frac{\partial}{\partial v_j} \left\{ (-\gamma v_j + \omega_c M_{jk} v_k) p \right\} + \sum_{jk} \frac{\partial^2 p}{\partial v_j \partial v_k} \frac{\gamma k_B T}{m} \delta_{ij}$$

And the eigenvalues are + or -, e to the power + - I psi. The 3 eigenvalues of this are 1, e to the i psi, e of the - i psi, okay. All right. So this is going to tell you what the rotation does, this process around this point. And of course if I expand this out, I am going to get a piece using M cubed is - M, I am way to get a piece which does not change, a piece along N and a piece along v0 cross N. Okay. So that is what this v of t should look like, it should be a vector. Now if you put this in a fluid, this comment particle come and ask what happens, due to the correlation, this velocity, average velocity goes to 0.

So all that happens is that the average v of t in a fluid becomes e to the - gamma t times e to the M omega Ct v 0. By this I mean, right this is a 3 by 3 matrix, write this as a column vector then operate on it. So this is all that happens for a Brownian particle, we were

deceived this. So let us see instead of trying to solve this problem explicitly, let us see if we can get a quick answer. So this is  $m \mathbf{jk}$ ... Pardon.

(12:42)

We want to write the FPA for this definitely. So what would the Fokker-Planck equation would look like, this will be  $\Delta P$  over  $\Delta t$  of  $\mathbf{v}$ , we 0, let us forget  $\mathbf{v}_0$  for a moment, it is understood. The initial condition on this is  $\mathbf{v}_0$ , equal to, so what should I write on this side? -, this is the drift term, this is the  $F$  here, right, so -  $\Delta v_j$  of  $-\gamma v_j + \Omega C M jk v_k$ , this fellow on  $P$ . Okay. So that takes care of the drift part. And then +, what should I write here? Clearly I should write, pardon me what should I write?

(13:57).

You, it is not  $\Delta^2$ , it is not  $\Delta^2$  because this thing is a Cartesian component, right and this is a scalar, this quantity here. So what should it be there, it is the diffusion matrix, does not, obviously, you will not have a diffusion matrix, so this will be some, let us use, let us use  $D$ ,  $D_{ij}$ ,  $D_{ij}$  for  $\Delta v$ , let us call it  $D_{jk}$ ,  $D_{jk}$ . And what is  $D_{jk}$ , this quantity here?

(14:47).

What should it be? We need to compute this quantity, we need to compute this quantity, we are not at home yet, we need to compute this quantity. So what you have to do to write this thing in terms of  $G$ ,  $G^T$ ,  $G^T$ , work out what that is and then compute this.

$G$  is  $\Delta$  (15:10).

So I am using bad notation here, let me for the moment, since when velocity is let us use this, let us use  $D_{jk}$ . And what is this fellow here, this is  $\gamma k$  Boltzmann  $t$  over  $M \Delta_{ij}$ . Because the different Cartesian components of this noise are appearing with the same strength, so the diagonal matrix, more than that it is actually a unit matrix times this. So half the square of this guy is what this is, this is what the diffusion matrix is in velocity space, in velocity space. Now it is a simple matter to see, it has an equilibrium distribution or stationary distribution, etc., it will turn out to be the Maxwell distribution was again.

We can solve this equation is by the way, this is like, it is a linear quantity here, so apart from the small complication is a different components are mixed up, this is (16:18) distribution,

is a solution for this problem. And it is a Gaussian distribution with a mean which is given by this. So it is  $e^{-\frac{1}{2} \mathbf{v} \cdot \mathbf{v} / \gamma t}$  and so on. Asymptotically it will go to the Maxwell distribution. So that part is quite straightforward. The next question is what is the phase space density going to look like,  $\rho(\mathbf{r}, \mathbf{v})$ .

Well, now it is a little more intricate, you have a 6 dimensional phase space, so these objects, this drift matrix and diffusion matrix will become 6 dimensional, etc. But, it really does not matter because you will have this matrix, 6 dimensional fellow will be of the form, there will be 0 here, 0 here, 0 here and then it is going to be just this, that portion is going to have this matrix here. So it is not, no sweat, I mean you will write down the big solution in this case, the full solution can be written down. Okay. But now we have an interesting question, what about positions space, what happens in positions space, what does the diffusion of the particle look like?

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$$\frac{\partial p(\vec{r}, t)}{\partial t} = D_{ij} \frac{\partial^2 p}{\partial x_i \partial x_j}$$

$$\int_0^{\infty} dt \langle v_i(0) v_j(t) \rangle$$

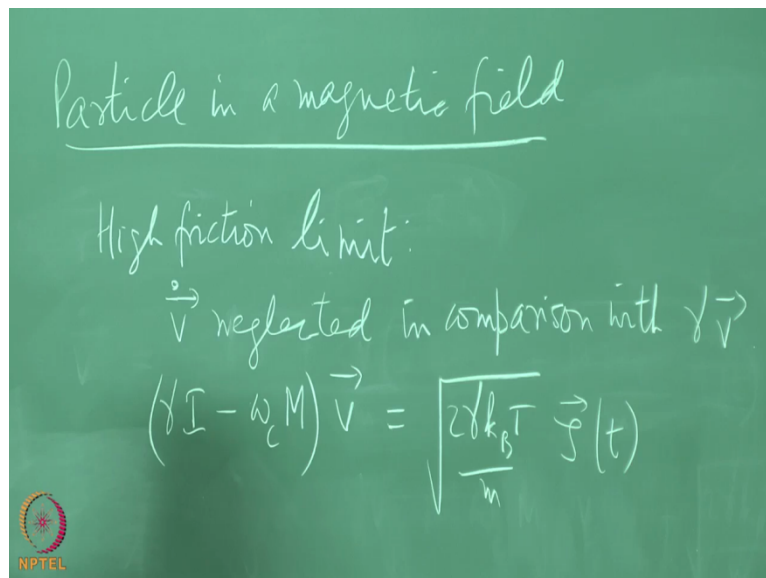
We already know that when you start with the Langevin equation phase space, if you go to the diffusion regime which means  $t \gg \gamma^{-1}$ , or take the high friction limit in which you neglect the inertia term in favour of the dissipation term and then pretend this is a Langevin equation with a velocity that is essentially white noise, delta correlated, then you can ask what does this Fokker-Planck equation look like, look like and it gives you a diffusion equation with a diffusion tensor. There was another way in which we did this, we solved this entire problem, I am going to retain some of the stuffs, I do not need this.



We solve the same problem in another way, we said look the displacement  $X$ , we call it capital  $X$ ,  $X$  of  $t$ ,  $X$  squared of  $t$  average, goes as  $t$  tends to infinity, we said that, we called it  $R$  square in 3 dimensions. This goes for  $t$  much much greater than  $\gamma$  inverse, this goes, like the diffusion constant, this fellow here will have some  $D_{ij}$ , etc., etc., right. But we found that the diffusion constant was different in the  $X$  and  $Y$  direction,  $X$ ,  $Y$  direction as opposed to the  $Z$  direction here. Okay. Now how do we get that? Well it is obviously arises from the following, it arises from the fact that the positional probability density  $P$  of  $R$ ,  $t$  will like,  $\Delta$  over  $\Delta t$  this fellow here, satisfies a diffusion equation which is not a homogeneous, which is not an isotropic effusion equation but must be of the form, now let us see what is the ordinary  $D$ ,  $D_{ij}$ ,  $d^2 P$  over  $dx^i dx^j$ .

And then you are guaranteed that  $R$  square goes like the sum of  $X$  square will go like  $D_{11} t + 2D_{12} t + 2D_{13} t$  and so on. We need to find this, what did we do, we use the Kubo formula in this case and argued that this quantity  $D_{ij}$  is equal to integral from 0 to infinity  $Dt$ ,  $v_i$  of 0,  $v_j$  of  $t$  equilibrium and that probably gave us what this diffusion tensor was. And we discovered that in the longitudinal direction it was not affected, it was  $k_B T / \gamma$  and  $\gamma$ , but in the transverse direction, it was moderated by a factor which is dependent on the relative side of  $\gamma$  and  $\Omega_c$ , the cyclotron frequency.

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I want to derive that results by starting here and just using this going to a Smoluchowski equation, okay, so let us see how to do that. In the high friction limit...

Somehow (( ))(21:02).

Exactly, exactly, yes. Okay. In the high friction limit, you are going to neglect  $v \cdot \nabla$ , neglected in comparison, in comparison with  $\gamma R$ . So we go back to this equation and say let us neglect this term compared to that, okay. And I bring this to the left-hand side over here, so what does it say and that it as a vector equation, so it says  $\gamma$  times the identity matrix -  $\omega_c$  times  $M$ , + this matrix acting on  $v$ , okay, is equal to this guy, is equal to on the right-hand side, square root of 2  $\gamma k_B T$  over  $N \zeta$  of  $t$ . Pardon?

(0)(22:22).

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$$\Rightarrow \frac{\partial p(\vec{r}, t)}{\partial t} = D_{ij} \frac{\partial^2 p}{\partial x_i \partial x_j},$$

with  $D_{ij} = \frac{k_B T}{m}$

$$\Rightarrow \frac{\partial p(\vec{r}, t)}{\partial t} = D_{ij} \frac{\partial^2 p}{\partial x_i \partial x_j},$$

with  $D_{ij} = \frac{k_B T}{m} \left[ (\gamma I - \omega_c M)^{-1} \right]_{ik} \left[ (\gamma I - \omega_c M)^{-1 T} \right]_{kj}$

$$\frac{\partial p(\vec{r}, t)}{\partial t} = D_{ij} \frac{\partial^2 p}{\partial x_i \partial x_j}$$

with  $D_{ij} = \frac{\hbar k_B T}{m} \left[ (\gamma I + \omega_c M)(\gamma I - \omega_c M) \right]^{-1}_{ij}$

$$M^T = -M$$

So that is the matrix equation, there is no  $v$  dot, but this is this crazy matrix acting on  $v$ . And this part of it is coming from the magnetic field. So formerly this is  $R$  dot equal to square root of  $2 \gamma K$  Boltzmann  $t$  over  $M$  times  $\gamma I - \omega_c M$ , the inverse of this matrix acting on  $Z$  of  $t$ . Okay. This is also noise, this guy is also noise and this part does not involve the velocity of the dynamical variables at all. So is this additive noise or multiplicative noise, if this is dependent on the dynamical variable, it is multiplicative noise, otherwise it is additive noise. So it is no drift, no drift and additive noise, okay. The only  $t$  dependence is from this white noise and this fellow is Delta correlated.

So if I call this whole thing some noise, some  $\eta$  of  $t$ , it is also Delta correlated, it is guaranteed to be stationary because that part of it comes from here. Okay. So it is stationary Delta correlated, it is not isotropic, I mean this fellow is sitting here, so you have to be careful about it. But if you call this  $G$ , the  $F$  term is 0, if you call this  $G$ , then we know immediately what the Fokker-Planck equations in this case looks like, it is exactly this. And what is  $D_{ij}$ , so this equation implies this with  $D_{ij}$ , equal to, one half  $j$  times  $j$  transpose and the  $i$   $j$ th element of it. So this is equal to one half and the half cancels against the 2, so it is  $\gamma K$  Boltzmann  $t$  over  $M$ , this matrix times its transpose, when you want the  $ij$ th element of it or  $j$ ,  $K$ th element of it.

So what is that equal to, this is  $\gamma I - \omega_c M$ , inverse,  $\gamma I$ , no, no, what do you see that?

The next one is transpose, so transpose of  $(\gamma I - \omega_c M)^{-1}$  (25:19).

Oh yeah yeah, sure, if I have written just G, I have to write G transpose. So the ijth element is this times ik and then Kjth element of the transpose, so this is again equal to gamma i - omegac M inverse transpose jk. Okay. But this matrix M is an antisymmetric matrix. Epsilon ijk, NK is antisymmetric in i and j. And what is the transpose of this guy, it just is the transpose of M because the unit matrix does not have any change. And that makes it a +. Okay. So permit that I can write this as a + and I have taken the transpose, so now we can simplify things, the whole thing is essentially the inverse of gamma i + Omega CM, gamma i - omegac M inverse and then the ij element of it.

(Refer Slide Time: 28:01)

$M^T = -M$

$$\Rightarrow \frac{\partial \rho(\vec{r}, t)}{\partial t} = D_{ij} \frac{\partial^2 \rho}{\partial x_i \partial x_j}$$

with  $D_{ij} = \frac{\gamma k_B T}{m} \left[ (\gamma I + \omega_c M)(\gamma I - \omega_c M) \right]^{-1}_{ij}$

$$= \frac{\gamma k_B T}{m} (\gamma^2 I - \omega_c^2 M^2)^{-1}_{ij}$$

NPTEL

$$\frac{\partial \rho(\vec{r}, t)}{\partial t} = D_{ij} \frac{\partial^2 \rho}{\partial x_i \partial x_j}$$

with  $D_{ij} = \frac{\gamma k_B T}{m} \left[ (\gamma I + \omega_c M)(\gamma I - \omega_c M) \right]^{-1}_{ij}$

$$= \frac{k_B T}{m \gamma} \left( I - \frac{\omega_c^2 M^2}{\gamma^2} \right)^{-1}_{ij}$$

NPTEL

I interchange the order, it does not matter in this case, this turnout with each other but I interchange the order because this was on the right, the inverse 1<sup>st</sup> and now we go to the next.

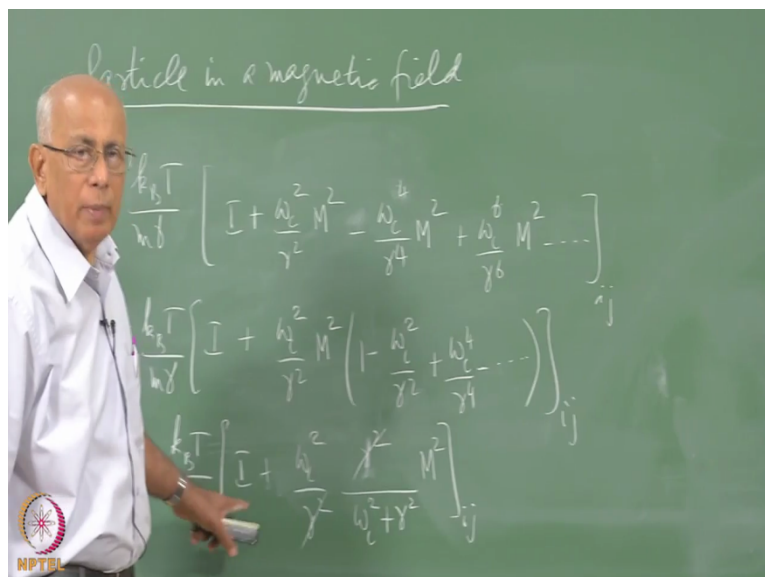
But  $M$  and  $i$ , is with each other, and therefore this is just  $\gamma^2 i - \omega_c^2$  and  $M^2$ . So this is equal to  $\gamma k_B T$  over  $M$ ,  $\gamma^2 i - \omega_c^2$   $M^2$  inverse. Let us pull out this  $\gamma^2$ , incidentally what is the guarantee that this one has an inverse to start with? What is the guarantee,  $M$  does not have an inverse, what is the guarantee,  $M$  does not have an inverse because 0 is an eigenvalue.

But what is the guarantee that this value has an inverse, what is the guarantee that this inverse exists?

(28:20).

Yes, you can treat this as,  $\gamma$  is an eigenvalue,  $\gamma$  or  $\omega_c$  is an eigenvalue of this fellow and there are no real eigenvalues. So as long as  $\gamma$  and  $\omega_c$  are real, this fellow can never, the inverse will always exist. Okay. There is no vector such that acting on it will give you a real number times that. Therefore this quantity has an inverse, okay, is that, do you agree, okay. All right. So let us pull out this  $\gamma^2$  and I will write it out as  $M \gamma$  and this goes away over  $\gamma^2$ . And then I want the  $ij$ th element of it, of this inverse. Now the matter is very straightforward, so I have  $D_{ij}$  equal to  $k_B T$  over  $M \gamma$ , notice this original diffusion constant as emerge here, but there is no really dependence on the (29:27).

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$$D_{ij} = \frac{k_B T}{m \gamma} \left[ \delta_{ij} + \frac{\omega_c^2}{\gamma^2 + \omega_c^2} (n_i \cdot n_j - \delta_{ij}) \right]$$

So inside you have  $i + \omega_c^2 / \gamma^2$ ,  $M^2 + \omega_c^2 / \gamma^2$ ,  $M^2$  but  $M^2$  is  $M^3$  times  $M$  and  $M^3$  is  $-M$ , so this becomes  $-M^2$ ,  $+ \omega_c^2 / \gamma^2$ ,  $M^2$  but that is  $M^3$  whole square and that is  $M^2$ ,  $i$   $j$ th element which is equal to  $k_B T / m \gamma$  times, there is an  $i$ , it goes and sits here  $+ \omega_c^2 / \gamma^2$ , you take that out and then it is  $1 - \omega_c^2 / \gamma^2 + \omega_c^2 / \gamma^2$  for  $- \dots$ . And then  $ij$ .


This alternating thing says it is  $1 / (1 + \text{this quantity here})$ . So this is equal to, equal to  $k_B T / m \gamma$   $i + \omega_c^2 / \gamma^2$  and then  $1 / (1 + \text{this squared})$  which is  $\gamma^2 / (\omega_c^2 + \gamma^2)$   $M^2$   $ij$  element. Okay and we are home. This cancels out and  $M^2$  we know, we know what the elements of  $M^2$  are, so  $D_{ij}$  equal to  $k_B T / m \gamma$ , that sits inside and here the  $ij$  element of the unit matrix, of course  $\delta_{ij} + \omega_c^2 / \gamma^2$   $n_i \cdot n_j - \delta_{ij}$ , that is it and that is the diffusion constant, what you have been simplifying a little bit. Alright.


So this tells you the transverse part and the longitudinal part, the coefficient of this portion here projects along the direction  $N$  when the other 2 guys, the rest of the tensor will project in the other direction. So that is a quick method, we do not have to do the velocity correlation or anything, although it is completely equivalent to this. So it is a check of the fact that Kubo formula is correct out here. So you do get this diffusion coefficient directly or it requires an inversion, inversion on this matrix here, this rotation matrix. Okay.

So once again in the presence of the magnetic field, the problem is completely solved over explicitly, it is diffusive into normal sense in spite of this velocity dependent force. And the diffusing constant is not the isotropic diffusing constant. Okay. Right, so that was one illustration, the right-hand side which we will not take up here. There is another aspect which I wanted to mention and that is the following. We have seen that in all these cases we started with a Langevin equation and went to the Fokker-Planck equation. Occasionally you may want to do the opposite in order to identify the kind of stochastic differential equation that the random variable will obey when you have, there would be a probabilistic distribution, description of it in terms of the corresponding conditional density. Okay.

(Refer Slide Time: 34:14)

Diffusion in 3D

$$\frac{\partial p(\vec{r}, t)}{\partial t} = D \nabla^2 p(\vec{r}, t)$$


$$p(\vec{r}, t) = \frac{1}{(4\pi Dt)^{3/2}} e^{-\frac{r^2}{4Dt}}$$




So here is a lasting example. Let us look at the problem of diffusion in more than one dimension, spatial dimension. You have no field and so on, so the diffusion equation in D dimensions would look like this, let us do it in 3 dimensions to be specific. So you have Delta P of r, t over Delta t equal to D del square P of R, t. I am interested in asking what is the equation obeyed by the distance from the origin, okay. I know what the equation is, what the equation, the langevin equation bring in this case for each Cartesian component. But I would like to know what the distance from the origin does, square root of X square + Y square + Z square, that looks fairly intricate but let us see how we could answer that.

So I look at the diffusion equation and I am going to look at the initial conditions which are completely spherically symmetric. So we start at the origin, we start with P of our 0 equal to Delta 3 of R and P goes to 0 as R goes to infinity in our direction. So this is the standard diffusion problem in which the solution is known to us, it is Gaussian. So we already know that, in the absence of boundaries, P of R and t is 1 over 4 pie Dt to the power 3 halves e to the - R square over 4 Dt. This is the fundamental Gaussian solution in 3 dimensions to the diffusion equation.

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$$p(\vec{r}, t) = \frac{1}{(4\pi Dt)^{3/2}} e^{-\frac{r^2}{4Dt}}$$

$$r = (x^2 + y^2 + z^2)^{1/2}$$

$$p(r, t) = \frac{4\pi r^2}{(4\pi Dt)^{3/2}} p(\vec{r}, t)$$

From here it follows that R square average is 6 D DM, so, okay, so I want to know what little r does the distance from the origin. So my random variable is this, okay, it runs from 0 to infinity and I want to know about its distribution, what it is stochastic equation is. This is a fairly messy thing to do because while the noise is not correlated from different Cartesian components, the moment you go to spherical, polar coordinates, the things become much



more complicated. While the 1<sup>st</sup> thing I do is to ask what is rho of R and t, this is the, sorry little R and t.

This is the probability density of the vector R, it is another matter that in this case there is no theta or phi dependence because I started with natural boundary conditions which are spherically symmetric and the initial conditions which are spherically symmetric, so the solution is also spherically symmetric because the equation is spherically symmetric. The differential operator del square, the initial condition, the boundary conditions, they all have spherical symmetry, so the solution also has spherical symmetry. Now I want to know the distance you are and that is of course the integral of this p probability density function over all angles and that will just give me a 4 pie factor. Right.

R square should come (())(37:47).

And then there is an R square, because you are not bothered about the duration but only the distance, so there is a phase space factor R square which is crucial, right. So this is equal to 4 pie R square over 4 pie Dt to the 3 halves p of R, t. Sorry, e to the -, e to the -, this is equal to 4 pie R square P of R, t, that is what we mean to say. This is guaranteed to be normalised from 0 to infinity in R. So you integrate from 0 to infinity R times, DR times this and you get 1. Now what is equation satisfied by this row, what is the Fokker-Planck equation satisfied by this row? You got to go back here to this and substitute for it.

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Diffusion in 3D

$$\left. \begin{aligned} \frac{\partial p}{\partial t} &= D \frac{\partial}{\partial r} \left( r^2 \frac{\partial p}{\partial r} \right) \\ \text{put } p &= \frac{P}{4\pi r^2} \end{aligned} \right\} \Rightarrow$$

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial r} \left( \frac{\partial P}{\partial r} \right) + D \frac{\partial^2 P}{\partial r^2}$$

$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial r} \left( \frac{2D}{r} \rho \right) + D \frac{\partial^2 \rho}{\partial r^2}$$

$$\text{LE for } r: \dot{r} = \frac{2D}{r} + \sqrt{2D} \zeta(t)$$

So let us do that, we are interested in only the spherical symmetric part of it, so therefore this del square I retain only the R dependent part of it, right. In which case the equation is Delta P over Delta t, this fellow here, is equal to B times 1 over R square Delta over Delta R, R square Delta over R of P. That is the equation be solved to get the Gaussian solution or whatever it is. This is the, so the radial part of the del square alternative, right. And now let us put t equal to, rho divided by 4 pie R square into this equation, okay. So this will imply an equation for rho which is precisely the Fokker-Planck equation for rho.

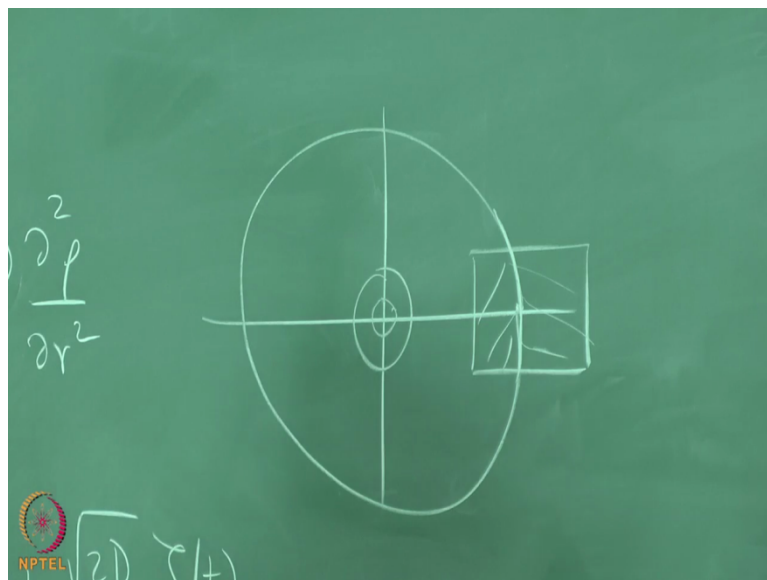
This is going to imply that Delta rho over Delta t, we get an equation for this guy here, by the way if I put that thing here and take partial derivatives, notice that if I put P over rho over R square, it is a partial derivative with respect to t, so the R square comes out, there is nothing to differentiate them. And then it will cancel against things over here. So this thing becomes relatively simpler, it becomes -, in this case I know the answer, Delta over Delta R 2D over R times rho, okay, + D times D2 rho over delta R 2. Check this out, I am not 100 percent sure but I believe it is correct. Whatever it is, this term is crucial, okay.

So what will this imply backwards now? It implies a langevin equation for little R, of little R which is square root of that crazy thing, this is going to be R dot equal to, this is F and G, right. And there is this term here, so we want - this fellow here, so this is 2D over R + the usual whatever it is, + the square root of 2D times white noise. Okay. So there is a drift, there is a drift here which is tending to increase R and there is no external force, but yet you have a drift. Where is this coming from? For the P there is no such thing, there is no drift, there is no applied force, no potential, nothing and therefore this had no stable equilibrium distribution, I just went to 0.

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$$\frac{\partial \rho}{\partial t} = -\frac{\partial}{\partial r} \left( \frac{2D}{r} \rho \right) + D \frac{\partial^2 \rho}{\partial r^2}$$

$$\Rightarrow \text{LE for } r: \dot{r} = \left( \frac{2D}{r} \right) + \sqrt{2D} \zeta(t)$$
 drift term!



But here I have done nothing, I just changed variables. And if this correspondence between Fokker-Planck and the stochastic differential equation is to be believed, you have a drift term. Okay. Where does this come from and how do we interpret this? It is telling you that independent of the noise, of course it is not independent drift, so notice that it is not like an external force or anything like that because  $D$  is sitting in there, it is very much there, it is the same  $D$  that is sitting here. So these are not unrelated to each other, we just changed variables but what is the definition of this term?

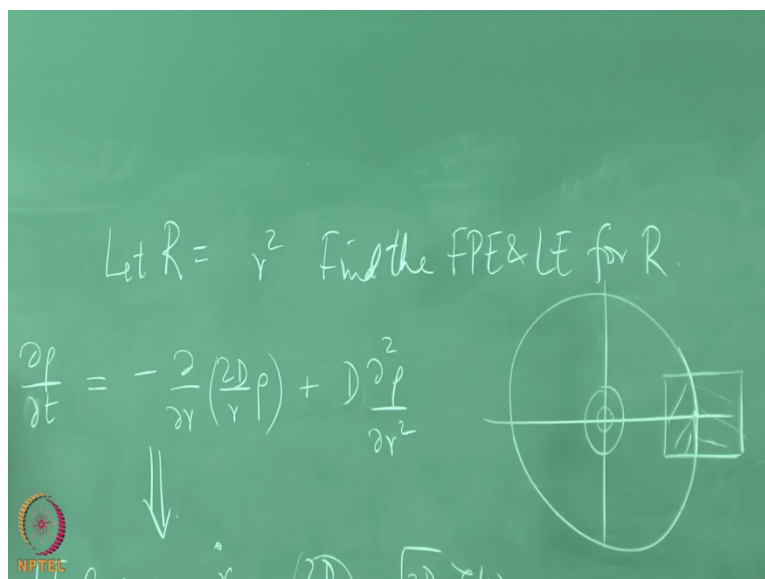
You notice that, you started the origin, this term is very large close to the origin, definitely push it away,  $R$  dot is positive, so it is tending to push it away. This means that if you do it in 2 dimensions, you see this immediately in the  $XY$  plane, this is like 2 Brownian motions

composed in the X and Y directions the forces are uncorrelated to each other and you have this motion, particle doing Brownian motion. But if you start here somewhere in this place, the tendency is to get pushed out, okay because this term is very large, it is going like 1 over R. And the reason of course is very clear, it says that if you start in a sufficiently small neighbourhood of this origin, then due to any fluctuation, R can only increase.

If R is sufficiently small in any fluctuation R can only increase, stately speaking at the origin any fluctuation will push it away from it, right. But that is actually true even if you are further away from the origin because suppose you are here at this point, you can go in any direction with equal probability and the forces that are uncorrelated are in the X and Y direction. So if you draw a little square like this, this is heuristic, a hand varying argument, right, now all points on the square are equally likely so to speak. But there are more points outside than inside, if you go inside it means R decreases and if you go outside, R increases. So that is the drift that is appealing here. Okay. This is the reason why it appears correlated in this case.

So you should not otherwise a priory you should not have such a drift but you do because of this simple geometrical fact. So while noise has this rotation symmetric, the variable you are looking at is spherically symmetric. Right. So you have a kind of drift effects even without an external force or potential. Similarly you could write down the equations for, if you had single variable, just X and it is undergoing Brownian motion, you can ask what happens to X square, what does this look like? Or in higher dimensions, what happens to R square, so that is an exercise, interesting exercise.

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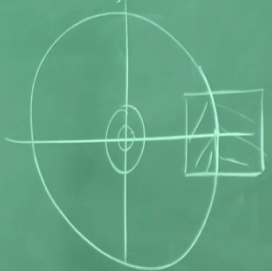



Let  $R = r^2$  Find the FPE & LE for  $R$ .

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial r} \left( \frac{2D}{r} p \right) + D \frac{\partial^2 p}{\partial r^2}$$

↓

LE for  $r$ :  $\dot{r} = \left( \frac{2D}{r} \right) + \sqrt{2D} \zeta(t)$

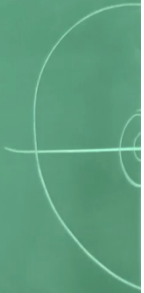




Let  $R = r^2$  Find the FPE & LE for  $R$ .

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial r} \left( \frac{(d-1)D}{r} p \right) + D \frac{\partial^2 p}{\partial r^2}$$

↓

LE for  $r$ :  $\dot{r} = \frac{D(d-1)}{r} + \sqrt{2D} \zeta(t)$

Find out what the stochastic equation satisfied by  $R$  square is. So consider  $R$  equal to, let  $R$  equal to  $r$  square, find the Fokker-Planck equation and Langevin equation for  $R$  without the square root in this case. So it is all the question of changing variables and again you would use the same trick, you start with the mass, the solution of the diffusion equation, the Gaussian solution, spherical symmetric Gaussian solution and rewrite that in terms of the density of probability density function of this  $R$ , keeping track of all the Jacobian and so on and so forth. And then having got that equation can be a first-order term as well, can be a drift term, go back and write the Langevin equation down for it in this case, okay.

By the way this thing here is easily generalised to  $D$  dimensions. What would happen if you have  $D$  spatial dimensions, where little  $d$  greater than or equal to 2, this becomes  $d-1$ , this becomes  $d-1$  here, this factor, this factor for  $\pi$  will change, it is a surface of the unit sphere

or whatever it is in  $D$  dimensions. So this will be some dimensionally dependent factors, but it is relevant for our purposes here, this fellow however becomes  $d - 1$  outlet and the constant, so let us write it as proportional to,  $P$  proportional to this guy. And what happens to the laplacean? This is going to be  $\Delta$  over  $\Delta R$  and then this is...

2 will become  $d - 1$ .

Exactly, so this factor becomes  $d - 1$ , this guy here becomes 2, sorry  $D$  into  $d - 1$  and this remains  $R$ . I do not remember if this is going to change not but you can figure that out. This constant but this one over  $R$  drift is still there, but this depends on this guy here. And of course this should be like this because when  $D$  equal to 1, the limit you just have, there is no drift, there should not be. Okay. Similarly you could ask about what happens to various functions of Brownian motion, various functionals of Brownian motion like the exponential and so on and so forth. And they have strong applications, there are many such applications but since we are not discussing stochastic processes per se, I am not going to discuss those here, okay.

The next thing we have to do again to fill up a gap is the following. I mentioned that throughout the langevin equation is an approximation, we made some statements about when it is valid and so on. And corresponding to the Fokker-Planck motion which is equivalent to langevin equation is an approximation in the same sense, okay. Can we go back and ask what a particle in a fluid is actually going to do? This is a very very hard problem it turns out, even classically. One could make the problem much simpler and ask what is the particular when it dilutes gas to? What happens if it is moved, knocked out of equilibrium and can be followed, find out what its time dependency is based distribution is, even the one particle stage, okay.

It turns out that you can derive an equation called the Boltzmann equation to describe this and from that you can find out what various transport properties are. You can make a connection between the Boltzmann equation and the langevin dynamics that we have talked about here and the specific assumptions but in a sense the Boltzmann description is more fundamental, it exposes more clearly stomach precisely what are the statistical mechanical assumptions here. So we will try to fill that gap, I will try to give a very short derivation of the Boltzmann equation for it dilutes gas. That will be the next topic, okay.