Physics of Biological Systems
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Lecture – 11
Solutions of the Drift-Diffusion Equations

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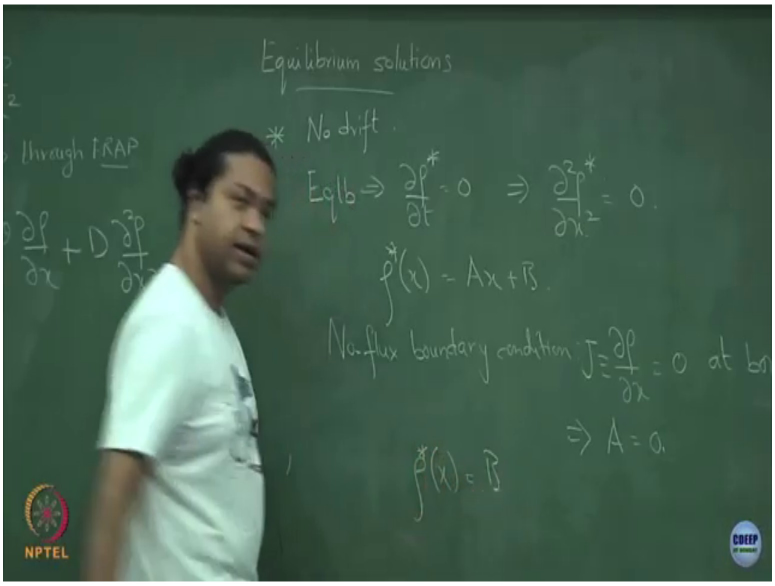

All right, now let us look at the Solutions of this Equation; let us first look at the equilibrium solutions. So, let us look at equilibrium solutions of this system and if I first take this standard diffusion equation without the drift ok. So, no force or no drift or whatever right. At equilibrium what will happen? Whatever probability or whatever density or concentration that you have that is not going to change with time anymore right.

So, this del rho del; so equilibrium or steady state whatever equilibrium implies that del rho del t is equal to 0 which means what you need to solve is delta 2 rho; del x 2 is equal to 0 right. So, what is the solution of this? So, we are just doing in 1 D; you can extend all of these to higher dimensions as you want.

So, if del 2 rho; del x 2 is equal to 0, I can write let me write rho star because this is what an equilibrium. So, rho star of x is some Ax plus B right. I need something else; I need some sort of a boundary condition in order to fully solve a different specify a differential equation. So, let me say I use a no flux boundary condition.

So, let me say I use a no flux boundary condition which basically means the current or therefore, equivalently del rho; del x is equal to 0 at boundaries. So, J or equivalently del rho the derivative of the concentration or density that is equal to 0 at the boundaries; so nothing flows in or out ok. If you do that then of course, what this says is that; what does it say? It says that A must be equal to 0.

So, if you impose this no flux boundary condition that implies that A equal to 0 and therefore, the equilibrium solution then becomes what you would expect? That it is a constant right, if you wait long enough the diffusion equation will take whatever in homogeneities you have in your profile and you will make it a flat profile.

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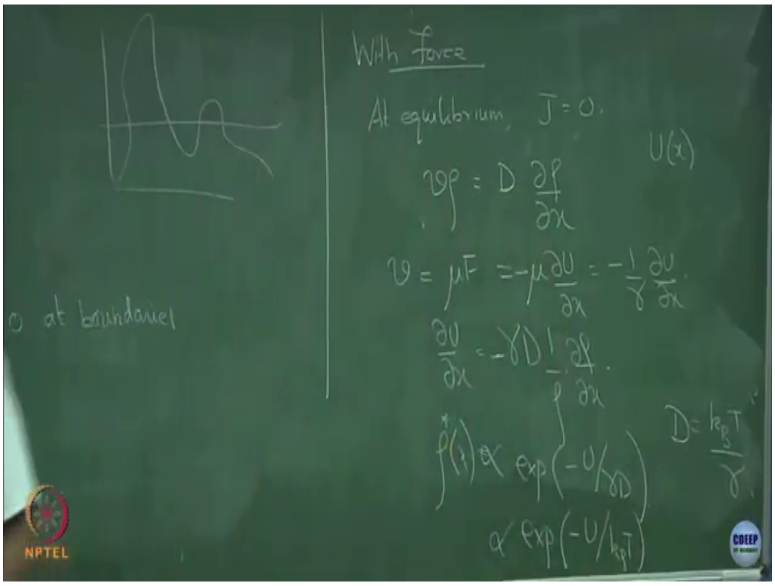

So, regardless of you start off with whatever if you wait long enough; it will go to this straight line, you will go to an uniform line. So, it is it is a boring equation in that sense all right; so that is the no drift case. But we can also do the case in the presence of in the presence of forces or in the presence of drift. So, with force alright; so we will solve the drift diffusion equation.

Now, if I have equilibrium; I will have no net current in my system right, everything is sort of stationary which means that. So, at equilibrium at equilibrium; the current is equal to 0 alright which means swap; remember the current is minus current is v rho minus D del rho del x all right.

So, if the current is equal to 0; there is no flow then what I have need to solve is this equation v rho is equal to D del rho; del x ok. Remember, that the velocity that if I had that was proportional to the force right. So, if the velocity; the drift velocity was proportional to the force. Let me assume for the sake of simplicity that this is a conservative force which means you can write it as the negative gradient of a potential right which means this I can write as some minus mu del u; del x right.

I have some potential U of x; the gradient of that gives me the force, the force causes a velocity ok. So, let me write the velocity in this form; it is minus mu del U; del x or if you want to write in terms of the friction minus 1 by gamma del U del x all right. So, now you need to solve that equation that is; so del U del x is equal to gamma D.

Let me write in terms of gamma; gamma D 1 by rho; del rho by del x ok. What is the solution of this equation? What is; so all of this are equilibrium. What is the solution of this equation? Here you have a del rho by rho; here you have a d U right; so therefore yes someone.

Student: Exponential.

Exponential right. So, the exponential of what? Let me write it is proportional exponential of?

Student: (Refer Time: 06:18).

Did I miss minus sign somewhere?

Student: Yes sir.

Yes, right that minus sign I missed. So, exponential of minus U by gamma D right and what does the Einstein relation should say about the relation between the diffusion coefficient and the friction? D is k B T by gamma all right. So, this is nothing, but proportional to exponential of minus U by k B T. So, recover back the Boltzmann ah; the Boltzmann distribution at equilibrium. So, you take this yes?

Student: (Refer Time: 07:03) Exponential.

This is the del rho by rho that will give you a log rho if you integrate right here you will get a U. So, then rho is e to the power of whatever you have that right. So, at equilibrium for this drift diffusion equation unlike this simple diffusion equation where you get a constant profile; here you recover back the Boltzmann distribution ok right. So, that was the easy part. So, this is the solutions at equilibrium; we can also write the full time dependent solution of the diffusion equation.

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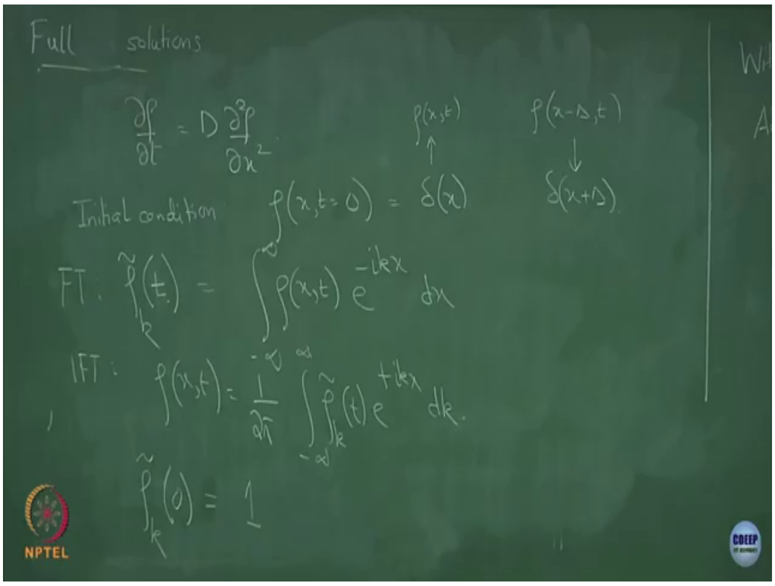

So, you can also write the full solution hm. So, that is what we will do next; it is good to know how to solve the diffusion equation at least completely in all cases alright. So, let me first solve this; the equation without drift and we will come to the drift part later. So, I will solve this one del rho; del t is equal to D del 2 rho del x 2 alright.

So, I need to specify some sort of an initial condition. So, I need to specify an initial condition and let me take a delta function for that. So, it is the particle started off at some given position ok. So, rho at x; at x comma t equal to 0, the initial condition is sum delta of x let us say. If you start off at some specified position and you want to know how does this probe; this particle which started off at this position which you know; how does the probability density for that evolve in time if it follows the diffusion equation.

This is a good probability density because this is automatically normalized right; if you integrate the delta function over space we will get one; yes it is normalized. So, what we will you can solve this in many many ways what we will do it we will do it using Fourier transforms. So, if I Fourier transform the density; I can write, so I will do a Fourier transform of rho rho tilde of k; that is rho x comma t; e to the power of minus ikx dx minus infinity to infinity.

You can also write the inverse Fourier transform of course, you can write inverse Fourier transform. So, rho of x comma t will be 1 over 2 pi ok; integral rho tilde k of t e to the power of plus ik x; d k alright. Everyone is familiar with Fourier transforms; all the department all right. Since I know the initial condition, I can find out this Fourier transform of the initial condition right.

So, this is not k, this is t sorry; so I can find out the Fourier transformation rho k tilde at time 0 ok. So, I just need to substitute the initial condition over here and that will give me the Fourier transform at 0 time. So, what is that? What is rho k tilde at 0 ok? What is delta x; e to the power of minus ikx; dx?

Student: 1.

1 so I know that yeah alright. So, what I will do is that I will try out a wave solution that is because this equation is translationally invariant. If I write down if corresponding to this I write down the solution rho of x comma t, then any other solution rho of let us say x minus delta comma t will also be a solution where this in e which corresponds to a shifted initial

condition x plus delta. So, it is a translationally invariant solution system which means that will admit plane wave solution. So, let me try you try a solution of this form.

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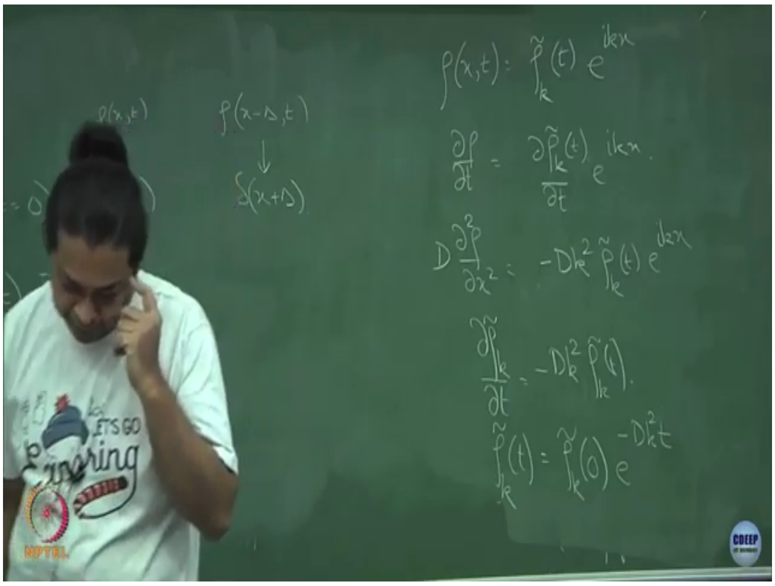

So, I will try out a solution of this form rho of x comma t rho of x comma t is rho tilde k t; e to the power of ikx ok. You can substitute this back into this equation; so this is my answers. You can substitute this back into this equation which means that del rho; del t is del rho k tilde of t; del t, e to the power of ikx and on the other side del 2 rho; del x 2 is what? Minus; so there is a D over here; so let me write that also.

So, minus D k square rho k tilde of t; e to the power of ikx all right; each differentiation will bring down an ik; ik into ik is minus k square. So, if I equate these two, then the equation that I get is del rho k tilde; del t is equal to minus D k; minus D k square; rho k tilde of t which I know how to solve; which has the solution that rho k tilde of t is equal to rho k tilde of 0; e to the power of minus D k square t right fine.

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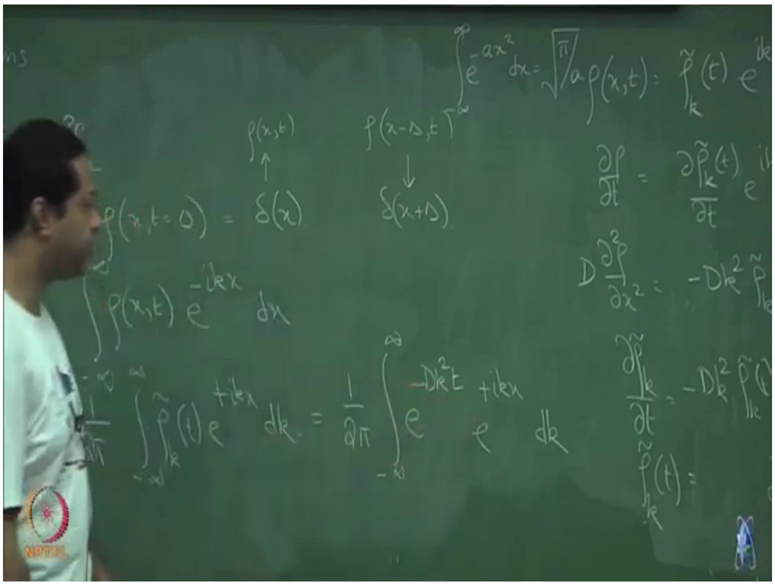

And this rho k tilde of 0 I have already found because I know what was the initial condition that is just 1, let me forget. So, I know what is rho k tilde of t; once I know what is the this Fourier transform, I can use the inverse Fourier transform to get back for my density. All I need to do is I need to substitute for that rho k tilde that I found in this equation. So, the rho x of t is going to be 1 by 2 pi integral e to the power of minus Dk square t; that is my rho k tilde.

Then e to the power of plus ikx plus ikx; dk from minus infinity to infinity ok. How would you do this integral? How does one do how does one do an integral like this? Anyone? Nithin?

Student: No.

No? What is this integral? e to the power of minus ax squared dx; this is the Gaussian integral right. So, what is the solution of this?

Student: (Refer Time: 14:40).

[FL] Root pi by a; this you should know by now. If you are not familiar with Gaussian integrals; just go back and look at them, it is a fairly standard. So, if you have an integral of this form; then what does one do? Complete the squares right, you add and subtract to multiply and divide by a term so that you complete the squares and then you recast it in this form in the form of a Gaussian integral.

So, please do this; what will you get? Krishna, what will you get? This is the diffusion equation, what will you get is the full time dependent solution of the diffusion equation?

Student: Gaussian.

Gaussian. So, what is the Gaussian; what Gaussian what is the normalization?

Student: 1 by square root of.

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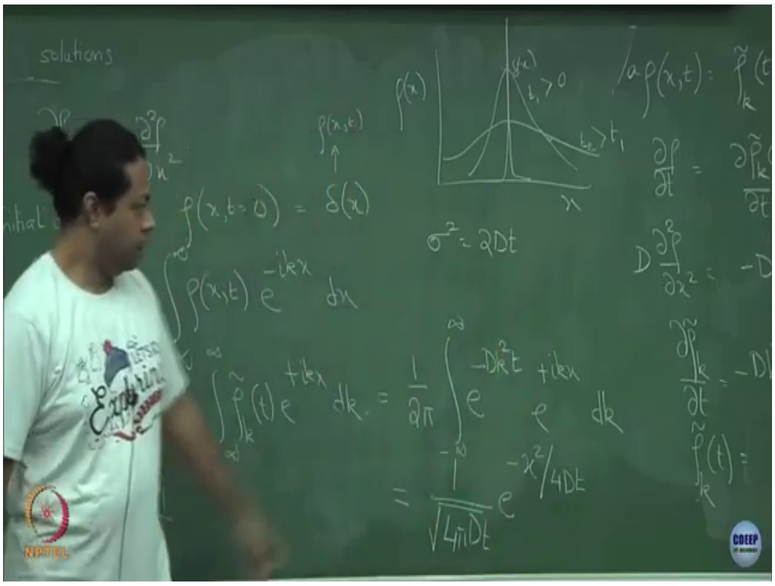

1 by square root of?

Student: 4 pi Dt.

4 pi Dt; e to the power of minus?

Student: x square by 4 Dt.

x square by 4 Dt. So, please do this; you complete the square ok, recast it in the form of a Gaussian integral, do that Gaussian integration and you should get this answer ok. So, this is a simple Gaussian e to the power of minus x square by 4 Dt with this normalization.

So, what does that mean? It means that I started off with this ok; if I plot this rho x of t; rho x versus x at time t equal to 0 I started off with a delta function right, this is delta of x. As time goes on, it will slowly smear out the probabilities and it will smear them out in the form of a Gaussian alright; this is at some time t 1 greater than 0; if you wait longer it will get smeared out even more. So, this is some time t 2 greater than t 1 and so on. After infinite time of course, it will become flat because that we have already seen that at equilibrium; it will go to a flat profile.

But how it goes? The full time dependence that it goes in the form of this Gaussian and the variance of this Gaussian of course, is sigma square is 2 Dt right which is exactly what we were doing earlier as well; the variance grew with the variance grew with the number of steps or the time that the random walker has walked for.

So, this plays the role of n in these earlier coin flip or drunkards walk examples that we do ok. So, that is the variance all right. So, this was the simple diffusion equation; what would you do for the drift diffusion equation?

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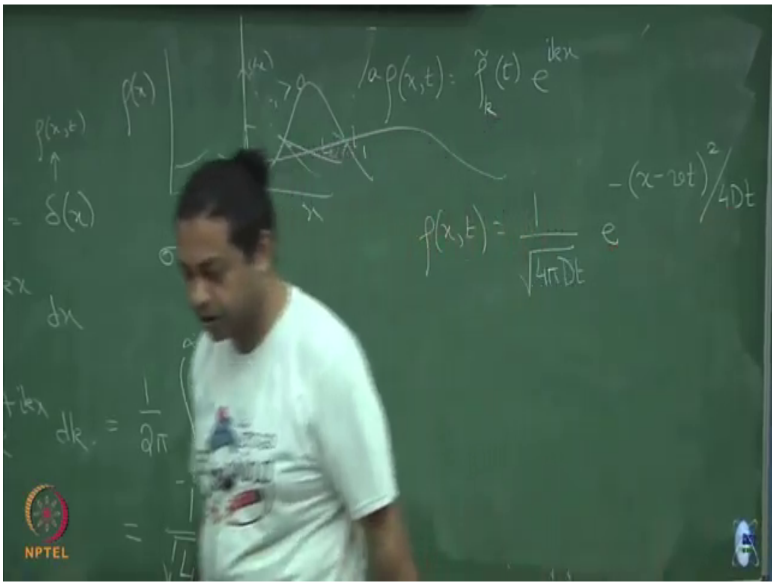

What; so, what would be rho x of t for the drift diffusion equation? Yes, can you just guess at the answer?

Student: (Refer Time: 17:58).

If you have something which is travelling with the velocity v; so remember here in this case the mean stays at 0 right; the peak is always at 0 right. So, if something is traveling with a velocity v, how would this change?

Student: (Refer Time: 18:13) x minus vt.

x minus vt. So, this you should again check for yourself that if you solve for the full drift diffusion equation; then the time dependent solution, the full time dependent solution is x minus vt whole square divided by 4 Dt ok. So here if you look at the mean that is going to be traveling with a velocity v ok. So, if this is what you started off with at some time; after sometimes if you would have shifted after sometimes it was shift even more ok; so that is the idea.

Couple of things this is of course, in a 1 D; generally here you will have a coefficient which depends on the dimensionality, the normalization will depend on the dimensionality and so on, but the technique the method or at least the salient feature that is going to be a Gaussian either stationary or a travelling solution like that that is going to remain independent that is going to remain unchanged all right. So, this is clear? So, this is a little bit about what I wanted to say formally before I come back to one more biological application.

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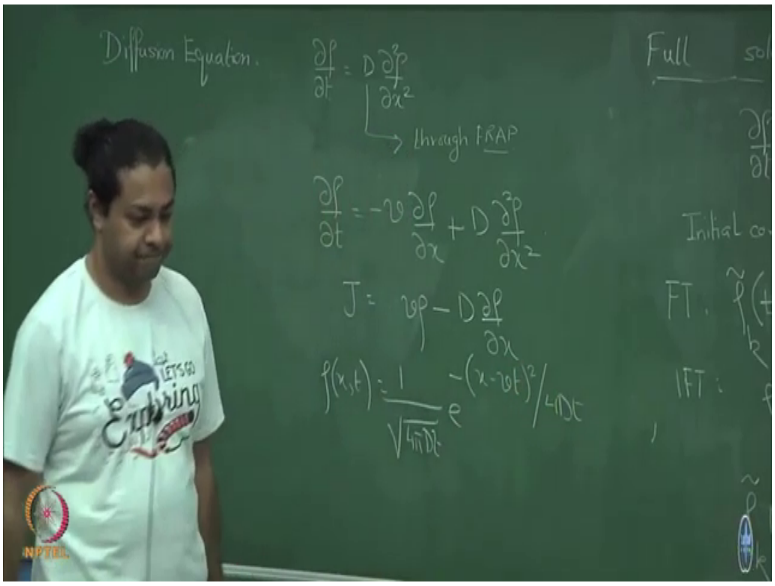

So, let me write this as well rho of x comma t is square root 1 by 4 pi Dt; e to the power of minus x minus vt.