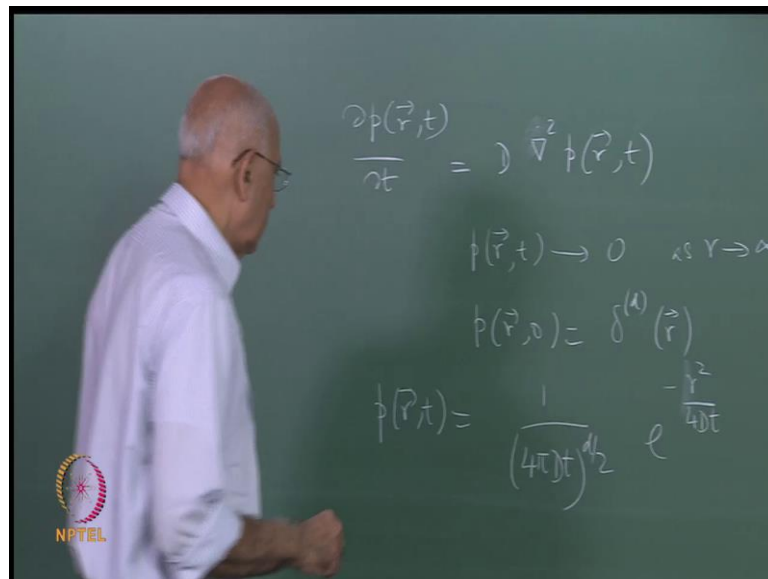


**Selected Topics in Mathematical Physics**  
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**Department of Physics**  
**Indian Institute of Technology, Madras**

**Module - 10**  
**Lecture - 26**  
**The Diffusion Equations (Part II)**

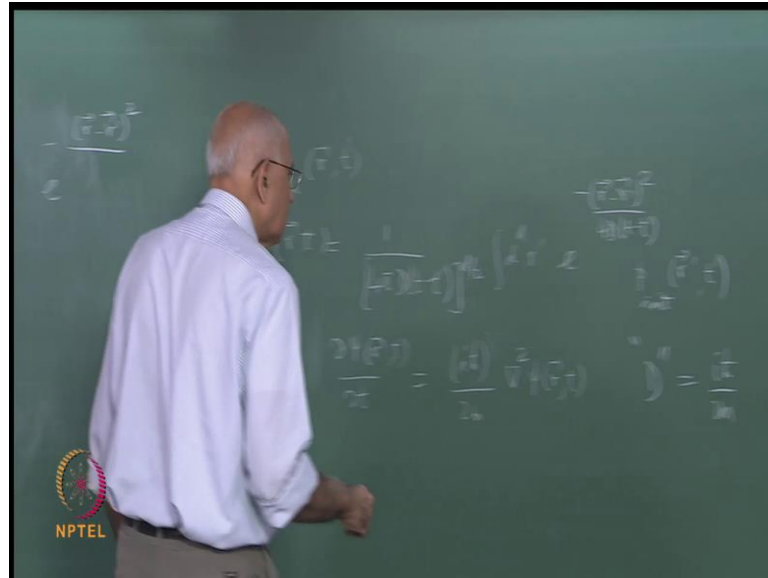
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We continue with our study of the diffusion equation and its solution. If you recall, we solve the problem of finding the fundamental solution of this diffusion equation,  $\frac{\partial p}{\partial t} = D \nabla^2 p$  subject to the boundary condition  $p \rightarrow 0$  as  $r \rightarrow \infty$  in all directions. And the initial condition  $p(\vec{r}, 0) = \delta^{(d)}(\vec{r})$  at the origin.

So, a particle starts at the origin, undergoes diffusion, and the question is, what is the probability density? And if you recall the solution to this was  $p(\vec{r}, t) = \frac{1}{(4\pi Dt)^{d/2}} e^{-\frac{r^2}{4Dt}}$ , that was the fundamental Gaussian solution. I pointed out that this is also the Green function, because this essentially solves the equation, it solves the problem for any prescribed initial condition.

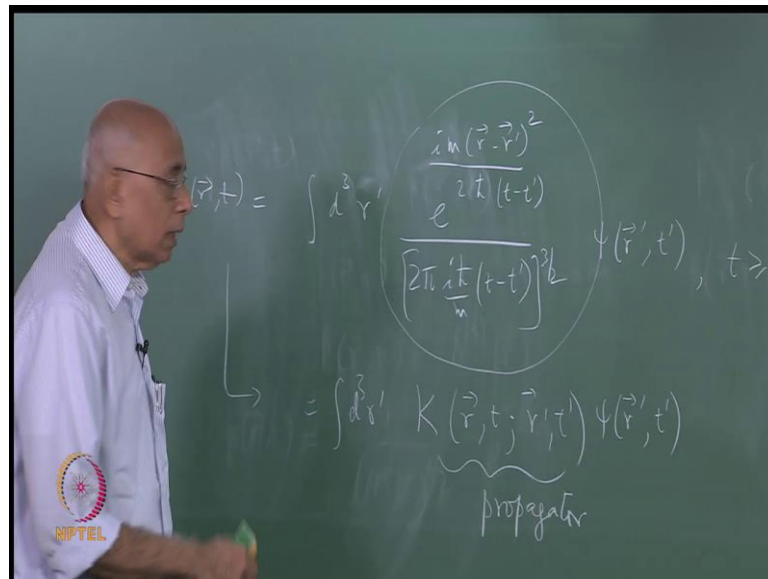
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So, if you tell me what  $p$  initial is as a function of  $r$  at  $t$ , if you give me this function at some instant of time  $t$  equal to  $t$  prime say? Then I can tell you what the solution is at any later instance of time by simply inserting it in this. So, the solution becomes  $p$  of  $r$  comma  $t$  equal to  $1$  over  $4 \pi D$ , and now it is  $t$  minus  $t$  prime to the power  $d$  over  $2$ , and integral  $d d$  of  $r$  prime  $e$  to the minus  $r$  minus  $r$  prime whole square over  $4 D t$  minus  $t$  prime multiplied by  $p$  initial which is prescribe to you  $r$  prime at  $t$  prime. So, what is happen is that we essentially found the fundamental green function to the diffusion operator  $\frac{\partial}{\partial t} - D \nabla^2$ , you essentially found the answer to that.

I want to you notice that if you wrote down the free particle Schrodinger equation for a single particle in the absence of any potential, that equation looks very much like this, it says  $i \hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi$ . This is minus  $\hbar^2$  over  $2m$ ,  $I$  ((Refer Time: 03:14))  $i \hbar$  cross the whole square, and if you remove one of this  $i \hbar$  crosses, then it is clear that it is likes the diffusion equation. It is exactly like the diffusion equation with quote and quote in imaginary pure imaginary diffusion constant, but the formal solution is exactly the same.

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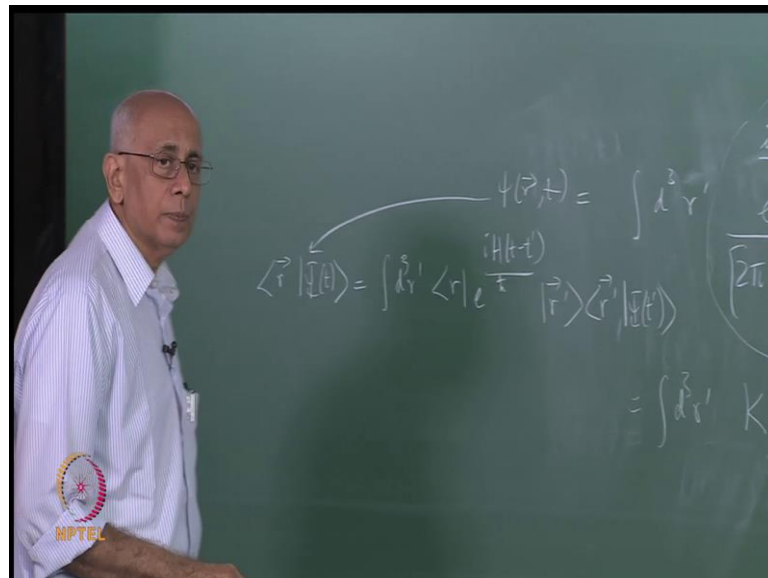
So, in fact what you could do is to say that for a free particle, the solution to the Schrodinger equation for any given initial wave function is  $\psi$  of  $r$  comma  $t$  equal to an integral. Let us write let us write this down  $d$ , let us work in free dimension for instance  $d = 3$   $r$  prime  $d = 3$   $e$  to the minus  $r$  minus  $r$  prime the whole square over  $4 D t$  and  $t$  is  $i \hbar$  cross over  $2 m$ . So, it is the  $i \hbar$  cross goes up, and you want 4 times that, so it is equal to minus divided by  $I$  am just trying to make sure that you had. So, this  $d$  is equal to  $i \hbar$  cross over  $2 m$  and we want 4 times that, so it is  $4 2 i \hbar$  cross over  $n t$ .

So, let us write this as  $i \hbar$  over  $2 \hbar$  cross times  $t$  divided by  $4 \pi D t$ . So, this is equal to  $2 \pi i \hbar$  cross over  $m t$  minus  $t$  prime to the power  $3/2$ 's  $\psi$  of  $r$  prime and  $t$  prime. So, at all later in since of time, this is what the wave function is given by. For any given initial way function if it is an  $l^2$  wave function for instance you guaranteed to remain  $l^2$ , and it transform and this it is given by this. So, what is essentially happen is that wave exponentiated the Hamiltonian ultimately this is what you done, because you know that this can also be written as equal to integral  $d^3 r$  prime, the propagator  $k$  which takes you from  $r$  prime at time  $t$  prime  $2 r$  at time  $t$  times  $\psi$  of  $r$  prime  $t$  prime.

This thing here is the propagator, and that is what this whole quantity is. So, we have essentially found the free practical propagator when you have a potential of course the

Hamiltonian is not just  $p^2$  over  $2m$ , and then you have to exponentiate that Hamiltonian. I hope you realize that this is essentially exponentiating the Hamiltonian and then finding certain matrix element.

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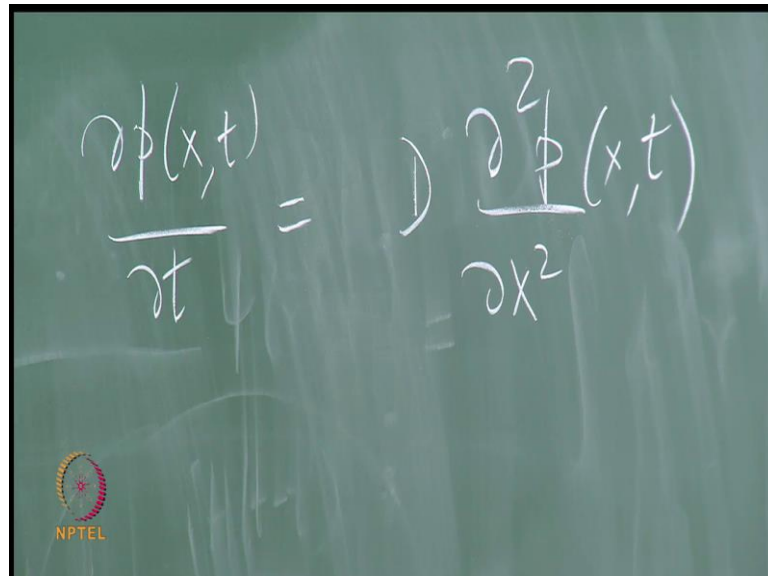
Because, if you write this in abstract notation what does happen is that  $\psi$  of  $t$  has been written in the form  $\int d^3r' \psi$  of  $t'$  that is what this quantity is has been written in the form  $\int d^3r' e^{i\vec{p}\cdot\vec{r}'} e^{-iH(t-t')} / \sqrt{(2\pi)^3}$ , and then there is an  $\int d^3r'' \langle \vec{r} | U(t) | \vec{r}'' \rangle \langle \vec{r}'' | \vec{r}' \rangle$  of  $t'$  in this fashion. And this quantity here is precisely the propagator that we are talking about, because this thing here is the wave function at time  $t'$ . So, what we found is in the position basis and explicit representation for the propagator by exponentiating the free particle Hamiltonian turns out to be this crazy function here.

Now, doing this for other Hamiltonian is nontrivial if you have even a potential like the harmonic oscillator potential, finding the propagator explicitly is a nontrivial exercise in general. But, for the free particle it is immediate and follows directly from the fundamental solution of the diffusion equation, that is a useful thing to know will come back to there is and discuss a little bit about this spread of the wave packets and so on.

So, now let us go back to our diffusion problem, and ask what happens if you have

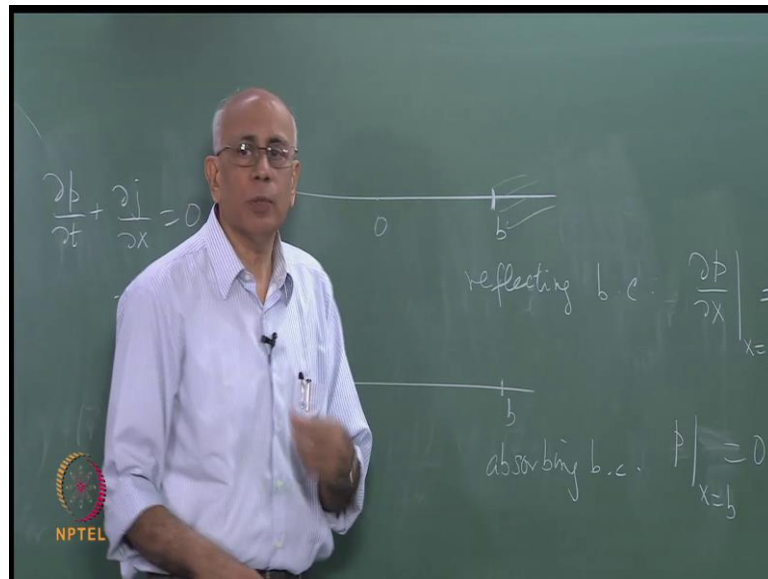
boundaries? We found the fundamental solution, but of course in practices we would like to have boundaries in the problem and then ask, what sort of boundary condition should you apply then you have various physical situations. Now, just to keep things easy, let focus now and diffusion in one dimension.

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

So, the basic diffusion equation is going to involve is going to be just  $d p$  of  $x$  comma  $t$  over  $\Delta t$  equal to  $D d^2 p$  over  $d x^2$  x comma  $t$ , and the question is what is sort of boundary conditions are we generally interested in. Now, one possibility is to say that you have a diffusion occurring in some interval finite interval, and at the boundaries you say the system does not diffuse out of it at all, and it does not get lost, it stays inside. If such a thing happens, then what kind of boundary condition would you put? You would say well there is no flux across that boundary. So, all you do is to set the flux at that point equal to 0.

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So, for instance you can write this equation as  $\frac{\partial p}{\partial t} + \frac{\partial j}{\partial x} = 0$ , where  $j$  is a current and this look like an equation of continuity, and what is the current this  $j$  by where a linear response that I already mention it is  $\frac{\partial p}{\partial x}$  more than that. And the boundary condition when we have a barrier, so on this line we have some boundary point  $b$  let say this is the origin, and you not allowed to go beyond this, this system comes and hits this and goes back, it remains to the left of it at all times. This is called a reflecting boundary condition.

It is equivalent to saying that  $\frac{\partial p}{\partial x}$  at  $x$  equal to  $b$  equal to 0 no flux through this point, and the physical reason is to the left of this point  $p$ , what would happen if I say. Well every time it hits the point  $b$ , it either escape or gets absorbed something, and I am no longer I no longer have the particle become extinct as far as the diffusion process is concerned to the left of this region, what kind of boundary condition would you put there? Where you would say this would be what is called on absorbing boundary conditions, and here you would say  $p$  at  $x$  equal to  $b$  equal to 0, because once it hits it that is it.

The probability of the existence of this particle is not there whatever, it is either lead through the boundary or it is when up absorb there and become extinct that is it. So,

these are the 2 common boundary conditions, of course you have a second order equation here in this phase variable, and therefore you can have a mixture of the 2 you can say it is partially absorbed, partially reflected and so on and so forth more complicated possibilities exists. We look at one more of these possibilities a physical problem, but these are the 2 common boundary conditions. Now, the question is how are we going to write down the solution to this problem in the present of this boundary condition here?

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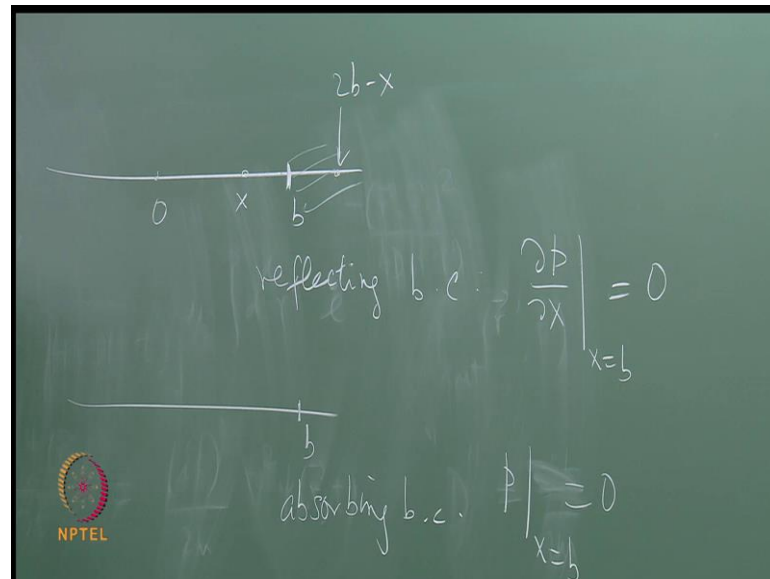
Semi-infinite region  $-\infty < x \leq b$

RBC at  $x=b \Rightarrow p(x,t) = \frac{1}{\sqrt{4\pi Dt}} \left[ e^{-\frac{x^2}{4Dt}} + e^{-\frac{(2b-x)^2}{4Dt}} \right]$

ABC at  $x=b \Rightarrow p(x,t) = \frac{1}{\sqrt{4\pi Dt}} \left[ ( ) - ( ) \right]$

So, the physical reason let say in the simplest case would be semi infinite region minus infinity less than x less than equal to b that is my region. And I ask, what is the solution to the diffusion equation with these 2 boundary conditions here? Now, the point is you can do this in many ways; we can solve this problem in many, many ways. The most common ways would be to either do separation of variables or to do the method of images etcetera.

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Now, the method of images is familiar to you from electrostatics, what you do to ensure that the flux 0 at that point is to say that you have another random walker. So, if instantaneously the position of the random walker or the diffusion particle is  $x$ , you pretend that there is another particle here. Solve this problem in the presence of these 2 particles, and ask what the probability density is, and then ensure that the boundary condition is maintained at that boundary. And once you do that then by the uniqueness theorem for solution, you have a unique solution exactly as in electrostatics.

Now, what would that be? Well, if this particle hits this boundary from this direction and the other one hits it from that side, the net flux is 0 that is the way we do it, all you have to do it is to add the probability densities. So, what we need to do is to ask where is this particle is a mirror image of this particle in this mirror at  $x$  equal to  $b$ , and if this is the origin it is clear that it is as far away on this side. So, this coordinate is there is a  $b$  and then this distance is  $b$  minus  $x$ , so it said  $2b$  minus  $x$ , the image particle is at  $2b$  minus  $x$ .



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Handwritten text on a chalkboard:

Semi-infinite region  $-\infty < x \leq b$

RBC at  $x=b \Rightarrow p(x,t) = \frac{1}{\sqrt{4Dt}} \left[ e^{-\frac{x^2}{4Dt}} + e^{-\frac{(2b-x)^2}{4Dt}} \right]$

ABC at  $x=b \Rightarrow p(x,t) = \frac{1}{\sqrt{4Dt}} \left[ \phantom{e^{-\frac{x^2}{4Dt}}} - \phantom{e^{-\frac{(2b-x)^2}{4Dt}}} \right]$

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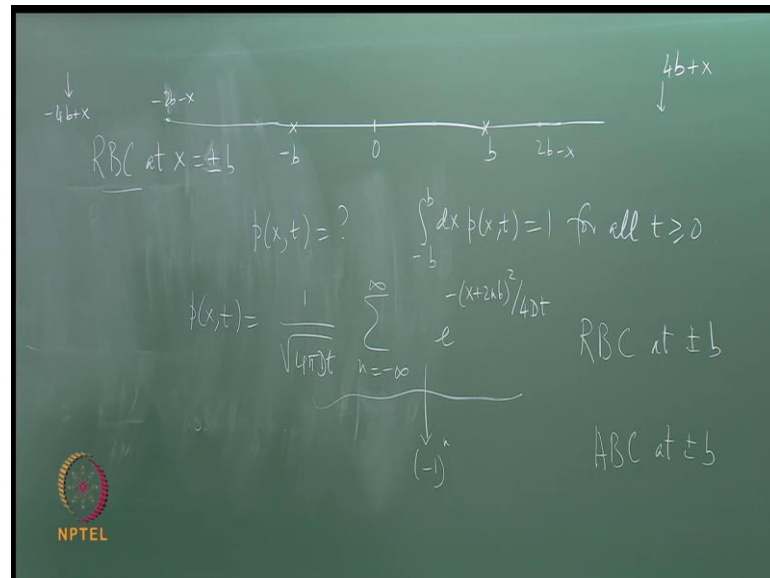
Therefore, I assert that with reflecting boundary conditions RBC at  $x$  equal to  $b$  implies that  $p$  of  $x$  comma  $t$  equal to  $1$  over square root of  $4\pi D t$   $e$  to the power minus  $x$  squared over  $4 D t$ , assuming as have done earlier that the particle starts at  $x$  equal to  $0$  at  $t$  equal to  $0$  this plus  $e$  to the minus the coordinate here is  $2 b$  minus  $x$  whole square over  $4 D t$  and that is it. I leave you to verify that this boundary condition will be satisfied at all instance of time, so the method of images unable such to write down the solution in the presence of a finite boundary failure to relay, if it is a reflecting boundary.

Well, what the absorbing boundary condition in just says that once you hit this point, the probability must be  $0$ . There of course, all you have to do is to say that these  $2$  walkers come along in this annihilate each other. So, it is a exactly the same solution absorbing boundary conditions at  $x$  equal to  $b$  implies  $p$  of  $x$  comma  $t$  equal to the same thing  $4\pi D t$ , this exponential minus the other exponential.

And of course if you set  $x$  equal to  $b$  you realize it these  $2$  will cancel each other completely, and that is a unique solution to the problem. So, in this problem it is completely trivial to write down the solution in the presence of a boundary at the point  $b$ ,

what happen if you have 2 boundaries an either side, you could have one which is absorbing, one which is reflecting and so on and so forth.

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But you already have familiar with what happens, so let look at one particular case where you have reflecting boundary conditions at x equal to plus or minus b, let us take it symmetrically just to make the algebra little easier. So, here is my reason here 0 there is a boundary at b which is a reflecting boundary, and another boundary at minus b. And the particle starts at the origin at equal to 0, and stays in this reason at all times and the question is, what is p of x comma t? One thing we know for sure, since the diffusion the diffusing particle does not disappear at all stays and side.

We sure that this is going to be true, integral from minus b to b d x p of x comma t equal to 1 for all t greater than equal to 0. So, it is normalize this normalize probability density must remain 1 at all times inside, no matter how long t is how large t is, it is still has to satisfy this conditions here. Now, how would you do this? Well, if instantaneously the particle is here, there is an image particle at this point 2 b minus x, and you add that contribution. Then of course it also gets reflecting in this barrier here. So, there is another image particle at minus 2 b minus x, and then this the image of this in that mirror out there.

So, there is going to be another particle somewhere here at  $4b + x$ , and another one here on this side at  $-4b + x$  and so on. There is actually infinite number of images, exactly as if you had a charge in there, and you had 2 boundaries in the electrostatics problem to write down the potential in this region in between, you need to have an infinite number of images. In exactly the same way, now the solution turns out to be  $p(x, t)$ , and I ask you verify this  $\frac{1}{\sqrt{4\pi Dt}} \sum_{n=-\infty}^{\infty} e^{-\frac{(x-2nb)^2}{4Dt}}$  for reflecting boundary conditions, so that all the contributions are added up.

And for absorbing boundary conditions, so this is for RBC and if you have 2 absorbers at plus and minus  $b$ . So, this is for RBC at plus or minus  $b$ , and if have absorbing boundary conditions at plus or minus  $b$ , it exactly the same formula except that there would be a minus 1 to the power  $n$  here, where  $n$  identifies a number of reflections. So, every time you reflect to put a minus sign there, and that is it nothing else changes. But, just that single minus 1 to the power  $n$  introduces a very different kind of a solution all together it a very different solution. For one thing you are sure that this particle is going to hit the boundary at some time or the other and disappear.

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Survival probability

$$\text{RBC at } \pm b \Rightarrow \int_{-b}^b dx p(x, t) = S(t)$$

Semi-infinite region  $-\infty < x \leq b$

$$\text{RBC at } x=b \Rightarrow p(x, t) = \frac{1}{\sqrt{4Dt}} \left[ e^{-\frac{x^2}{4Dt}} - e^{-\frac{(2b-x)^2}{4Dt}} \right]$$

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So, it is clear that this quantity with A B C at plus or minus b implies that this quantity minus b to b d x p of x comma t with start of at 1, because p of x comma 0 is delta function at x equal to 0 will decrease as a function of time. It is clear that as time goes along this must decay to 0, and it is of interest to ask how it goes to 0 will compute this quantity. Now, this thing has a simple name, what is this equal to? It could call this S of t, the survival probability that the particle is still in this region between minus 1 and 1. So, this thing here is of interest it is, and this number must decrease to 0, starts at 1 at equal to 0, and then decays to 0 as t goes along.

So, this normalization cannot be maintained this thing is a decaying function of t, and this quantity is S of t which decreases as time goes long will find out what it is at least for free diffusion. The other interesting thing that happens is you could ask All right, if there is going to be absorption here or there. And this is for instance a physical problem would be if you had 2 chemical species, and when they meet they react or something like that. You have the reactant one of the reactant sitting at one of the boundaries, and the other particle diffusing in between, you could ask what is the means time before this reaction take place, what is the average time if I start of somewhere. Now, what would that b?

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$$\int_0^{\infty} q(t) dt = 1$$

$$q(t) = -\frac{dS(t)}{dt}$$

$$-\frac{(2b-x)^2}{4Dt}$$

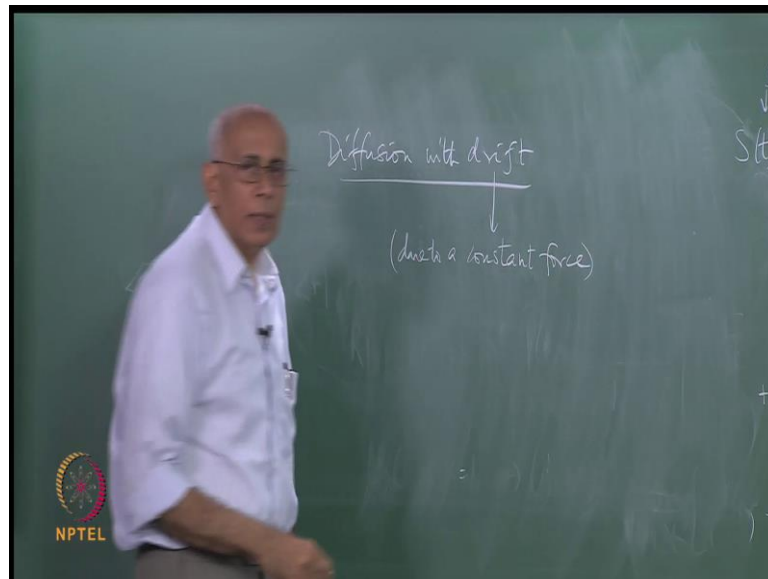
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Well, you can compute the time, you can compute the distribution of this time by saying that if the particle hits the boundary between  $t$  and  $t + dt$ . Let us call the probability density  $q$  of  $t$  that it hits  $e$  the plus or minus  $b$  for the first time without having hit the other boundary between  $t$  and  $t + dt$ . Then this quantity integral from 0 to infinity  $dt$  this is equal to 1, because it suppose to hit it for sure, and you could ask what is the mean time it takes, and that the first movement of this distribution, and what would this quantity  $q$  of  $t$   $b$ ?

This is just  $-dS(t)/dt$ , it is the rate at which the survival probability decreases with a minus sign, because  $S$  of  $t$  is in a decreasing function minus  $ds$  over  $dt$  is positive, and that is just the rate at which that is just the distribution of the first hitting time here. So, it is of interest to find this quantity is in various physical applications, we try to do that at least for unbiased diffusion, what we have do is to start with this solution and then compute this number which is in interesting exercise. So, in this manner all sorts of makes boundary conditions and so on can all be handled.

Now, the same diffusion problem we can extended just a little bit to take care of some very interesting physical problem, one of them would be what happens if this diffusion occurs under uniform external force for instance. Suppose, this is gravity that is acting downwards and the diffusion is in the vertical direction, then the question is what does the diffusion equation look like in that case for the probability density function, and what is its solution look like, and what does it do asymptotically.

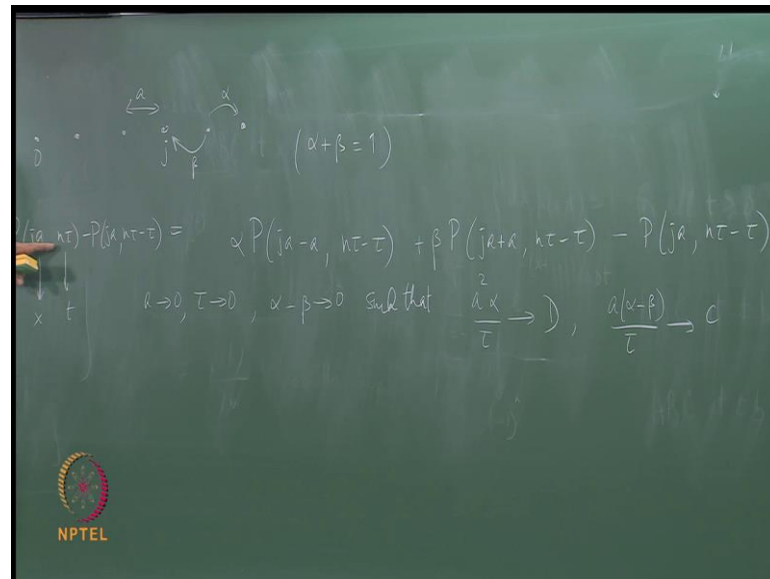
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So, we could ask that question and to get to that question, this is the problem of diffusion with drift, so diff let us call it that diffusion with drift. And the drift I have in mind is cause by a constant force uniform due to a constant force. There are more complicated situation where the force itself will depend on the position of the particle, but let us look at the simplest case, but you have a constant force acting. Now, how would you meaning that, and let us do this from first principle let us write to derive this equation from first principle.

As usual I already pointed out that if you took a random walker on a linear lattice, and when to the continue a limit in which the step size goes to 0, and the time step goes to 0 suitably then you can derive the diffusion equation. Now, let us do that in the presence of a bias, this would play the role of a constant free force in some direction. If I say that the probability of a jump to the right is greater than that of a jump to the left, and that is true at every site in exactly the same way, then that clears that there is a drift to the right hand side a constant of a constant bias fixed bias.

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So, let us look at the problem of a random walker walks on a linear lattice. These steps are label by this index  $j$  by this integer  $j$ , and let us say that the steps size is  $a$ , and the time step is  $\tau$  let me put the time step in, and then take the limit in which the time step goes to 0. So, now I ask what is the probability  $P$  that is act the point  $j$  or other  $j + a$  in the  $x$  direction. So, I start with some 0 here at time  $n$  time steps  $n$  or if you like at time  $n\tau$ . So, this, this space point and this is the time here, what this equal to?

Well in the previous step he should have arrived at one of the 2 neighbors either the neighbor to the right or neighbor to the left. And then we need to know, what is the probability of a jump to the right and what is the probability of a jump the left? So, if the probability of a jump to the right is  $\alpha$  and that to the left is some number  $\beta$ , such that  $\alpha + \beta$  is equal to 1, then clearly he should have arrived at  $j - a$  at this point in the previous time step. So, at time  $n\tau - \tau$ , and then with the probability  $\alpha$  he jumps to the right to get to this point plus  $a$   $\beta$  times  $P$  of  $j + a$  at  $n\tau - \tau$ , that is the difference equation.

And you can put in any initial condition we could start at the origin at  $t$  equals to 0, and we have to solve this set of double recursion relation, because these are recursion relations both in  $n$  as well as in  $j$ . And the solution will give us the answer to the random

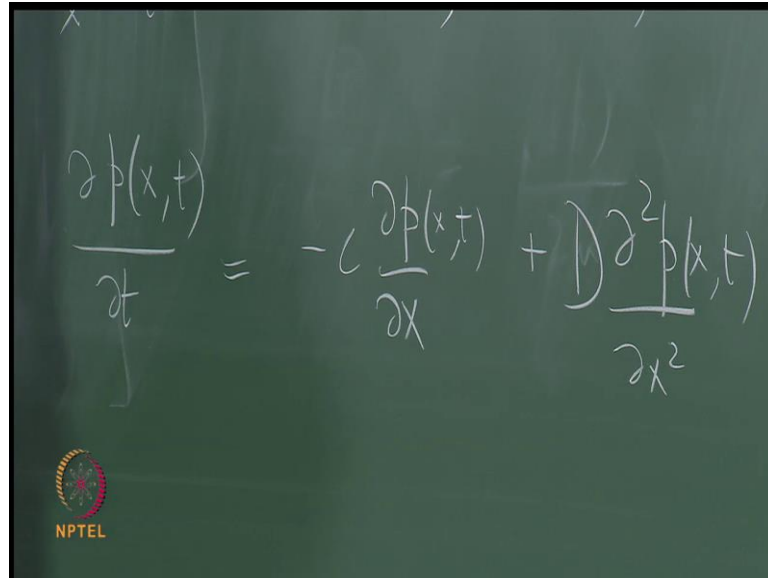
of problems, but we are interested in finding what they continue limit of this whole thing is. So, the obvious things to do is to subtract from this, because I want an equation and time  $P$  of  $j$  a  $n$  tau minus  $P$  of  $j$  a  $n$  tau minus tau subtract this from both sides. I am going to obviously divide this by tau and then claim that as tau goes to 0, this goes to  $\frac{\Delta P}{\Delta t}$ .

So, I am going to leave this as an exercise to find out what this limit is just a little piece of algebra, but the limits you need are the following. You going to need  $\alpha$  goes to 0, tau goes to 0, the time step goes to 0, the space steps the spatial steps goes to 0, and the bias goes to 0,  $\alpha$  minus  $\beta$  goes to 0 such that we can almost see what is going to happen. So, here is an  $\alpha$  this  $\beta$  here you write this as  $\alpha$  minus  $\alpha$  minus  $\beta$ , and then you combine it with this  $\alpha$  here. And this coefficient minus 1 you write it as  $2\alpha$  minus  $\alpha$  minus  $\beta$ , and when you play with that and separate this terms etcetera.

Then in this limit  $\alpha^2$  over tau goes to  $D$  the diffusion constant, we call in the absence of bias this was a half and we said  $\alpha^2$  over  $2\tau$  went to  $D$  the diffusion constant. And  $\alpha$  times  $\alpha$  minus  $\beta$  over tau goes to  $C$  some finite number  $C$ , in this limit this different equation will go over into a partial differential equation for the probability density  $p$  of  $x$  comma  $t$ . And of course, you also need to say that  $j$  a goes to  $x$ , and  $n$  tau goes to  $t$ ,  $j$  goes to infinity,  $n$  goes to infinity such that this goes to  $x$  any point  $x$ , and this goes to  $t$  here.



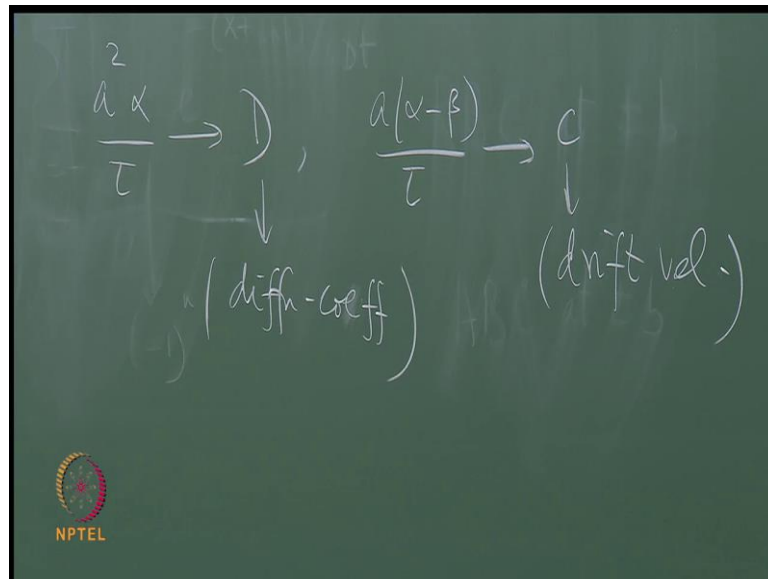
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$$\frac{\partial p(x,t)}{\partial t} = -c \frac{\partial p(x,t)}{\partial x} + D \frac{\partial^2 p(x,t)}{\partial x^2}$$

And then this probability density goes to  $p$  of  $x$  comma  $t$  in a specific way by satisfying a partial differential equation, and that equation looks like this  $\frac{\partial p}{\partial t}$  equal to minus  $C$   $\frac{\partial p}{\partial x}$ ,  $x$  comma  $t$  plus  $D$  in this fashion. Now, you can interpret this things in a very easy way, this  $D$  is the diffusion constant that is exactly what they was free diffusion in the previous case it is sitting here as a coefficient of the second order term, what are the physical dimension of this  $D$ ? Well,  $a$  is a lattice constant, it is a length and this is a time step.

So, it is  $l^2$  over  $t$  diffusion constant, what are the physical dimensions of this quantity  $C$ ? It is length over time that is a velocity. So, what is happening is that  $D$  is playing the role of diffusion constant of course, but  $c$  is playing the role of a drift velocity in average drift velocity. There is a systematic drift to the right if  $\alpha$  is greater than  $\beta$ , and the systematic drift to the left if  $\alpha$  is less than  $\beta$ , and when  $\alpha$  is equal to  $\beta$  there is no drift it is unbiased diffusion on either side.

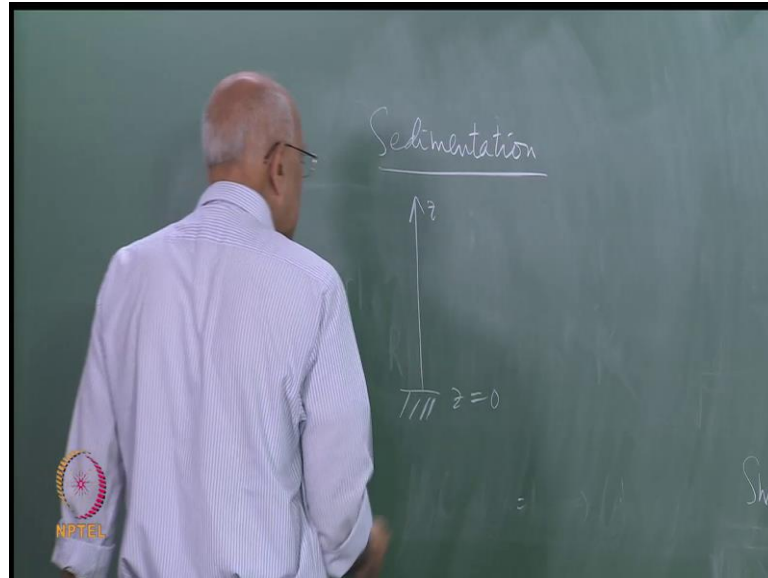
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So, you have a modification to this thing, and this C by the way is the drift velocity and this of course as usual is the diffusion coefficient, and you have a diffusion equation which has this extra term here first order term here, this equation is called the Smoluchowski equation. So, diffusion in the presence of constant drift in under a constant field of force is described not by the original diffusion equation, but by an equation in which there is also a first order term which gives you the drift contribution. And in the absence of a bias these like having no force, no external force at all you have the pure diffusion equation.

So, you no longer expect the solution to be what it was earlier is going to be little more intricate. It could solve this equation, but we will see what it is in some simple instance physical instance. Now, one application that comes to mind immediately is what happens when you have diffusion in the vertical direction under gravity. So, you have a fluid like air for instance, and you have a diffusion particle in air which would tend to come downwards because of gravity, and we could ask what does it do asymptotically. So, we need not solve this full equation, but we need to know what the boundary condition is?

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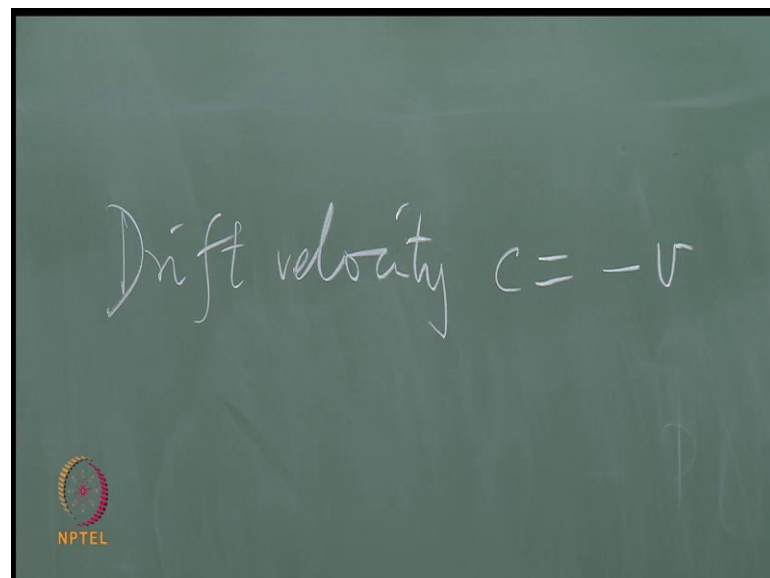
We let us ask this problem, it is the problem of sedimentations is a diffusion under gravity. And let say you have the ground here, it is called  $z$  is equal to 0,  $z$  axis is vertically upwards, and I would like to know what does a particle diffusing in a medium under gravity to, we not interested in the  $x$  and  $y$  coordinates only in the  $z$  coordinate of this particles.

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$$\frac{\partial p(z,t)}{\partial t} = -c \frac{\partial p}{\partial z} + D \frac{\partial^2 p}{\partial z^2}$$
$$\frac{\partial p}{\partial t} + \frac{\partial j}{\partial z} = 0, j(z,t) = c p(z,t) - D \frac{\partial p(z,t)}{\partial z}$$
$$\frac{\partial p(x,t)}{\partial t} = D \frac{\partial^2 p(x,t)}{\partial x^2}$$

So, it would satisfy an equation of this kind, so let us what that equation is. So, it would satisfy  $\frac{\partial p}{\partial z} + \frac{\partial j}{\partial t} = 0$  or  $\frac{\partial p}{\partial z} + D \frac{\partial^2 p}{\partial z^2} = 0$  in this fashion by the way you can write this as a continuity equation once again, because you can still write this as  $\frac{\partial p}{\partial t} + \frac{\partial j}{\partial z} = 0$ , where  $j$  of  $z$  comma  $t$  is equal to  $C$  times  $p$  as  $z$  comma  $t$  minus  $D$  times  $\frac{\partial p}{\partial z}$  that is the current. Now, we are interested in the problem of sedimentation which means that you have the field of force acting downwards in the direction of decreasing, decreasing  $z$ . So, the velocity the drift velocity is in the opposite direction here.

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So, to keep track of that, let say that the drift velocity in this problem just shows the notation is clear. Let us could drift velocity put a minus some  $v$ , and what would this  $v$  actually be for a particle in a fluid medium ((Refer Time: 34:02)) medium. It would be the terminal velocity, because the system is actually an equilibrium thermal equilibrium. So, the drift velocity is the terminal velocity for which we know, what the answer is from hydrodynamics for instance, but let see what by this gets as here.

We need to solve this, but the question is what boundary condition I am going to put here. In this column of fluid I am not going to allow the particle should go through the floor, and not I am going to allow the particles should get destroy, they just going to

bounce back from the floors. So, I need a reflecting boundary condition, and what is the reflecting boundary condition in this case? It is not  $\Delta p / \Delta z = 0$  at  $z = 0$ , it is  $j = 0$ , the current equal to 0 at that point.

(Refer Slide Time: 34:57)

The chalkboard contains the following equations:

$$\frac{\partial p(z,t)}{\partial t} = -c \frac{\partial p}{\partial z} + D \frac{\partial^2 p}{\partial z^2}$$

$$\frac{\partial p}{\partial t} + \frac{\partial j}{\partial z} = 0, \quad j(z,t) = c p(z,t) + D \frac{\partial p(z,t)}{\partial z}$$

$$\text{B.c.} \quad v p(z,t) + D \frac{\partial p(z,t)}{\partial z} \Big|_{z=0} = 0$$

An NPTEL logo is visible in the bottom left corner of the chalkboard image.

So, the boundary condition is  $c$  which is minus  $v$ . So, we want  $v p$  of  $z, t$  plus  $D \Delta p$  over  $\Delta z$  at  $z, t$  at  $z = 0$  equal to 0 that is the boundary condition. So, it is a mixed boundary condition not just on the probability density function  $p$ , but on  $p$  plus a combination of  $p$  and a derivative of  $p$  that is equal to 0 at this point, and we need to solve this diffusion equation with that this Smoluchowski equation, that is a little bit of a technical task, but we can make a life little easier for us by saying what happens after very long time in equilibrium. Suppose you have this huge fluid column which is in thermal equilibrium at some fixed temperature  $t$ . So, let us takes this to be the simplest case you have a fluid medium, it is called a viscosity you have a diffusing particle in it, and this system is in thermal equilibrium completely.

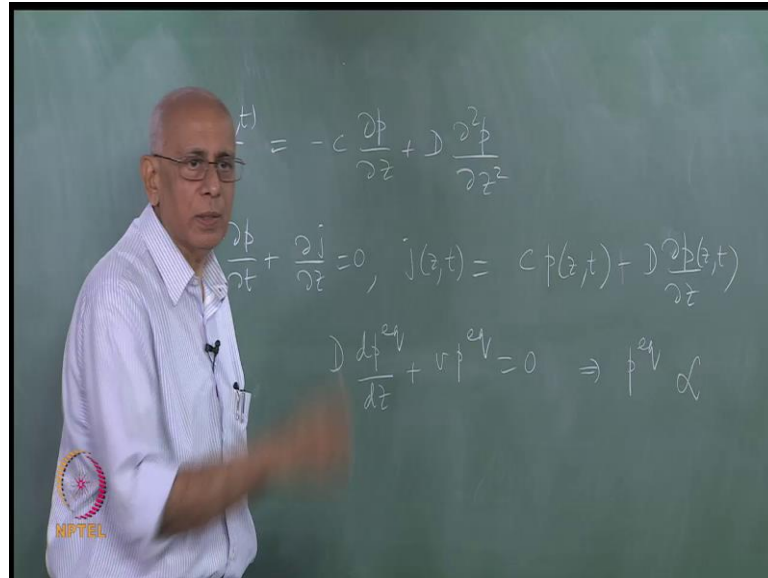
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$$p(z,t) \xrightarrow{\text{equil}} p^{\text{eq}}(z)$$
$$\frac{dj^{\text{eq}}}{dz} = 0 \Rightarrow j^{\text{eq}} \text{ is indep. of } z$$
$$\text{B.C. } j^{\text{eq}}(z=0) = 0 \Rightarrow j^{\text{eq}}(z) = 0$$

Then what is the distribution, and this is something we know already, because remember let me know that in equilibrium  $p$  of  $z$ ,  $t$  tends in thermal equilibrium to  $p$  equilibrium has a function of  $z$  alone. The distribution does not change with time, because it is in thermal equilibrium, we want the final asymptotic distribution, that means this term is 0, and then the equation simply says  $d$  over  $d z$   $j$  equilibrium is equal to 0, but what is that imply?

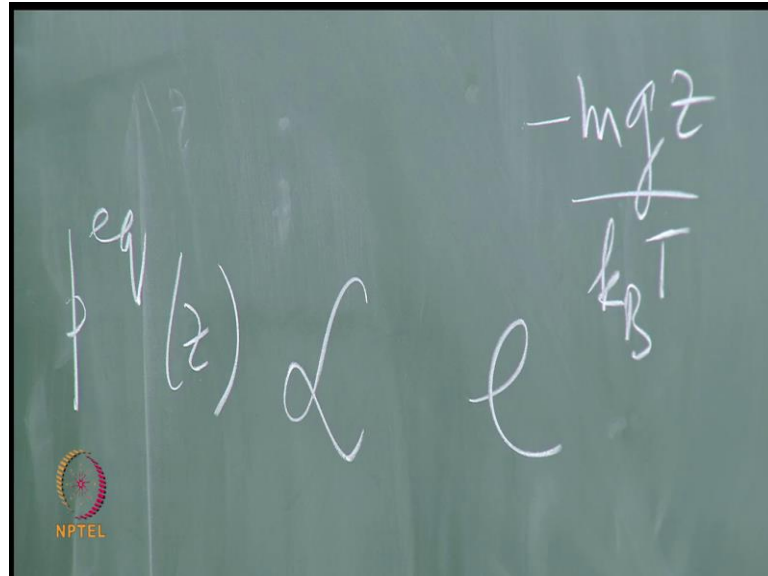
It is says that the current is independent of  $z$  completely. So, it says  $d j$  equilibrium, it is a independent of  $z$ , but at the boundary the current is 0 that equation alone  $d j$  over  $d z$  equal to 0 just says  $j$  equilibrium is a constant independent of  $z$ , but at the boundary it is 0, therefore it 0 everywhere. So, the boundary condition for all  $z$  that is triviality itself, because it immediately says that you can solve this problem.

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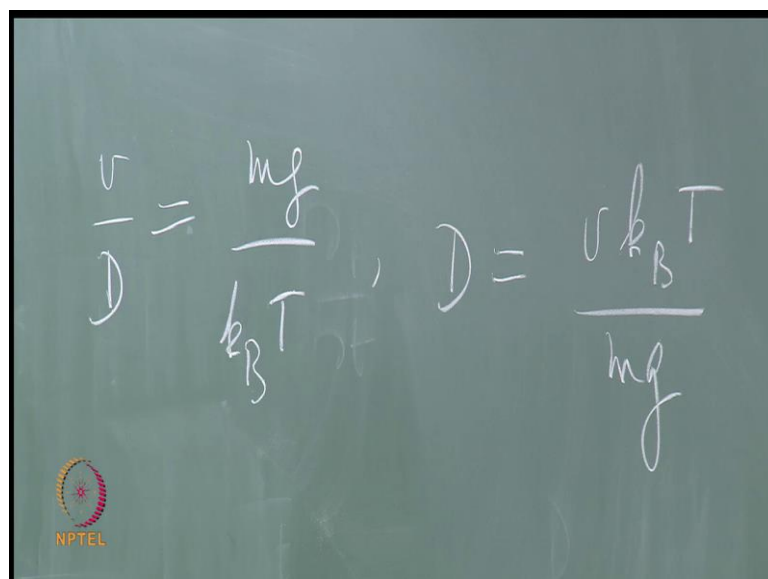
And all you have to do now is to notice that  $D \frac{d^2 p}{dz^2} + v p$  equilibrium over  $d z$  plus  $v p$  equilibrium equal to 0, it is a first order differential equation and we known have to work very hard to solve this equation, what is the solution here is proportional to apart from some normalization will normalize it you into or something like that is proportional to  $e^{-\sqrt{v/D} z}$ . It is an exponentially decaying distribution and just says that the most probable value is the ground level, and then it decreases exponentially in this fashion which is exactly what you would expect. In fact, since this system is in thermal equilibrium you would say, well the probability of being at some height  $z$  is proportional to  $e^{-\beta U(z)}$  where  $U(z)$  is the potential energy at that height, and the energy is just potential energy here and solving interested.

(Refer Slide Time: 39:05)


$$p^{eq}(z) \propto e^{-\frac{mgz}{k_B T}}$$

So, we already know this is called the barometric distribution. We already know that  $p$  equilibrium of  $z$  is proportional to  $e$  to the minus if  $m$  is the mass of the particle, then it is  $m g z$  over  $k$  Boltzmann  $T$  that is the barometric distributions for the atmosphere at constant  $T$ . And now let us compare that with this.

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$$\frac{v}{D} = \frac{mg}{k_B T}, \quad D = \frac{v k_B T}{mg}$$



So, it says therefore it says  $v$  over  $D$  must be equal to  $m g$  over  $k$  Boltzmann  $T$  or  $D$  equal to  $v$  times  $k$  Boltzmann  $T$  over  $m g$  that is the usual relation, and what does that say now further, what is  $v$ , how are we going to find  $v$ ?

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$$D = \frac{v k_B T}{mg}$$

$$= \frac{k_B T}{6\pi R \eta}$$

↓  
(viscosity)

Stokes' relation:  
 $6\pi R \eta v = mg$   
(Einstein - Nernst - Sutherland relation)

Well, if this is a viscous particle and let us assume it is as a spherical particle of radius  $r$ , and it is a terminal velocity, you know that there is an relation stokes relation which says  $6 \pi$  times a radius times the viscosity of the fluid times the terminal velocity must be equal to the force  $m g$  on it. So, you put that  $n$  and then this becomes equal to  $k T$  over  $6 \pi R \eta$  this is the viscosity of the fluid, and that is the radius of the particle. The  $6 \pi$  comes, because you assumes spherical particle and you assumes in specific boundary conditions, you assumes stick boundary conditions.

In another words you assume that here is this object of for radius  $R$  moving in this viscous fluid and the velocity of the fluid at the surface is  $0$  that is called a stick boundary condition. If we change that to a slip boundary conditions saying that it is not  $0$ , it is perfectly slips by in this becomes a  $4 \pi$ . If it is not a spherical particle, but in ellipsoidal particle then this factors change a little bit depends on the aspect ratio and so on. But whatever it is, the viscosity of the fluid appears here in the denominator in the temperature appears appearing, and the diffusion constant is related directly to the search

measure up directly from this. This relation was derived by Einstein.

So, it is Einstein in his brown in motion paper, but coincidentally it was derived a couple of months earlier by an Australian physicist called a Sutherland not as well known, and knows names is also associated with it is, so let us call it give everybody the due and an alphabetical order it is caught other name, it is caught it is an example of what is called a fluctuation, dissipation theorem and so on, but this is a very, very simple physical argument that we been through. And we actually found explicitly what the solution is by applying the boundary condition solution to this sedimentation problem at least on equilibrium.

The time dependent problem is a little harder, but it can also be done, this can also be explicitly solve it involves error functions and so on, because you got a finite boundary, but nevertheless this is the explicit asymptotic solution this here. It shows that when you have a reflecting boundary you can have a non trivial equilibrium distribution asymptotically as  $t$  tends to infinity which is normal strength unit. You know that if have done this, you have to go back now and look at what happens when you have.

Now, let us look at what happens when you have observing boundaries at the 2 ends, 2 finite ends and let us look at what the survival probability does? This is part of very, very significant part of the theory of diffusion random box namely it is related to the so called first passage time problem, problem of finding out when will in event occur for the first time given that it definitely does happen. And this problem of hitting the hitting probability of hitting one of the boundaries getting captured, getting trapped and so on is of direct physical significance in a large number of applications.

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$$S(t) = \int_{-b}^b dx p(x,t)$$

$$p(x,t) = \frac{1}{\sqrt{4Dt}} \sum_{k=-\infty}^{\infty} (-1)^k e^{-\frac{(x+2kb)^2}{4Dt}}$$

$$p(x,0) = \delta(x)$$

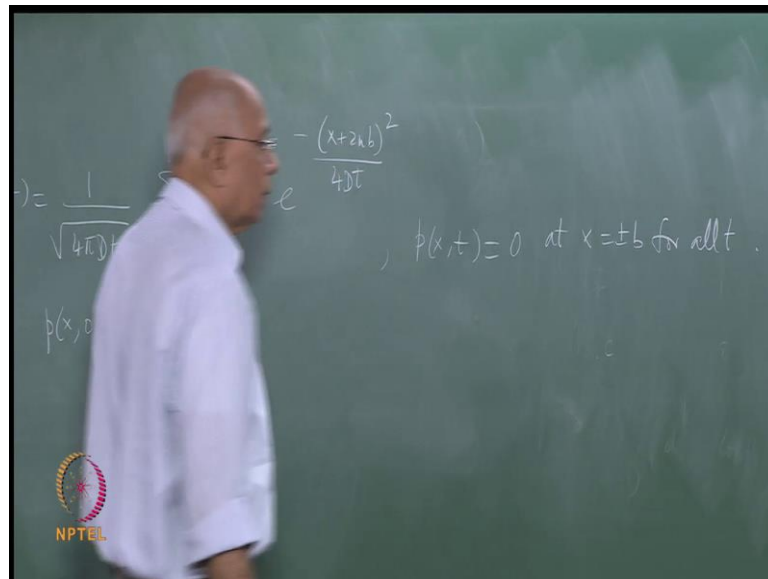
A diagram shows a horizontal line with points  $-b$ ,  $0$ , and  $b$  marked.

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So, we are going to look at this problem, and asks what  $S$  of  $t$  equal to explicitly for boundaries at minus  $b$  and  $b$  d  $x$  p of  $x$  comma  $t$  by this has 2 boundaries which are absorbers at  $b$  and minus  $b$  and the particle starts at  $0$  at  $t$  equal to  $0$ , we going to compute this number explicitly, and see what it does? Now, as I have said already  $p$  of  $x$  comma  $t$  is this quantity minus  $1$  to the power  $n$  e to the minus what is call it  $4Dt$ .

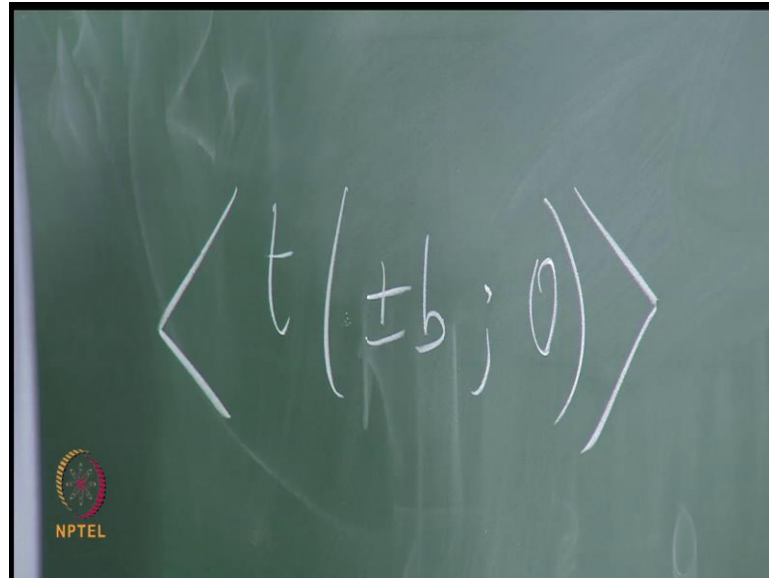
By the way although it does not appeared immediately from here, as you go to  $t$  going to  $0$ , this would generally vanished for all finite values of  $x$ , but it singular, because our boundary condition remember was  $p$  of  $x$  comma  $0$  was equal to delta of  $x$ . So, this is the spike at the origin of unit strength. And this formula tends to that tends to the singular quantity the delta function as  $t$  goes to  $0$ . There is a  $t$  sitting in the denominator here, there is a  $t$  sitting here and there is a big sum here overall length, but it goes to this point here.

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I urge you to check that this boundary condition is immediately satisfied  $p$  of  $x$ ,  $t$  equal to 0 at  $x$  equal to plus or minus  $b$  for all  $t$ . So, those are the boundary conditions they absorbing boundary conditions, and this is the problem we have to do. We have to do this integral due to compute this quantity, and find out what the rate of change of this is the minus sign that will give us the mean hitting times and so on, what do you think will happened? I want to know the following; I am asking the question given that the particle let say it is start at 0. So, let us even ask what is the survival probability for a particle which definitely starts at the origin, what it is going to do as time goes along. I would like to know, what is the mean time that you think the particle will take?

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$$\langle t(\pm b; 0) \rangle$$

So,  $t$  for a particle with starts at 0, and hits the point either plus or minus  $b$ . For the first time having started at the origin at  $t$  equal to 0, and I want the average value of this quantity. And what is the average over, all possible random box all possible excursion of this particle. I would like to calculate this quantity, what do you think it is going to be, and let us look at the problem with no bias. So, it is very immediately simplified normal satisfies the  $b$  satisfies the diffusion equation without any bias stop, what do you think it is going to be? Ask the combos question, if you had free diffusion on a infinite line then you could ask All right, how does the variants of the particle, how does its distance change as a function of time.

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0 at  $x = \pm b$  for all  $t$ .

$$\langle x^2(t) \rangle = 2Dt$$
$$p(x,t) = \frac{e^{-\frac{x^2}{4Dt}}}{\sqrt{4\pi Dt}}$$
$$\sigma^2(t) = 2Dt$$

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So, you know the following, you already know that if it starts at the origin at  $t$  equal to 0, and it is got an infinite line to diffuse, you can ask the questions what is  $x$  squared of  $t$  equal to? All you have to do is to take the second moment of this Gaussian distribution, you know the answer is a Gaussian distribution, and you know that  $x$  of  $t$  average is 0 for all  $t$ , so it is triviality itself. Remember that in the case of free diffusion  $p$  of  $x$  comma  $t$  was  $e$  to the minus  $x$  square over  $4 D t$  divided by square root of  $4 \pi D t$  that is a normalized Gaussian, and what is the variance of the Gaussian, sigma square of  $t$  equal to  $2 D t$  ((Refer Time: 48:33)) you are in one dimensions, so it is  $2 D t$ .

So, this is equal to  $2 D t$ . So, it is clear that  $x$  square of  $t$  is increasing linearly with  $t$  proportional directly to  $t$ . So, what you done there is to say at a fixed time I asked on the average what is the mean how far does it gone, what is the square of the distance that it is gone the mean value. So, there the time is fixed, and the distance is a variable random variable. Here, in this problem the time is the random variable, it starts here the distance is fixed.

It is called move a distance plus or minus  $b$  in go to a point plus or minus  $b$  on either sides, so it is got to move a distance  $p$  from it is initial point. And now you are asking, what is the mean time it takes to move that distance, what would you expect this answer

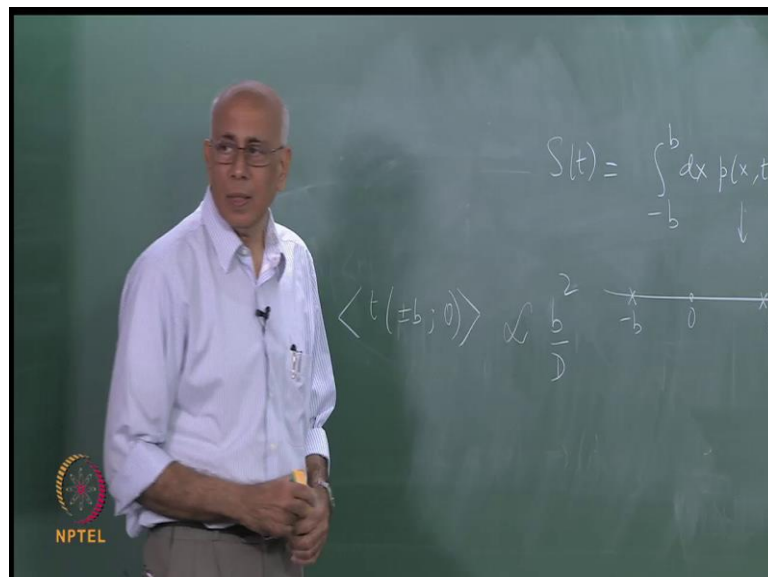
to be? There is only 1 parameter in this problem the natural parameters a diffusion constant, and what are the dimensions of that diffusion constant?

Student: ((Refer Time: 49:51))

Length squared over time that is the only parameter with dimensional parameter that you have in the problem. So, what would you expect this to be?

Student: ((Refer Time: 50:00))

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I would expect this to be proportional to be proportional to b square divided by D exactly. So, even before I begin the problem I know this is what I am going to get at the end, what constant of proportionality there is remains to be seen, but this is the only possibility nothing else. And we will be see how this is borne out by very simple trick will use a little trick to solve this problem, and the problem is very clear it says you start here, and now you ask what is the meaning time it takes to go either here or here for the first time.

So, it should hit this point or this point without hitting the other point, because if it hit the

other point earlier it will be absorbed completely. So, we need to solve this problem, and we will do that the next time. We could then ask what happens if I move this fellow away to minus infinity then how long will you take to hit this point, and the answer is infinite the mean time will become infinite, but with barriers on both sides it becomes finite we will see how that comes.