Physics of Biological Systems
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Lecture – 14
Capture probability of reflecting sphere

So what is the question so, let say that the question is that I release this at b and I want to find out and I my reflecting sphere is of radius a.

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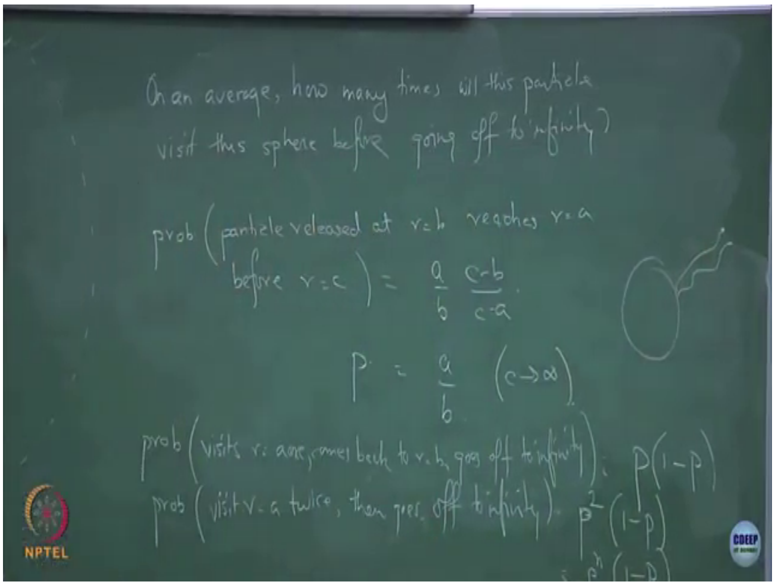

So, I want to ask that on an average how many times will this particle visit this sphere; will this particle visit this sphere before going off to infinity ok. So, it comes once it hits maybe it comes back again it hits and then maybe it just goes off away so, that is 2.

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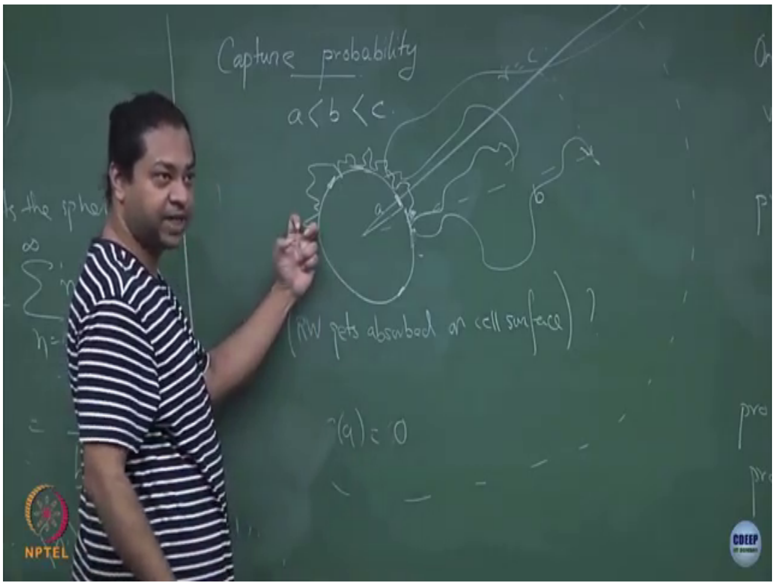

That is so, it does this 2 times if you do this again and again and again and you take an average you will find some average number of times of the particle visits the surface of the cell before it wanders off. So, let see if we can calculate that.

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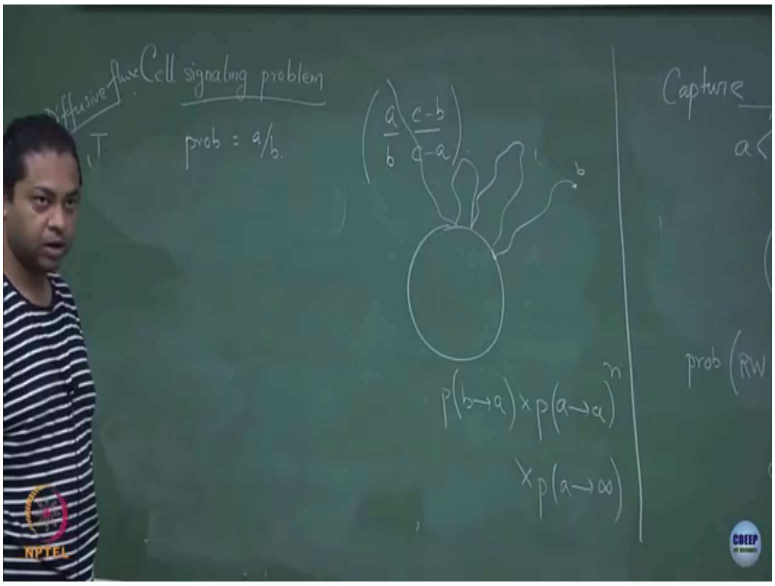

So, what we will do is that we will use this absorbing result, but little carefully. So, this particle that is doing the random walk it does not really know whether there is an absorber sitting here or not right. It only realizes that the surface is absorbing once it comes and hits this surface alright. If it was reflecting the point until it reaches it does not know, but once it hits it knows that it is not an absorbed then it goes back. So, this probability this a by b, c minus b by c minus a I can recast this that. So, this is I can interpret this in this case as the probability that the particle released at r equal to b reaches r equal to a before r equal to c and that is then this c minus b by c minus a is this clear.

So, until it hits this it does not know it is an absorbing; it is an absorbing boundary condition. So, I can reinterpret this problem that this particle which was released at r equal to b it reaches this distance r equal to a before it reaches this outer sphere that r equal to c that is that probability is going to be the same as what I calculated right a by b into c minus b by c minus a and therefore, if it that c if I cook it to infinity that probability is a a over b.

So, then this is the probability that it reaches the surface before it wanders off the infinity. So, let me call this P let me call this P. So, then if I want to ask that what is the probability that the particle visits r equal to a visits r equal to a comes back to r equal to b comes back to r equal to b and then goes off to infinity and then goes off to infinity to this part the visits r equal to a that is this probability right before and then the part that it goes off to infinity that is whatever is remaining right.

So, this is visits r equal let me be more explicit visits r equal to a once you can do this recursively. So, you can ask that what is the probability that this particle visits r equal to a twice and then goes off to infinity and then goes off to infinity right. So, you release it come goes here over here once that probability is P.

Student: Ok.

Because, it is reflecting it does not get absorbed it again wanders back and you ask what is the probability, it comes back again that is another P so, P squared and then you say it goes off. So, that is P square into 1 minus P and similarly if you ask what is the probability that visits thrice and so on. So, the probability that it visits n times before it wanders off it is going to be P to the power of n into this final 1 minus P yes.

Student: (Refer Time: 05:09) whether it once it is going that is (Refer Time: 05:15).

Ideally you should so, this is an approximation ideally what one should calculate is here is my sphere. So, I can break it up this is my r equal to b. So, what is the probability that starting from b it goes to a. So, it reaches here and then the probability that starting at a it comes back to a.

So, it reaches it hits it once like this then what is the probability of something like this and something like this and then finally; so, this let say n times and then finally, the probability that it goes from a all the way up to infinity right. So, this is not this so, this is an approximation in that sense it is a sort of classic approximation by Burke in his 1977 papered.

Student: Why 1 minus P?

Student: 1 minus P.

So, once you have released the particle here it has 2 things to do it, it can come over here or it can go off right. So, if the probability that it comes here is P, then the probability that it goes off on the other side is 1 minus P so, in that sense. So, this is an approximation. So, get back to this question it is a little bit uncontrolled um. In fact, I will derive it using this, but then in the assignment you will see that there is there is exact problem.

But, a simulation and you can compare what you get with the results that I will derive here and you will see there is some discrepancy between what we will derive here and what we do at least I think there is some there should be some discrepancy ok. So, once I have done this I can say, that therefore what is the average number of times that this particle visits the sphere.

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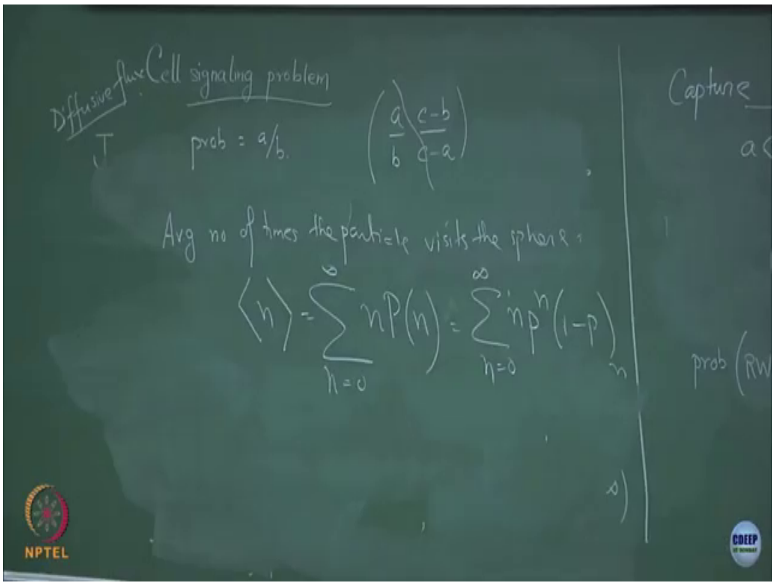

So, what is the average number of times the particle visits the sphere. So, this average n that is going to be n times the probability that it visits n times summed over all n right n equal to 0 to infinity. So, what we have written down over here in using this approximation is this P of n. So, therefore, this is nothing, but n P to the power of n 1 minus P n equal to 0 to infinity ok.

Student: (Refer Time: 08:09).

Yes.

Student: Here we using that (Refer Time: 08:16) r is equal to a (Refer Time: 08:21).

Yes. So, that is the approximation I am saying that that is what Suprith was also asking that I am saying that it does it I release it here it comes over here and then I am assuming that it again somehow wanders back and I am starting the calculation from this point again. So, that is the approximation ok.

So, if I do this what is this average? Someone quickly, what is this? This is geometric series come on, what is this Nithin? What is this sum? What do you know? (Refer Time: 09:06) what is the sum, geometric series come on man this is P by 1 minus P n goes up to infinity.

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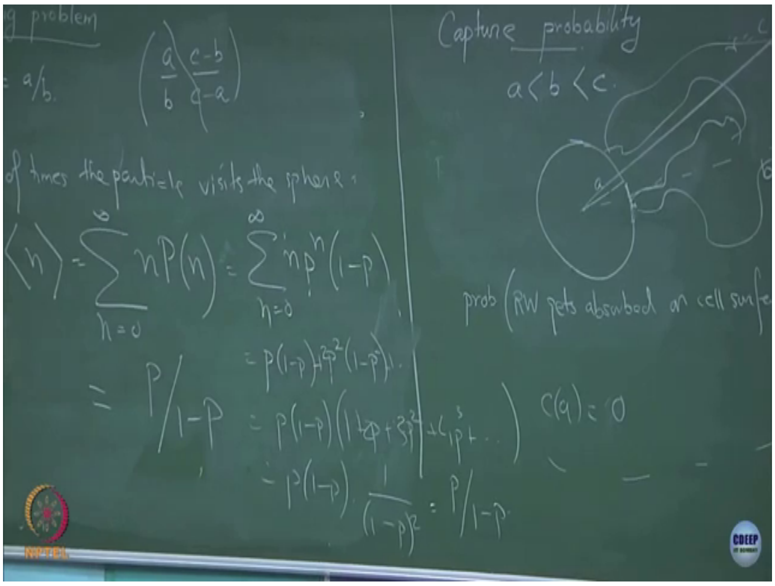

Student: (Refer Time: 09:20) n is a (Refer Time: 09:24).

I do not understand n is a.

Student: n is not.

N is being summed over.

Student: (Refer Time: 09:32).

So, what is this so.

So, this is let me say n equal to 0 is not there. So, P into 1 minus P plus P square into 1 minus P plus so on. So, if I take P into 1 minus P common this is 1 plus P plus plus P square and so on right 1 plus wait this is 2 1 plus 2 P plus 3 P squared plus 4 right.

Ha. So, in this series sum is what this is this is P into 1 minus P this series is 1 minus P whole square. So, it is P over 1 minus P so, but this P n what P I know right P is a over b which means that this is nothing, but this is nothing, but a by b minus a right.

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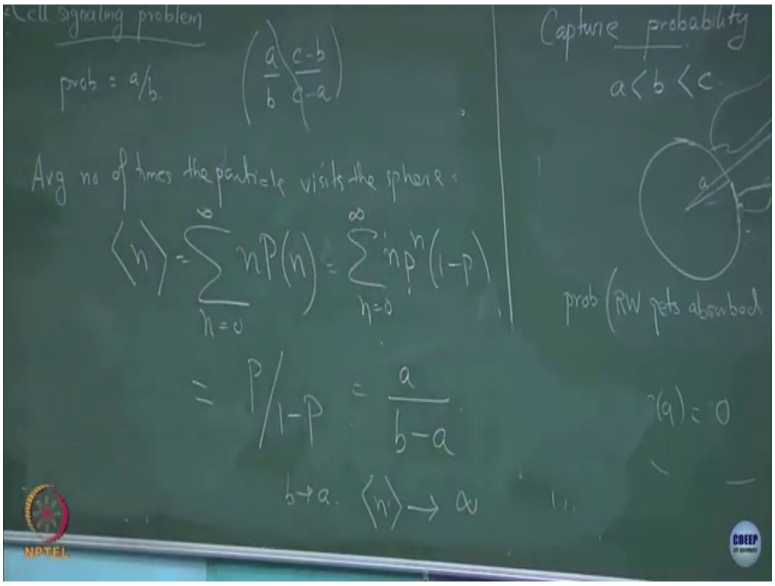

So, the average number of times that the particle visits this sphere, if you release it at b is going to be a over b minus a which means that if you are releasing the particle very close to the surface of the sphere. So, in the limit that of in the limit that b tends to a right the average number of visits the mean number of visits that tends to go to infinity ok.

So, which is what I mean when I said that you did not need a very large concentration of absorbers if you release, if a particle reaches somewhere over here. Then it is very likely it will wander very many times hitting, this sphere many times until it sees one of these patches and gets absorbed at one of those patches.

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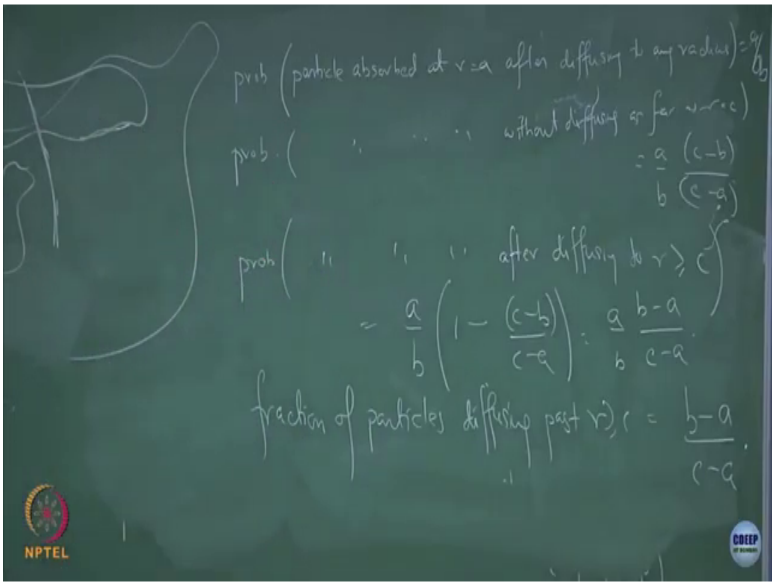

So, if I say that so, let me write the probability that a particle is absorbed at r equal to a absorbed at r equal to a, after diffusing to any arbitrary radius after defusing to any radius is a by b a by b right. On the other hand the probability that is it is absorbed at r equal to a without diffusing as far as r equal to c without diffusing as far as r equal to c is a by b c minus b by c minus a. So, this is the infinite case if I take the sphere to infinity then this gives me the probability that it gets absorbed regardless of how far it has gone.

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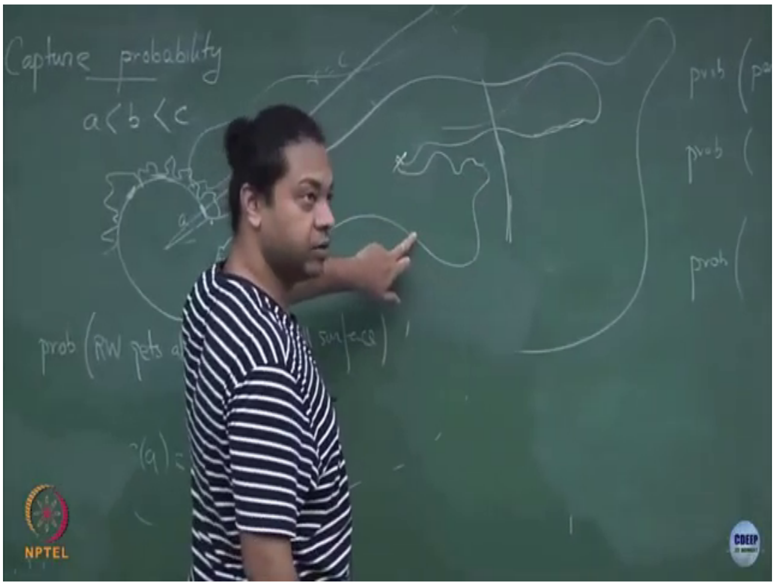

So, it can start with born up to here, but then again comes back. So, all of these combined is a over b, on the other hand if the c was finite if I had a finite thing then this is equivalent to the probability that it gets absorbed at r equal to a. So, I have too many skidlid lines all around that. So, here is my it starts off it can go up to here, but it does not hit this sphere and then it comes back to a that is this probability a by b into c minus b by c minus a right, it gets absorbed on the inner sphere without hitting the outer sphere.

So, it has not gone as far as r equal to c. So, if I wanted to calculate what is the probability that it is absorbed at r equal to a. So, this part is still the same after diffusing after diffusing to r greater than equal to c right. So, all a trajectory like this it starts off it goes beyond this r equal to c and then comes back and gets absorbed ok, that would be the difference between these 2 right. This is the first one is all trajectories, the second one is all trajectories that do not go up to r equal to c and therefore, the difference between these 2 are all trajectories that do go beyond this and then comes back.

So, that is whatever a by b 1 minus c minus b by c minus a and this is a by b b minus a by c minus a ok. So, the fraction of particles that does this that diffuses beyond this point is going to be. So, the fraction of particles diffusing past r equal to c that is going to be this number divided by this total number that gets absorbed. So, that fraction is b minus a by c minus a.

So, this is the probability of going beyond this and getting captured this is the probability of all trajectories. So, therefore, the fraction of particles that go beyond this sum r equal to c that you set and then gets absorbed this b minus a by c minus a ok. So, I just wanted to do this to just put in some numbers. So, let me put in some numbers now.

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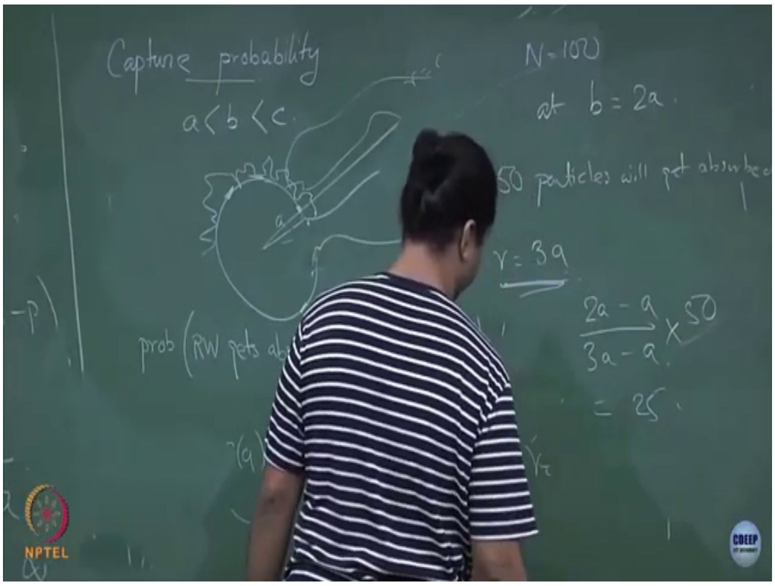

So, let us say you put you release some 100 particles you release some n equal 100 particles at some distance which is 2 a ok. So, this is my starting point I release 100 particles from there. How many particles will get absorbed at a?

Student: (Refer Time: 15:35).

A a by b is the probability right so, that is half. So, 50 particles will get absorbed at a 50 particles will get absorbed all this is the sum of all trajectories ok. So, out of these 100 particles that I release 50 will come and get absorbed 50 will wander off.

Student: Ok.

So, let say I want to just get a sense of how far these particles can go before they come back and get absorbed. So, if I want to say that how many particles have wandered beyond r equal to 3 a ok, before it comes back and gets absorbed that would be this fraction. So, b is 2 a so that number would be 2 a minus a and the c in this case is 3 a minus a of so, that is the probability of the total number that gets absorbed is 50. So, that is 25.

So, out of these 50 particles that get absorbed 25 of them on an these are all average quantities 25 of them would have gone past this 3 a and then come back and got absorbed ok. So, if I ask what is sort of roughly on an average sense the maximum distance that it goes before it comes back and gets absorbed that you can.

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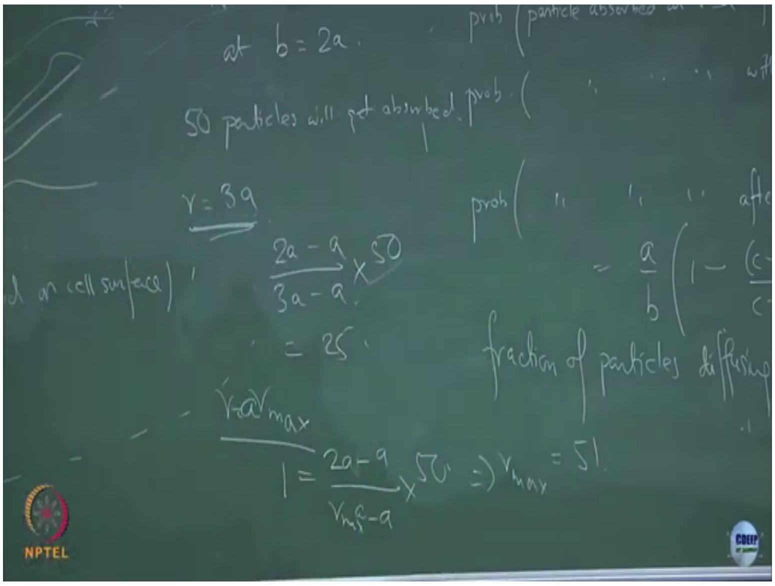

So, if I want to find what is this r equal to let say r max then that I can say that let say that one particle is going to do that. So, that is 2 a minus a by r max minus a into 50. So, you can solve for this r max alright. Let me write it as a function of a so that I can cancel out this a, the r is equal to r max a times r max ok. So, then this is what is this give in this gives r max is equal to 51 r max equal to 51 right, but; that means, is that you have one particle that has gone up to 51 times this distance before it has come back and gotten absorbed over here.

So, because this diffusive because this is diffusion there is no memory associated with it you can have particles which very very far off and then come back and get absorbed on the surface of this sphere I just wanted to do this to give a feel of that alright. Let me try to formalize this little bit so, I talked. So, let me try to write an equation for this captured probability. So, I want to know what is the probability that.

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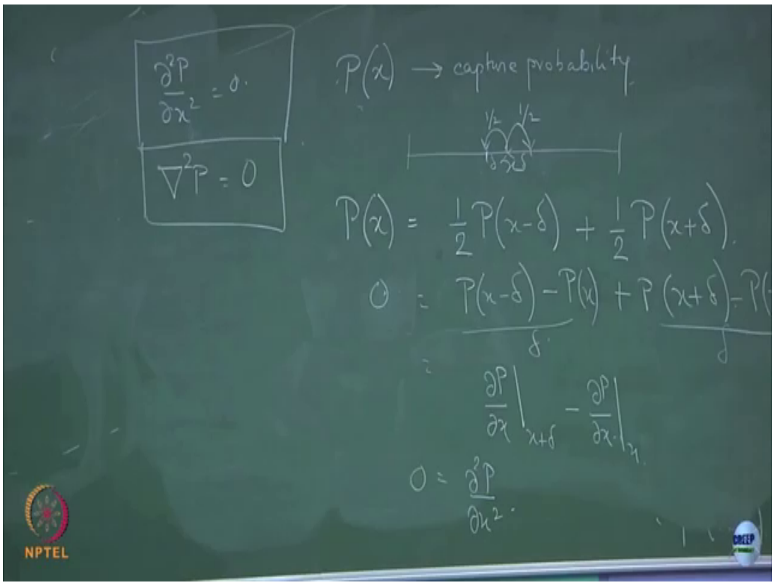

If I release a particle from x r is equal to x let us say what is the probability that particle is going to get captured ok. So, this is the capture probability this is what I computed for this specific geometry, but let me see if I can just write down an equation for this right. So, let me say that this is a random walk. So, let me do it in this simple one d case that I have a random walk which can hop to the left or hop to the right each with probability hop and I want. So, this is my starting position x, I want to calculate what is the probability that a particle released from x will get capture ok.

So, if I release a particle from x it has a probability of half to go to the left right. So, it has the probability of half to go to the left once it has gone to let say my lattice spacings are delta ok. So, each hop is of length delta. So, once it has gone to the left it has reached a position x minus delta and then the probability of getting captured at that position I will just write as P of x minus delta right. So, that is one part that it can do. The other thing it can do is that it can hop to the right that also has a probability half and once it is hop to the right it is at x plus delta and has some capture probability P of x plus delta.

So, now I can take the continuum limit of this. So, 2 P x is P of x minus delta plus P of x plus delta right, let me subtract minus P x here minus P x here which means that basically you have taken this left hand side to 0 right, what is this. So, if I divide throughout by delta over here and delta over here this is del P del x at x plus delta minus del P del x at x right which is del 2 P del x 2 right ok.

So, I start with this recursion relation I take the continuum limit or that gives me is this equation for the capture probability, but the capture probability obeys this del 2 P del x 2 is equal to 0. I did this for a one d random walk you can do this in general and in general it will satisfy that the Laplacian of the capture probability is equal to 0 and you can verify that this is correct. So, let us just solve it for this case that we already did so, painstakingly this sphere.

So, if I want to solve it for this sphere I solve Laplacian of this capture probability equal to 0 I want to know what is. So, I want my surface at r equal to a to be. So, I want to know the probability that it gets captured at r equal to a.

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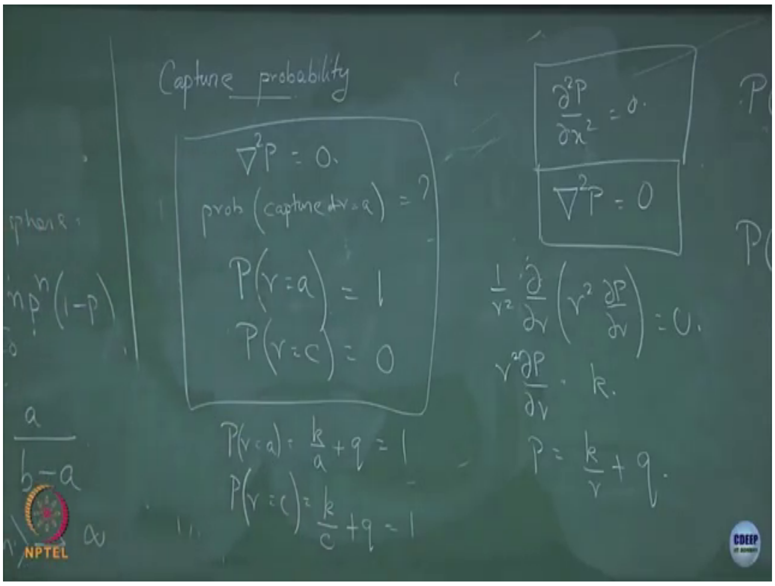

So, probability that it gets captured on the surface of the cell; so, at r equal to a that is what I want to know, which means that what is going to be my boundary condition. So, if I if it starts off at r equal to a then what is the probability it will get captured.

Student: 1.

1 right, we will definitely get captured. On the other hand on this other side I will set r equal to c if I put a finite thing let us say I do not wanted to be captured there. So, these are my boundary conditions. So, I can solve this equation subject to these boundary conditions and see what I get. So, again this if I assume this is spherically symmetric. So, 1 by r square del del r of r square del P del r is equal to 0 which means r square del P del r is equal to some

constant. Let say k which means P is equal to some k by r plus another constant something like this right and then I can put in I can substitute these boundary conditions.

So, if I put r equal to a P at r equal to a is equal to k by a plus q is 1 and P at r equal to c is k by c plus q is equal to 1. So, you can solve for k and q and you can tell me what is P of r, yes this is P x minus P x minus delta right.

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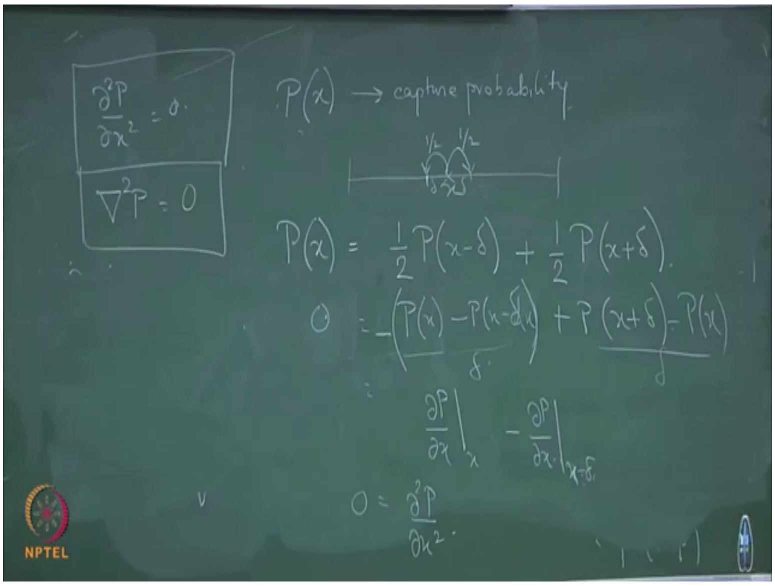

If I just write the if I write this with a minus sign then this is P of x minus P of x minus delta this I am calling as minus del P del x at x.

Student: (Refer Time: 24:50).

No.

Student: (Refer Time: 24:53).

So, you want me to call this at x minus delta that is right. So, then this is at x, but is there an overall minus sign.

Student: (Refer Time: 25:04).

There is not a wrong oh you mean which one I put in the limit fine, but this is this ultimately this is the second derivative at x right.

Student: (Refer Time: 25:18).

Yes it is not a reflect it is not a reflection condition the reflection is del P del r at r equal to c is equal to 0.

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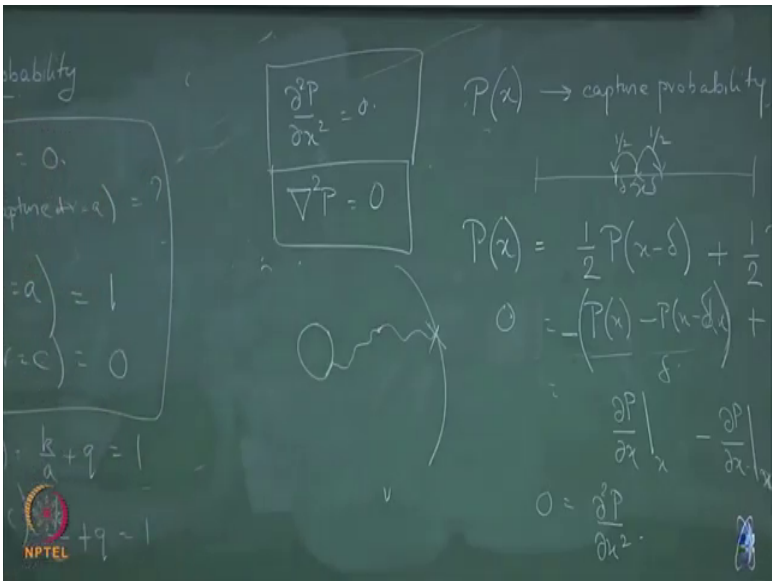

So, what I am saying is that I have my r equal to a, I have my r equal to c right and I am starting off from here when it reaches here the inner sphere I am that is what I am going to count as my absorption, when it reaches this I am going to throw away that trajectory. Because, I am not interested in those trajectories which are getting absorbed on the outer sphere, but it is not a reflecting boundary condition that is different that is del P del r at r equal to c would be equal to 0. So, while I have been doing this what is k and what is a q?

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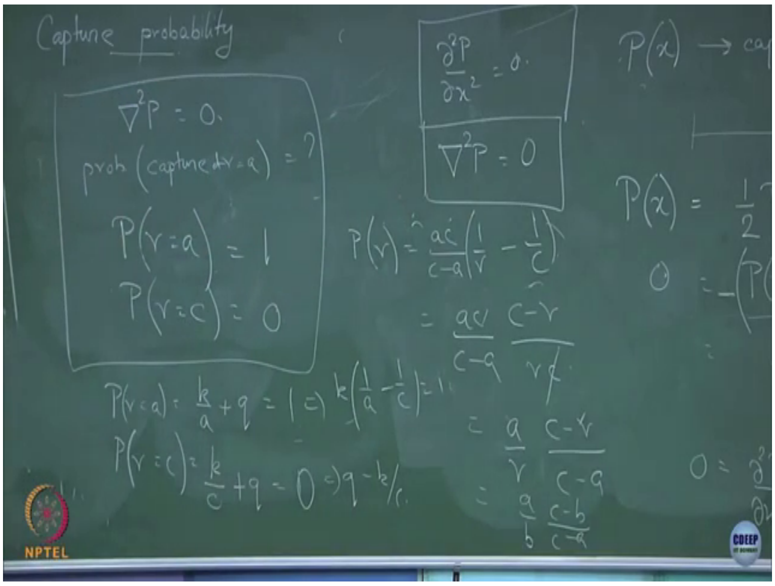

Sorry this is 0 right P at r equal to c. So, q is minus k by c which means this is k 1 by a minus 1 by c is equal to 1 which means k is a c by c minus a which means my P of r is equal to a c by c minus a into 1 over r and q is minus k by c minus 1 c. So, I hope yes correct me if I am doing anything wrong a c by c minus a c minus r by r c. So, this is a by r c minus r by c minus a ok. So, this is the probability that it gets captured at the inner sphere if you have released it starting at r.

So, in the setup P was releasing it at r equal to b. So, if you put r equal to b you get exactly what we had earlier, a by b c minus b by c minus a right. So, you can set up the problem as this solution of this equation this Laplace this equation with P being the capture probability and then solve it using the appropriate boundary conditions. So, for example, just to do the simplest case actually if I do take this 1 D problem.

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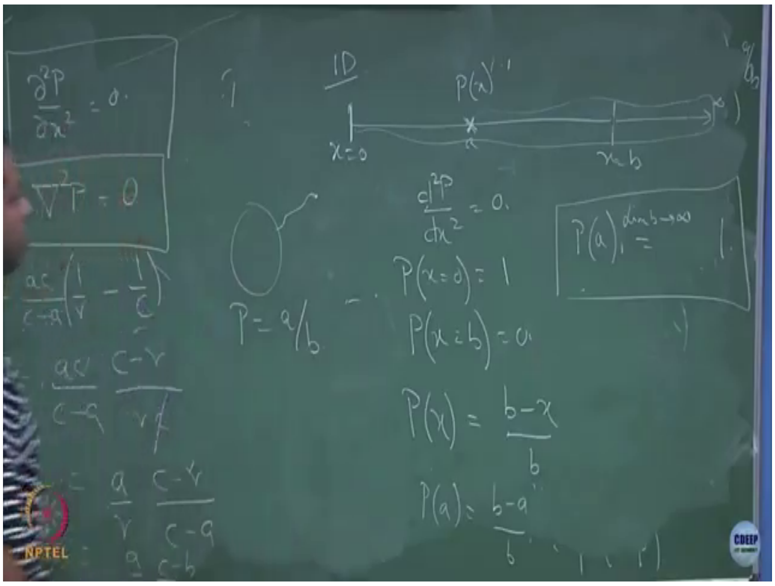

If I take this diffusion on a 1 D line let say I have this line between x equal to 0 and let say x equal to b and I release the particle from some random position and I want to ask what is this p of x ok, if I release it from x. So, I have to solve d 2 p d x 2 is equal to 0 and let say I am interested in the absorption and this boundary then what is the probability it will get absorbed here which means that my I will set this as my boundary condition, x equal to b is equal to 0, what would be the solution of this? What would be P of x? This is just a x plus b right d 2 p d x 2. So, if you put in the boundary conditions what is what does it give ok.

So, let this will give you b minus x by b ok. So, if you release it from some particular position a then the capture probability will be b minus a by b, remember this is the probability that a particle release that x equal to a is going to get absorbed at this boundary x equal to 0 not at the other boundary. One nice thing to notice so what would be this probability if I move this boundary away to infinity. So, what would this P of a b in the limit that b goes to infinity, yes what is this Nithin?

Student: 1.

1 right this is 1 which means that as opposed to the 3 D case right when we took a sphere and I released a particle here and I move this outer sphere away all the way to infinity only a fraction a by b ultimately got absorbed. As opposed to this in the 1 D case if you take remove this boundary all the way up to infinity if you wait long enough eventually everything is going to get absorbed, it might wander off very far, but it has to come back and get absorbed over here.

So, if you calculate the time of absorption that may be large, but if you calculate the probability of absorption the probability of capture in the limit that b goes to infinity that is necessarily always going to be 1, in a 1 D case you are bound to have a capture whereas, in a 3 D case you are not in a 3 D case this is a by b.