Selected Topics in Mathematical Physics
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Module - 10
Lecture - 27
The diffusion equation (Part III)

So, today what I would like to do is to go back to the diffusion equation - the one-dimensional diffusion equation and introduce you to the idea of first passage times, survival probability and so on.

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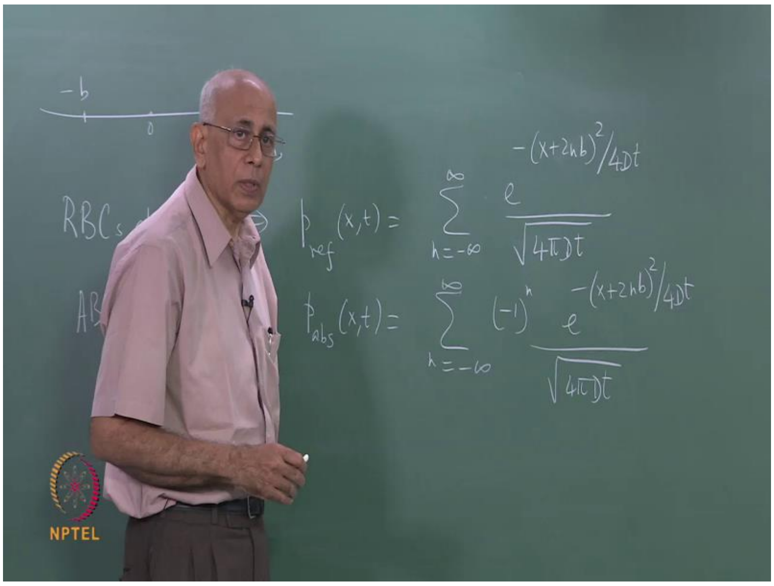

So as to get some feel for what the diffusion equations solution look like in the presents of boundaries finite boundaries. And the first of these problems is something we already mentioned. So, on the x axis, you have the diffusion particles satisfying the ordinary diffusion equation, here the origin and thus the barrier at the point b and another at the same minus b. In this case, symmetrically placed on either side, and these barrier is either reflecting or absorbing (( )).

Now if it is reflecting boundary conditions, at x equal to plus or minus b, this implies that the solution to the diffusion equation p. And let me call it reflecting just to keep track of this fact x t is equal to a summation over all integers minus infinity to infinity e to the minus x plus two n b whole square over four D t divided by the normalization factor four pi d t as usual. So, this is the function that is the unique solution to the diffusion equation in this region, satisfying the boundary condition that there is no flux across this point or that point. So, delta p over data x vanishes identically at these two points.

On the other hand, if we had absorbing boundary conditions at these points this implies that p absorbing of x, t is summation n equal to minus infinity to infinity. And then all you have is a minus one to the power n over and above the original expression divided by the same normalization. But the fact that you have this minus one to the n, and you have absorbs here which means probability density vanishes at these two points makes a huge difference. These are very different functions over they look like very similar to each other. The fact that you have this factor here makes these functions very different.

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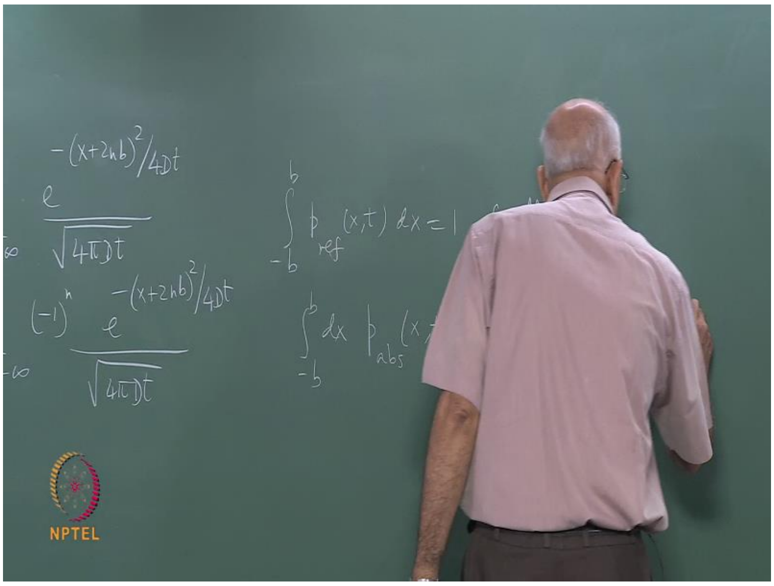

For instance, in this case and guaranteed that p reflecting of x,t from minus b to be integrate over d x equal to one for all t greater than equal to zero that is no longer true when you have absorbs at the two ends. Because it means that the diffusing particle could hit the end point either of the two end points and get absorb after that the diffusion process comes to a halt. Or it could lead through this barrier and get out of this region of interest. In either case, this quantity minus b to b d x p absorbing of x, t is not equal to one, it is start at one at t is equal to zero, because my initial condition has always been p of x, zero is equal whether it is an absorber or reflector. So, or equal to delta of x is also is equal to p absorber x, zero.

So, I start with the particle at the origin and I say let go and satisfy the diffusion equation. So, the initial condition is the exactly the same for both. So, this quantity at if t equal to zero is obviously just the integral of a delta function that is equal to one, but because of this factor a decreases us time increases as will see explicitly a particular fashion. And this is equal to the total survival probability that the particle is still here in this region between minus b and b without having absorbed. And that survival probability let me call it s till time t, and this is to indicate where the barriers are given that is started at the origin at t is equal to zero.

So, let me call it S of t, but I put in these year tell me where are the barriers and where did it is starts. It is depends on where it is started, we took a nice symmetric initial condition. So, this thing here is the survival probability, in the region, in the open region minus b to b. So, it says in this interval without hitting the end points.

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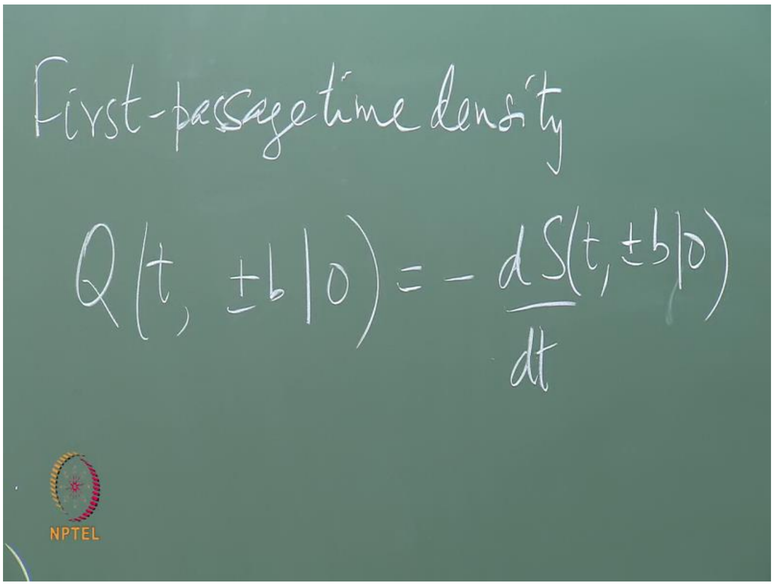

Now, what to be expect of S of t plus or minus b. So, if I plot this as a function of t, if I plot this S here, I expect that t equal zero it of course one then I did expected die down as a function d some fashion. We would like to know exactly how it dies down it turns out it dies down exponentially fast and we must see that explicitly. Now you could also asked what is the probability that this particles hits this boundary or that boundary for the first time at some time intervals time instant t between t and t plus dt. For the first time and the moment is hit it its absorbed, this is called exist time or a hitting time or a first passage time, first passage to the points plus or minus.

And what would that p well if I called the first passage time density and let us called it Q of t. So, it happens between t and t plus d t. Given that you had barriers of plus minus b and given that you started at zero, exactly as in this case the question is what is this quantity is equal to that is of interest, because if I find this quantity is normalized in t between zero and infinity, its integral must be equal to one. If I say that absorption is sure event this integral must be equal to one that is the first point and second point is if i find the average value of t with respect to this density then I have mean time it takes to hit the barriers that the two ends.

Now this thing is very easily computed this thing here is equal to minus d s over d t (( )). because after all you could go back here and write it from small infinite decimal difference delta t and you could ask what is s of t plus delta t, what is the probability that is a survived till t plus delta t. And you add to that the probability that is absorbed between t and t plus delta t that is Q of t times delta t together they must be equal to S of t, because system survival till time t, probability S of t. And then it has two possibilities after that either it gets absorbed or it continues and survives. So, that immediately tells you that S of t minus S of t plus delta t divided by delta t in the limit is just the Q. So, that why put a minus sign here, this thing is decreasing function of t I expected to this. So, minus is a positive quantity and that is the first passage time density in these points.

Let see we would like to compute this quantity Q for this problem. Now this can be done in number of ways the many ways of doing this as I said, but this is not a very good representation for it, because as you can see the t appears in the denominator here, and as t increases, this denominator makes becomes larger and larger. So, these exponential tends towards one, e to the zero which tends toward one, and then you have very slow decade due to this guy here. And it is not at all clear what is the actual the behavior of this quantity as t goes to infinity, this is a very bad representation. Near t is equal to zero, it is pretty good because tells you both singular starts with the develop functions and then its spreads out, but the question is what is do for very large t, it is not a great thing, but we already have the hint on how change this representations.

You see this is a sum over integers in this fashion and now it is clear that if you use the parts of summations formula you can tried to bring this t in the denominator to the numerator, if you write in terms of a Fourier transform. But instead of doing that let us do this little more directly, let us solve the diffusion equation once again in this region. We wrote the solution down using the method of images from the fundamental solution, but instead of doing that lets start again with the diffusion equation and solve it by the time honor elementary method of separation of variables, where obviously do and let see what happens then.

And the reason I want to do that is because of the following hope. The diffusion equation is first order in time and if I use separation of variables, I would get a first order differential equation with possibly and exponentially decaying solution. And once I have an exponential decaying function of time, I know what it does for large values of t, it just goes to zero. So, let us see that borne out or not and let us start again and I am specifically interested in absorbing boundary conditions.

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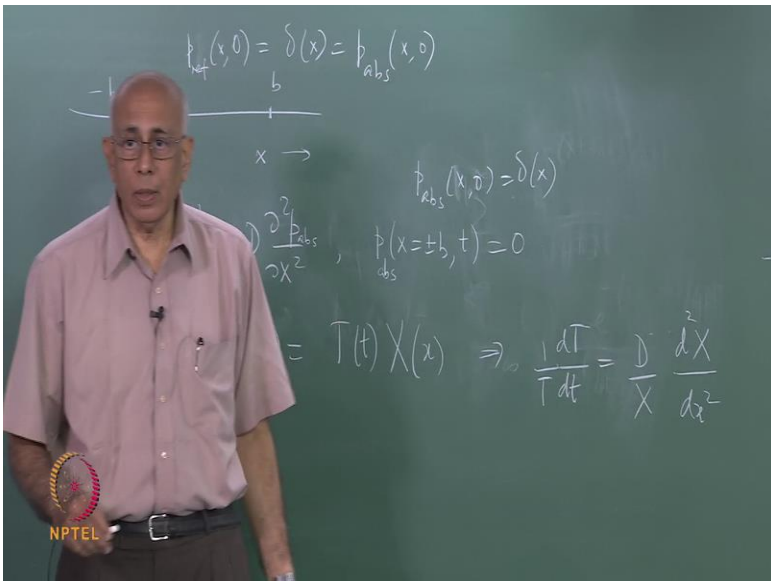

So, we will focus on just that. So, I have delta p over delta t equal to D d two p over d x two and p at x equal to plus or minus b t equal to zero go for all. And the initial conditions, this is p absorbing, and initial condition is p absorbing of zero x, zero is delta of x. So, what does one normally do it is say well this p absorbing of x, t, you would assume this to be some T of t, function of t alone multiplied by some function capital x of little x alone that is the simple assumptions. And then this equation would implied the capital x times delta t d p over little d t. So, capital x times d T over little d T equal to D times T times d two X over d x two and then the obvious things to do it should divide by x t. So, you have a one over T and then a d over X, this should be equal to that, but this is a function of time alone, and that is a function of little x alone, that is only possible if each side is a constant the same constant.

So, let us write that constant out is equal to minus I want to say minus, because I want exponentially decaying solutions. You can take any arbitrary constant alpha, but it will turn out to be negative number. So, let us put that into start with by saying minus C square some constant, I expect C to be a real number, so that this will be a damped function. And then what is that means it says T of t equal to e to the minus C square t times T of zero this is straight forward solution to this. And what is the solution to this fellow here, it is says x double prime plus C square over d x equal to zero. So, it immediately says X of little x equal to sum A cos C square. So, it is C over root d x plus B sin C times x over root D, that is the solution to be X equation, that is the harmonic oscillator equation.

But you see I am starting with that is the delta function condition which is symmetric in x, and the barriers are placed symmetrically on either side. So, the boundary conditions a completely symmetrical, it is a same boundary conditions at plus b and minus b the initial condition is symmetric under x to minus x. The boundary conditions are invariant under x going to minus x, and the diffusion equations invariant under x to minus x, because it is second order in X. So, I expect the solution to the symmetric as function of X. A moment I see that this thing goes away by symmetric, x to minus x, there is no b and then you have a cosine which is an even a function of x.

And the next thing to do is to put in what the boundary conditions are and we want p to vanished at boundaries. So, this implies that cosine C over root d times b equal to zero that is the boundary conditions, whether I put plus b or minus b does not matter, the cosine and I want this to vanished. And what exact implies it says this thing must be n plus half time pi otherwise its cosine does not vanished. So, this will immediately implies that c over root b equal to n plus half pi or C equal to 2 n plus one pi root D over root 2 b, where n is an integer. Now this integer and principle could be plus or minus but the fact is I have taken to the solution to the cosine and sine. So, I do not have to go to the negative integer at all. Had I taken an exponential here then of course, had I have to keep the both the positive and negative integer and the moment I say cosine or a sine then it does not matter, because one again relate cos n plus half the with the negative n to positive half odd integer.

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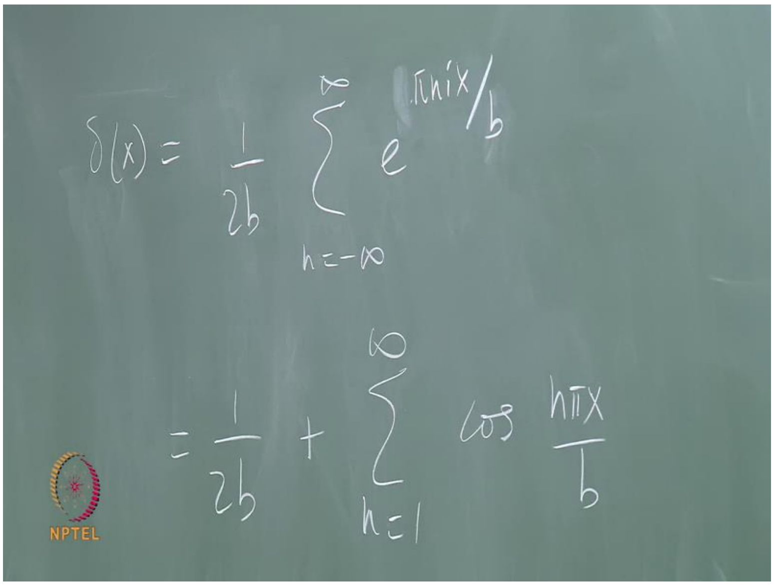

So, this immediately implies now that we have a solutions, the solution is p absorber of x, t equal to a summation over n equal to zero to infinity some coefficients A n which will still have to discover times cosine of c x over root d, but we know what C is, it is two n plus one pi x over two b. The square root D cancels, because C over root D is sitting here multiplied by exponentials and those are e to the minus C square t times e to the power minus and c square is two n plus one whole square pi square D t over four b square that is a solutions. Now it is still have to find out what it does at x equal to zero. you still have to put in the initial condition and make sure that you can determine the initial the coefficient and that easily done.

Because all you need and I am not going to do that, but all you need for that it that note know that initial conditions delta of x, we know the delta of x as a Fourier expansions. We know that is one over l summation over all n equal to minus infinity to infinity e to the two pi nix over l. Now put l equal to two b, and end up with two b here, and the two b here, so this thing cancels. So, we have a representation for a delta function in terms of exponentials, but now I have n equal to zero upwards. So, let's take terms says this is one over two b, I take the n equal to zero from out plus a summations n equal to one to infinity and I have half of this plus with the same with minus there that is equal to cosine, so this is equal to cos n pi x over root b.

So, use this fact in here, use the fact there a t equal to zero it must reduced to this thing here. and compare to write down what the coefficients are, this is the simple exercise, and the answer turns out to be just one over b. So, verified this, check this. Whatever we have now an explicit solution in terms of decaying exponentials out here where n run over all the integers zero to infinity and it got the right dimensions the probability density must on over length as the dimensions and that (( )) and this is it. So, as you can see from here immediately this quantity actually vanished as t tend to infinity including n equal to zero terms that to has a non zero exponent of here. Therefore it is not surprising that when you integrate this from minus b to plus b, the answer is trivially, you can write this not trivially it would still d k.

So, let us write that down that let see what S of t plus or minus b zero equal to this is equal to integral for minus b to plus b dx p absorbed of x, t. What is that equal to that is equal to one over b and then let's integrate n equal to zero to infinity e to the minus 2 n plus one to the square pi square D t over four b square and then I have integrate this point to be between minus b and plus b. So, that is equal to sine two n plus one pi x over two b from minus b to b, and then it is divided by two n plus one pi over two b and the b cancels in the two goes on top. So, let's take out two over pi and write like this and that is a sine function, which is going to changed sine from b to minus b and I am going subtract the value of minus b. So, this is an extra factor of two may that four and is just a value at plus b. So, the b cancels and you have this which is n plus half pi.

That sine n pi cos pi over two is zero plus cos n pi and sine pi over is one; cos n pi is minus to the n this whole thing that is the exact solutions. So, we have this as I promised this survival probability in this region is a decaying some of decaying exponential. In the leading term goes like e to the minus pi square d t over 4 b square and it is the added to it or even more rapidly decaying exponential. And we have whole spectrum of relaxation times by it which decays. And you guaranty this convert to extremely rapidly, because you have this e to the minus n square sitting here definitely goes to zero very very rapidly. Now of course, you can ask is it true that this things sure, namely the definitely hit the point or not well what is the answer to that.

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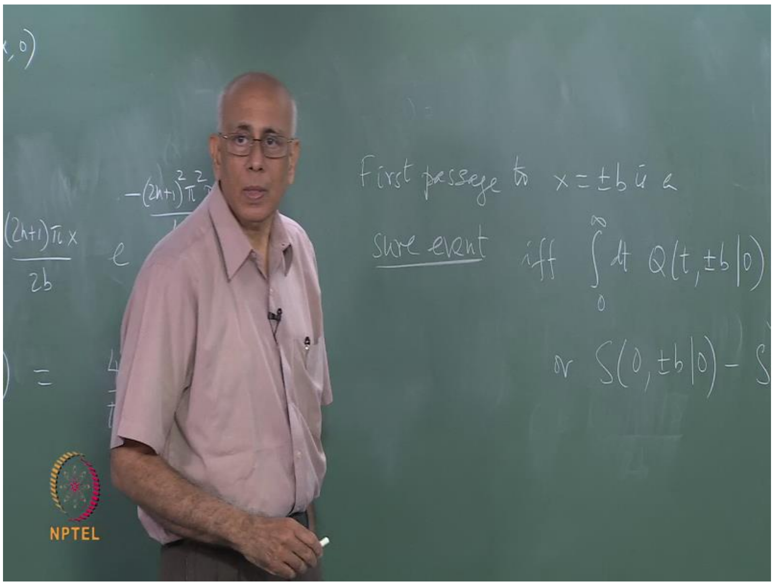

You definitely going to hit it, if s goes to zero because first passage to x equal to plus or minus b is a sure event which will occur with probability one always provided the survival probability goes to zero as t tends to infinity. So, now let it going to hit. So, it a sure event integral zero to infinity d t q of t plus minus b zero is equal to one if and only if this is clear because it is says this is the probability that between time t and t plus d t and if a integrate that between zero to infinity. So, some over all the times and is equal to one then you know the event you go to it probability one. So, you just need condition, but if put that in here he put this in here than this is the same as saying yes of infinity well say minus sign.

So, it is says of zero plus minus b zero minus s of infinity plus minus b zero is equal to one that the same condition all am doing into integrating respect to t, but this quantity zero. So, you have ensure is that the survival probability is one at equal to zero you started equal to zero if the particular; obviously, it is a . So, you need to put the equal to zero and this and ensure that we get one has one sure.

What happen you put the equal zero this goes to and we have the minus to the n plus point what is the value of that c d c one minus plus one third plus one fifth its five over fourth this time hearing this . So, we knows this minus one and by the by this equal to times is equal to one it just the r tangent see this madava series this r time and its value five or four. So, in need this is the true. So, we have sure first passage does. The next question is all right now the first passage as here what is the average time he take for its happen for that you need to little more work they need to find out what is q they still not find out what is q from this things.

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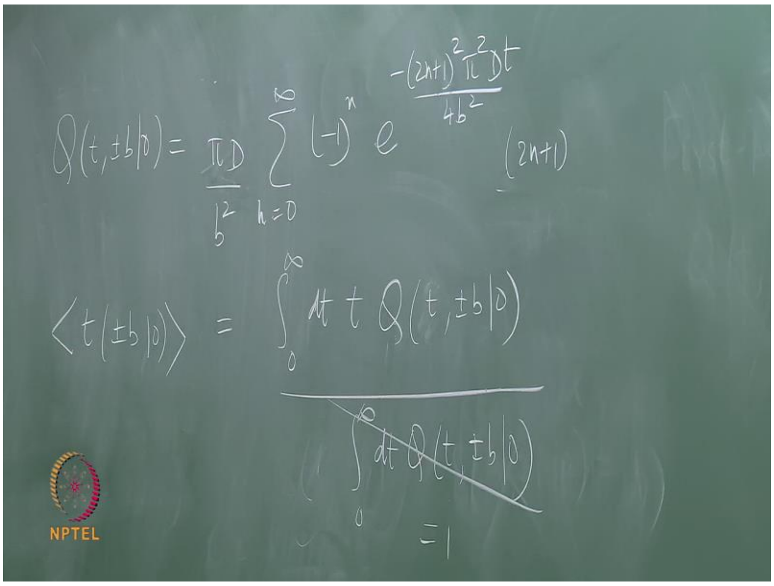

So, let us complete the first passage time density itself that turns to be Q of t plus or minus b to zero. This is the derivative minus the derivative of this function with respect to t. So, this is equal to four over pi summation n equal to zero infinity this things converges absolutely. So, we can differentiate inside the integral sing minus one to the power and then e to the minus 2 n plus one square pi square to D t over four b square over 2 n plus one times this thing here, so that gives me 2 n plus one square pi square D over four b square. And I differentiate (( )), so all we have do is to differentiate this one, and you just bring this factor down and let's get rid of things. So, four goes away, there is the pi, D over b square, and then 2 n plus one on top, and that is it.

And we are not overly concern about the factor that is the 2 n plus one sitting here because this things here is the very strongly done exponential e to the minus n squares. So, whatever power of n appears here is relevant, in fact all movement of this function will exist now, so that is Q. And then the next step is to find out what is the mean time it takes. So the average time over all possible diffusion process, all realization of this diffusion process that you are going to hit plus or minus b having started at zero, for the first time you going to hit plus or minus b having started at the origin as zero. And let us call these angle of bracket, the average over all random box all diffusion process. This thing here is equal to an integral from zero to infinity d t T times Q of t plus or minus b starting at zero divided by the normalization, it is zero to infinity d t Q of t plus minus b zero, but this is the one, the denominator is one.

You normalized the probability, because S of zero was equal to one. So, this is the differently normalized unity. And you have to do this, you have to do this integral, you have to differentiate, you have to put this in and integrate this. Now previously we had e to the minus some a t has the integral. Now you got t e to the minus a t as the integral that is also a doable. And then you have to do this sum, but you know there is the short cut do this business and that is the following.

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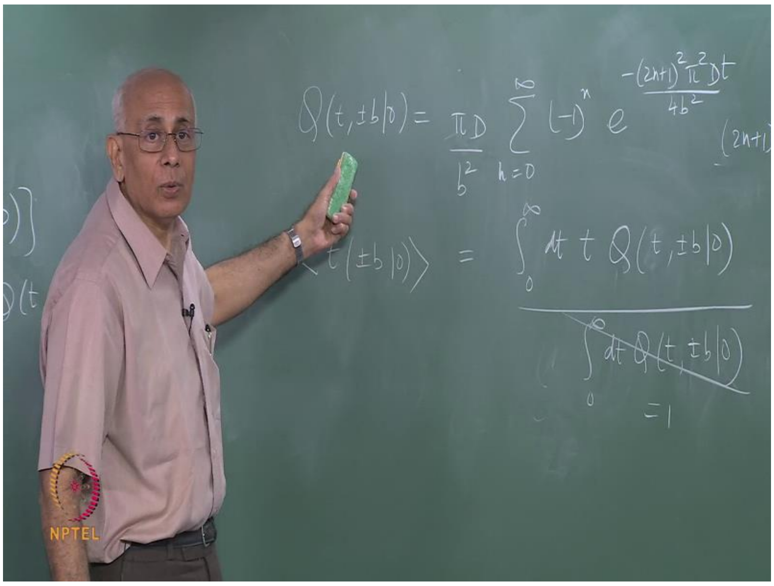

Suppose you define, you want to find the moments of this t, suppose you define the Laplace transform with respect to t of this Q. So, let us define q tilt of s plus or minus b of zero to be the Laplace transform of this Q of t plus minus (( )). And this is equal to integral zero to infinity d t e to the minus s t Q of t (( )), that is Laplace transform of this function. What is the value of this Laplace transform at s equal to zero. You put S equal to zero, you get this integral, but that is the sum over all probability that is one.

So, if the event is the sure event, the corresponding Q must be Q tilt must be equal to one at s equal to zero. And that is easy to check, because we already verified this quantity is one. So, this we know for sure that at s is equal to zero, this quantity is one. But we now need this integral (( )), what should I do for that integral, I need to bring down a t here, I take it derivative with respect to s of this Laplace transform; that brings on a minus t and then I put s equal to zero, so this goes away.

So, it is obvious that this quantity is also equal to minus d Q tilt over ds s plus minus b is zero evaluated at s equal to zero. And I am just lazy I could do the integral t e to the minus a t, but I want to do this because it easier to do and write the answer down immediately. Well we can write down Q tilt here without too much do, because each terms is like e to the minus a t, and what is the Laplace transform of e to the minus a t, one over s plus a. So, we have write Q tilt of s plus or minus b zero equal to pi D over b square summation n equal to zero to infinity minus one to the power n over is plus whatever it is, this is 2 n plus one sitting outside s plus two n plus one square pi square D over four b square.

And of course, it is not hard to see that again if you put s equal to zero, you going to get one that is very clear, because you put s equal zero, you get again pi over 4 from this series, which cancels the four over pi and gives you one. But now you go to differentiate this with respect to s and then said s equal to zero. So, I differentiate it, I am going to get the same thing squared with the minus sign, but that minus is killed again this minus sign and then I said s equal to zero. So, d Q tilt over d s minus this whole thing s equal to zero is the square of this at s equal to zero. So, it gives me let’s write it carefully 2 n plus one to the power four and then four square that gives me pi cube in the denominator and in the d square that gives me D out here, and then it gives me a sixteen b to the four. So, the b square and this goes away, and this things here becomes the q, that is the result. This is the not such a trivial series as that, but we have a exact answer.

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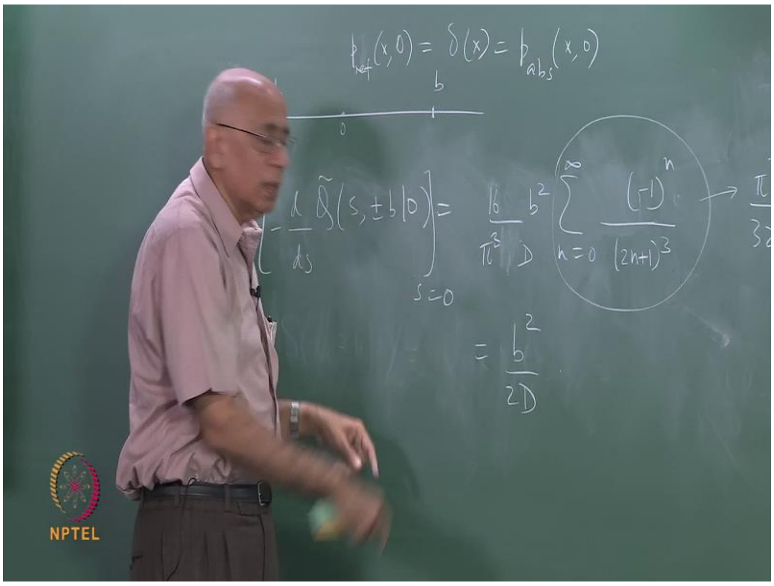

I mean this is exactly equal to t plus or minus b zero, average over all possible random without any bias of course, now as expected I already pointed out that this time must be proportional to b square over d, because that is only time scale in the problem. So, in d this proportional that the b square over d, the d (( )), so the d square in the denominator. So it is in fact proportional to b square over d times this series here.

Now we need a little bit of information, we need the value of this series. This is not so trivial to obtain, but it is doable the series here. It turns out this series is pi cube over 32. You compare to look at the tables the class, but it is possible to do this by the means as well. I am not going to waste time doing that here. It is little tricky because of the cube here, had it been a fourth power then we could have use various contour and tricks and so on. But because it is cube little tricky, but it smooth in terms what are called Bernoulli number.

So, here we are and this is the equal to b is square two b, so remember that I said that l square over d over region l is the diffusion time to reach a distance l. Now what is happened here, exactly that we know that the root means square displacement will go like two d t that is thing for the displacement as the random variable. On the other hand, the time is the random variable for fixed distance b on either side of the origin then the time is average time is precisely b squared over two D. So, this ties in because complementary piece of the information to what we had earlier, (( )) in the fact that length the times scale in this problem is indeed b square over D, including this factor two turns of that is because of artifact it is a symmetric initial condition, but in any case this is the exact answer.