Selected Topics in Mathematical Physics Prof. V. Balakrishnan Department of Physics Indian Institute of Technology, Madras

Module - 10 Lecture - 28 The Diffusion Equation (Part IV)

So, you see how this first passage time density behaves as a function of time. In fact it is interesting to ask how this guy behaves this q till the itself which we got there just a function of dam to exponentials. Now you could ask a slightly harder question, we did this problem with two boundaries on either side with a nice symmetric initial condition, suppose you do not have one of the boundaries you have just one boundary in the other side goes all the way to infinity say on the left what happens, then when something very very different happens? And let us do that problem with no barrier here at all, but without loss of generality. Let us take one barrier somewhere, and I again start with same initial condition.

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And I ask the same question as before I have a single observing barrier here that reason is forbidden I start at the origin I do not have to do that I can start anyway, but it start at the origin says. So, there is a delta function at t could zero, and then I let the particle diffuse, and I ask what is the average time it takes to hit this point, but before you answer

that you have to answer the question is it going to hit this point at all with certainty is this a sure event or not that is the first question we have to answer after we make sure that it does happened, then we can start averaging over the density whatever density it is. So, we need to find the survival probability first, and find out if that really does go to zero as t times to infinity in this in this problem. So, let us do that. So, now, let us write the solution now.

So, you have p observing of x comma t equal to, and this one here does not there is a trivial application of the method of images which four pi d t e to the power minus x squared over four d t minus, because there is a barrier here put an image point at through be minus x. And then next e to the minus x minus two b whole square over four d t, and the whole thing is divided perhaps, but you must remember that the physical region is minus infinity less than x less than equal to b that is the region of interest, and they guaranteed that the x equal to b b vanishes identically showing that it is an observing barrier. Now if I want the problem of when does a diffusion the diffusion particle hit a particular point b, then I pretend.

There is an observing barrier there, and ask what is the survival probability, and if that probability goes to zero as t tends to infinity, then I know that it is sure to hit this point. So, that is the strategy. So, we have the solution, and what I need to conclude is a survival probability, and what is that in this case s of t till time t, and there is a barrier at only b.

So, let me just write a b here I start again at the origin, and this is equal to an integral from minus infinity up to b d x p absorber of x comma t that is my s of t, and we need to find out if as t goes to infinity this goes to zero or not well you could say look as t goes to zero this goes to one that goes to one we cancel each other this fellow goes to zero one over infinity and so s s of t does go to zero, it looks like it is definitely going to hit this point looks like it, but with these t's in the denominator you got to be very careful be very very careful here. So, we got to do this properly let us see what happens let us see whether you can. In fact, compute this quantity or not well what I actually lead is the first passage time density. So, let us write that down I need q of t b starting of zero to minus d over d t of this now let me write just to make the algebra easy let me write this in terms of these two functions we put that n, but I do not want to carry this huge mess around all the time.

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And let me write p of x comma t equal to e to the minus x square over four d t over square root of four pi d t just for a moment, let me write that down just to show that this is the fundamental solution to the diffusion problem on an infinity line both side infinity know. So, what I have here this p observer is p of x comma t minus p of x minus two b comma t. So, this is p of x comma t minus p of x minus two b comma t, and what I need is minus the time deliver to of that. So, that becomes inside here delta p over delta t with a minus sign outside minus delta p over delta t of this fellow minus is outside.

So, let us... In fact, write this as minus this gum plus this guy, and now it is a bit of the new sense we have to differentiate this with respect to t put that n, and little bit of algebra you have to do this, but as lazy people you do not want to do that. So, you try to see if you can make do this a little shorter after all these fellow satisfies a diffusion equation. So, instead of this limit just write it in terms of the right hand side of the diffusion equation, and write this as a d times d two p over d x two in this function, and this is p two p, and x two that is readymade for doing the x integration, because it just a second derivative right. So, we immediately get this is equal to d times delta p over p of x

comma t over delta x between with a minus sign between minus infinity, and b, and then applies delta p over delta x x minus two b, and t between minus infinity, and b. So, I do not have to do any integrals, and I have this thing just a differentiation with respect to x will be, but I know the solution I differentiate with respect to x you gone to pull down an x over t. So, you gone to pull down a t to the three halfs here, and then you gone to put a minus sign here, and put x equal to b you going to put a plus sign here, and put x equal to b which gives me the same thing, because it is again a argument is minus b. So, it is clear these two guys are going to add up in this case.

And in they do on the solution turns out to be by the by we going to put x equal to b which will give us e to the minus b square over four d t in both cases that is it that is the solution. So, this tells you that the probability density that diffusing particles starting at origin here hits the point b any arbitrary point b to the right for the first time between t, and t plus dt is given by this density which is now a probability density in time goes like this it looks exactly like the solution to the diffusion equation exactly like that multiplied by b over t, because is the t q by takeout t square is b over t, but b over t is like a velocity the distances b, and the time is t. So, it is look like b over t very deceptive, because the velocity of this particles is really infinite formally off course it diffuse a process, and the first derivative, and t is balance to the second derivative, and x. So, it is clear remember also that in the random of model the latest constant a had to go to zero in the time stepped how had to go zero to zero such that a squared over two tau was finite. So, a over tau is actually infinite. In other words a diffusing particle has formally got an infinite velocity why, because after all you can think of it basically at this fashion you start with a particle at the origin.

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So, the probability density is the delta function at the origin, and at any t no matter how small for any positive t, it is a Gaussian very narrow Gaussian to start with. And then broadens. So, no matter how small t is there is a finite probability of finding the particle arbitrary far away that can only happen if you an infinity velocity. So, brown in particle brown emotion this is brown emotion has formally an infinite velocity in practice there could be damp, and there could be viscosity and so on, and that would this equation would only be true in the. So, called diffusion regime, but we would not talk about that right now in the fact is that as a mathematical model the diffusion equation describes the motion random motion of a particle with infinity velocity. So, this is now the first passage time density we need to know what it does as large as t becomes large, and a t is small.

So, let us plot this the function of t here is q as t goes to zero this goes to one e to the minus infinity which is zero, goes to zero sorry, and this thing goes like one over t to some power. So, this dominates, and you have an extremely plat zero at the origin. So, does this, and then it takes off, and dies down very slowly essentially like one over t to the three halfs, and we need to ensure that the integral of this quantity from minus infinity from zero to infinity should be one, I am not going to do that, but I assert that it is. So, so I assert you can check this that q of t b zero integral d t zero to infinity is equal

to one. So, it is a sure event, it will happen definitely will happen as you can see also by looking at the survival probability, and saying whether goes to zero or not as t tends to infinity. So, the fact that it hits the point is for sure.

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But the question is what is the mean time it takes to hit the point, and then there are in for a big surprise, because the mean time t to hit the point b starting from zero is equal to an integral t q of t b starting from zero, then divided by the normalization which is unity in this case, but what happens to this integral what would happen to this integral we have to put this in here, then you faced with an integral which goes like zero to infinity d t there is a t here there is a t q here.

So, there is a t to the half e to the minus b squared over four d t, and what is the value of this integral what happens to it, as t tends to infinity what happens to the exponential goes to one the exponential just goes to one, and it does not do anything for conversion at all what happens to the denominator that is t to the half, and when you integrate to the half in the denominator it becomes t to the half in the numerator in the it blows up at infinity. So, this is infinity. So, here is a process which is guarantee to happen, but the average time it takes for it happen is infinity the mean itself is a infinity this is a nice probability density distribution that is called a levy distribution with exponent of half by the way this thing here anything which goes like one over the random variable to the power three halfs e to the minus a positive constant over the random variable is called the levy distribution, it is one of the stable distributions, like the Gaussian etcetera levy distribution that exponent half, but it is first moment happens to be infinity. So, therefore, it is hire moments are even worst the variants and so on you are familiar probably with distribution where the mean is finite, but this variants s infinite formally like a distribution, but here is a case where even the mean is infinite in this problem. So, such a random process first passage to this point is said to be a null recurrent process in the fact that it is recurrent it does happen passage to that point is for sure, but the mean time is infinite similarly one can show that the mean time to return to the origin is also infinity etcetera, etcetera on the infinite line first passage from any starting point to any final point is for sure you know always happen given enough time the process will always happen with probability one, but the mean time to do.

So, is infinity in the absence of a bias, and that follows directly from this where is that here the fact at this mean has become infinity this thing here is a levy the gaussian is also a stable distribution with exponent two, and in this case this thing here is the exponent half this case mean is infinite in this case. So, there many other such problems that that one could tackle using a some of the tools that I have given here the key point is that there several ways of finding the first passage time distribution, and we saw at least two of them here is one from the method of images you find the survival probability tool this the other method is the separation of variable you find the probability density, and from their you find the survival probability etcetera. So, in neither case as you can see this will give you a definite answer over the averages over all possible random box all possible fusions. Now what happens? When you have a bias is very interesting we did this in the absence of the bias you could ask what happens if the equation.

That is describing that describes this p of x comma t is not the original diffusion equation, but delta p over delta t equal to minus c delta p over delta x plus d d two p over d x two what happens if you have a drift as well as a diffusion, then you have yeah. Yes, that is the connection with this semi circle law. So, on which I am not talk about here at the moment, but actually one should not write b one should ask what is the first passage to any point b? Suppose b has been in the opposite side. We could have done that too you could have said I have an infinite line, and I want to know what is the time of first passage from zero to some point minus b here on this infinite line. So, I start on this line, and I say there is an absorb here it hit's it for the first time it is gone be now it is immediate clear from here that this does not depend on the sign of p. So, the first thing that happens is that one should write mod b here, and one could look what are its property is as a function of b over t one can scale and so on and so for, yeah I do not want to get into that right now, but the point is that in this diffusive process we know that x squared the square of the length variable scales like a time.

You saw that in two different ways the mean squared this placement this proportional to time the mean time is proportional to the distance squared for a fixed distance right is a complementary pieces of information in this case. Now turns out that when you have a Gaussian distribution for a random variable, you could ask what is the distribution of one

over the square of this random variable? And that has a levy distribution of exponent half, and since x squared is scalding like t that is what has happened here for the t essentially this is happened. So, there is a duality between the stable distributions with different exponent which I have talk some other occasion, but that is essentially what is happened in this problem now we have to solve this equation here, and ask, but let me just coat what the result would be unless without loss of generality say there is a point here which you want to it b, and now I ask what happens? If I have A bias walk if I have a drip velocity in this direction as oppose to one in this direction or no bias at all. So, far we have seen that if you no bias at all in the diffusion do not have this term, then first passage to this point is a sure event, but the mean time is infinity, if there is a bias in this direction in other words if there is a dripped in this direction you would expect this to be even more true. So, first passage to this point is in the sure event, and there is a finite time a mean time over which it goes, and exit which can be computed, but if drift is in this direction the opposite direction, then even first passage to a point on the right is not a sure event in other words if you compute this integral over q you do not get one the survival probability does not go to zero as t tends to infinity.

There is a finite probability that you will escape capture forever no matter how long you wait, then off course the mean time to hit this point does not make sense, because it is not a properly normalize random variable, if you could still ask a question like what happens if I take all those realization where the particle does go, and hit it what is the mean time, then over those realization that is doable we can do that, and you can have answers. In fact, what you could do this you put a barrier here, and how do things go as a functional of this barrier if you put barrier at some point minus l, and ask what is in the absence of bias what is the main time to start a zero, and hit b for the first time the answer become proportional to l. So, l goes to minus infinity where it goes to infinity rather in this this sign convention this diversion. So, that is the diversion we just discovered on the other hand if there is a bias in this direction, then this answer goes like e to the power l.

So, as l goes to infinity this becomes even more diversion on this side conversely e to the minus l if you have bias in this direction etcetera. So, one can put in all these drills one can put in this extra details work out this first passage time problem, but this is already giving you a hint that is to what is going on is the reflecting one yeah. So, it is than off course by the by as a sort of toy model of this fact that you may escape all together.

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If you word a bias in the wrong direction there is a famous story about which I believe talking about some time ago. So, you have, and then you start at zero, and let say there is an observing barrier at one on this side, and a probability of a jump to the right is say p, and a probability of a jump to the left is q, and the random occurs start at zero tosses a coin with probability p he get's head he move on the right probability q, he get's he move to the left in the question asked is what is the probability that he is gone to hit this point one which is an absorber. So, what is the total probability, and is that probability equal to one or not as a function of little p this bias p now this is a solvable problem. So, we want probability p that the walker hits one at some time total probability at if this over one, then is a sure event if is less than one it is not on the question is it is as a function of little p what is it equal to we just seen that when p equal to half, it is like the random walk analog of an un bias diffusion, and then it was a sure event.

So, we know for sure that p equal to half the value is one is capital p of p must be one the question is what is it for other values of p as p increases it is clearly gone to remain one it cannot be a bigger than bigger than one right question is than what is the value as p become less than one you can do this fast let me do that in a minute. So, what are the possibilities p of little p equal to what is p, because in one step it goes from zero to one that is it the problem is over plus q times a once it is q; that means, he jumped here, and from here to be captured at that point for the first time sorry. So, from zero you jumped probability p there probability q here.

So, if he jumps to minus one in the first step, then to be captured at all at once we has to go here, and then go here for sure, but the total probability that is start at minus one, and goes to zero is the same as the total probability is start at zero, and goes to one, because it translation in variant on this side it is an infinite that is on the side that is crucial know. So, this is q times p of p multiplied by p of p, and that is it all possibilities are exhausted, because you took further step is either to the right or the left, and then we have summed all possibilities. So, this says p squared q p squared minus p plus little p equal to zero, and the solution off course is p equal to one plus or minus square root of one minus four p q over two q, but q is one minus p. So, this is four p plus four p squared let us write this or properly

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We have p of p equal to one plus or minus square root of one minus two p is a whole square over two over twice one minus p, because q is one minus p in this sense, but here is what we have to be careful this square root of a square is a modulus or whatever is inside to be very careful there. So, this is equal to one plus or minus modulus one two p over twice one minus p, and that is equal to depending on whether p is bigger than half or less than half you get two different answers.

If it is less than half by the by there is also an ambiguity here plus or minus you have to have a definite answer, but we know for sure that p of zero if there is no probability is going to the right at all, then this p of zero is zero we never jump to the right, because never going to be captured at one right. So, you need to do that, and the correct root here is that for the minus sign. So, you have to eliminate this, and use the minus sign that is the correct root, and now if p is less than half this is one minus one plus two p. So, it is equal to p over one minus p p less than half, but if p is bigger than half its two p minus one, and it is two p. What it what happened yeah it is one minus two p plus one once again which is twice one minus p over twice one minus p.

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So, this is equal to two minus two p equal to one if p is bigger, and half, which is what we expected we already knew p equal to one this has to be one anyway. So, if you plot that as a function of little p here zero here one, and here is p of little p here is the value one beyond half its equal to one at p equal to zero it zero which is what you expect never get captured, and then it increases linearly till at p equal to half it becomes equal to one. So, it joins up in this passion, and your sort of face transition at the point half you know very different behavior all together there is a at this point now we can assert that for p greater than equal to half capture is sure, but for p less than half, then is a bias to the left even the first passage to that point is not sure is not a certain event and. In fact, is to zero by this graph here, but we solve this problem very trivially, but it is a non trivial problem, because we really average over all possible random walks, and why did this magic happen that if there is a bias to the left you may never be captured, because there is a infinite amount of space available to the left, and they could be random box where it dis disappears arbitrary far to the left, then he can never come back.

No matter how long you wait does not come back again. So, it is an interesting problem simple problem in this case, but we use this principle of inviting the problem, we essentially said crucial step was to say that, because of this translation variance the probability of going from minus one to zero for the first time is the same as going to zero to one for a first time you use that fact, and then there was a clever trick which gave the solution here, but this helps you illustrate what goes on in the continue a diffusion case in the presence of a bias I did not solve this equation in that case, we can do that, but this already tells you what is going to happen qualitatively.