Physical Applications of Stochastic Processes

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Lecture-27
Non-Markovian Random Walks

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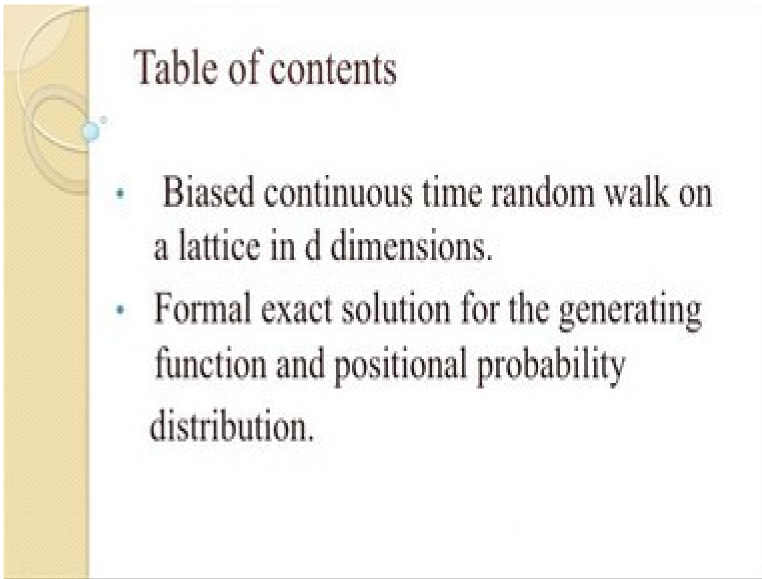

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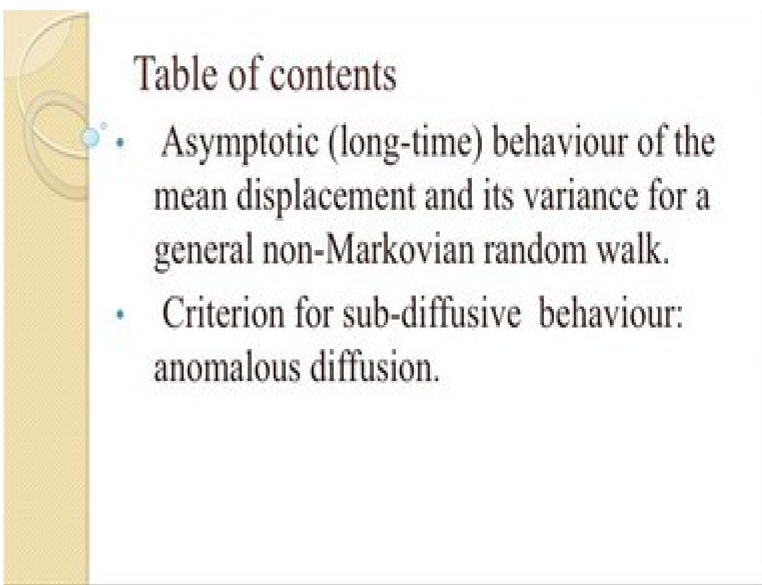

All right today let us formally solve this problem of a continuous time random walk on a lattice in d dimensions. Just to be specific let us take a hyper cubic lattice.

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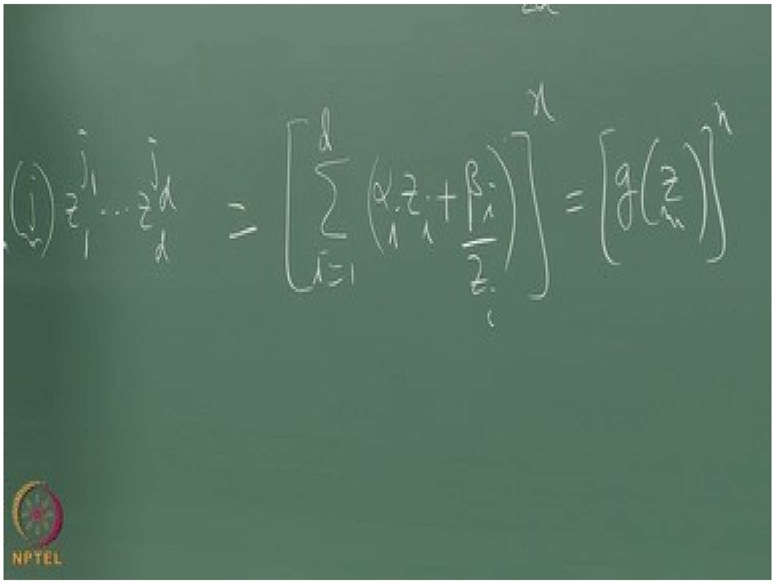

So, here is the problem we are going to solve it is a continuous time random walk on a hyper cubic lattice in d dimensions and we could specialize should be = 1, 2, 3 etcetera. So, just to recapitulate we already know a lot about this, what I had like to do is to write the formal solution down it is fairly straightforward to do it for a class of continuous time random walks governed by some renewal process in time.

And then we will look at the diffusive behavior the first moments and second moments of the displacement and so on and understand how diffusion comes about in this case. So, all the while we will have the Markov case as a check on our calculations because we must reduce to the known results in the Markov in random walk case which we have solved completely okay. So, here is what happens.

Let me denote by j and an element of hyper cubic lattice in d dimensions labeled by the integers infinite lattice so this j stand is shorthand for j1, j2 up to jd where these are all integers. So, that is a lattice point and we are going to look at walks which by translation invariance we start at the origin in this d dimensional lattice and we take steps in time. Now the first thing is we ask what is the probability of being at the site j at time n?

So, just to avoid the confusion with what happens in continuous time let me put the subscript outside to show that this is = the probability of being probably probability of being at of the walker being a j at time n given that the walker was at the origin at time 0 okay. We already know this we know this is some combinatorial factor it depends on whether there is a bias in the problem or not. We already know what this quantity is it is some multinomial coefficient.

Because remember that when in the case of 1 dimension it was just a binomial coefficient with some factors which depended on the bias to the right or to the left etcetera. We could as well take a bias in this problem also. So, let us suppose that you have bias factors alpha i and beta i = 1 - alpha I, so these are bias factors but i is any 1 of these directions okay. So, in the dimensionality 1 to d any 1 of them could have a bias.

But we also need to know the total probability must be 1, so we also need to write summation i = 1 to d alpha i + beta i sorry Phi and beta i in general after you sum this is = 1. So, in each Cartesian component we have a bias and the total probability of a jump out of a site into any 1 of its nearest neighbor sites is = 1 okay so, each of these is a fraction. The unbiased case would be every 1 of these factors is = 1 over 2d alpha i.

So it says if you are in 3 dimensions for example there are 6 nearest neighbors and the probability of jumping right or left each of these is 1 6th or top or bottom etc. So, this is some multinomial coefficient in fact we know what this fellow is explicitly. We looked at its generating function and let me call the generating function let us call that G sub n of z1 up to zd this is = a summation over all components of j elements of zd over all the integers for each component P n of g z1 to the j1 dot zd to the jd that is the generating function.

What is the random variable here j is the random variable you are given a time and this components the components of j they are random numbers they are random integers you want to know which side to ended up at etcetera and this is the generating function. This coefficient here as we know is a multinomial coefficient right. We already know what this Pj looks like we know what this generating function looks like.

Remember for 1 dimension this was P times z alpha times z + beta times z inverse to the power n. So, in the general case this quantity here is = summation i = 1 to d alpha i zi + beta i over zi the whole thing to the power n because this is the generating function for a single step which could be in any 1 of the 2d directions. So, we already know this and therefore what you are asking for is of this quantity when you take this fellow and you expand it in powers of each of the z's the coefficient of this combination is this quantity which you want here.

So it is a multinomial coefficient, so let us call give it a give this fellow a name this is the = g of let us collectively call it g to the power n okay. I want to make the notation straight that is the reason I am taking pains to do this. So, that this is just a shorthand for z1, z2 up to zd okay. Now let us introduce so this in a sense this problem is trivial we know how to solve it once you know how to make a multinomial expansion this identifying this quantity is 2. Now let us ask what happens we put continuous time on this right.

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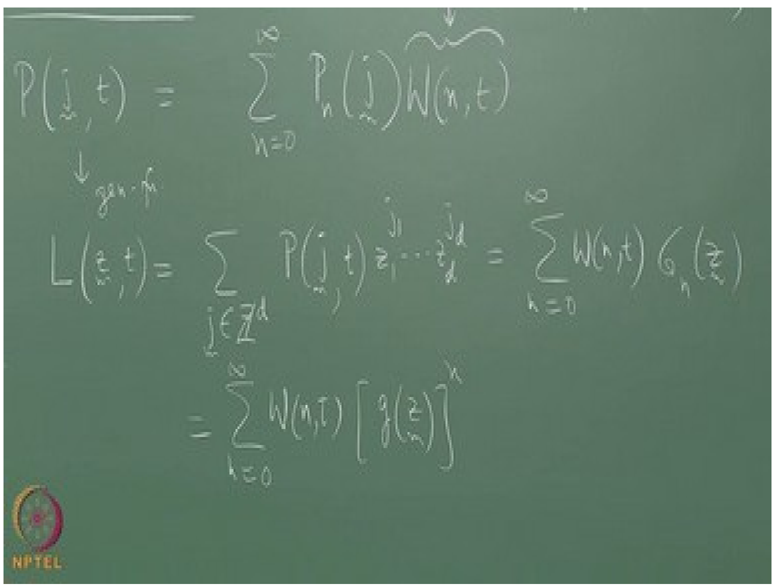

So, let us go to continuous time and the way to do this is very simple now I ask what is the probability of being at the site j at time t since t is a continuous variable I put this index inside this is obviously = a summation over n from 0 to infinity in principle P n j times W of n , t where this fellow here is the probability of n jumps in the time interval exactly n jumps and you are going to allow for all possibilities so is sum over n okay.

Remember the different jump events are independent events so the probability that you have 10 jumps in time t this is distinct from the probability that you have 15 jumps and so on these are mutually exclusive events the number of jumps and therefore I sum over all these guys. So, I have separated out the special and the temporal parts all the time dependence is sitting here the space part is right here and that is just pure combinatorial factors.

Now you can generalize this to other lattices you do not need this high per cubic lattice you have to tell me what is the quote unquote generating function or characteristic function for a single event jump event and that is what this quantity is. So, on any lattice we can find out what are the nearest neighbor vectors etc and find out what this quantity is and after that you are guaranteed that since the jumps are independent of each other this is the generating function for this probability distribution.

Now you could ask what happens if the system remembers its previous jump and so on. All that is happening in time so that is going here that input is going here. So, the jumps could all be uncorrelated correlated with each other and that will show up in W of n, t. So, as it stands this is the very general framework out here. Now we can ask what about what can we say about the generating function for this.

So, let me call; I need a new symbol so let us call it L of z, t to be = the generating function for this, this is = summation over j all lattice points j over zd P of j t times z1 to the j1 z e to the j that is this fellow here it is the continuous time analog of this generating function here. So, instead of P of P n ,t. So, what I have to do is to multiply this by z1 z2 etcetera this factor and sum over all the j's components of j's and when I do that this becomes = summation n = 0 to infinity W of n , t.

And then here I have to multiply this by these factors and some it but that factor we already know explicitly it is this guy G and so it is just Gn because I multiply this by these things and sum over all the j's and that gives me this but this fellow is already known to me in terms of this characteristic function. So, finally I get this is = summation n = 0 to infinity W of n, t g of z to the power n, I still do not know anything about this I have not specified anything about it at all.

But I have a formal expression of this kind now W of n, t is the probability of the distribution of a random variable n which is the number of jumps in any given time interval t. So, we can define a generating function for that quantity.

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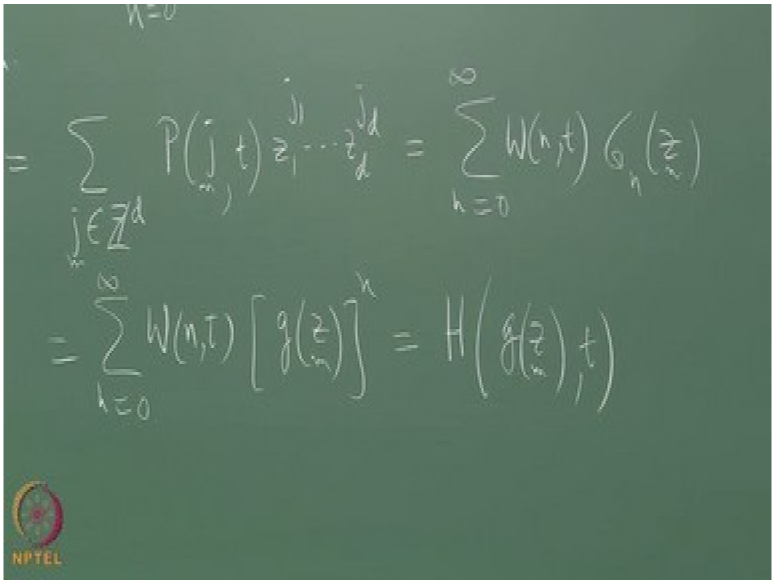

So, let us define so W of n, t generating function H of Zi and t this is = summation n = 0 to infinity W of n, t some Zi to the power n I do not want to put a z here as n here because I use that for the space variables conjugate. So, this is the definition of the generating function of this probability distribution in n. So, once I do that it is clear what this is this is by definition now = H of g of z, t because it is just this to the power n.

So, in principle the problem is solved because if you give me this characteristic function or generating function little g which depends on the lattice structure what are the nearest neighbors etc and you give me the statistics of this number of jumps in time t I computed a generating function and there it is and I write that in that expression that gives me the generating function for P of j , t which is what I want to find.

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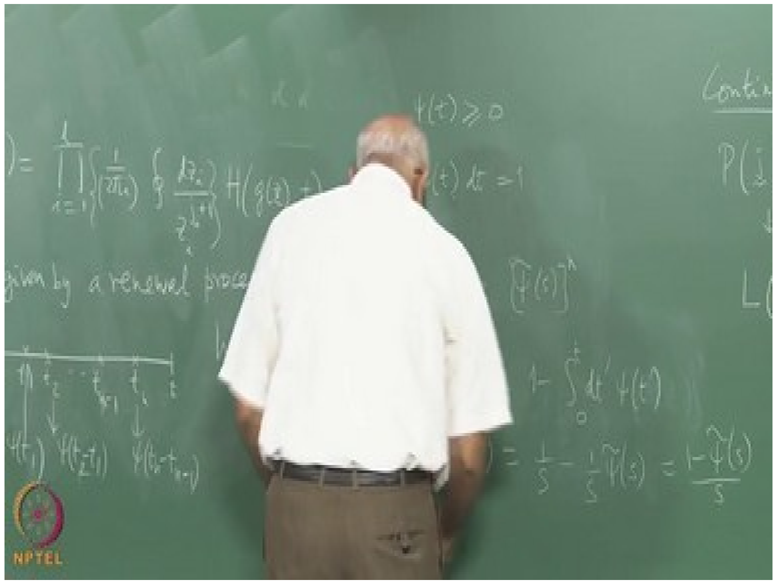

So, once you have this L which is this crazy power series in multiple variables formally formally we can write what its inversion is so piece of j , t is = the coefficient of z_1 to the j_1, z_2 to the j_2 etcetera till z_d to the power j_d right and the moment you have an expansion of this kind it is a Laurent's expansion because there are positive and negative powers of each z. This can be written now as a product from i = 1 to d 1 over 2 Pi and integral around the origin be z_i over z_i to the j I + 1 times this guy here H of g of z product acting on that.

So, just inverting this Laurent transform this Laurent series to find the coefficients this is around a small circle around the origin in the Z_i plane and you got to do this for each of the Z_i is in principle you got the answer. Or you have to differentiate it a sufficient number of times it is some suitable derivative of this quantity or of this quantity with respect to each of the z_i's will get and $z_i = 0$ will give me the coefficients right.

But the difficulty with that is that you have got negative powers of z. So, therefore that is not a trick which is easily doable this is a much more reasonable format. So, that is it this solves a problem but now let us see whether we can do something more in this model. In particular I want to say something about W of n, t and I want to say that it is a renewal process W of n, t given by a renewal process that is what a continuous time random walk is.

In other words there is a certain function a waiting time density which tells you the density that in time for the random interval between two jumps. So, the idea is that if you give me time 0 and t the first jump may occur here the second may occur here he and he n - 1 and so on. This interval between jumps successive jumps is given by specifying a waiting time density which is the same for all the intervals okay.

We introduce a waiting time or holding time density waiting time density let us call it Psi of t, so it says if you start at t = 0 then the probability that you have a jump between t and t + dt is Psi of t dt and it is obvious that Psi of t must decrease as a function of time clearly wait long enough there is going to be a jump. It is a density, so Psi of t must be non-negative it is integral from 0 to infinity must be 1 it is a normalized probability density function.

So, these are the properties we require of it the Markov case is given by an exponential waiting time density as I mentioned and it is not hard to see then the W of n, t will be a Poisson distribution with intensity lambda. But we will do it more generally than that does not have to be exponential just has to satisfy these conditions.

What happens then because the waiting time density is the same for all of these guys that is why it is called a renewal process with a common waiting time density. I could generalize this a little bit by saying this jump has a waiting time density different from the second different from the third etcetera. But in the simplest instance that is not what we look at we look at just the simplest case where you have got a common waiting time density okay not necessarily exponential okay.

Then it is clear that in this geometry here t1 is less than t2 is less than etcetera, it is clear that this t1 appears anywhere between 0 and t2, t2 appears anywhere between t1 and t3 and so on and it is in the form of a convolution. Because these intervals the size are the arguments for the size right. So, it is immediately clear that if you take Laplace transforms and you write W tilde of n, s, s being the transform variable.

It is a convolution after all this guy here has a Psi of t1 this fellow here has a Psi of t2 - t1 because that is the time you waited for and so on till out here you have a Psi of tn - tn - 1 and it is a convolution of all these fellows because each ti is bounded by the next ti + 1 in the upper limit right so the end of these guys. So, it is immediately clear that there is a Psi tilde of s to the power n but we got to be a little careful that is not W tilde of n , s because you can ask what happens if n is 0.

Then you need the probability that in the time interval t no events have occurred at all nothing has happened at all and what would that probability be because if I just took this to be the case W tilde of 0, s is 1 and the inverse Laplace transform of 1 is a delta function that is not what is happening at all right. So, what is the correct situation what is the correct W tilde of W of 0 t what is this = nothing should happen in this interval right.

If a jump occurs it occurs with density Psi of t so this must be = 1 - integral 0 to t dt prime Psi of t prime that is the total probability that a jump occurs in time t + 1 - that is a probability that no jump occurs. What is the Laplace transform of this guy what is the Laplace transform of 1, 1 over s yeah 1 over s - the transform of this guy is the convolution of 1 times i of t.

So, it is 1 of 1 over s times i tilde of t there are + transform of this integral Psi tilde of s over s when you differentiate you multiply by s when you integrate with you doing. So, this in fact is the correct answer so this is 1 – Psi tilde of s over s and check this check this against the case we already know against the Markovian case.

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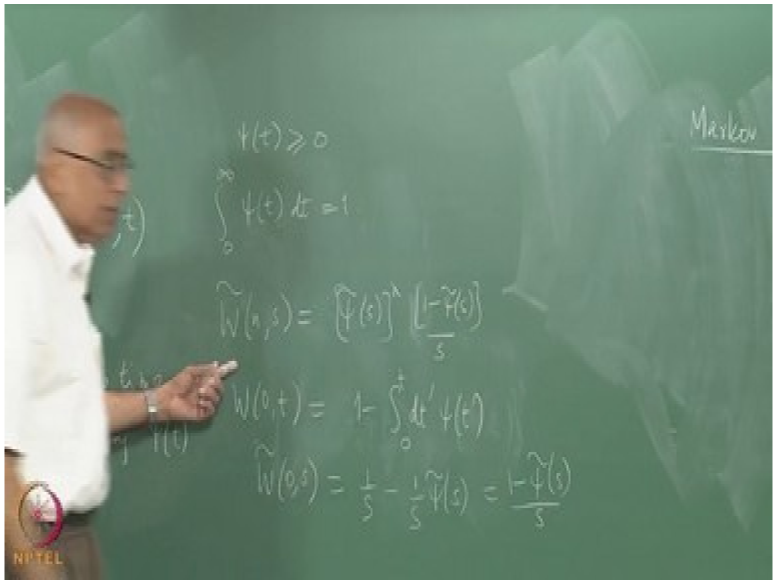

Markov Psi of t = lambda e to the - lambda t well I am just some positive constant right. This is guaranteed to give you immediately to be able to check that W of n, t is going to be the correct answer which is a Poisson distribution and what is W of 0, t when you have such a Poisson distribution W of n, t is lambda t to the n over n factorial e to the - lambda t so what is W of 0, t e to the - lambda t you should it should come out.

Because this will imply that Psi tilde of s lambda over s + lambda 1 – Psi tilde of s over s is this fellow here it is 1 over s + lambda, so that tells you that w of 0 t = e to the – lambda t, so that checks that checks so indeed that is the correct answer for W tilde of 0 , s otherwise you end up with this inconsistency that you have a delta function it jumps immediately which is not, W of 0 , t has a delta function at t and then it is 0 thereafter it is not true okay.

So, what is the correct expression now for this W tilde of n , s we took into account a jump here a jump here and jump here a jump here with this convolution but we must be careful we want W of n , t is the probability density the probability that exactly n jumps have occurred in time interval t. So, nothing should happen here, so if I call this the probability that nothing happens here call it Phi of t.

So W of 0, t actually you have to multiply by that that also is in the convolution right. So, the correct expression is this times 1 - Psi tilde of s over s that is the correct expression for W tilde of course you put n = 0 you end up with this. So, we are all set we have an expression for W tilde and therefore we know what H is and let us put that in and see what happens.

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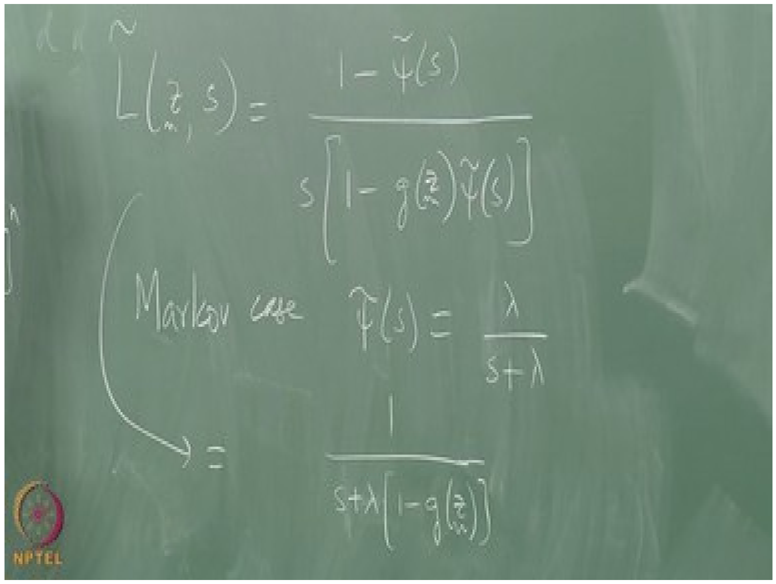

So, we have H of Zi t = summation n = 0 to infinity W of n t is i to the power n but this is 1 - so therefore H tilde of Zi is = summation n = 0 to infinity W tilde which of course is very conveniently 1 - Psi tilde of s over s times Zi times Psi tilde of s to the power n which is a geometric series so that is trivially sum and this gives you 1 – Psi tilde of s divided by s times 1 - Zi times Psi tilde of s and therefore finally we have our L of z , s Laplace transform this is the generating function for P of j , t.

Now I take it so class transform instead that is = 1 - Psi tilde of s divided by s times 1 - not Zi but g of Zi right Psi tilde of s and that is the Laplace transform with respect to time of the generating function of my probability distribution P of j, t quote unquote all I have to do is to invert this transform and to invert the power series itself I mean the Laurent series itself but in principle that is a solution that actually finishes it completely explicitly.

What we need to know or now do is to ask how do we extract information from this in principle we can solve this once again but let us first check the Markovian case quickly and see whether this works or not. So, again Markov case Psi tilde of s = lambda over s + lambda so what does this give you for L this is = 1 - this guy is s over s + lambda and the s cancels out. So, it is 1 over s + lambda 1 over 1 - g of Zi titled of s.

So, there is a lambda sitting there over s + lambda so let us take this and write it as s + lambda - this guy and this s + lambda goes away and I take out this lambda and I get 1 - g of Z and of course we can invert this transform in time 1 over s + anything s + a constant independent of s is e to the - that constant times t right.

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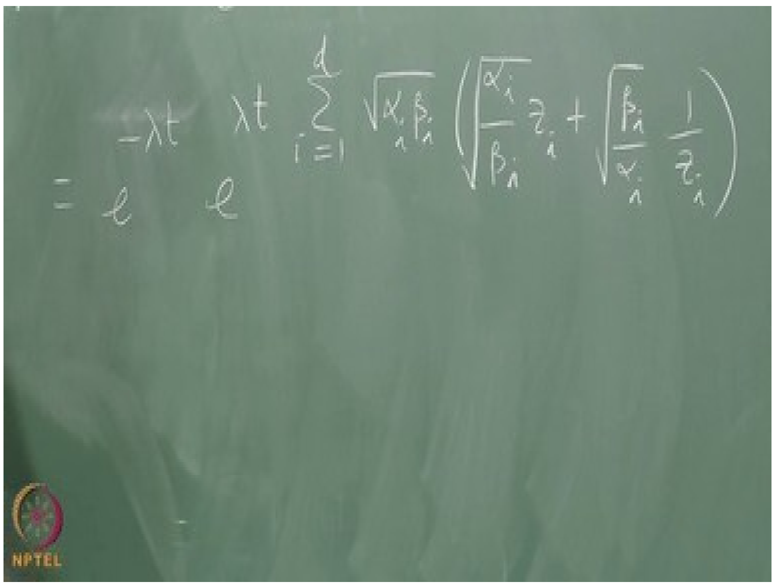

So, that immediately tells us so it says tilde L of z t = e to the - lambda t e to the lambda t that is it of course if you look at the case we are looking at this is e to the - lambda t on the cipher cubic lattice e to the lambda t summation i = 1 to d alpha i zi + beta i zi inverse and what is the usual trick well take out alpha i beta i so write this as alpha i beta i times alpha i over beta i square root zi + square root beta i over alpha i 1 over Zi and that is the generating function for pardon me for which one.

Yes, so what is the function that you get this is a generating function for the modified Bessel function we know that goes right so recall exactly this Kellum distribution.

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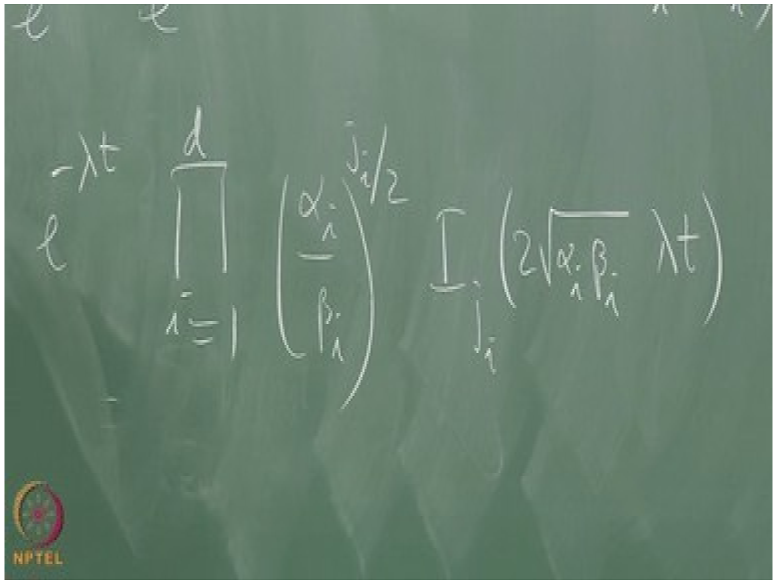

So, we call that e to the power is Zi over 2z + 1 over z = summation j = - infinity to infinityi j of Zi is z to the power j and that is the modified Bessel function on the with the integer order and i - j is identically = i + j so this is a product is = e to the - lambda t product i = 1 to d should not forget this factor so alpha i over beta i to the j i over 2 that is sitting there and then I j sub i of twice root alpha i beta time.

So, it is a product of these Bessel functions that is the solution to the biased random walk in a hyper cubic lattice, the Markov in case. So, this general answer this guy here reproduces that immediately. But you do not always have such a simple function to invert unless this is 1 over s + lambda or something simple this is not such a trivial matter to invert this always. In general the solution could be much more complicated.

In particular we are interested in the asymptotic behavior of both the mean displacement and the mean square displacement other variants now we know by symmetry that if you do not have a bias in the problem if each alpha = beta = 1 over 2d then there is no bias at all and the mean displacement should go to 0. Let us see if that emerges let us see if that emerges from this general case even without inverting the transform.

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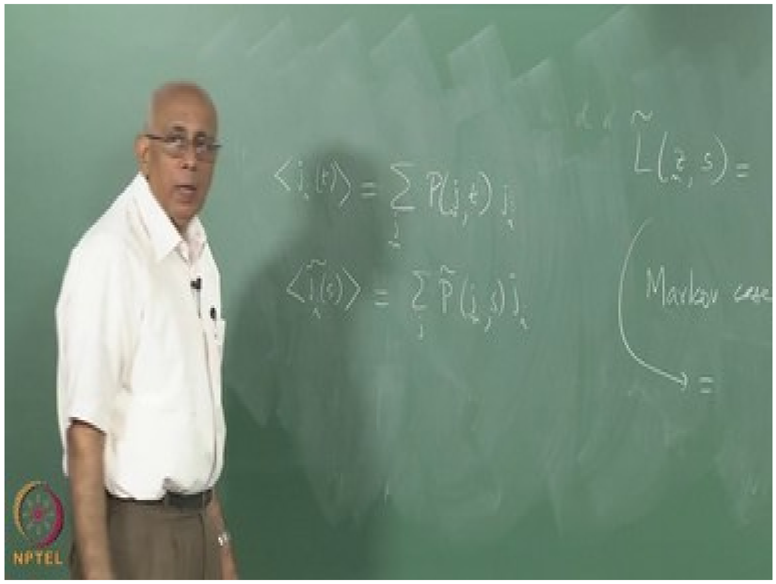

You see what I want is j any 1 of the j so ji as a function of t this is = a summation over all the j's P of jt time j’s of i by any particular ji. So, the transform of this guy ji of s transform in t is with a P tilde appears over j P tilde j’s of subprime i need to pull down a ji how do I do that from the generating function.

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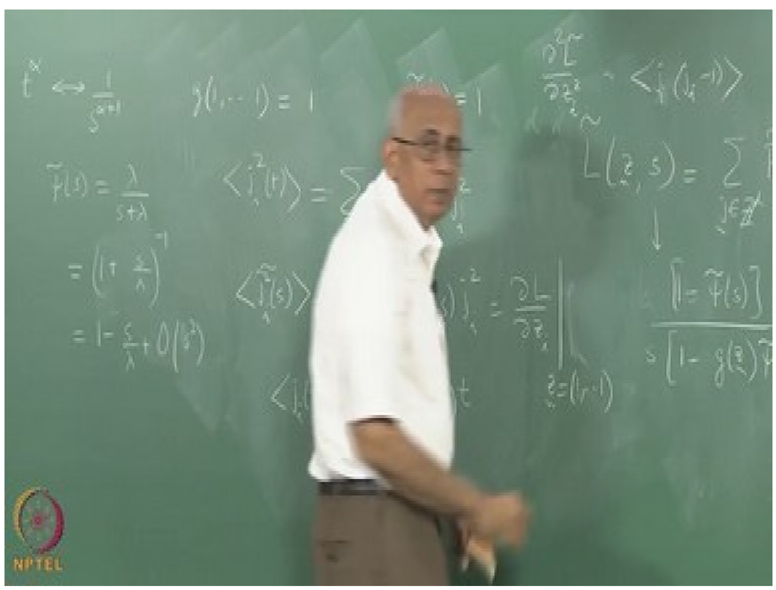

We already have a generating function because this fellow here if you recall this guy = summation over j element of d dimensional lattice P of j, s and then z1 to the j1 zd to the jd, I want to pull this down and pull the 1 power of ji down what should I do differentiate with respect to that particular z and then set all this as = 1. So, this is = Delta L over Delta zi at all the z = 1, so this is 1, 1, 1, 1 all they all z components are = 1.

Now when I differentiate that what is going to happen recall that we had a formula for this fellow here this was you have to remind me of that what this formula was 1 - Psi tilde of s in general divided by s times 1 - now I am not very sure what really happened there was a g of z and then Psi tilde of s right and we have to differentiate this and then set z = 1 all there is that components = 1. You differentiate this guy remember that so if you differentiate this fellow here Delta L over Delta zi d1.

It is going to have all these factors as before hmm but it is going to have a g prime of z on top with respect to that particular z and this g so I would not belabor the point very much because if you put g all the z is = 1 what do you get here. You get summation alpha + beta which is = 1. So, it is very clear that g of 1 = 1 right. So, after you differentiate you are going to put g = 1. So, you are going to get 1 - Psi tilde divided by this fellow squared you put g = z = 1 it cancels 1 factor between top and bottom.

But you want to have this factor here and remember the corresponding z depend i dependence was in the form alpha zi + beta over zi + other stuff but when I differentiate this I get alpha zi - beta over i squared and I put all zi is = 1. So, it is immediately clear that this fellow is going to be proportional to alpha i - beta i that is going to come out as a factor indeed it should because if there is no bias in that direction that particular coordinates average value must be 0.

So, this is where it is coming from moreover if it is a Markovian walk we know it must be linear and that emerges also because what is Psi tilde of 0 = that is the integral of Psi of t from 0 to infinity so it must be 1 right, so this must be 1. But now I ask what a Psi tilde; so you got to be careful when you put s = 0 this blow vanishes here. So, you have to ask what is the small s behavior of Psi tilde of s?

Now it is clear that in the Markov case if Psi tilde of s = lambda over s + lambda this is = I pull out a lambda = 1 + s over lambda inverse this is = 1 - s over lambda + order s square near s = 0 be careful because we have got factors like 1 - i tilled office so we better be careful. So, now look at what happens if you differentiate this guy gives me alpha - beta multiplied by a Psi tilde.

But that is = 1 if I put s = 0 this gives me a 1 over 1 - Psi tilde between this and the square of this so that gives me a factor s this gives me an s. So, the whole thing for small s is going like 1 over s squared what is the inverse Laplace transform of 1 over s squared it is a ramp function it is t. Because we know that the t to the power alpha the transform is 1 over s to the alpha + 1. So, if you have large t behavior like that you have small s behavior like this, that is a useful thing to remember.

So, you have got a 1 over s squared so the whole thing it will tell you that ji of t average for t tending to infinity will go like this in general. As long as Psi tilde of s has an expansion 1 + order s as long as they do it this factor is not relevant I mean the fact that in this case it happens with this is not relevant. So, if Psi tilde of s is analytic at s = 0 the leading term must be 1 at s =1 0 by conservation of probability.

The next term if it is analytic must be of order s there is a Taylor series which exists then you immediately get this result. Now look at what happens to diffusive behavior in the case of diffusive behavior let us let us we must look at the variance but let us be simple and look at just the mean square displacement let us put the bias factor = 0. So, all alpha is = beta i's and so on. And then this g of z just becomes zi + 1 over zi some over 1 over 2d outside common factor.

So, let us look at the unbiased case and see how diffusion comes out so we want ji squared of d, so ji squared of s has a square here you still have this but now you want twice ji you want to differentiate right what should you do if you differentiate once you are going to get a ji if you differentiate a second time you are going to get a ji times ji – 1.

So, second derivative is really d 2 tilde over d zi 2 is going to give you this moment ki times ji – 1. But that is ji squared average - ji average but if there is no bias ji average is 0.

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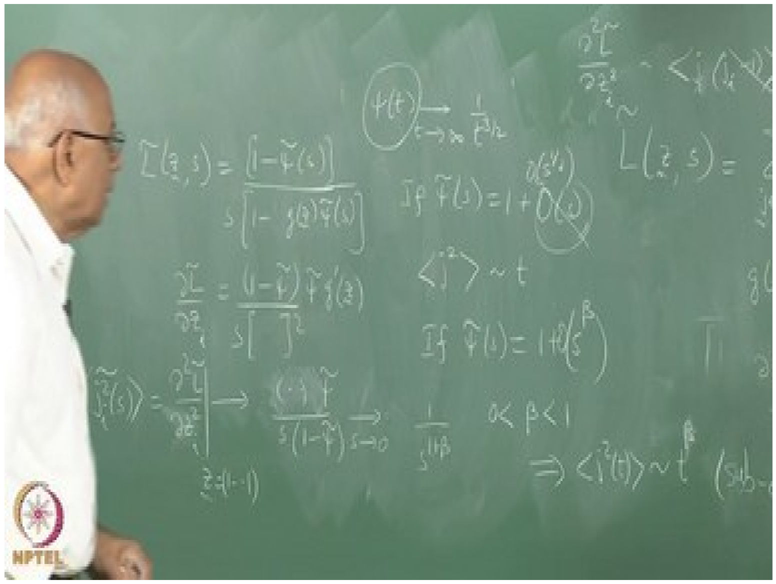

What does that imply that says g prime remember this no bias implies g prime of z = 1 = 0 because each time you differentiate this fellow you get alpha - beta over z squared but if alpha = beta this is 1 - 1 over that square you put z = 1 it is goes to 0 right. What I am saying is g of z is 1 over 2d alpha 1 + z1 + beta 1 over z1 + dot, dot, dot. If I differentiate this guy in the in the unbiased case it is just this.

If I differentiate this g prime of zi = 1 over 2d if I differentiate with respect to 1 of these ends its zi - 1 over zi squared this is Delta, so g prime if I put z = 1 vanishes in that stage therefore it is sufficient to take the second derivative of this guy and that will tell me what the behavior of this is at long times immediately. So, let us go back and quickly do that I have L tilde of z is = 1 - Psi of s over s times 1 - g of z Psi tilde of s.

I have to differentiate this twice I differentiate it once I am going to get a g Prime on top this follows squared and then I am going to get Psi tilde times g prime I use prime for the partial derivative with respect to 1 of the zi’s for the moment I differentiate second time I differentiate this guy and I am going to get another g prime factor on top. But g prime is = 0 at z = 1 so that does not contribute.

And in the second derivative it is only the second derivative of this that contributes but what is the second derivative of this it is just 2 over zi 2 and I put z = 1 so it is just some number 2 some finite number. So, this guy goes the second derivative of this fellow at z = 1 1 this goes to 1 - Psi tilde times a number here and s into 1 - i2 the square this goes away that is it times the number into some number times that there is no s dependence.

That this is now what this is = ji squared what does it do for smallest that will tell me what this guy doesn't lock the inverse transform does it long t what does it do it small what does this fellow do at s = 0 this is 1 so this is harmless and you just have this. So, all we got to do is to look at this small s behavior of this guy here. If Psi title of s = 1 + order s analytic then this gives you an s here you get an s squared and the inverse Laplace transform of s squared is t diffuse the behavior.

You have normal diffusion everything therefore depends on the smallest behavior of this or the large t behavior of the waiting time density if it is exponential or anything which has got a Laplace transform which is analytic at s = 0 the first term is order s other than 1 then immediately you have diffused the behavior in general. But suppose it turns out that if Psi of s = 1 + s to the beta order s to the beta less than 1 not analytic like square root of s.

For example what is going to happen is that this whole thing is going to go like 1 over s to the 1 + beta because there is 1 cancels and you have s to the 1 + beta and what will it imply for the mean square displacement which is sub defusing this is the famous anomalous diffusion. It is entirely therefore dependent on the long tail behavior of Psi of t because what does it mean if for instance Psi of t went like 1 over t to the 3 halves.

What would it mean for the Laplace transform you have to take the Laplace transform of t to the alpha where alpha is – 3 halves, so that is 1 over – 3 halves + 1 which is zi to the half. So, this will immediately tell you that this fellow here would not be true you would get s to the half that will immediately lead to sub defusing behavior which says the mean square displacement will go like the square root of the time rather than the time itself.

So, the root mean square behavior will go like t to the 1 4th in that case it is slower than normal sub diffuser and there is a huge literature on anomalous diffusion the practical implications of anomalous diffusion etcetera. We will say a little more about this but this is 1 mechanism by which you can see a huge variety of behavior will emerge and it is essentially exact an arbitrary lattice and we have seen that everything depends finally on this waiting time density.

What its long tail behavior if it has a long tail then you have a normal s diffusion. If on the other hand it cuts off exponentially then its Laplace transform is analytic at s = 0 and then you do not have any problem you have normal diffusion. The process is still non-Markov as soon as you do not have an exp1ntial waiting time density but it could lead to all kinds of anomalous diffusion if this has a long term t.

So we have done this without actually writing down a master equation for P of j, t which we cannot in the normal in most non Markovian cases so we did this by this trick of writing down generating functions and then looking at the statistics of the time the step distribution separately from that the geometrical problem of anymore where you are on this lattice. We can go ahead with this and find first passage time distributions current properties and so on and so forth.

The matters of detail but I thought this will give you some idea of how anomalous diffusion arises how this non analytic behavior entices let me stop you.