Selected Topics in Mathematical Physics
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Module - 10
Lecture - 25
The Diffusion Equation (Part I)

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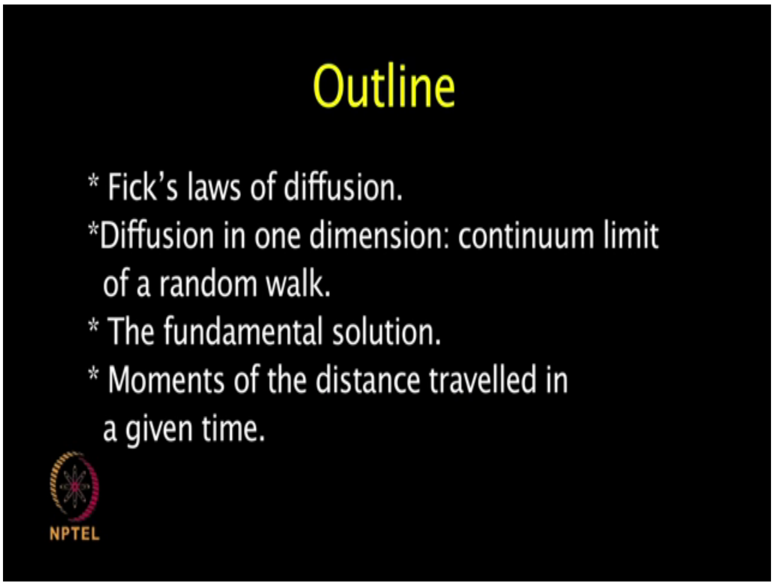

We start now with the study of the diffusion equation which is the next in the progression of mathematical physical equations of relevance. The reason I chose the diffusion equation rather than the wave equation is technical one, this is the little easier to handle and then we move on from here to the wave equation. Now, the equation itself is fairly easily return down, but we need little preamble about where it is come from, what the physical significance of this equation is?

This is going to be a slightly different kind problem than the problem of Poisson's equations which typically we had kind of charge distribution. We try to find the potential here; you have an operator which again involves the del squared operator, but there also time that comes in here. So, it is a partial differential equation which involves both space and time variables. Now, if you recall from elementary a physical chemistry i guess you have told that when you have substance like a solid put inside diffusing substance put inside liquid for instance ink in liquid.

Then, this due to molecular collusions this ink spreads out is diffuses throughout. So, if you have a concentration of some molecular species inside some solvent this would typically spread out and diffuse and uniformly find itself throughout the liquid as in the case of ink in water. Then, there are certain empirical laws which tell you how this process occurs and these are known as Fick's laws of diffusion the first of laws and what are these laws for?

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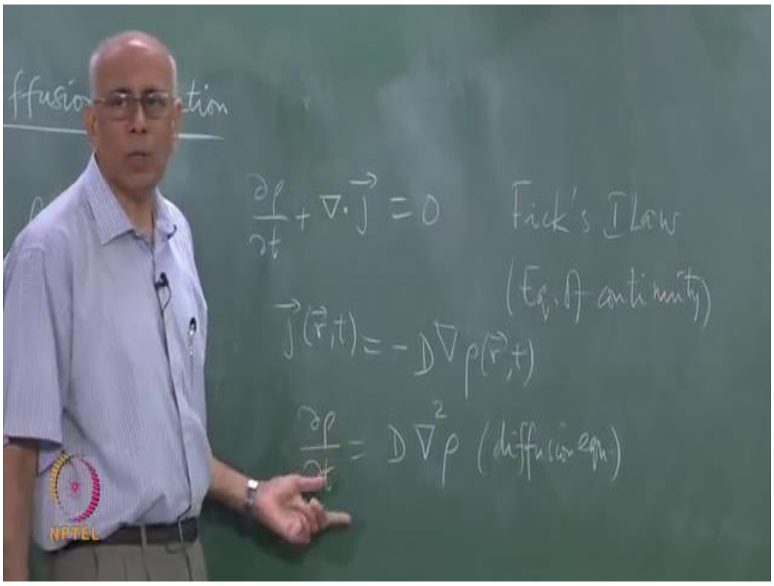

You would Like to find out the concentration rho as a function of space and time of certain species, and this function this concentration is suppose to obey an equation called the diffusion equation which easily derive if we make two assumption. The first is this material never disappears it is always there, so you write in equation of continuity for it right away which says delta rho over delta t plus the divergence of a current equal to 0. This gives you the flux of this substance per unit area per unit time in any given direction this is Fick's first law it is also the equation of it is just the equation of continuity conservation of matter if you like.

The real physics comes in the second law because you would like in equation for a rho a loan there for you need something which relates j to rho. The statement made is empirical observation tells you the diffusion process this current flows from a region of higher concentration towards the region of slightly lower concentration. So, the assumption is that j as a function of r and t is equal to the gradient of this rho of r and t, but with the minus sign to show that is the going direction in which the function increases most rapidly. It decreases the most rapidly and of course your dimensions are completely wrong here these two have different dimensions.

So, you fix that by multiplying by constant here call the diffusion constant, now this if you like this number of molecules or maths depending upon the density of looking at per unit volume this already length here one over length sitting here. So, these quantity as and these is amount of material crossing per unit area per unit time. Therefore, this thing here has dimensions of square of the length divided by t if physical dimensions of d or l square over t. Now, this d depends on what kind of diffusion of numerical value depends very much on what kind of diffusion we looking at if it is diffusion in an electrolyte it is one set of values in the gas.

It is a very different set inside a soil it much lower and so on and so far this d ranges over huge number of orders of magnitude in practice whatever it is if you put back in here. Then, it immediately says delta rho over delta t equal to d times del square of rho and that is the diffusion equation. We need to solve this with some boundary conditions with some kind, we also need to specific the initial condition because it involves time first order in time.

By the way this is the first of the equations which introduces irreversibility in the problem because its first order and time it is not reverse its not reversible this equation is not invariant time and the t goes to minus which is another way of saying. Let us put in a drop of infuse in the water, then we come back in technical terms the facts of the second order in space and first order in time means that is classified what is called a parabolic differential equation as a differential equation Laplace's equation was. So, that makes a huge difference, but we will see what the differences are?

Now, what are like to mention is the following instead of looking at the concentration this is the macroscopic picture this is after all the average number of molecules in unit volume at any given time. Instead of looking at the concentration, we could ask for macroscopic interpretation of equation in terms of what each molecule does and each of these molecules of this diffuse substance is being hit by whatever in the flow in the medium in random direction. So, then we cloud asked what is the probability that any instead of time given molecule some position are and some time and it essentially above basic same equation these probability density same equation.

We can also see this by going to this diffusion equation starting with the random walk model for a particle, and just to keep algebra simple just to write a line in one dimension and to generalized higher dimension.

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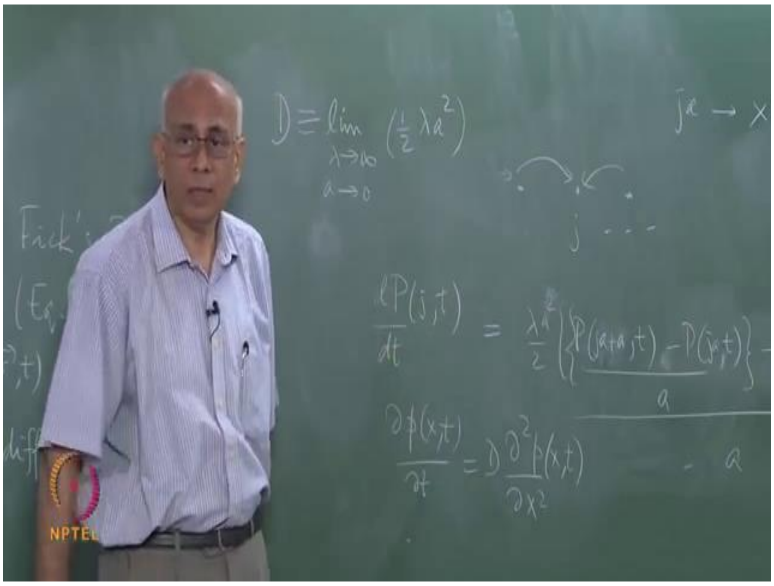

So, if you recall on line in fact look at lattes on a linear lattes if we look at unbiased un biased random walk, we labeled the points on the linear lattes by this integer j j running is minus infinity to infinity and ask the questions. Suppose, this random walker tosses the coin, if it is heads and most of the rights if it is tales most of the left probability equal probabilities in the simplest instance. Then, we ask this question of what is this quantity equal to d p over d t that is how does the probability that is the point j at time t how does the change as a function of time. We got the master equation it is a this is equal to the average rate at which they jump circle that is a quantity lambda.

Then, there was a half, because that is the rate lambda over two related which jumped probability rate jumps to the right and lambda to left. So, this trended out be lambda out to it could jump either form the right or from lift to this point, so you either had flip like this like this and a from here of course he could jump out. So, that was a lost term and that was minus twice, this was the master equation for the probability of being ad a point j at time t. Then, he start all this which some entails condition say you started at the origin at is equal to 0 in which case p of j coma 0 just at chronic delta j coma 0.

Now, how do you go from here to diffusion equation well what I am go to argue is that this lattes constant which have taken to one here is gone to 0 having a unique steps point 1, 2, 3 etc and introduce lattes constraint. So, call this distance a m going, let a to 0, so become a continue line and a same time am go to little lambda go to infinities or the main time between jumps go to 0, the mean rate of jump is lambda. So, the mean time between jumps is one over the call it some tau for something, so am let lambda go infinities and a go to 0 and ask what happens to this equation here this as you can see, so j time a go to x continues.

Then, a probability will became a probability, then city and leave our work out intimate steps out, but as you can see I could have written at in the flowing way I could have written this as this minus p of j coma t minus p of j minus coma t and by j. I really mean j a plus a because that the lattes constraints this is j a coma t this j a this j a minus a on this side that is multiply by a and divide by an a here this. The first difference and a is going to go to 0, so what is that? What does nothing go to this is going to go become write their better of the of x coma t this going to go left. What happens to take the difference of those two divide by another await the second write.

So, multiply by another a different a square in the hole things could be divided by another a processed to the limit appropriately. Then, it is cleared this probability will become a probability then city, because now have a continue its variable and equation will read delta p of z coma t o delta t equal to d d to p is d x and what is d equal to d limit lambda d a goes to infinities a goes to 0 such that half lambda is defined it.

So, that should go away from discrete random walk discrete lattes to diffusion process on a continue side now you can do that same. Thing to higher mention and it is very obvious immediately that you had square lattes. For example, you can jump in here from in this side see their three dimensions from all three directions this is gone to became a del squared operator.

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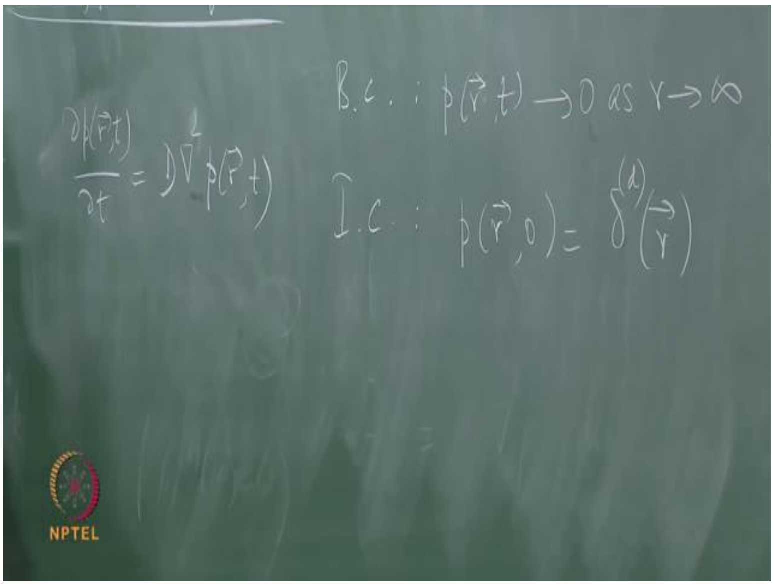

So, instead of this you get in a equation which is essentially say delta p of r coma t or delta t equal to b del squared and that is the diffusion equation. So, there is the microscopic picture of each particle undergoing some kind of random process random collusions defecting or average the concentration itself that is the more microscopic picture essentially. So, let us solve this equation let us see how we gone to what is boundaries condition we should per what should initial condition we should per. So, this is gone to depend on this one is system and what kind of boundary put let us take the natural boundary condition.

Let us stay the space in finished and the boundary condition is the probability then city 0 infinities 5, 9, and then p of coma r t 10 to 0 is r 10 to infinities in any direction so that all boundaries condition. We need than initial condition so boundary condition b f r coma t and 0 o might as solve the problem in 1, 2, 3 or any number of damnation. We will do same thing as a before solve in dimension, space dimension in one shot and what the initial condition that we like put where this depends. It depends on what your initials profile is what your initial construction profile is, but let us start it is with the picture of the single particle at the origin.

Since it in infinities space and put good any point at the origin any 5, 9, so let us started origin in the dimensional space and the lest go in this, so the initial condition is p of r 0 equal to delta function at the origin without any lose analyses change. Some are not does not matter and all solve into d dimensions, so this del square id the d dimensional the passing the d is 1, 2, 3 etcetera. So, that is the problem you want to solve and so well post problem having initially condition should we have to any condition to unity in these conditions. So, the first step this problem is a initially value problem so little t transforms 0 to infinity.

I want the conversion of partial into some kind of multiplication what times from should I take past trans from not full trans form because t is 0 from infinity. So, lapace transform from respective the t value and fasitial variable to off course once minus to infinity module directions. So, then natural thing is to take the ferial infinity, let us do that into two steps. Let us first say of p r some of t equal to p delta r s that is the first step that is put into the right the pass transform of b r from t easy equal to p delta of r minus p equal r from 0 in unit that is initially condition put d, del square this del square is because respective special by does not anything to the placing, it goes right through.

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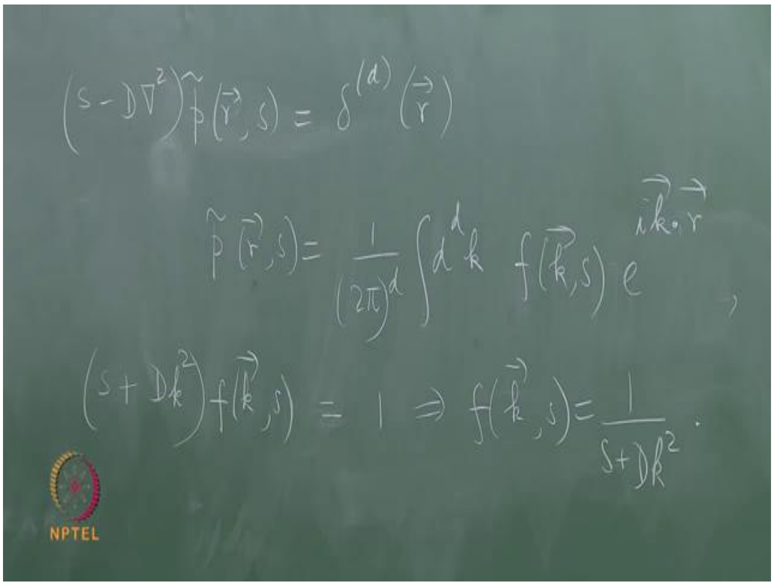

So, we will put that in and end up with s minus b del square p tilda of r s equal to delta d that was the initially condition. So, I moving to that I still have the del square, now I do a transforms, so let me write lets you some other symbols already finished of this till there here. So, let me write p delta of r comma s equal to 1 over 3 pi to power into b k f of k comma s that is the ferial and off course stands for f of k comma of s easy equal to d d r it was the minus i k delta f p this is ferial stands for and then what happens in del square?

It is hit only this and give minus case quit time to same thing here, so end of with s plus d k square on f of k and s deducted here. The Fourier of placing of now of the p and this del square of e place from minus c square becomes this square b k square and that on right on side the Fourier stands for that is the function and what is that my coral stands for conventional 1 over 2 by to the d d k is i k y a data function. So, this is equal to which off course immediately implies that f f k and it could be 1 over s plus b k square right. Now, we have job of invite this from this invite Laplace stands form we need to invite to know which one, we do first we did the Laplace one and then Fourier.

So, which would you do now first? In try, but in Fourier stands form you have to do this you have to do this you have to put to this and you have to do this integral with respective kind here. You have to do d dimensional integral that is found the k minus one top even though this is function. Only one case do you got do angler integration and there is and there pawls in the nominator and in look into function of case the pawls are plus or minus square root of and the movement of you s or d the movement of root of us. This means that is the branch point in their playing and you cannot do the invasion because incredible complicated you end of having fine the of transform rood of us this is very bad news on other hand suppose you invert Lpalace transform what would happen?

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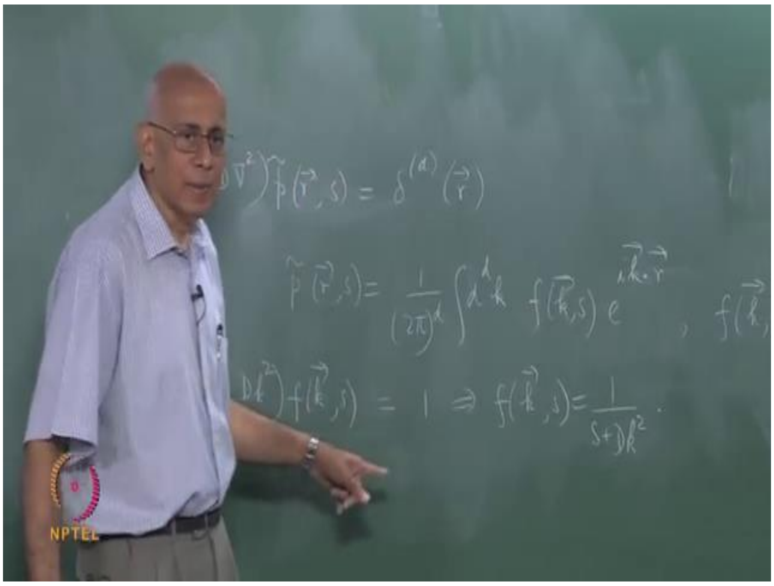

The Laplace's stands form is a 1 over s plus a and Laplace transform one over a plus a is e power minus a t.

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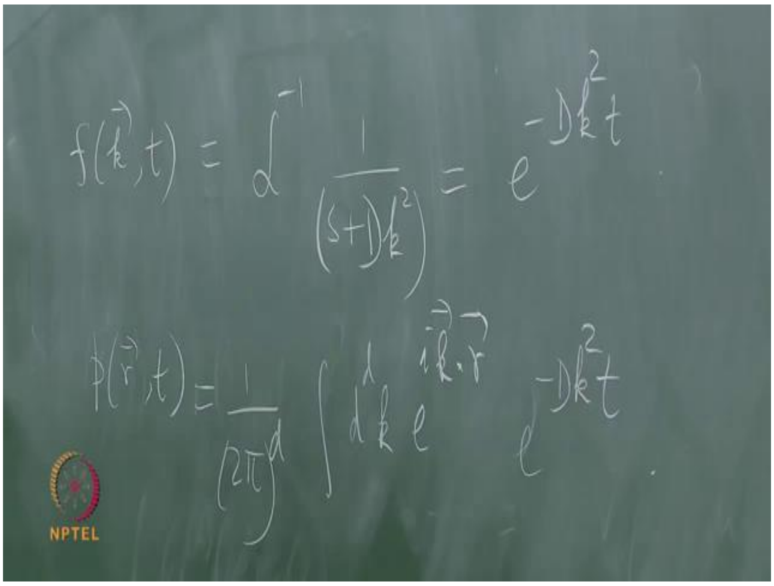

This immediately tells you that the inverse Laplace transform let me call as f f k t want a better word m, I should call to some tilde so that you know that is the stands for some kind. So, f f k t without delta in this place this kind here easy equal to Laplace in the 1 over s plus d k square and this is e to the minus b that is it. This does not depend upon the dimensionality of space you just plus stands form invited in that is it. Now, we need to invite Fourier transfer form that is all, so we have to do p f r comma easy equal to 1 over 2 by to the of d is b k k dot r sitting there.

Then, the invite this minus d this also looks pretty bad because you see you got this factor here which is gone give you angler integral and so on, but you also have the case and you have to do it, what is the k square mean? Remember that k square equal to k 1 square plus k 2 square d square d dimensions some squares of incase how suggest to do this integrity, what coordinated system I choose m? I should choose because these thing factors immediately these choose fellow coordinate as one template to when you are stuck completely really got a mess with. If I choose Cartesian coordinates, it is exactly the same integral for one of every one of them all multiple together because what does this imply?

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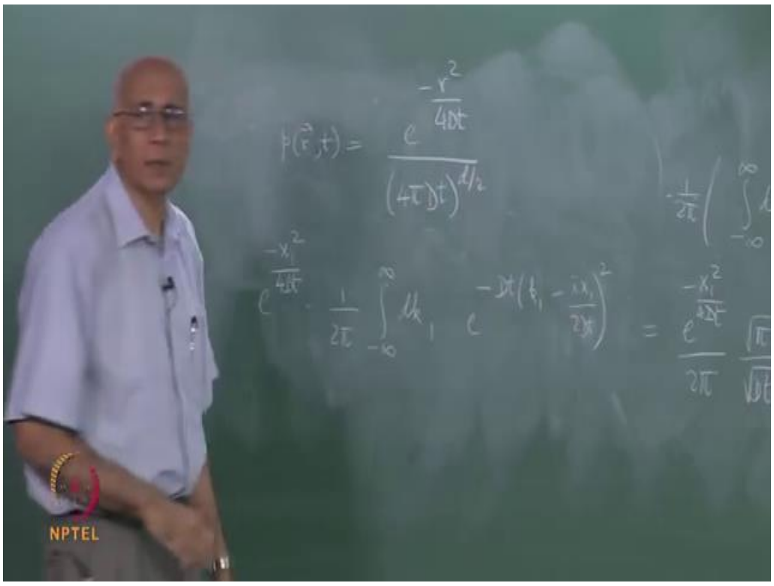

P of r comma t equal to 1 over 2 pi to the power b and then there is a d k 1 e to the i x 1 this is the minus d k 1 square t and second thus multiply just do a minus time into the b. So, just the integral the same integral with x 2 and x 3 and so on right integral d k into the i k d x b minus b k d square. What is the range of integration these of Cartesian coordinate its minus, so it is same integrate in which the final x 1 or x 2 or x c that is it, but doubt in integral in do that because that take a typical integral here. This, here integral minus to the infinity d k 1 and take a 1 over 2 5 along with the going to here as same factor for each integral minus the d t the k 1 square minus i k one is b t x 1 and then you complete the square.

So, this becomes i square k 1 square x 1 square sorry not k 1, so its i square x 1 square over 4 b minus i square x 1 square and what is this its k 1 minus i x 1 over d t the hole square i by x 1 of 2 d t to the hole square. So, its k 1 minus i x 1 the hole square and then very carefully you got a keep this, now this became a plus sigh, but there is an i square here and out comes e to the minus x 1 square over 4 d t outside the integrity. So, e to the minus x 1 square over 4 d t outside the integral multiplying this whole thing that is it that is this integration to each of these an fact at 2 phi and what you done is this factor that is equal to this.

Now, this requires a little careful handling buts this doable you shift variables you shift k 1 minus this over here then the counter of integration moves up parallel to the x axis, but the contribution from the two ends of the rectangle it can showing to be 0. You can bring back to the real axes when I stick y and I will not to try that out independently, but this just a in integral. You can write this again independent of this its equal to e to the minus x 1 square over 4 d t and 1 over 2 pi and integral minus infinity to infinity e to the minus d t k 1 square that is like e to the minus a x square in the answer is square root of pi over here 1 second yeah student.

Whether it also d t multiplying it, there is also d t multiplying it so that canceled d t here so that is it, so this is equal to e to the minus x 1 square over 4 d t divided by square root of let us take this 2 n 4 phi d t. Now, we have an answer for the full probability distribution it is just this guy here x 2 square x 3 square etcetera, but you add up all those exponents and you get r square.

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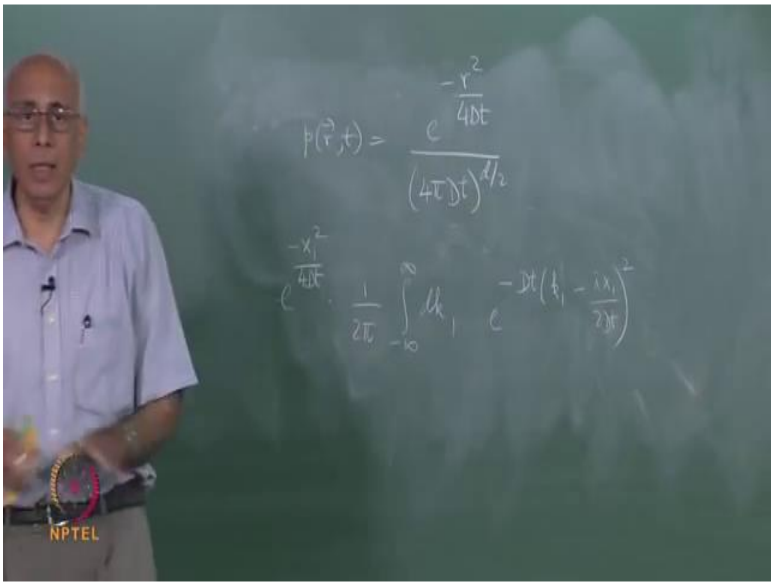

So, it is says this finally, says e to the minus r square over four d t divided by 4 phi d t and that is it and that is the solution this is the fundamental Gaussian in solution to the diffusion problem, what does it look like, what does it profile look like? That is easy to answer you can see that it is a Gaussian in R and width increases nearly the variance increases nearly in time.

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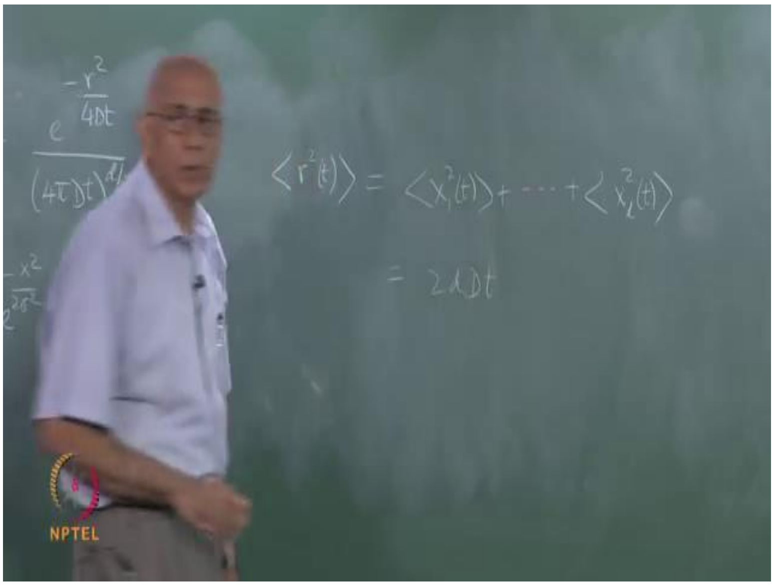

Then, what is the average value r square this as the function of t what is the definition of this guy by the way what is the average value of vector r what you think it is going to be i will be 0 because you have e to the minus r square. Then, you take x square plus y square z square etcetera, you take the average value of x or y or z that is in odd function immediately which is reasonable because if you doing push back. Then, on the average and displacement will be actually 0, but mean square displacement is to be another story altogether because this thing here is equal to the average value of x 1 square of t plus etcetera plus the average value of plus d square of t and what each of these guys?

Well, for each of them the other variables are irrelevant, so you could write is as e to the minus square over 2 four d t 4 phi d t to square root that an normalize goosing. I ask what the mean square value is? Does the mean value is 0 and the answer we know its two d t because it normalizes Gaussian. So, we call we call that in a Gaussian distribution when you have square root of 2 phi sigma square e to the minus x square over 2 sigma square this is the variance here or in this problem the means square simply because the mean itself is 0. So, it immediately this is four d t is, so the sigma square is 2 d t and that true for each of these 2 d d t.

So, if you are in two dimension in its four d t if you are in three dimension its 6 d t and so on and one dimension you get the 2 d t again. This is true for all time at all times this problem is so simple that is defuse a behavior sets in from t is equal to 0 onwards t is equal to 0 onwards and you get this linear behavior in for the mean square displacement. So, root square displacement proportional to the square root of the time, which is the typical of dip use a behavior typical of randomness due to this molecular.

You can compute all moments from here because you have a nice all its moments exist you can compute every one of them. So, what you done is to solve this deputation equation with the given initial condition the initial condition was that you are delta function distribution at the origin, but that precisely the equation satisfy by the green function.

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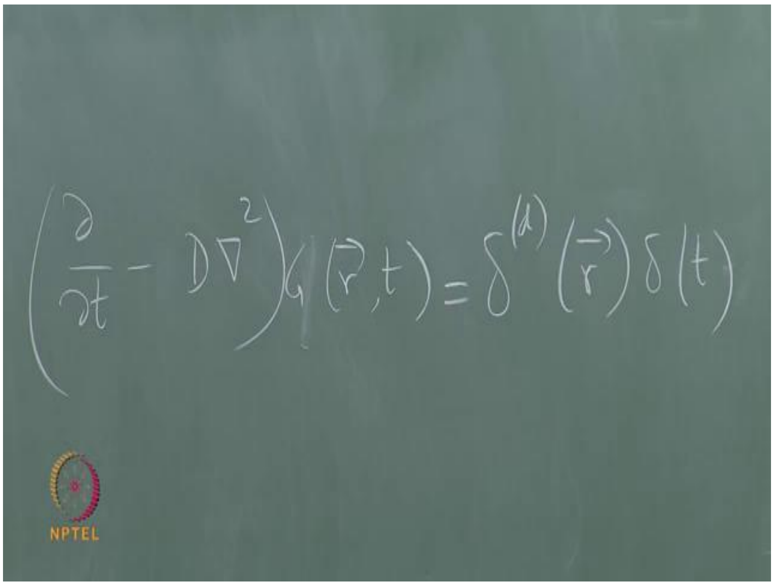

So, you see if you have we found delta over delta t minus d del square p of r comma t for the form this was true, but the green function for this problem would look like this delta of t. That would be the equation satisfy by green function for this problem right, but this is the problem which have sought here.

So, in solving the delta function initial condition at the origin, we actually solve the general problem. So, what happens if you start with an arbitrary initial distribution because this equation in variant under translation in time you shift into t minus t 0 nothing happens you shift r minus r 0 nothing happens then? What does this problem give you?

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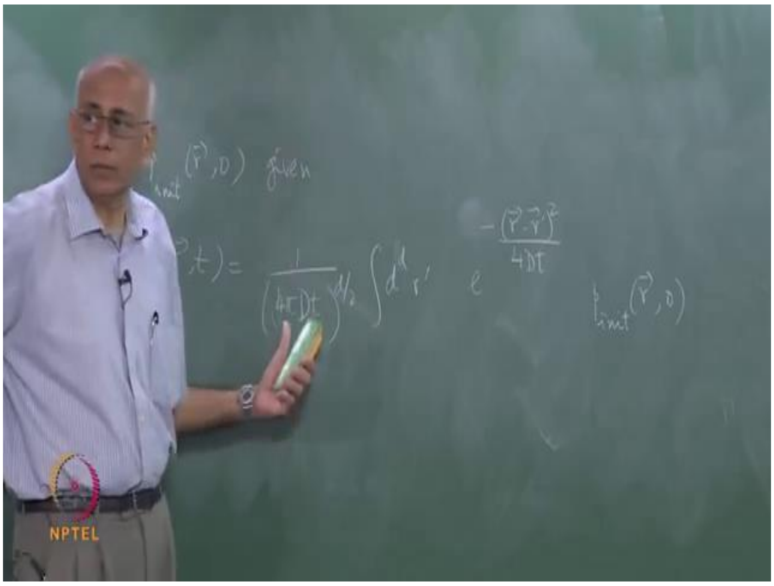

Suppose I had t initial of r 0 given and now I go to ask you, I give you this at t is equal to 0 and ask what is the probability distribution at any finite time t. So, what would you say you just integrate over the green function times this guy here, so this would implies that p of r comma t equal to 1 over 4 phi d t to the power d over 2 integral d d of r prime of all directions times e to the power minus. Now, you would say r minus r prime holes square over 3 d t multiplied by p initial of r prime that is it.

That is the whole power of the green function that is y kept saying with you finding the fundamental green function fundamental solution to this equation because this now gives you over this Gaussian. If you integrate your initial distribution however it be you get final answer for the actual distributer. Suppose, I had started not at t is equal to 0 buy just change the t t at t is equal to some t not what would the solution look like for t greater than t naught.

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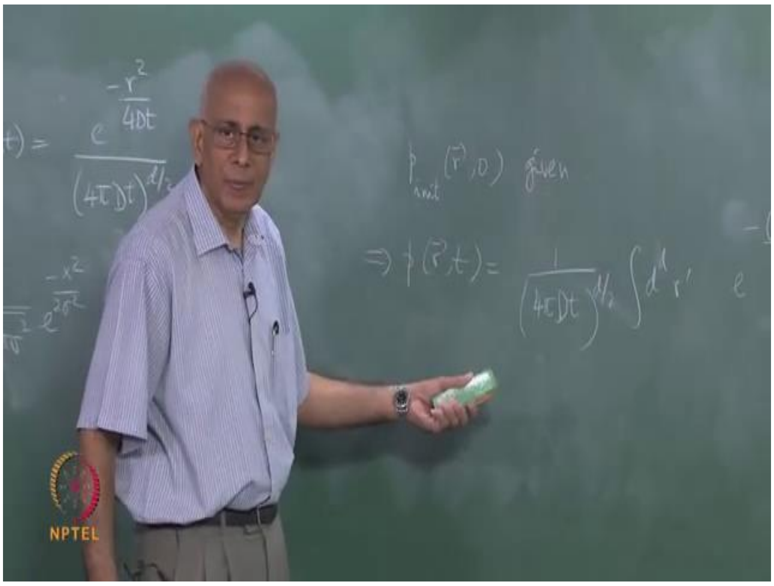

So, my initial point is sometime t not and I want the solution for all T greater than equal to t not t equal to t not is singular how would I write? What would I write here? T to t minus t not this is t minus t not and this is t minus t not that is it, so this fundamental Gaussian solution is the green function for the diffusion operator delta over delta t minus d square. Essentially, what we found now off course real diffusion problem you would like to also put boundary condition you would like to say this is an finite medium and what happens in the ends of the medium and so on.

We need to able to say suppose all thing is trapped inside a you want to say that flux zero does not go out its stay inside then you need to put certain conditions inside and there after interest are down, we will discuss a little bit some detail, but let me ask you.

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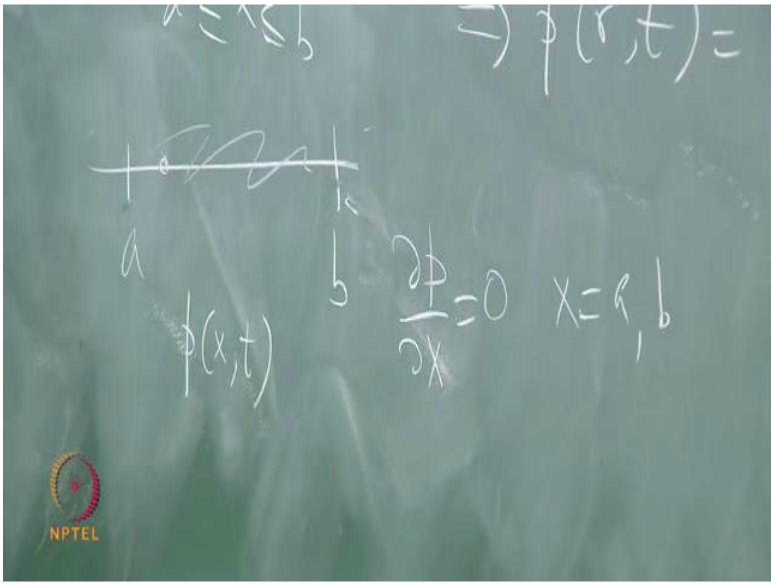

Suppose you had a one dimensional problem and you are confine to this region inside here the diffusion is confined to this region. What condition you would put at this end or this end? On this or on the concentration road like what condition goes both side same both side same. No reason why they should be the same really etcetera as in I means if I start at some point here and I imagine this random problem it is clear that I am likely to hit this earlier I am going to hit that right. So, the profile need not always be uniform off course you wait a long enough time I expected to be uniform.

We will to the we will see how it comes about, but it easier to think about it in one dimension what would be the boundary condition appropriate boundary on p of x comma t at the barriers at the barriers, suppose you had a here and b. So, you have a less than x less than equal to be and you are solving for p f x comma t given that you started at some point or some point inside here, what would be the appropriate boundary condition? On this p at the points a and b what would be the physical boundary condition given that the material does not go out does not escape, what happens? That partial hit the boundary its get reflected back gets back here, so the appropriate condition is not that p 0 at the ends as you do in the problem of a box.

When you put in the infinite potentially you say the patens you say the wave function are 0 at the ends these are knows at the end here we would not say that its reflected back. So, what is physical what the physically happen at their is no flux of particle across there is no current across and what is the current given by in this problem delta p over delta x. So, the boundary condition you would impose is that at this end the condition impose the delta p over the delta x is equal to 0 and x equal to a n. These are called a reflecting boundary conditions, on the other hand suppose you say the particle dies as soon as brought in paper on the both sides. Then, what would you say this is nothing disappears as soon as it takes the end say p 0 at the ends the moments.

That comes at the particles becomes extinct then u impose p equals to 0 in the sense then one side reflecting one side absorbing and so on and so forth. So, you can right down the proper boundary condition. If we start 0 somewhere yeah initially p will be 0 at the boundary, it will also say that it will be always be 0 right why do you say that you want to ask what happened this is the argument you are following. So, see if you put p equal to 0 and x equal to 0 at the end points does it remain 0 at all times, but remember differential equations has to be satisfied. So, what the ultimately meant will see the solution means what it does what meant by imposing the boundary condition on the differential equation the equation itself is satisfied their at that point.

You would like to have some physical condition put at that point and difference between these two called you 0 that is what you call a boundary condition in a qualitative way. We will see, will write down the solution when you have a boundary and see what happens at that point is p identically 0 at that point the answer is no, but the flux is 0 at all times is that need to, so partial differential equation. We are property in the sense this is another variable this also t variable, so will write this down, but condition is already there I was not intending to do that, but will try to solve this problem by the method of a measures. One can do that by one dimension you can always solve such problems by the method of images because what it does is to give the function satisfy the proper boundary condition.

Ultimately, what we do in the electro static as well right what do you how do you argue you the potential is unique once its well post problem and you have a solution. Then, you replace the surfaces on which you fix potential etcetera by fictitious charges by which will give you the same potential on those surfaces. Then, you will say there is a equivalent problems and therefore, will solve one and solve the other and write the solution down by uniqueness the uniqueness around going to do the same thing here.

So, the method of images is not restricted to the static problems it works for all these green function problems and we will try to find out the green functions. When you have two barriers reflecting or absorbing etcetera in terms of what the method of images that do this very briefly. If you have an example of absorbing i here, then you pretend that there is another walk here such that when this point meet at will kill each other, and you will write the solution for that that will give you guarantee to the right answers, we will do that.