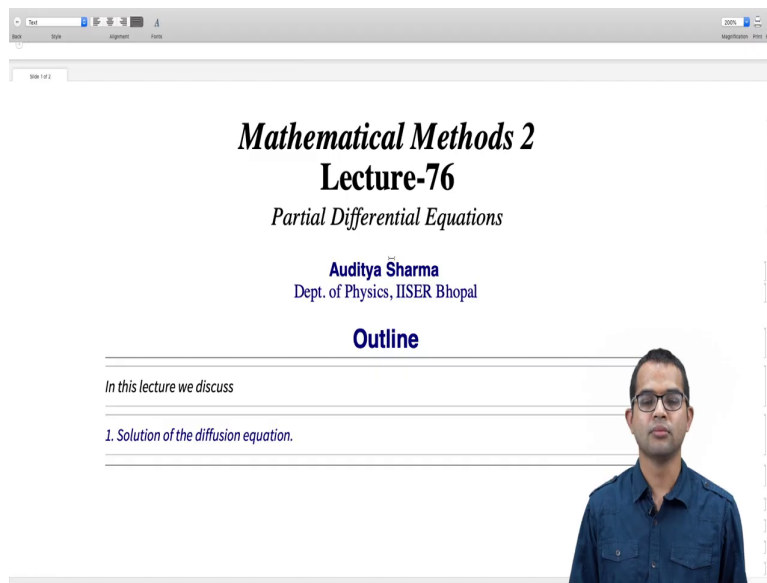


Mathematical Methods 2
Prof. Auditya Sharma
Department of Physics
Indian Institute of Science Education and Research, Bhopal

Module - 08
Partial Differential Equations
Lecture - 76
Solution of the diffusion equation

(Refer Slide Time: 00:19)



Mathematical Methods 2
Lecture-76
Partial Differential Equations

Auditya Sharma
Dept. of Physics, IISER Bhopal

Outline

In this lecture we discuss

1. Solution of the diffusion equation.

So, in this lecture, we will solve the diffusion equation in 1D using a very general approach.

(Refer Slide Time: 00:29)

Solving the diffusion equation.

Let us find the solution for the one dimensional diffusion equation:

$$\frac{\partial p(x, t)}{\partial t} = D \frac{\partial^2 p(x, t)}{\partial x^2}.$$

It is a partial differential equation, and to solve for it, we must specify both the boundary conditions and the initial condition. Let us say that the particle is initially localized at the origin, so we have:

$$p(x, 0) = \delta(x).$$


As time progresses, we would expect that a wider and wider region of space will have non-zero probability of finding the particle. So we impose the natural boundary conditions:

$$p(x, t) \rightarrow 0 \text{ as } x \rightarrow \pm\infty.$$

The time variable starts from zero, while the spatial variable goes from $-\infty$ to $+\infty$, so to proceed, we take the Laplace transform with respect to the time variable, and a Fourier transform with respect to the spatial variable. Let us denote $p_L(x, s)$ to be the Laplace transform of $p(x, t)$ with respect to time, and $n(x, s)$ to be the Fourier transform of $p_L(x, s)$ with respect to space. Then the diffusion equation becomes:

$$s n(x, s) - n(x, 0) = -D \frac{\partial^2 p_L(x, s)}{\partial x^2}.$$

5:06:12



So, the diffusion equation in one dimension is just $\frac{\partial p}{\partial t} = D \frac{\partial^2 p}{\partial x^2}$. So, the initial condition that we will choose is such that it will actually allow us to consider other kinds of initial conditions as well. We will come to that later on. But let us say that our particle is localized at the origin at time $t = 0$. So, there is no chance for the particle to be found anywhere else at time $t = 0$, it is localized at the origin.

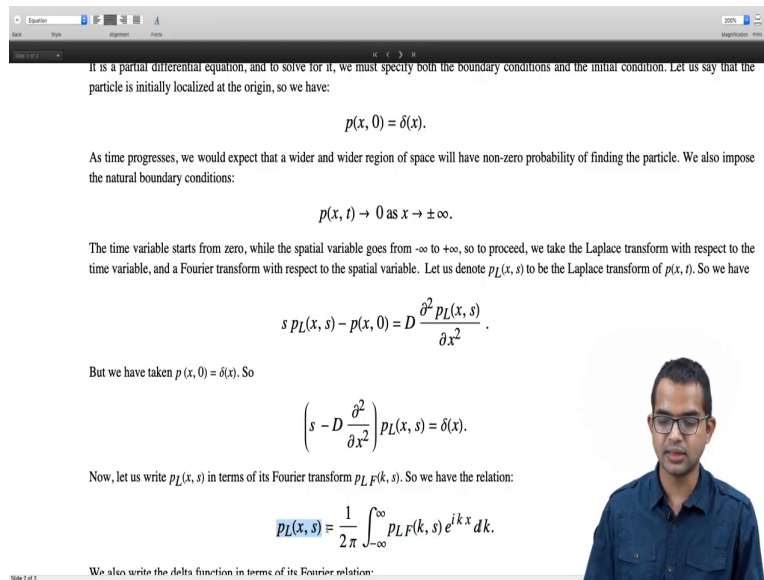
Now, we write this down as $p(x, 0) = \delta(x)$. So, this is the density, probability density is just given by $\delta(x)$. Now, as time progresses, we would expect that a wider and wider region of space is going to be covered, so there is going to be a non zero probability of finding the particle.

And so we also impose these natural boundary conditions which are very physical. So, the probability of finding this particle you know goes to 0 as x tends to plus infinity or minus infinity. So, as you go further and further away from the origin, the probability of finding this particle is going to be vanishingly small.

So, the time variable starts from 0, and the spatial variable also goes from minus goes from minus infinity to plus infinity. So, you solve this problem by taking a Laplace transform with respect to time which goes from where the variable t goes from 0 to infinity, so the Laplace transform is a suitable transform to take here. And on the other hand, with respect to the

spatial variable which goes from minus infinity to plus infinity, we will take a Fourier transform right.

(Refer Slide Time: 02:17)



It is a partial differential equation, and to solve for it, we must specify both the boundary conditions and the initial condition. Let us say that the particle is initially localized at the origin, so we have:

$$p(x, 0) = \delta(x).$$

As time progresses, we would expect that a wider and wider region of space will have non-zero probability of finding the particle. We also impose the natural boundary conditions:

$$p(x, t) \rightarrow 0 \text{ as } x \rightarrow \pm\infty.$$

The time variable starts from zero, while the spatial variable goes from $-\infty$ to $+\infty$, so to proceed, we take the Laplace transform with respect to the time variable, and a Fourier transform with respect to the spatial variable. Let us denote $p_L(x, s)$ to be the Laplace transform of $p(x, t)$. So we have

$$s p_L(x, s) - p(x, 0) = D \frac{\partial^2 p_L(x, s)}{\partial x^2}.$$

But we have taken $p(x, 0) = \delta(x)$. So

$$\left(s - D \frac{\partial^2}{\partial x^2} \right) p_L(x, s) = \delta(x).$$

Now, let us write $p_L(x, s)$ in terms of its Fourier transform $p_{LF}(k, s)$. So we have the relation:

$$p_L(x, s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} p_{LF}(k, s) e^{ikx} dk.$$

We also write the delta function in terms of its Fourier relation:

So, let us start with finding the Laplace transform. We will denote this as p_L of x comma s instead of from p of x comma t . So, we take a look at this differential equation, and then when you take the Laplace transform. On the left hand side, it becomes s times p_L of x comma s minus this p of x comma 0 you know as we know from Laplace transform theory.

And on the right hand side, it is just basically the same; in place of p of x comma t we write it as p_L of x comma s right. It is just this function alone which is getting whose Laplace transform is being taken. So, it is just simply replaced by a different function here. And in place of t , we have s here.

Now, I mean p of x comma 0 is of course given to us to be just delta of x right. So, we can write this as s minus D times d^2 by $\text{d}x^2$ p_L of x comma s is equal to the initial condition which is just delta of x . Now, we want to take the Fourier transform of you know this function as well. And so it is convenient to actually write p_L of x comma s in terms of its Fourier transform.

So, right the relation that we are going to invoke here is actually the inverse Fourier transform. So, p_L of x comma s can be written as 1 over 2π integral minus infinity to plus infinity p_{LF} of k comma s so the e to the ikx dk right. So, p_L of F is it has both where it is

the function where both the Fourier and the Laplace transform has been carried out. So, p_L of x comma s can be replaced by this expression.

(Refer Slide Time: 04:02)

$$p_L(x, s) = \frac{1}{2\pi} \int_{-\infty}^{\infty} p_{LF}(k, s) e^{ikx} dk.$$

We also write the delta function in terms of its Fourier relation:

$$\delta(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk.$$

Plugging back in, we have:

$$\left(s - D \frac{\partial^2}{\partial x^2} \right) (p_{LF}(k, s) e^{ikx}) = e^{ikx},$$

so

$$(s + Dk^2) p_{LF}(k, s) = 1,$$

and thus

$$p_{LF}(k, s) = \frac{1}{s + Dk^2}.$$

Taking the inverse Laplace transform, we have

$$p_F(k, t) = L^{-1} \left[\frac{1}{s + Dk^2} \right] = e^{-Dk^2 t}.$$

So, and then we also use this integral representation for the delta function which is simply given by this integral right. So, if you plug this stuff in, so we have on the left hand side s minus D times $\text{doubled squared by } dx \text{ squared } p_{LF}$ of k comma s , then e to the ikx is the same as e to the ikx right. So, we have compared the integrands on both sides right.

So, this stuff has this integral, and then this stuff also has an integral. So, we can go ahead and write s plus Dk^2 $p_{LF}(k, s)$ is equal to 1 right. So, this is a simplification which ensues, and then we can go ahead and solve for p_{LF} of k comma s right. So, this is immediately seen to be 1 over s plus D times k^2 right.

So, all we have done is some simple jugglery involving you know taking a Fourier transform and a Laplace transform, and then simply arguing that the integrands are the same. And then some simplification and we immediately have s plus Dk^2 times this is equal to you know the e to the ikx can be removed, and it is this quantity is seen to be 1. So, p_{LF} of k comma s is equal to 1 over s plus Dk^2 .

Now, if you take the inverse Laplace transform of this function which is straightforward to do, we get e to the minus $Dk^2 t$.

(Refer Slide Time: 05:51)

$$p_F(k, t) = L^{-1}\left[\frac{1}{s + Dk^2}\right] = e^{-Dk^2 t}.$$

Now we have to just evaluate the inverse Fourier transform to get

$$\begin{aligned} p(x, t) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} p_F(k, t) e^{ikx} dk \\ &= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-Dk^2 t} e^{ikx} dk \end{aligned}$$

This is just a familiar Gaussian integral that we can carry out, and we get the answer:

$$p(x, t) = \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{x^2}{4Dt}}$$

This is a plausible result, and a familiar result. The probability density spreads like a Gaussian, whose variance goes linearly in time. The linear time-dependence of variance is symptomatic of diffusion, and is a result of remarkable generality.

Although we solved the above problem for the specific initial condition where the particle is initially localized at the origin, the solution holds the seed for the general solution of the problem for an arbitrary initial condition, provided the initial condition is localized. The key idea is to realize that we have not the Green's function since we have not

And then we have to take the inverse Fourier transform of this function to get back $p(x, t)$. If you do this, then you have this integral to be performed $\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-Dk^2 t} e^{ikx} dk$ which returns to us this familiar Gaussian integral. So, this is a Gaussian integral, and then you get a Gaussian as the final answer.

So, this $p(x, t)$ is equal to $\frac{1}{\sqrt{4\pi Dt}}$ and $e^{-\frac{x^2}{4Dt}}$. So, this is a plausible result and something which is familiar right. So, we saw the discrete version which had this Gaussian appearance, and indeed the general solution also is Gaussian in nature right.

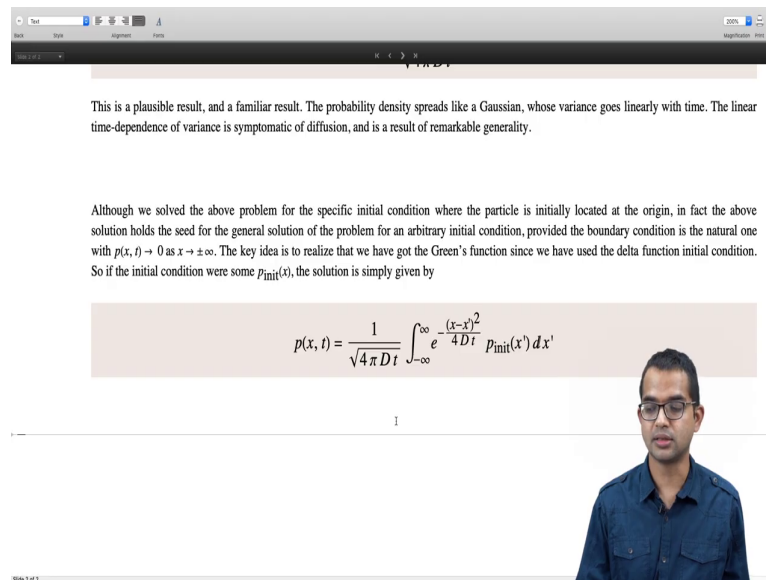
So, initially our particle was localized at the origin, and then we see that the probability density keeps on spreading. And in fact a key point to notice here is the width which is given by this variance. Variance goes as is linear in t , it is which is very its characteristic of diffusive motion right. So, what is called ballistic motion is characterized by you know the spread being proportional to time, whereas here it is the variance which is proportional to time right.

So, in diffusive motion, if you if a walker takes n steps you know he is typically covered and steps, whereas in ballistic motion it covers steps which is proportional to. And whereas in diffusive motion, n steps will probably give him only square root n of order of square root n ,

so that is symptomatic of diffusion; it holds in different dimensions, it holds in the continuous version, the discrete version and so on.

Now, we have solved this problem with some very specific kind of initial conditions, but this initial condition is such that it is amenable to generalization.

(Refer Slide Time: 07:58)



This is a plausible result, and a familiar result. The probability density spreads like a Gaussian, whose variance goes linearly with time. The linear time-dependence of variance is symptomatic of diffusion, and is a result of remarkable generality.

Although we solved the above problem for the specific initial condition where the particle is initially located at the origin, in fact the above solution holds the seed for the general solution of the problem for an arbitrary initial condition, provided the boundary condition is the natural one with $p(x, t) \rightarrow 0$ as $x \rightarrow \pm\infty$. The key idea is to realize that we have got the Green's function since we have used the delta function initial condition. So if the initial condition were some $p_{\text{init}}(x)$, the solution is simply given by

$$p(x, t) = \frac{1}{\sqrt{4\pi Dt}} \int_{-\infty}^{\infty} e^{-\frac{(x-x')^2}{4Dt}} p_{\text{init}}(x') dx'$$

1

Slide 1 of 1

So, in fact, if we pause and think a little bit what we have found is really what a Green's function right. So, we worked out the solution for the delta function. So, if you have some other initial condition, if your initial probability density is some p in it of x , so we can just use the Green's function prescription and immediately write down a formal expression for the full solution p of x comma t is going to be $\frac{1}{\sqrt{4\pi Dt}}$ times this constant from minus infinity to plus infinity.

Now, you have to shift this e to the minus x minus x prime of the whole square divided by $4dt$ times this right. So, this comes about just from Green's function theory which we are familiar with. So, the advantage with the initial condition we have considered here is that we have worked out the full solution here.

And therefore, it automatically leads us to a more general solution assuming these natural boundary conditions, which is that this probability must die down to 0 at plus x equal to plus and minus infinity. We look at some other interesting boundary conditions. And we will solve the same PDE by a different method in the lectures coming up, but that is all for this lecture. Thank you.