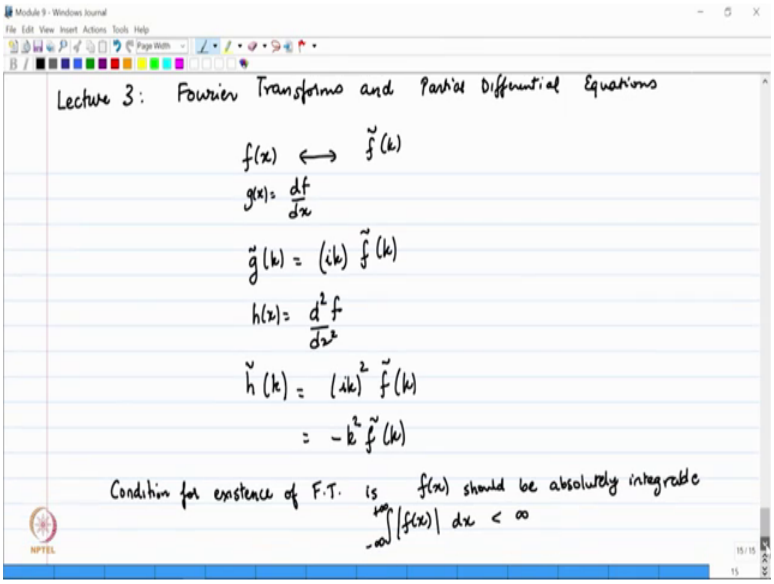
Advanced Mathematical Methods for Chemistry
Prof. Madhav Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Module - 09
Lecture - 03
Fourier Transform and Partial Differential Equations

In this lecture I will show the use of Fourier transforms in solving partial differential equations. I will take the example of partial differential equations, but you can use it for any differential equations.

(Refer Slide Time: 00:38)

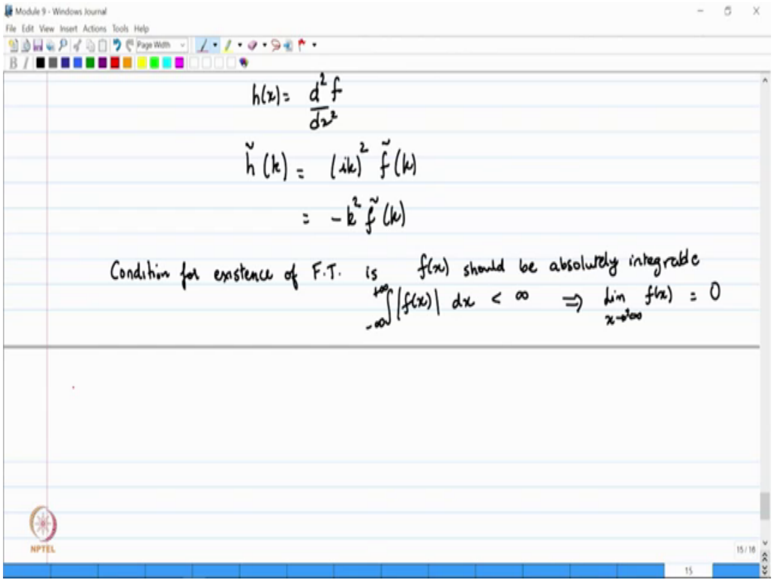


In the last lecture what we saw is that if we had f of x whose Fourier transform was f tilde of k and you had the g of x equal to D df by dx of derivative, then what we had was that we saw that g tilde of k was equal to i k times f tilde of k.

Suppose you had a second derivative; suppose you had h of x is equal to D square f by dx square then h tilde of k you can show that this is just ik square f tilde of k that is equal to minus k square f tilde of k. And in general, so every derivative introduces a factor of i k. So, if you take n derivatives you have to introduce n factors of i k. Now one of the things about Fourier transforms is that it should be absolutely your function should be absolutely integrable so condition for existence of Fourier transform is f of x should be absolutely integrable.

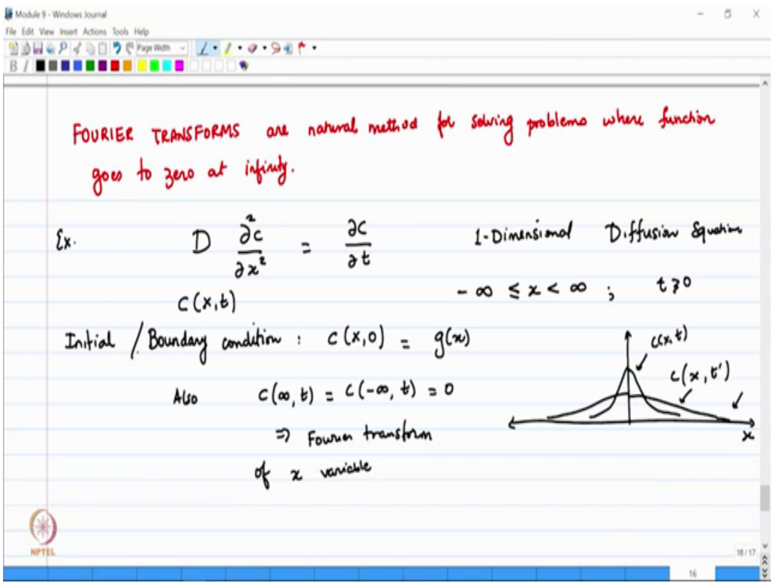
In other words your integral f of x absolute value of x dx from minus infinity to plus infinity should be less than infinity it should be finite. And this can happen only if limit as x tends to infinity f of x; x tends to plus or minus infinity f of x equal to 0.

(Refer Slide Time: 02:14)



So, if your function does not go to 0 then you can clearly see that the area under the function will go to infinity.

(Refer Slide Time: 02:39)



So, what I want to emphasize is that Fourier transforms are natural methods for solving problems where function goes to 0 at infinity.

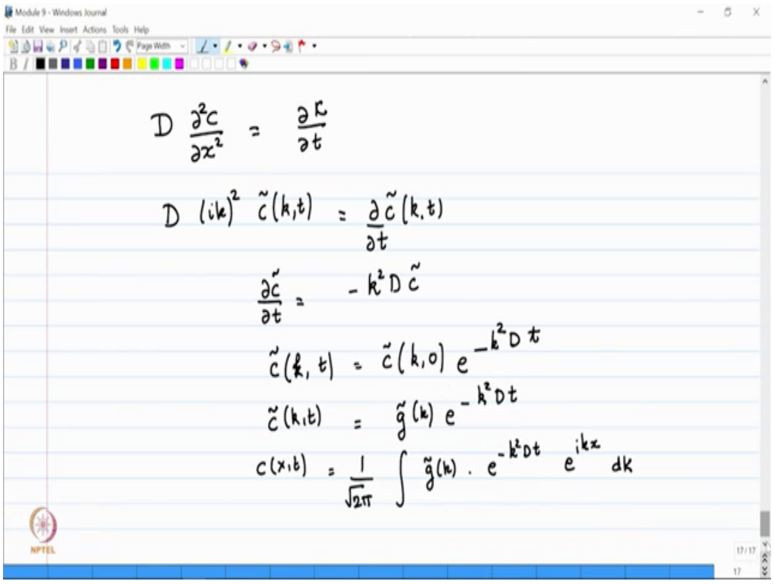
So, what I mean is suppose you have a differential equation let us take an example. So, example: suppose you had an equation D times dou square C by dou x square equal to dou C by dou t. And here you have this is this is called a 1-dimensional 1-D 1-dimensional diffusion equation the conditions are minus infinity less than equal to x less than infinity and t is greater than 0 greater than or equal to 0 and this partial. So, this is a partial differential equation it is called the 1-dimensional diffusion equation minus infinity is less than x less than infinity t has to be greater than equal to 0. Now the boundary condition C of 0 C is. So, remember C is a function of x and t C is a function of x and t. So, boundary condition I can write C of x 0 at t equal to 0 this is some function I will just call it g of x it can be any function g of x.

So, with this boundary condition can we solve this 1-dimensional diffusion equation and this will illustrate a lot of interesting properties of interesting things that come with Fourier transform. Now notice that let this also C of infinity equal to infinity at any time minus infinity at any time equal to 0. So, basically as x tends to infinity as you go very far away in space the C, C is typically the concentration of some species and that goes to 0 as when you go very far away.

So, typically the kinds of problems that we look at are those in where you start where you where you might start with some initial concentration. So, this might be C of x x t and when what you will have is that that concentration will spread out as t goes to infinity as C of x t prime. So, t prime is greater than t it might go it might look as something else, but basically it goes to what I wanted to say is that it goes to 0 at infinity.

So, such equations are naturally solved by Fourier transform. So, so this implies that you do a Fourier transform x variable. So, you do a Fourier transform of x variable. So, there are 2 variables x and t. So, you leave t as it is and do a Fourier transform of x variable. Now, let us get back to our equation.

(Refer Slide Time: 06:18)

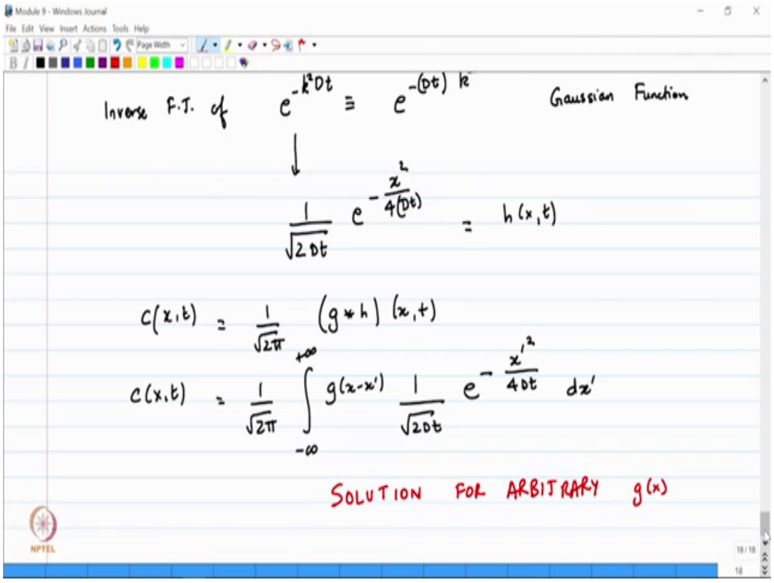


So, our equation D times dou square C by dou x square equal to dou C by dou t now if I do Fourier transform now Fourier transform of derivative is nothing, but or let me. So, if I take Fourier transform on both sides then I can through see that Fourier transform of second derivative as I k square and now I have C tilde of k and t this is equal to C tilde of k t dou by dou t. So, what I get is a differential equation in time.

Now I can solve this differential equation in time. So, I can write dou C by dou t is equal to minus k squared D C, I can write C is equal to or C of C tilde of t tilde here of kt is equal to C tilde of k 0 e to the minus k square dt. So, this is a solution of this differential equation and time and this is the constant of integration I have put as a pre factor to this exponent now C tilde of k 0 is we had a boundary condition C of x 0 was g of x. So, C tilde of k 0 is nothing, but g tilde of k e to the minus k square dt g is some function of k. So, g is some known function of k. So, you are you are told some function that way that depends on whatever initial condition you take.

I should say this boundary condition is an initial condition. So, this is the solution. So, so we have C tilde of k now if I wanted to calculate C of xt this is inverse Fourier transform of this inverse Fourier transform of this. So, so I just go ahead and calculate it one over root 2 pi integral what I want is a inverse Fourier transform of g tilde of k times e to the minus k squared dt e to the i k x dk. Now what you are doing is you are taking the inverse transform of a product of functions. So, we are going to use the convolution theorem, but first let us find the inverse Fourier transform of e to the minus k square dt.

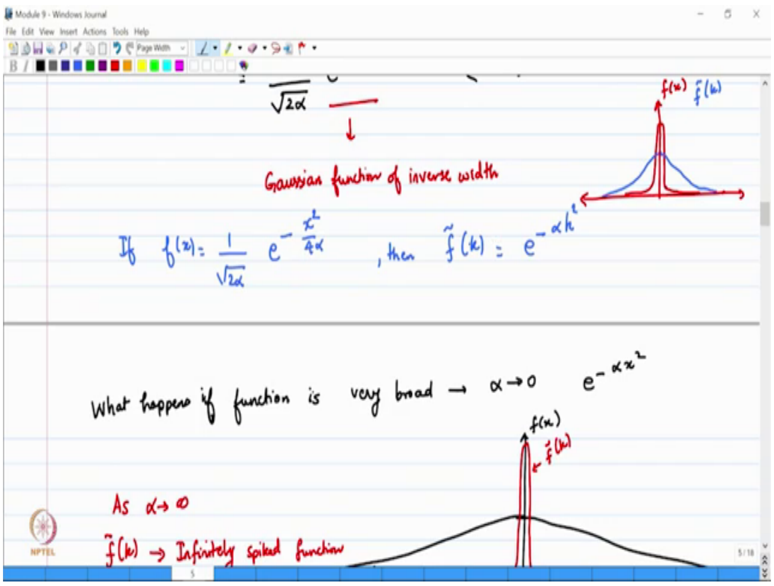
(Refer Slide Time: 09:33)



So, what is inverse Fourier transform of e to the minus k square dt and this we can use or we can use our result for Gaussian.

So, this is basically this is equal to e to the minus dt into k square this is a Gaussian and we know the Fourier transform of a Gaussian. So, we just go we just go to our Fourier transform pairs.

(Refer Slide Time: 10:18)



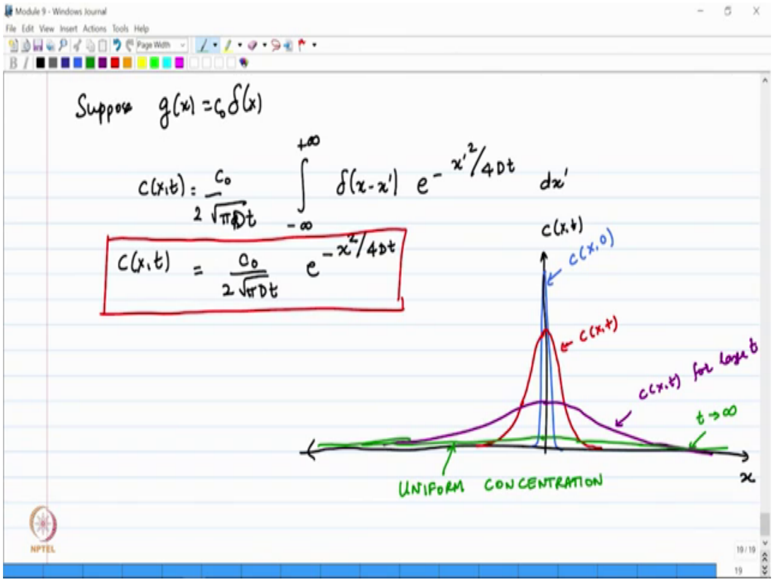
So, let us just go back to the first lecture of this module where we did the Fourier transform for Gaussian. So, what we said was that if I had e to the minus alpha k square then the Fourier transform is one over square root of 2 alpha e t to the minus x square by 4 alpha.

So, now instead of alpha I have D times t. So, I should have one over square root of 2 dt e to the minus x square by 4 dt. So, I just have, so this Fourier transforms. So, it will be one over square root of 2 now alpha is dt e to the minus x square by 4 alpha square alpha square is dt square 4 sorry not dt square x square by 4 dt. So, so this is the Fourier transform of this and now what we get is that we can write C of x t. Now we can use we can use the convolution theorem.

So, by using the convolution theorem what we will get is that if you if you let us go to the convolution theorem inverse Fourier transform for product of f tilde g tilde is one over square root of 2 pi times the convolution. So, if I take this product that we had. So, C tilde of kt was a product of g tilde of k and this e to the minus k square dt. So, we have the inverse Fourier transform of this. So, let me call this h of x. So, so this is just 1 over square root of 2 pi g star h of x h of x comma t.

So, this is one over square root of 2 pi now I will write it as g of x minus x prime times 1 over square root of 2 dt e to the minus x prime square by 4 dt dx prime from minus infinity to plus infinity. So, this is the solution. So, I mean this is an integral if you know g of if you know this function g you can perform this integral and what we have shown is how you can solve this partial differential equation using the method of Fourier transforms and we solve it for an arbitrary g. So, this is the solution for arbitrary g.

(Refer Slide Time: 13:17)



Now, let us look at an example suppose. So, so suppose g of x is equal to delta of x times let me call it C 0 C 0 times delta of x C 0 is a constant then you can see that C of xt is equal to. So, so let me take the one over 2 square root of pi D dt and what I have is integral minus infinity and I will take the C 0 outside minus infinity to plus infinity. Now what I have is delta of x minus x prime e to the minus x prime square by 4 dt dx prime. Now, integral over the delta function of some function is just the function evaluated at x prime equal to x. So, this just becomes C 0 by 2 square root of pi dt e to the minus x square by 4 dt. Now, this is the solution. So, what does this solution mean physically? So, the physical interpretation of the solution is the following.

So, what you have is you have let me show x here and you have C of x t. So, at t equal to 0 at t equal to 0 C of xt is g of x which is a delta function in x. So, at t equal to 0 it looks like this C of x 0 now as t increases it becomes a Gaussian now. Now if you take this Gaussian and put t equal to 0 then you basically the limit of this Gaussian as t goes to 0 is the delta function. So, as t becomes larger this Gaussian goes its width as t becomes larger the width of the Gaussian becomes more. So, your Gaussian becomes a wider function. So, as t becomes larger.

And this is C of xt as you increase t as you increase t it gets wider and wider C of x t for larger t and you can you can also see that as t goes to infinity as t goes to infinity your Gaussian. So, notice that the prefactor also is inversely proportional to t. So, as t becomes very large your pre factor becomes very small this becomes e to the 0 almost goes to a constant. So, as t goes to infinity your species basically spreads like this all over t tends to infinity. So, basically it goes to a constant.

So, this is a nice illustration of the use of Fourier transforms to solve. So, what you have is initially you have some species might be let us let us imagine that you have some species that is there only at x equal to 0. So, that is there only at a particular point and what we are seeing is how this how this species spreads in space as time goes as time increases. So, this is what the diffusion equation says. So, suppose I imagine that I take a perfume bottle and I open it. So, at t equal to 0 all the perfume at the initial time the perfume is all localized in one region, but as t as t becomes larger this perfume will spread and. So, this is how 1-dimensional spreading that you are seeing through this diffusion equation.

So, I will conclude this lecture here in the next lecture, I will mention about some other integral transforms such as the Laplace transforms and I will just mention how they can also be used to solve differential equation and in which cases you should use Laplace transforms which cases you should use Fourier transforms. So, that will be the next lecture of this module.

Thank you.