Advanced Mathematical Methods for Chemistry
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Module – 10
Lecture – 04
Recap of Module 10, Fourier Transform Solutions of PDE

Now let us just recap what we learnt in module 10. So, module 10 was dedicated to partial differential equations, and initially in the first lecture I told you about the different kinds of partial differential equations and I tried to give you some physical idea of where partial differential equations appear in various applications and the different kinds of partial differential equation.

In the second lecture I talked specifically about a technique that we learnt to solve partial differential equations that is call the separation of variables, and we said that this is the technique that basically converts a partial differential equation into an ordinary differential equation. And we looked at some simple examples of separation of variables and then in the third lecture which was a fairly long lecture, we took the two dimensional wave equation and we solved it using the separation of variables.

You for two different geometries one where we had a rectangular geometry and the other where we had a circular geometry, and what we saw was that in the rectangular geometry which has got sines and cosines whereas, in the circular geometry we got we got Bessel functions. So, we had to use the power series method which we learnt and when we learnt the solution of ordinary differential equations. So, we had to use that method to get the solutions for the circular problem and what we saw is that just by using spherical plane polar coordinate system, we got equations that looked very different that had additional terms and it did not look like a simple wave equation, it look more like a Bessel equation . So, that is what we did.

So, in some sense we have been doing examples throughout this module because as such there is only one technique that we actually learnt now. So, today I will do one more example which is the diffusion equation, which we have already seen when we saw Fourier transforms. So, again now Fourier transform is another technique used to solve partial differential equations. So, we will look at this diffusion equation how that is solved in using Fourier transforms. Now I have been doing all this you can find very good references in the mcquarrie chapter 16 is partial differential equation, 17 is Fourier transform.

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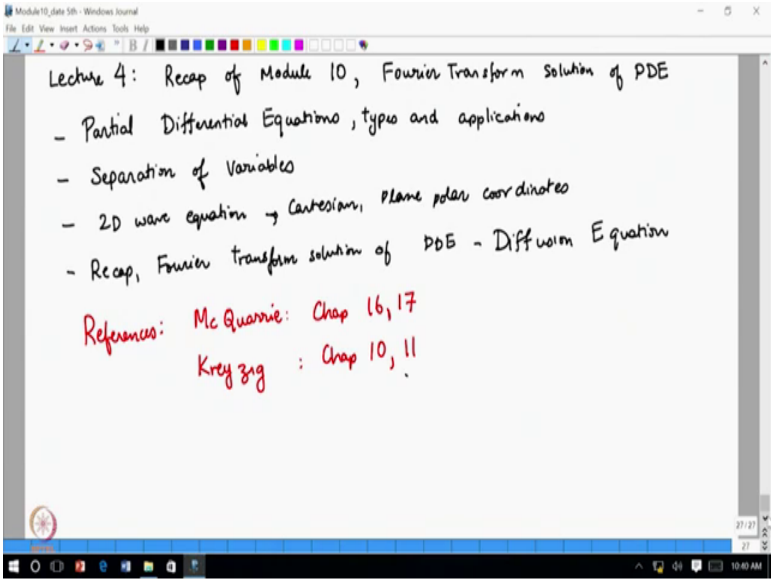

So, at least what we will be doing today you will find in chapter 17 in krey zig chapter 10 is integral transforms and chapter 11 is partial differential equation.

So, in these places you can find, but in any case these are very standard topics. So, you will find lot of sources on the internet and other places.

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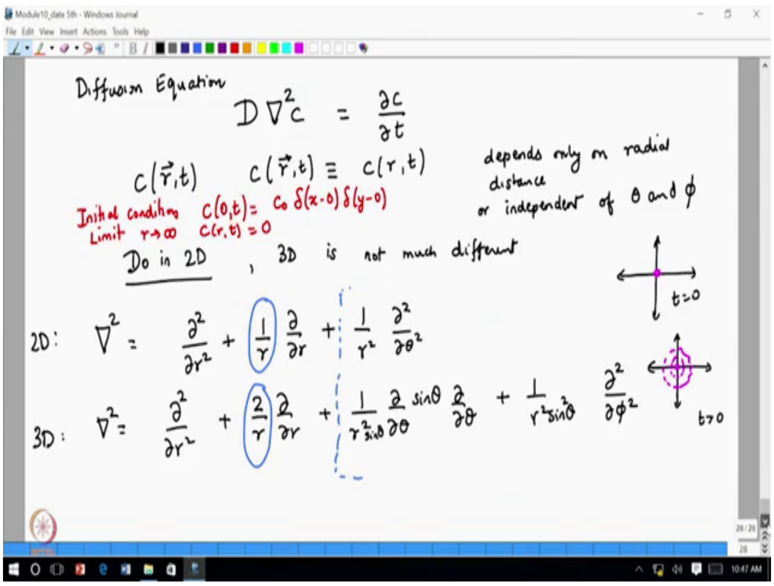

So, now, let us look at the diffusion equation. So, the diffusion equation is written as D times dou square c is equal to. So, D is a constant of positive constant and this is dou c by dou t. So, it is just a first derivative. So, in a wave equation you had a second derivative here in this equation you have a first derivative let us look at the following case ok.

So, we look at. So, c is generally a function of r and t and we will consider the case when c of r t can be written as c of rt so; that means, in other words depends only on a radial distance or independent of theta and phi. So, we look at this particular case. So, let us try to solve this now whether you solve it in 2D or 3D they will be a difference. So, let us take the case where. So, for simplicity we will do this in 2D 3D is not much different. So, just to emphasize. So, if you see the Laplacian. So, in 2D your Laplacian looks like D square by dou square by dou r square plus 1 by r dou by dou r, 1 by r square dou square by dou theta square. In 3D your laplacian looks like. So, if I expand it I can write it as dou square by dou r square plus 2 by r dou by dou r plus 1 by r square dou by dou theta of sin theta dou by dou theta plus 1 by r square sin theta dou square by 2 phi square r square sin theta here r square sin square theta ok.

So, that what we looks like; so if you have a function that is independent of theta and phi then this term will go away and in the in 2D in 3D all these terms will go away. So, these terms will go away. So, the only difference is only difference. So, if you take away the theta and phi parts. So, if I take away all these parts then I am left with only this part and the only difference between 2D and 3D is that in 2D you have 1 by r in 3D you have 2 by r. So, that is the only difference. So, we can do either in 2D or 3D you will get exactly the same solutions, but let us do it in 2D just for convenience and what we will do is we will put some more conditions we will put some initial condition.

C of 0 t is equal to delta or let me put C 0 times a dirac delta function of r minus 0, r minus 0 I will write as x, x minus 0 delta of y minus 0. So, delta of x delta of y and we will also use the fact that limit as r tends to infinity c of rt equal to 0. So, we will. So, we will also say that the c of rt goes to 0 as r tends to infinity.

So, what is the physical problem that we have? So, we have at t equal to 0 I have some concentration of some species I (Refer Time: 08:06) and the species is only at x equal to 0 y equal to 0. So, if I show it here. So, at t equal to 0 everything is right at the origin this is t equal to 0. So, all the species is let me do it in a slightly different color. So, everything is right at the origin, as t goes as t becomes greater than 0 what will happen what you would expect to happen due to diffusion is that this the species that was there only at the center will spread out it will spread out, but if you go very far away you would not have any species it will go to 0. So, that is the idea.

So, it is spreading out from the center and it is eventually it will go to 0 very far away. So, that is the picture. So, this is t greater than 0. So, this is the two dimensional diffusion that we are going to analyze. So, now, let us explicitly write out the equation. So, we have see ok.

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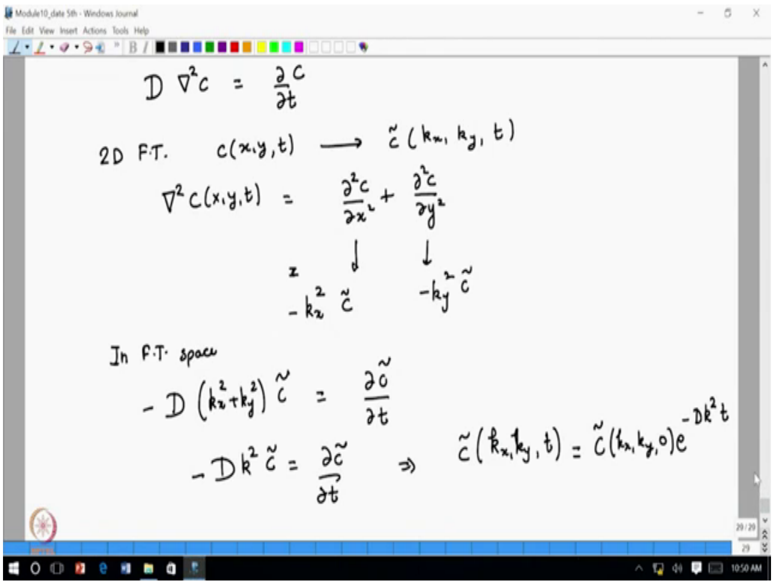

Now, what I will do is I will set I will take a Fourier transform. So, take 2D Fourier transform c of x y t take it to c of k, ky t and if you do this then what will happen is del square of c of xy, t this is basically dou square c by dou x square plus dou square c by dou y square and this I can write as. So, now, what will happen is this will transform to kx square c, c tilde let me call it tilde and this will transform to ky square c tilde. So, if you do a Fourier transform, Fourier transform of derivative gives you a factor of with the minus sign minus kx square minus ky square. Ik a factor of ik comes before and if you take a second derivative then you get ik square ik the whole square that is minus

So, then my in Fourier transform space my differential equation looks like D times. So, I will have kx square plus ky square c tilde is equal to dou c tilde by dou t and let me call this kx square plus ky square as k square. So, I can write it as Dk square c tilde is equal to dou c tilde by dou t are this implies c tilde of kx, ky 0 is equal to c tilde of kx, kyt c tilde of kx ky 0 e to the minus sign minus D k square t where k is k square plus ky square.

So, this is the time part and now we can write the special part of the diffusion equation.

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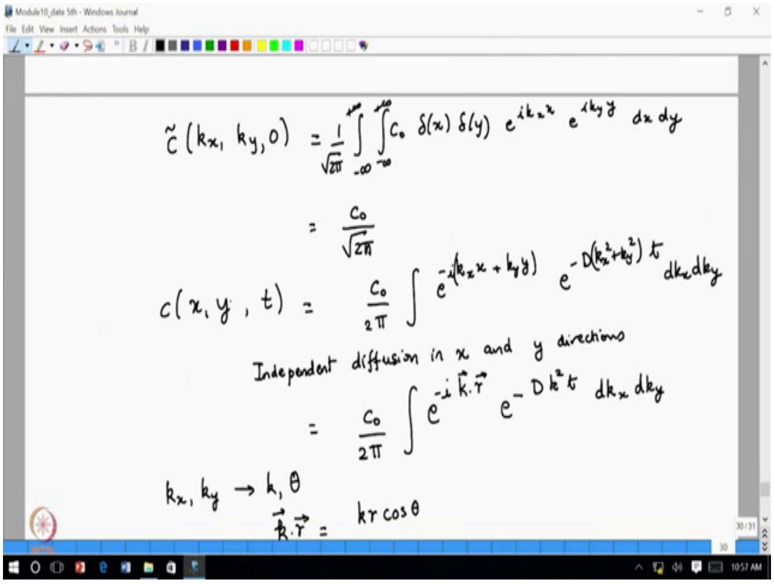

So, if you want to solve the diffusion equation all you need is c tilde of kx ky 0 and this at t equal to 0 you have the condition that at t equal to 0 your c of 0 t is c 0 delta of x minus 0 delta of y minus 0. So, this is nothing, but Fourier transform. So, this is Fourier transform of c of Fourier transform. So, you have c 0 delta x, delta y e to the i kxx e to the i kyy and then put a 1 over square root of 2 pi if you want, minus infinity to plus infinity you have two integrals dx dy. So, what you will get is that you will get c tilde of. So, we can evaluate this ok.

Now, the delta function will basically gave nothing here. So, this is just give me c 0 by square root of 2 pi. So, the integral of the delta function will give me one and you will have a square root of 2 pi there delta x delta y. So, when you put x equal to 0 this will go to one x y equal to 0 this will go to one. So, each of these integrals will give me 1, you have a factor of c 0. So, then what we get is c tilde of kx ky at time t is equal to C 0 by 2 pi I have integral e to the I k dot or kxx plus kyy minus dkx dky.

Now, the so, in if you had independent diffusion in the x and y directions then you could write it in this form. Now suppose on the other hand. So, this is the independent diffusion in the x and y directions, and it I got I should not forget e to the minus d kx square plus ky square t dkx dky. So, this is what it will look like if you had independent diffusion in x and y directions ok.

Now, suppose in this case I can write this in a slightly different form, I can write it as c 0 by 2 pi integral e to the i minus i k c 0 by square root of. So, that 2pi it will become 2 pi. So, you have an additional factor of 2 pi coming there. So, now, you have k dot r, I am just writing it as k dot r e to the minus d k square t dkx dky now what I will do is change from kx ky to k k theta k and k theta. So, it is you are changing the kx and ky to plane polar coordinates, then what you get is I can write k dot r , I will just call it theta I want I do not want to call it call it k theta. So, k dot r I can write as k r cosine of theta. So, then my c of k theta c of sorry sorry I think this should be c of xyt this should be c of xyt because I took the inverse Fourier transform of c of c tilde of ct. So, this is c tilde of kx kit.

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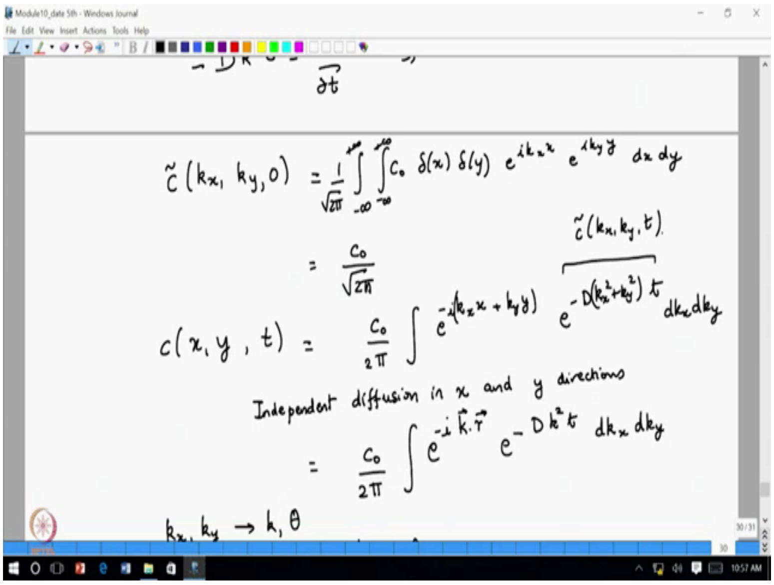

And I am taking the inverse Fourier transform of that. So, this multiplied by this c 0 by 2 pi c 0 by square root of 2 pi and then when I take the inverse transform I will take I will get this.

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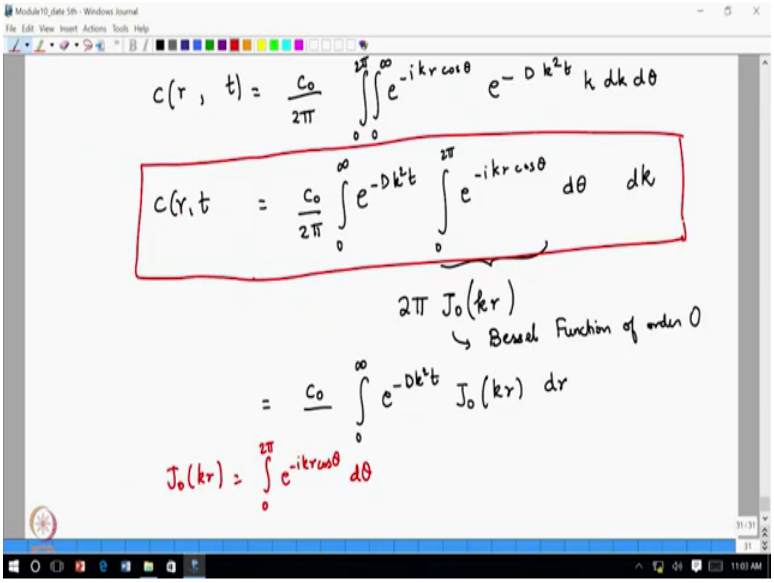

So, now, if I write c of k theta t it will look like c 0 by 2 pi and I have integral e to the minus i kr cosine theta e to the minus d k square and now dk I can write as k dk d theta. So, dkx dky I can write as k dk d theta. Now if you just look at the theta integral. So, theta goes from 0 r goes from 0 to infinity theta goes from 0 to 2 pi. So, if I just look at the theta integral 0 to infinity now e to the minus d k square t and then I have integral from 0 to 2 pi of e to the minus i k r cos theta d theta . So, essentially this represents the solution. So, this is the solution of this of this wave equation.

Now this integral is a function of k it is a function of k and a function of r d theta and I have a dk. So, this is a function of k and a function of r and what you can show is that this this whole integral is a function of k and its a function of r. In fact, its a function of kr together and you can show that this is exactly equal to 2 pi j 0 of kr j 0 is this Bessel function. So, what you can show by this I mean you can actually work this out, I mean you can you can show that j 0 kr can be written in this form you can do it term by term, you can do an expansion of this in the series and you can show that each of the terms with this factor of 2 pi will is exactly equal to j 0 of kr ok.

So, my final solution has this form c 0 by 2 pi integral 0 to infinity e to the minus Dk square t j 0 now the 2 pi 2 pi I can cancel with this 2 pi j 0 of kr dr. So, by Fourier transforms you can get this solution now if you had not used Fourier transforms if you had used spherical if you had used plane polar coordinates like how we did in the in the previous problem, like how we did in the case of a circular membrane if he had use plane polar coordinates instead of using this Fourier transforms, we would have directly got it in terms of j 0 of kr. We would have we would have got our results in terms of the Bessel functions just as we would have got Bessel when we do the separation of variables, you would have seen Bessel functions appearing and you would get the solution in this form ok.

Now, the connection between the Fourier transforms method; in the Fourier transform method you end up with you end up with this with this this is what you end up with in the Fourier transform method. So, c of k now it is sorry this is not k theta this should be c of r theta t this theta is actually of of rt its independent of theta. So, c of rt. So, this is c of rt and this was equal to this. So, this is what you will end up if you do Fourier transforms, and then you have to do this integral. So, you have the small matter of doing this integral when you actually work out this integral then you will get exactly the bessel function. Now if instead of that you had started by converting to spherical polar coordinates you would have got you have directly got it in terms of Bessel function you directly got it in terms of integral of the Bessel function and you would have gotten this result.

So, actually the two approaches will lead to the same result, but in order to make the connection you have to know that this integral you have to know that. This integral that is the crucial connection is that J 0 of kr is equal to can be expressed as integral 0 to 2 pi e to the minus ikr cos theta d theta. So, this is the crucial connection between the two methods. So, if you know this connection then you can show that you know whether you do using Fourier transforms or you do using using plane polar coordinates and you know actually solving the equation just as you solved in the other case you would get the same solution.

So, with this I will conclude this module. So, I will talked about partial differential equations and essentially there is only one method to solve it that is separation of variables. So you do separation of variables, you can you can use various techniques in some case you can use power series methods you can change your coordinates you can use Fourier transforms, but basically exactly the techniques that you use to solve ordinary differential equations, can be used. So, with this we will conclude this module here.

Thank you.