Advanced Mathematical Methods for Chemistry
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Module - 10
Lecture - 03
Two-Dimensional Wave Equation, Bessel Functions Part 2

Now, what I want to do next is to take the same 2 dimensional wave equation, but instead consider the case where the domain is a circular. You can think of this as the equivalent problem of particle in a circular region; particle that is confined to a circular region, but the other physical problem that you can think of is that of a drum you can think of a vibrating drum which is a circular drum and we are looking at the at the vibrations of that circular drum.

So, now this is what I want to do. And in doing this we will see the power series method of appearing.

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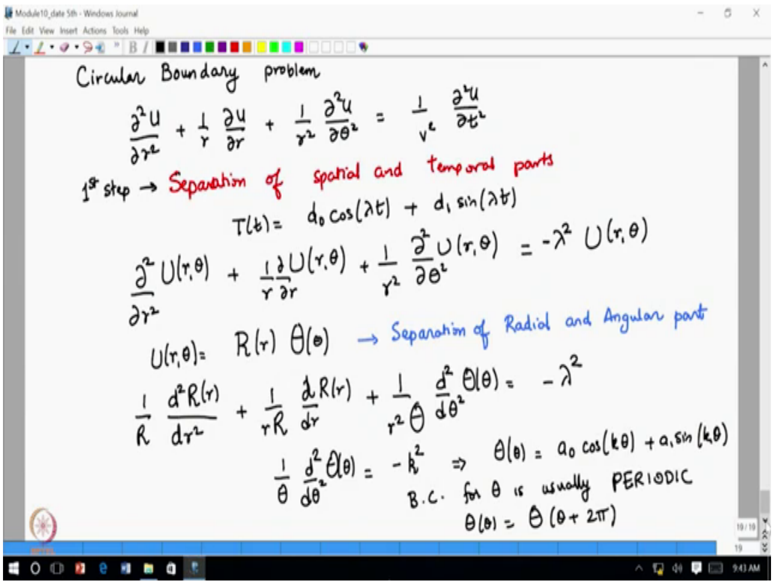

So, we will see the power series method appearing for the solutions and we will see Bessel functions appearing, so circular boundary problem. So, here what we have is our equation looks like d square u by dou r square plus 1 by R dou u by dou r plus 1 by R square dou square u by dou theta square is equal to 1 by v square dou square u by dou t square.

So, the first step when you do the separation of variables remains the same. So, first step is the separation of spatial and temporal parts. So, this will yield the same solutions as we had before. So, we will get t of t is equal to a 0 will I can let me call it d 0; d 0 cosine of lambda t plus t 1 sin of lambda t which will be d 0 and d 1 will be determined by the initial conditions.

So then that gives you the differential equation in terms of spatial coordinates. So, that will be d square by d r square and what will write is capital U of r theta plus 1 by R capital U dou by dou r capital U of r theta plus 1 by R square dou by dou square by dou theta square of capital U of r theta this is equal to lambda square U of r theta or minus lambda square.

So, now what will do is will write U of r theta is equal to R of r into capital theta of theta. So, if you do this separation of; so this is the next separation of radial and angular part. So, if you separate the radial and angular part then this equation if I substitute and divided by r times theta, what I will get is dou square rather d square R of r divided by dr square into 1 by R plus 1 by R times R d by dr of R of r plus 1 by R square capital theta d square by d theta square of theta of theta is equal to minus lambda square.0 Now the only theta dependence is in this; so theta dependences only in this part.

So, the first thing you will say that this should be a constant. So, since you have all this is dependent only on r. So, the theta dependences only there here, so this whole thing should not right hand side is not dependent on theta. So, therefore, you conclude that 1 by theta d square by d theta square of theta of theta is equal to constant; constant I will call it as minus k square a constant. It can be any constant, it need not be equal to lambda square we will just call it minus k square.

So, what this gives is. So, this implies theta of theta is equal to I will call it say a 0 cos k theta plus a 1 sin k theta. So, will just leave it at this; this is the theta part that is solved and you and a 0 and a 1 can be determined using the boundary conditions. In fact, in this case you have a boundary condition that that theta at theta and theta at 2 pi theta at theta plus 2 pi both should be identical.

So, in this case boundary condition for theta is usually periodic that is theta of theta is equal to theta of theta plus 2 pi. So, you have a periodic boundary condition in theta.

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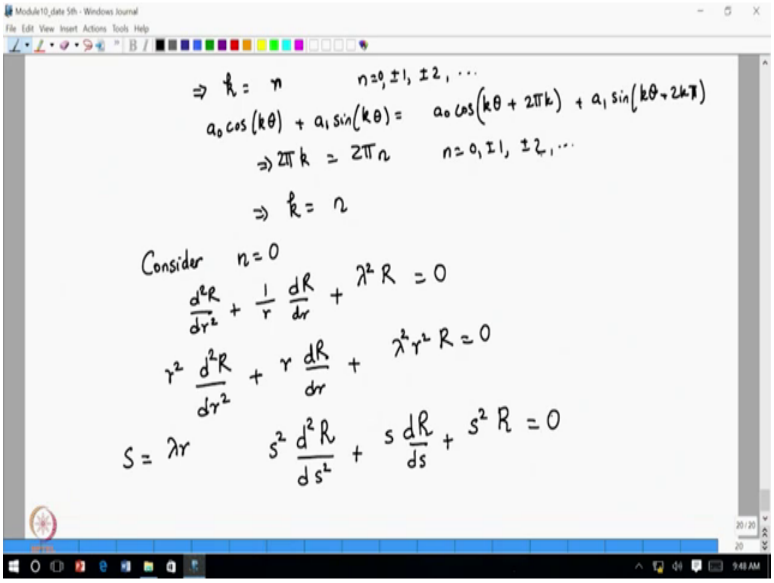

And you might have seen this. So, if you want a periodic function then this implies k is equal to 2 n pi n equal to plus minus 1 plus 0 plus minus 1 plus minus 2 and so on.

So, k has to be an integer multiple of 2 n pi and you can write the solutions. So, it has to be equal to n where n equal to 0 plus minus 1 plus minus 2 etcetera. So, k has to be an integer because you can you can see this by when you apply this boundary condition you will get a 0 cosine of k theta plus a 1 sin of k theta is equal to a 0 cosine of.

Now, you will get k theta plus if you put 2 pi if you if you replace theta by theta plus 2 pi plus 2 pi k and plus a 1 sin of k theta plus 2 pi k 2 k pi. So, if these 2 have to be equal and if you say each of the cosine and sin terms have to be equal. So, this implies that 2 pi k should be equal to 2 pi n where n is an integer so, on. So, this implies k is equal to n. So, this is what we said.

So, the theta part is done now suppose you have an integer there then what does this look like what does the remaining r part look like let us look at what the remaining r part looks like. So, you have if this is equal to n if this is equal to equal to n n can be 0 plus minus 1 plus minus 2. So, let us consider the case n equal to 0 consider n equal to 0 will just take this as an example you can do for other ends also.

So, if n equal to 0 then what you will then this last term d square theta by d d theta square is 0. So, this last term goes to 0. So, what are equation for r our equation for r simply becomes d square r by d r square plus one over r dr by dr plus lambda square r equal to 0 this is what the equation for r becomes.

Now, let me just multiply out by r square. So, I will write this as r square d square r by dr square plus r dr by dr plus lambda square r square r equal to 0 now put let me choose let me choose a variable. So, let me say put I will call it r s is equal to lambda r then r square will be r square will be s square divided by lambda square, but d square r by d r square will be d square will be lambda square d square r by dr square.

So, what I will get is if I make the substitution I will get s square d square s by d or d square r by ds square plus s dr by ds plus now lambda square this is just s square times r equal to 0. So, we get. So, we get a homogeneous second order ode. So, we will try to solve using power series method.

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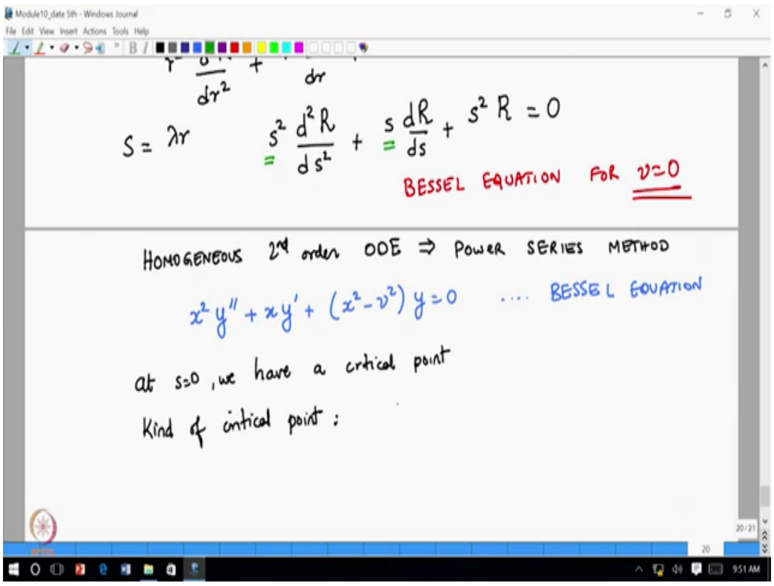

Now, this equation is actually very well known this equation. So, the equation where suppose you had suppose you had suppose you had x square y double prime plus x y prime plus x square minus nu square y equal to 0 this is called the Bessel equation. So, what we have here what we have in this case is the Bessel equation for nu equal to 0.

Now, you can solve this by the power series method. So we can solve this by the power series method and I will just outline a few steps in this solution. So, we notice that s equal to 0. So, at s equal to 0 we have a critical point and it is a and what kind of critical point it is. So, if you want to know the kind of critical point you we divide; so to know kind of critical point.

So, if you recall from what we did when we did when we were solved the power series method we said that we take the ratio of this quantity of this quantity to this quantity.

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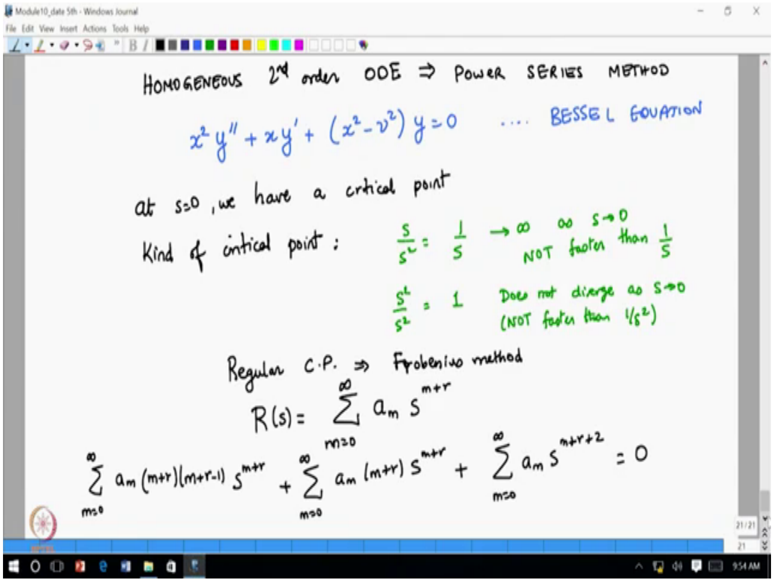

Now, that gives me. So, s by s square equal to 1 by s tends to infinity as s tends to 0 not faster than 1 by s. So, it is not a power of s that is greater than 1. So, this tends to 0 0 as s tends to infinity not faster than 1 by s.

Similarly, the the other term, so, if you look at if you look at s square by s square equal to 1 this does not diverge as s tends to 0. So, in this case you do not even have to worry I mean it is not it is definitely not faster than 1 by s square. So, this is a regular critical point. So, this implies Frobenius method can be used.

So, what will do is r of s is equal to sum over n equal to 0 to infinity I will say m equal to 0 to infinity and what we will say is that will write a m s raised to m plus r s raised to m plus r and now and now and now we will use a usual power series method and will substitute in this equation and I will skip a few steps I will just write what happens. So, you take the second derivative and you multiply by s square.

So, then what I will get is sum over m equal to 0 to infinity am m plus r m plus r minus one s raised to m plus r minus 2 plus sum over m equal to 0 to infinity am m plus r s raised to m plus r oh sorry no we had an r square. So, that goes away m plus r again plus sum over m equal to 0 to infinity am s raised to m plus r plus 2 equal to 0 and this we can we can immediately see that the power of s raise to r.

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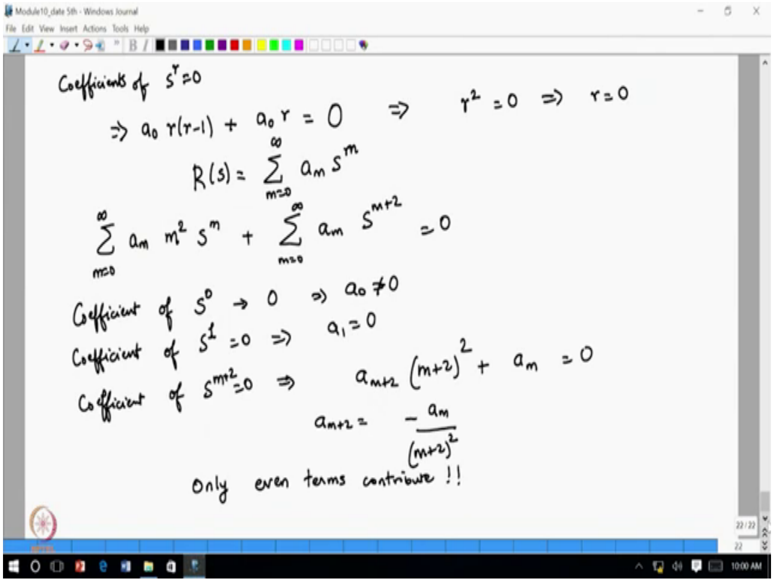

So, if you if you look at the coefficient or rather I should say coefficients of s raise to r. So, the coefficient of s the sum of coefficients of s raise to r on the left should be equal to 0. So, this implies. So, if you want s raise to r then m has to be 0. So, you get r r minus 1 r r minus one and then and then you have s reservoir now here also m has to be 0. So, a 0 plus a 0 r equal to n.

Now, here if you want s raise to r then m has to be minus two, but m cannot be negative, so you do not get any contribution from here, so, this has to be equal to 0 and this you can immediately see that this implies r square. So, if you add up these 2 with the you will just get a 0 times r square a 0 times r square equal to 0 or r square equal to 0 this implies r equal to 0.

So, r equal to 0 and then the solution has this form r of s is equal to sum ocer m equal to 0 to infinity am s raise to r. So, it just looks like a regular power s raised to m and now we can substitute in the equation. Now, let us go back to this expression. So, your equation becomes some over m equal to 0 to infinity am r m minus 1 s raise to m let me combine these 2 terms.

So, I will just write am times m minus 1 and you have m here. So, if I add those 2 I will just get m square s raised to m plus sum over m equal to 0 to infinity am s raised to m plus 2 equal to 0 now. So, what we see is that is that you have s raised to m and s raise to m plus 2. So, basically you can you can look now you look at coefficient of let us let us let us look at. So, we have already seen the coefficient of s raised to 0.

So, we have already seen that. So, this is clearly this goes to 0 goes to 0 now if you look at coefficient of s raise to one equal to 0 implies a 1 equal to 0 because if you want s raised to one then m has to be equal to 1. So, m has to be equal to 1 then you just get a 1 times one and here you will get here you can never have m raised to one. So, this implies a 1 equal to 0. So, this 0 is not equal to 0. So, we assume that a 0 is not equal to 0 a 1 equal to 0 a 0 we will choose arbitrarily.

Now, what about what about coefficient of s raise to m equal to 0 implies am m square or let me say m plus 2 let me put m plus 2. So, if I put m plus 2 equal to 0 then what I will get is now I want m plus 2. So, what I will should get is a of m plus 2 m plus 2 square should be plus a of m equal to 0 because then each of these will be the coefficient of s raise to m plus 2.

So, what I will get is a m plus 2 is equal to minus am over m plus 2 square so. So, now, what you get is. So, obviously, only even terms contribute which we have already seen and what you get next is that is that I can write I can write.

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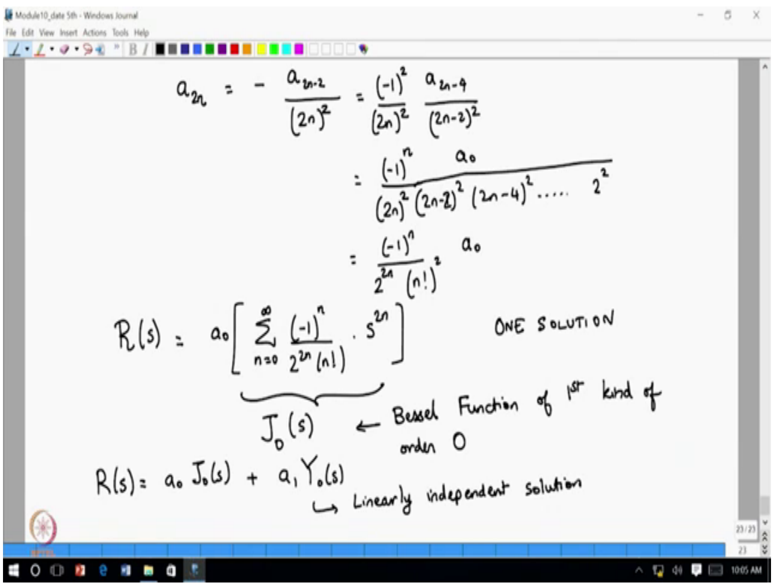

So, if I want to write a of 2 n m m is 2 n. So, n is an integer. So, m is an even integer. So, I am writing it as 2 n.

I can write this as minus a of 2 n minus 2 divided by 2 n square. So, and I can write this further as minus one square a of 2 n minus 4. So, what I am doing is I am writing this as a of 2 n is minus one into a of 2 n minus 4 divided by 2 n minus 2 square and I can I can go on I can write this as minus 1. So, I keep doing this.

So, 2 n minus 4 I will replaced by 2 n minus 6 and so on. So, I go all the way up to all the way up to a 0 when I reach a 0 then I cannot go any further. So, I can write it as minus 1 raise to n divided by 2 n square 2 n minus 1 square 2 n minus 2 square 2 n minus 4 square all the way up to 2 square times a 0.

So, I can write a 2 n in this form and what you can write this as. So, I can write this as minus 1 raise to n divided by I have 2 raise to 2 n into n factorial square, so, n factorial because I have n n minus 1 n minus 2 and so on. So, I take the 2 common and I can write it in this form a 0. So, this series; so, the solution r of s is equal to a 0.

I will let me call, so a 0 times one or I can just write sum over n equal to 0 and this series does not terminate anywhere it goes all the way to infinity. So, 0 to infinity minus one raise to n over 2 raise to 2 n n factorial this is see when n equal to 0 this whole thing becomes one. So, it also works for n equal to 0 times s raise to 2 n. So, this is what the series looks like.

Now, now this is only one solution incidentally this quantity is called Bessel function of order 0 j 0 of s this is Bessel function of first kind of order 0. So, its denoted as j 0 of s now in general we started with the we started with the second order differential equation. So, there should be 2 linearly independent solutions. So, the second linearly independent solution is found by variation of parameters.

So, general solution r of s is written as a 0 times j 0 of s plus a 1 times what I will call this y 0 of s this is the linearly independent solution, but this linearly independent solution.

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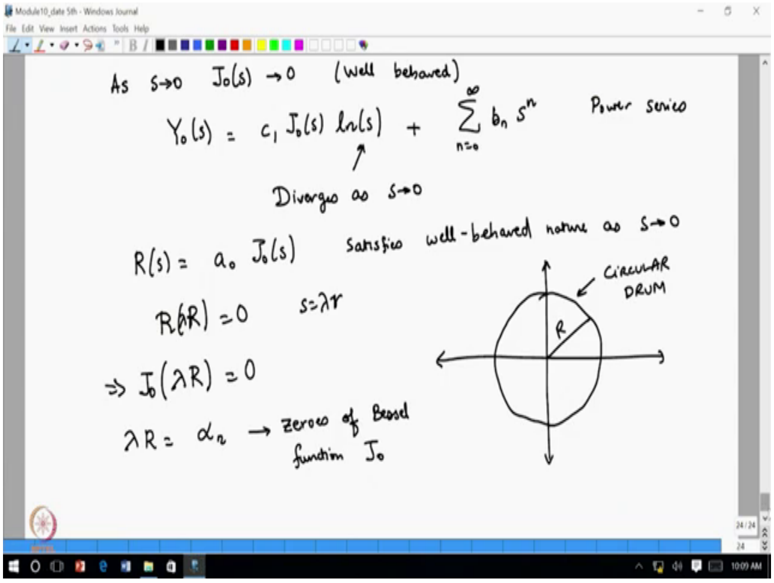

So, now, we notice that as s tends to 0 j 0 of s tends to 0 this is well behaved.

But if you look at y 0 of s y 0 of s if you do by variation of parameters what you will get is you will get you will get something like c one times j 0 of s times natural log of s plus sum over n equal to 0 to infinity you will get you will get some other series. So, well just call it bn s raised to n this is another power series.

Now, the issue with this is at ln of s diverges as s tends to 0. So, as s tends to 0 this goes to infinity. So, if you want well. So, if you want r of s to be well behaved as s tends to infinity then we have to set a 1 equal to 0 we have to set this coefficient to go to 0. So, r of I should not call it a 1 maybe I should call it something like c one some other constant some other constant. So, it is a linear combination of these 2 linearly independent solutions.

So,. So, for the problem of interest that we have r of s equal to a 0 j 0 of s and now this is the spherical system now there must be some other boundary conditions. So, this satisfies well behaved nature as s tends to 0. So, we are going to get a solution that looks like this now in order to apply the other boundary condition we need to we need to consider the domain.

So, typically we do this in a circular domain. So, typically you choose a as I said a 2 dimensional wave equation is like a circular drum and we will set this radius r. So, we will set R of r of r equal to 0. So, in other words what will get is this implies j 0 of s is basically lambda times r equal to 0. So lambda, remember s was equal to lambda r s equal to lambda r.

So, now, what this implies is that lambda is equal to. So, what this implies is that lambda times r equal to alpha n what are these alpha n alpha n are called 0s of Bessel function Bessel function j 0. So, what is the physical meaning of this the meaning of this is a following if you look at if you look at j 0 j 0 of some variable as a function of whatever that variable is ok.

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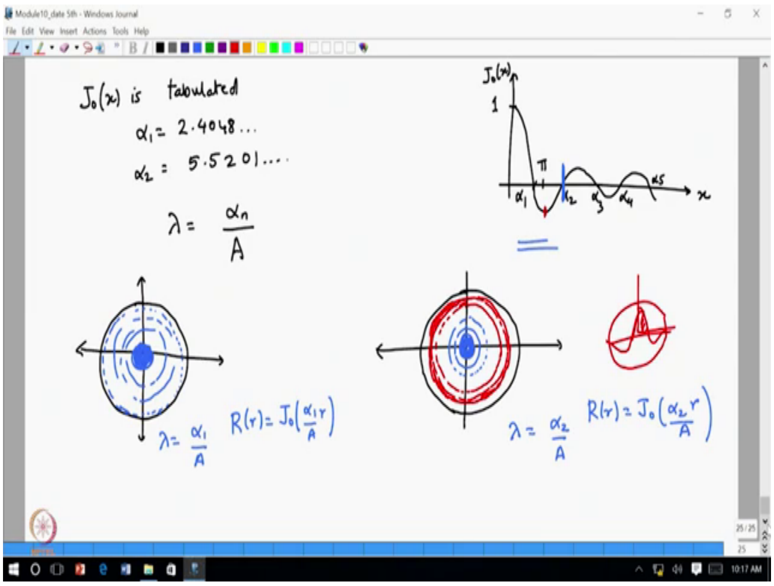

So, this looks this has this form. So, it starts at one when a when x equal to 0 it goes to one and then and then it has a form that looks like this. So, this is what your j 0 looks as a function of x this is fairly well known I would not going to derive this value is about pi is somewhere here and. So, on I do not I am not worrying about the exact values, but this is called alpha one alpha 2 alpha 3 alpha 4 alpha 5 and so on.

So, these are called the 0s of the Bessel function. So, Bessel function is actually the j 0 is a j 0 of x is tabulated. So, since it involves an infinite series. So, for any value of x you have to write it as an infinite series. So, j 0 of x is basically this function. So, you can write it as an infinite series and you have to calculate it for each value of x this has been done and tabulated numerically and it has this form.

So, what you get is that alpha one works out to about 2.4048 and alpha 2 is 5.5201 and so on I will just; I will not write the remaining. So, what we have is that your lambda times capital R should be equal to alpha n. So, therefore, lambda should be equal to alpha n divided by R; R is the capital R, let me take a different name. So, the radius I will put it as capital A.

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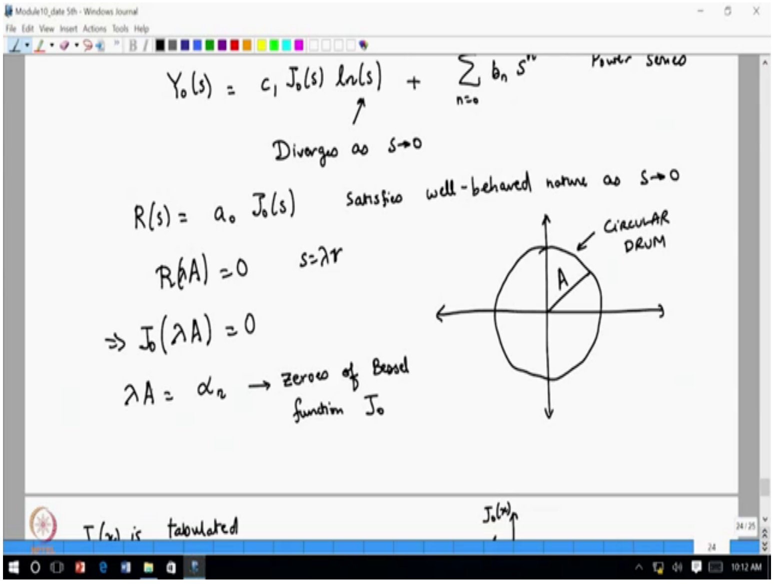

So, let me change the name not to confuse with this capital R. So, I will just call it capital A everywhere that is the radius of your drum and so lambda has to be the 0 of the Bessel function that is 2.4048 divided by capital A or it can be 5.52201 divided by capital A.

So, this will ensure what will happen is that this will ensure that when you take lambda times a then you will get a 0 of the Bessel function lambda times a is a 0 the Bessel function. So, therefore, the wave r of s the wave function will go to 0 at that at the boundary. So, this will ensure that the wave that the function the amplitude of the wave will go to 0 at the boundaries.

So, what this will look like if you we have completed the solutions now if you if you look at it pictorially this will look like this. So, you have a drum you have a circular drum. So, what you have to think is you have this function you have this j j function and it is going out. So, the first case you just have a you just have a wave whose amplitude is largest in the center, but it is the amplitude is largest in the center.

So, I will just show it via dark color and then and then it goes it becomes smaller and smaller before it becomes very very small and goes to 0 at the boundary. So, this is this is the function correspond to correspond to lambda equal to alpha 1 by a. So, in that case R of r is equal to some constant times j 0 of alpha 1 by a r. So, this is a solution what I am showing is that the amplitude is largest here. So, it is lot of lines then the amplitude decreases slowly decreases and here, it becomes very very small.

Now, the other the next, next wave looks like this. So, now, if you have lambda is equal to alpha 2 by a alpha 2 by a is right here. So, what you can see is that the amplitude goes it crosses 0 and then becomes negative and then it and then it again comes to 0. So, here your R of r is equal to j 0 of alpha 2 r by a. So, here again your amplitude is largest in the center.

So, this is then becomes less and less positive and at when r is equal to at some point it goes to 0 and then after that it becomes negative it becomes negative and it actually increases in negative before it becomes 0 again. So, I will just show in red the region where it is negative. So, it becomes more and more negative. So, it becomes at some point these are negative actually becomes quite a large amplitude. So, that is right here and then and then it goes back to 0.

So, it looks like this and you can you can sort of imagine this if I show a side view you can you can think of it look exactly like the Bessel function, but you imagine that it is this is on the on this on the on the on the circle. So, it looks like this. So, this is what the solutions of this of this wave equation in a circular boundary conditions look like.

Now, I just want to emphasize a few things again. So, before I conclude this lecture I just want to emphasize a few things.

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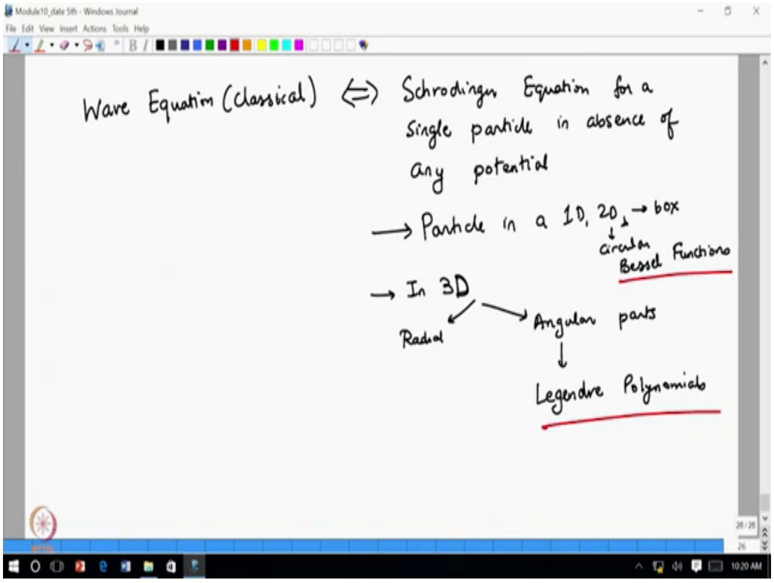

So, first is that the wave equation classical is identical to a to a Schrodinger equation for a single particle in absence of any potential. So, this is harmonic oscillator. So, sorry this is particle in a box in 1D, 2D box, if you have a circular box then you get Bessel functions.

Now, actually there is a very nice thing. So, in 3D; 3D; so, what is done is the angular part in 3D; we have the radial and angular parts. The angular parts give you Legendre polynomials these are these are the angular part of the waves in angular part of these waves in D. So, this is angular part of the wave in 3D.

So, here we saw that if it is rectangular. So, if it is circular, you get Bessel functions and in the angular parts we saw there Legendre polynomials the radial part is I mean that has to be worked out, but what I want to emphasize through this whole discussion is that is that when you solve partial differential equations.

Then especially those that have typically; the partial differential equations have a spatial part and a temporal part the spatial part typically you define a domain over which it is applicable you might define a circular domain you might define R going from 0 to infinity or 3D infinite space or you might define a box or you might; you know, you can you can choose your domain and based on that domain; the solutions have different forms and these have been extremely worked out because their classical wave solutions in all these domains have been worked out.

So, the Legendre polynomials that you get for classical waves in 3D; these are referred to as a spherical harmonics. So, they are the angular part of the classical wave in 3D and so this wave equation is something that is very fundamental to physics and you know you can use it not only for to study drums and strings and in such instruments.

But, you can also use it for example, you can think of suppose; there is an earthquake then you have these you know you have these waves that are going through the earth and the maximum and if you have one epicenter of the earthquake from where all these waves originated and if you if you think of a at least locally you think of it as a 2D region then you will see you will see that the waves go out like Bessel functions.

So, there are; whole lot of engineering problems in which in which Bessel functions and Legendre polynomials appear very naturally. So, I have kept this as a slightly longer lecture and we have already done examples. So, in the next lecture, what I will do is I will just recap what you have learnt about pds and then I will just do one under the other example; where we use a slightly different method to solve pds where we use Fourier transforms.

Thank you.