Advanced Mathematical Methods for Chemistry

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Module - 10
Lecture - 03
Two- Dimensional Wave Equation, Bessel Functions Part 1

In the last lecture we saw a technique of solving partial differential equations, which we refer to as the separation of variables. And what we saw is that by using this technique a partial differential equation can be converted to a set of ordinary differential equations. Now what I want to do is an application of this method, and this method I will apply it to a problem which is called the wave equation.

And we will apply it in 2 dimensions. And what I want to emphasize through this method, is that, is that I mean first I want to illustrate how this method work. And then the next thing that I want to do is to really show you how do doing this 2 dimensions based on the boundary conditions, you will get solutions that look very different, even though they are solutions to the same physical problem that of a wave going in 2 dimensions.

So, what we will see is that by imposing the boundary conditions, we will change the nature of the solution, and we already saw in the first lecture that the geometry of the problem decides on the coordinates that you use. And the coordinates that you use we will actually affect the solutions. So, this is what I will show in today’s lecture. So, today’s lecture will be a slightly longer lecture. So, it will be actually substantially longer. So, it will be almost one hour lecture. So, after this we will go straight to the final lecture of the module. So, this module will have only 4 lectures and today’s lecture will be a slightly longer lecture.

So, let us start this module will start by writing down the 2 dimensional wave equation. So, in general I can write the wave equation in the following form right.

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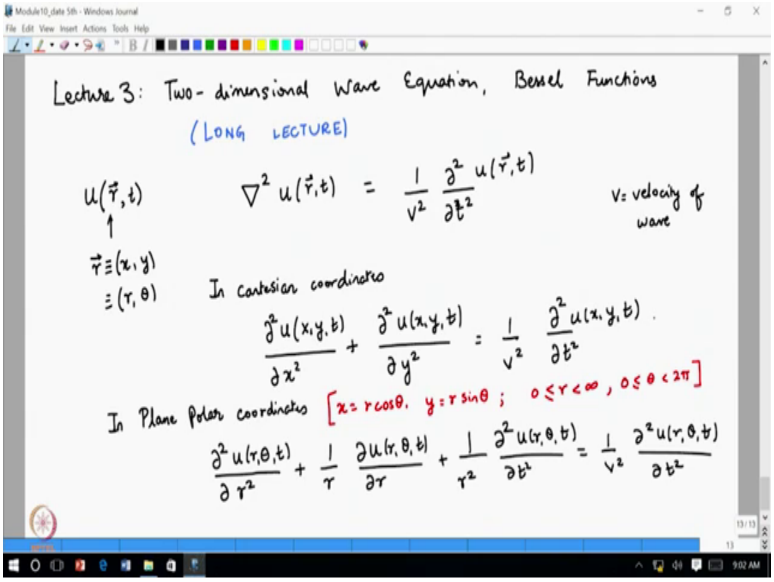

Let me write u as the amplitude of the wave. So, if I write u as the amplitude of the wave. Then u is a function of I will just say r, r is a 2 dimensional vector and is a function of time. So, r has r is composed of coordinates x and y or equivalently you can write it in terms of r and theta, in terms of either polar coordinates or Cartesian coordinates. Then what the wave equation does is it relates the Laplacian, this is a Laplacian in 2 dimensions of u, u of r t it relates it to the second derivative with respect to time t square of u of r t and between these 2 there is a factor the factor is related to the velocity of the wave. So, v square v is the velocity of the wave ok.

So, this is the, this is a general 2 dimensional wave equation. Now in Cartesian coordinates this takes a form second derivative with respect to X of u of x y t by dou x square, plus second derivative of u of x y t with respect dou y square this is 1 by v square dou square by dou t square u of x y t.

So, this is what the wave equation looks like in Cartesian coordinates, in plane polar coordinates, where we say and just to remind you plane polar coordinates have x equal to r cosine of theta and y equal to r sin of theta and you know r, r goes from 0 to infinity and theta goes from 0 to 2 pi. So, this is the plane polar coordinate. And so in these coordinates what this becomes it takes a following form. So, it becomes dou square u of r theta t divided by dou r square plus 1 over r dou u of r theta t divided by dou r plus 1 over r square dou square u of r theta t divided by dou t square is equal to 1 over v square dou square u of r theta t divided by dou t square.

So, we have these 2 forms one is in Cartesian coordinates and one is in plane we in plane polar coordinates. Now let us first look at the case. So, the wave equation we have we have this xy coordinates.

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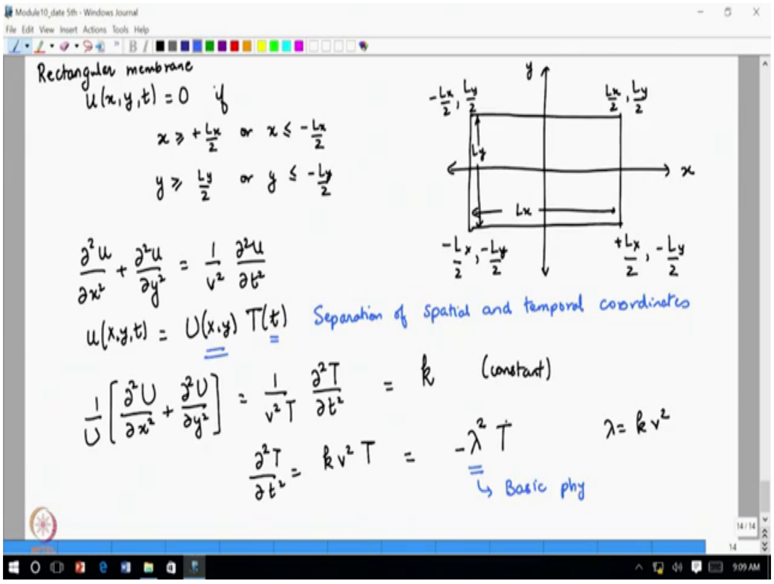

This is the 2 dimension of space. So, 2; so this is a 2 dimensional space and the wave equation is something that is satisfied in this 2 dimensional space.

Now we look at 2 examples the first example, we look at where the boundary conditions are along x and y. So, what will say is that you have a rectangular region where the wave equation is satisfied and just for convenience I will take this rectangular region to be symmetric about the over the axis you do not have to. So, we have this rectangular region. Let me call this minus L x to plus L x, L x by 2. Therefore, the length along the x direction is L x. And let me call the y coordinate is minus L y by 2 this becomes plus L y by 2. So, this is minus L x by 2 L y by 2. This is L x by 2 L y by 2. So, these are the coordinates of these 2 points.

So, what I am saying is that this distance along the Y direction is L y along the x direction is L x. So, this is L x and this is L y. So, what I want to do is I want to say that the wave equation is only satisfied in this region and outside this region the wave equation is not satisfied. In other words what I am going to say is that u of x y t equal to 0 if x is greater than equal to minus or plus L x by 2 or x is less than equal to minus L x by 2. And y is greater than equal to L y by 2 or y is less than equal to minus L y by 2.

So, in all these cases the u goes to 0. So, basically outside this region outside this rectangular region u is exactly equal to 0. So, this is for the rectangular membrane. And the why I call it a membrane is because there is a wave equation. So, if you just had a 1 dimensional wave equation that would look like a string that would look like oscillations like the vibrations of a string. If you have a 2 dimensional region that is like a rectangular membrane. So, in this case we have fixed the boundary. So, we have fixed the edges of the rectangle. So that the u goes to 0 at those edges and now we want to solve what is the equations of these waves of these waves inside this region.

So now let us let us look inside the region we have we have dou square u by dou x square plus dou square u by dou y square is equal to 1 over v square dou square u by dou t square. So, what will do first is u of x y t is equal to we will call it as a capital U of xy times capital T of t this is a first separation of variables that we are going to use. So, separation of spatial and temporal coordinates. So, in other words the t is the time and these 2 are spatial coordinates.

So, we separated the spatial and temporal coordinates. And when you do this then when you make the substitution in the equation then what you will get is you will get dou square u by dou x square plus dou square u by dou y square into 1 by u is equal to 1 over v square t dou square t by dou t square. So, we did the substitution we divided by u times t and accordingly you will get such an equation. Now the right hand side is a function only of t the left hand side is a function only of x and y.

So, therefore, each of these should be equal to a constant. And so we will just call this k constant. So now, the temporal part is very straightforward. So, we have dou square t by dou t square is equal to k v square t. And we will call we will set this equal to minus lambda square T where lambda is equal to k v square. So, we assume that k is negative and k times v square is we write it as minus lambda square. This is I mean there is a there is a very intuitive reason why this should be true. There is a basic physical reason. And you can you can sort of understand this because this looks like a harmonic oscillator. And if you if your harmonic oscillator had had it has to have it has to have the it has to have a frequency then this should be a negative sign. So, if it is not a negative sign it just becomes exponential function. So, then this t will just be exponential functions it would not represent a wave. So, there is a basic physical reason why this should be negative.

Now, what you will get if you solve this equation this is a straightforward equation, you will get t is equal to.

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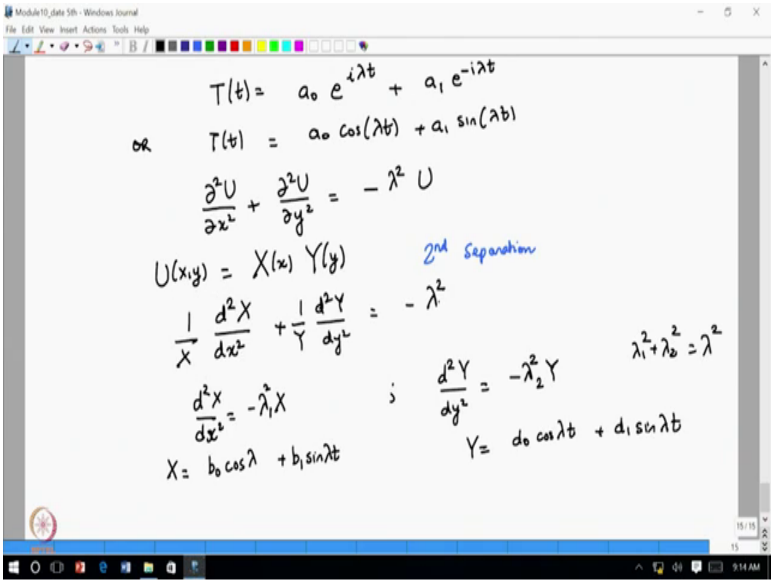

So, let me put the time explicitly, T at time 0 e to the I and a t more because you can have either plus or minus lambda. So, I can write as a 0 e raise y lambda t plus a 1 e raise to minus i lambda t or T of t is equal to a 0 cos cosine of lambda t plus a 1 sin of lambda t. Now these two a zeros are not the same. You can write it an either of this form. But it is basically either a sum of sins and cosines or a sum of lambdas, or a sum of exponentials e exponential with imaginary coefficients.

Now, let us look at the other equation. So, the other equation has this form dou square u by dou x square plus dou square u by dou y square is equal to minus lambda square u. Now this is not separated yet. So, you assume that u of x y is equal to X of x times Y of y. So, this is the next second separation of variables. So, we are separating the x and y parts. And now what you will get is you will get if you substitute this and you again divide by x y, what you will get is those or I should write d square x by d x square times 1 by x plus d square y by dy square times 1 by y is equal to minus lambda square.

So, each of these is each of these has to be con this give the first term depends only on x next second term depends only on y, a right hand side is a constant. So, if you have a function of x that depends and a function of y and they add up to give a constant then each of these should be independent of x and y each of these should be a constant. So, what you have is 1, what I can write is I can write 2 equations I can write d square x by d x square is equal to minus lambda square x and I can write d square y by dy square is equal to minus lambda square y. So, I have these equations.

Now, each of these I can I can solve this. So, I can write X is equal to a we call it b 0 cos lambda t plus b 1 sin lambda t and y is equal to let me call it d 0 cos lambda t plus d 1 sin lambda t. So, these are the equations that you have and no sorry. So, this there is there is one point I should I should I am mention I will call this lambda 1. And I will call this lambda 2 and what I will say is that lambda 1 square plus lambda 2 square equal to lambda square. So this.

So, this has to be a constant it need not be equal to lambda. So, it has to be a constant it can be lambda 1. So, I will just call it lambda 1. And this has to be a constant it can be lambda 2: so lambda 2 y lambda 2 y and so lambda 1 and lambda 2 should satisfy the relation that lambda 1 square plus lambda 2 square should be equal to lambda square. And further we are saying that x should be of this form. So, if x is of this form then will have d square x by dx square should will give you minus lambda 1 square x. Similarly if y has this form then we will have d square y by d x square equal to minus lambda 2 square y ok.

So now we can do more. So now you impose boundary conditions. So, when we impose the boundary conditions, so what will say is that X of minus L x by 2 equal to X of plus L x by 2 equal to 0.

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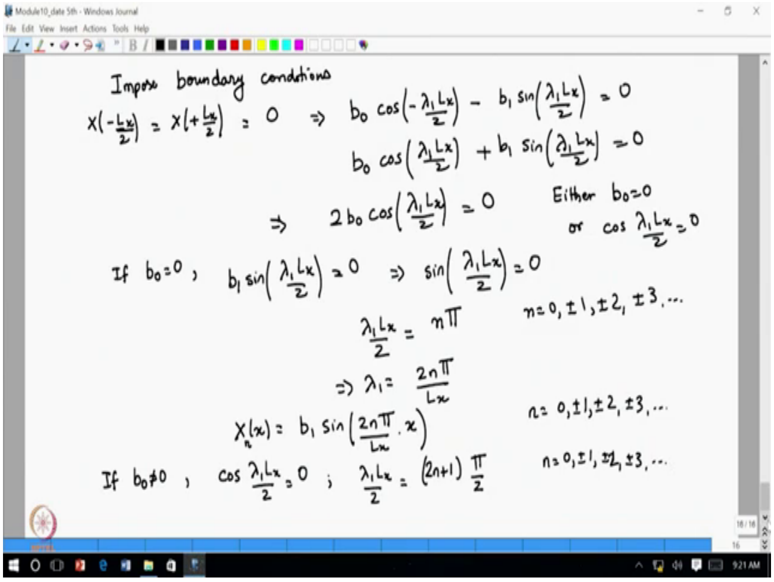

So, when we impose this condition what will find is the following. So, first let us So, what we will get is that this implies b 0 cos minus lambda 1 L x by 2 plus b 1 sin. So, sin of minus I can write as minus sign. So, I will write minus sin lambda 1 L x by 2 equal to 0, and the other equation will get so this is from putting at minus l; if you put at plus l then you will get b 0 cosine of lambda 1 L x by 2 plus b 1 sin of lambda 1 L x by 2 equal to 0. And if you add these 2 equations we will immediately if you if you add these 2 equations. So, you will get 2 b 0 cosine of lambda 1 L x by 2 equal to 0.

So, either you can have b 0 equal to 0 or lambda 1 and L x by 2 equal to 0, you can have you can have a higher of these cases. Now So, either or cosine of lambda 1 L x by 2 equal to 0. So, these are the 2 possibilities.

Now, if b 0 equal to 0, then we have then we should have b 1 sin lambda 1 L x by 2 should be equal to 0. We should all have this additional condition; so if b 0 equal to 0 now b 1 cannot be 0. So, if b 0 equal to 0 b 1 cannot be 0. So, this implies sin of lambda 1 L x by 2 equal to 0 or what you will get is. So, this implies. So, sin equal to 0 when lambda 1 L x by 2 is a multiple of pi n pi n equal to 0 plus minus 1 plus minus 2 plus minus 3 and so on. So, whenever this is equal to a integral multiple of pi then the sin of that goes to zero.

So, in this case So, what this implies is that lambda 1 is equal to 2 n pi by L x, where n can be 0 plus minus 1 plus minus 2 etcetera. So, then the u of or rather X of x is equal to b 1 sin 2 n pi by L x into x. So, this is what it looks like. So, lambda can take only these values and x can take any of these values, what will do is now this is indexed by n; so will just put an n here. So, n is 0 plus minus 1 and so on.

So, this is one kind of solution you can get. Now the other solution you will get is if b 0 not equal to 0. So, if b 0 is not equal to 0 then what you get is that, you will get you have to have cosine of lambda 1 L x by 2 equal to 0. And if you have cosine of lambda 1 L x by 2 equal to 0 then what you can get is you will get lambda 1 L x by 2 is equal to 2 n plus 1 pi by 2. So, it has to be n it has to be a ma it has to be a multiple of it has to be an odd integer multiple of pi by 2 ok.

So, you will get at pi by 2 3 pi by 2 5 pi by 2 and so on. So, n is equal to 0 plus minus 1 plus minus 2 plus minus 3 etcetera. Now in this case in this case I can write so b 0 is not equal to 0. I have I have this additionally and We should have b 1 sin lambda 1 L x by 2 equal to 0.

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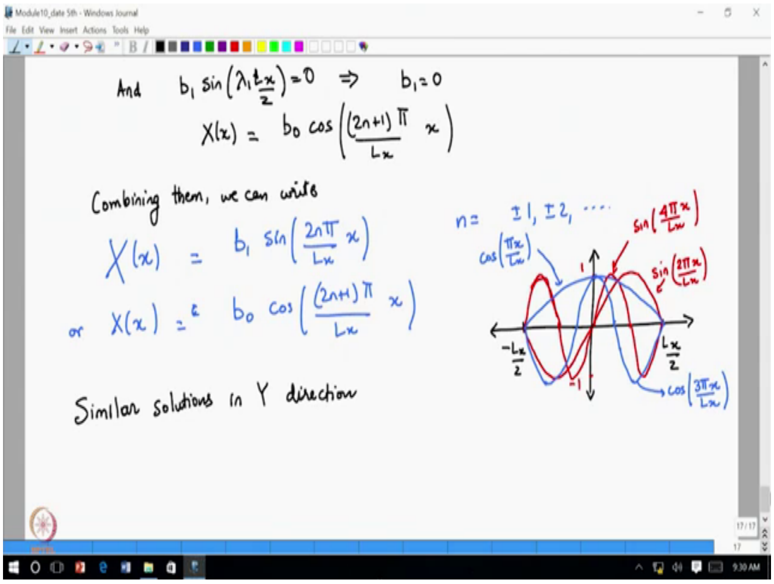

So, this implies we can choose b 1 equal to 0.

Now, now since we already had a condition, since we already had a restriction for lambda 1, we would not have lambda satisfy this other relation. So, lambda we already chose to be an odd multiple of pi by 2. So, it cannot be it cannot be an even multiple of it cannot be it cannot be a multiple of pi. So, therefore, what you will get is the solution X of x looks like b 0 cosine of 2 n plus 1 pi, pi by L x into x. So, what you will get is lambda has to be 2 n plus 1 pi divided by L x and so, and so you will get such a relation ok.

So, what are the possibilities? So, in general and then we can write and let me make this in blue. So, X of x is equal to either it is will call it b 1 sin 2 n pi by L x into x and so on. Or easy or is it equal to or same if you go to b 0 cosine of 2 n plus 1 pi by L x into x. So, all these are possible. So, what does say what do these waves look like. So, if I just plot them. So, let me basis minus L x, L x. So, first let us consider the case lay let us consider the first equation. So, will consider the sin terms let me show it in red and I will just take b 1 and d 0 I will just consider them as one just for convenience. So, this is 1 and minus 1.

So, what does sin if n equal to 0 sin 2 n pi by L x looks like this in this region, it looks like this is when n is sorry, any n equal to 0 is not is not valid. So, n equal to 0 will make the wave function make this function go to 0. So, n equal to 0 should not be taken. In this case you can take n equal to 0. So, for the sin case you cannot take n equal to 0, because n equal to 0 means the function itself will go to zero. But in the case of cosine you can take n equal to 0 because n equal to 0 will still give me pi by 2.

So, this is n equal to 1. So, this is a sin with n equal to 1, and then let us, what about sin with n equal to 2? With n equal to 2 the sin will look will look like this, this is the equation. So, this is sin 4 pi x by L x sin 2 pi x by L x and this is sin 4 pi x by L x and so on you can take. So, sin 6 pi x will have will have 3 will have 3 completed, I mean I mean 3 oscillations in the x direction and 3 in the Y direction or 3 in the minus x direction.

Now, let us look at the cosine. So, what does the cosine look like? So, I will draw this in blue; so the cosine if you again assume b 0 equal to 1. So, when n equal to 0 then you have cosine of pi x by L x. So, when x equal to L x by 2 then this becomes cosine of pi by 2 equal to 0. Oh made a mistake, this will be minus L x by 2 plus L x by 2. Now, when x equal to 0 this equal to 1; so it goes so it starts this way and it goes to 0 here, starts this way and goes to 0 here. So, this is for cosine of pi x by L x. So, this is cosine of pi x by L x.

Now, when you take the next one when you take cosine of 3 pi x by L x, then when x equal to L x by 2 it goes to a cosine of 3 pi by 2. So, cosine of 3 pi by 2. And so what will happen is that it will go it will go to 0 and then it will become negative and then I will go back to 0. So, this will look like this. So, these are what the waves looked like and notice that they all go to 0 at minus L x by 2 and plus L x by 2.

Now, I do not need to do the same thing again for the Y direction. So, I will just write So, we will get very similar solutions for the Y directions in Y direction. Now let me just mention one small thing which, which you might recall from your quantum mechanics. So, I will just mention this.

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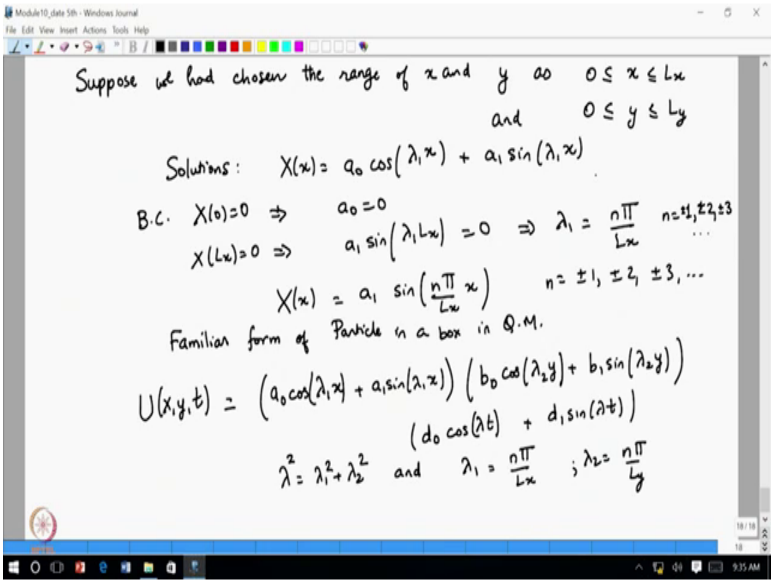

Now suppose we had chosen the range of x and y as 0 less than equal to x less than equal to L x and 0 less than equal to y less than equal to L y. Will just take x just to illustrate the point. The solutions would have been X of x equal to a 0 cosine of lambda 1 x, x plus a 1 sin of lambda 1 x. So, we will just look at the x direction and just I will just illustrate this point. Now boundary conditions X of 0 equal to 0 implies a 0 equal to 0. Because when you put x equal to 0 the sin term goes to 0. So, will just left b left at a 0 and that has to equal 0. So that directly implies a is 0 equal to 0 now X of L x equal to 0 implies a 1 now a 1 cannot be 0. So, sin of lambda 1 L x equal to 0 and this implies lambda one is equal to n pi by L x n equal to n, n cannot be 0 in this case because n equal to 0 will mean the function itself is 0 n equal to 1 plus minus 1 plus minus 2 and plus minus 3 and so on ok.

So therefore, we will directly get the solution in this form. So, we directly get the solution of X of x is equal to a 1 sin n pi by L x into x. N equal to plus minus 1 plus minus 2 3 and so on. So, what we see is that is that the this is this is this is familiar form, form of particle in a box particle in a 1 d box in quantum mechanics. So, what I want to say is that the wave equation is essentially the same as the Schrödinger equation. It is the wave equation if you look at the spatial part it looks same as the Schrödinger equation for particle in a box. And you can get the solutions in exactly this way ok.

So, the general solutions if we write; so let us just write. So, we will write the general solution u of x y t is equal to So, you have a 0 cosine of lambda 1 x plus a 1 sin of lambda 1 x, b 0 or we called it b 0 cosine of lambda 2 y plus b 1 sin of lambda 2 y. This is the x part multiplied by y part and multiplied by a time part; the time part is we just call it d 0 cosine of lambda t plus d 1 sin of lambda t. Where lambda lambda square equal to lambda 1 square plus lambda 2 square and lambda 1 is equal to n pi by L x. If the domain is from if the domain is from 0 to L x, lambda 2 equal to n pi by L x if the domain is from if the domain is from 0 to L x lambda 2 equal to n pi by L y. Again if the domain is if these are the domains, if these are not the domains then you have to you have to write you write the solutions in this other form.

So, what we have seen here is that is that the 2 dimensional wave equation is can be solved by the separation of variables, and the 2 dimensional wave equation is actually very familiar to us because when you do the particle in a 1 dimensional box in quantum mechanics, the solutions looks exactly like this. The equation that you get has exactly this form inside the box. And we are used to seeing these solutions.