Advanced Mathematical Methods for Chemistry

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Module – 08
Lecture – 02
Fourier Expansions And Differential Equations
Part B

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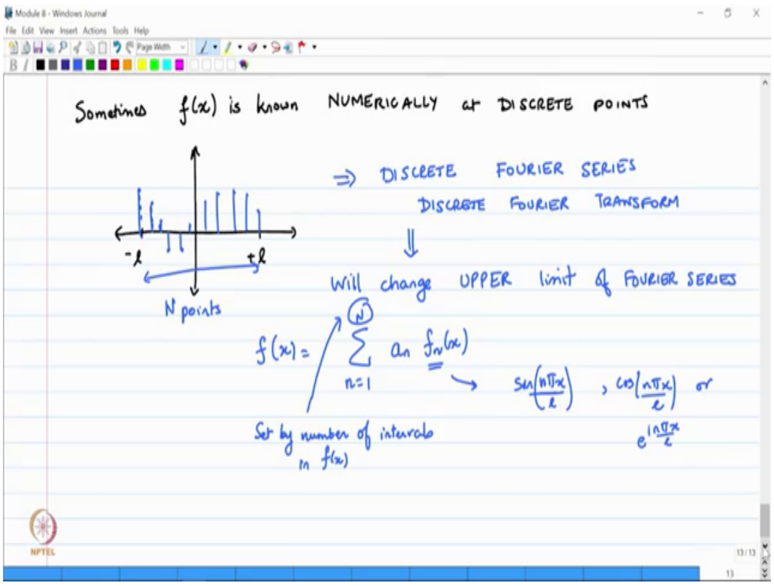

The next important point that I want to make is that sometimes f of x is known numerically at discrete points. In other words your f of x instead of being so, suppose I take minus l to l, now I might I might have a function which I know only at discrete points, I might only know it at discrete points this is the problem that often happens numerically. So, you know it only at discrete points you do not know it at all the points.

So, then you can use a version called the discrete Fourier transform discrete Fourier series or its often called a discrete Fourier transform. What this will do is I mean we will discuss this later when we are talking about Fourier transforms, this will convert the will change upper limit of Fourier series. So, what I will get is I can write f of x is equal to sum over n equal to we might get from 1 to N; now what you will get is A n and you will get fn of x.

So, I have used fn to denote the basis function in this case, in this case fn will be your either your sin n pi x, x by l or cosine n pi x by l with the factor or you can write as e to the i n pi x by l, but the important thing is that the upper limit, this n its usually set by number of intervals m f of x. So, basically this number of points there are n points. So, there are n discrete points in f of x you will have n terms in the Fourier series.

So, this is something that we will discuss later when we are talking about Fourier transforms, but what this means is that you can do you can use these ideas of Fourier series, even for functions we can use for functions that are discontinuous we can also use for functions which are not known at all the points, which we know only at discrete points and this is something that happens in lot of numerical calculations.

So, now, let us take a differential equation and see what happens when you do a Fourier expansion.

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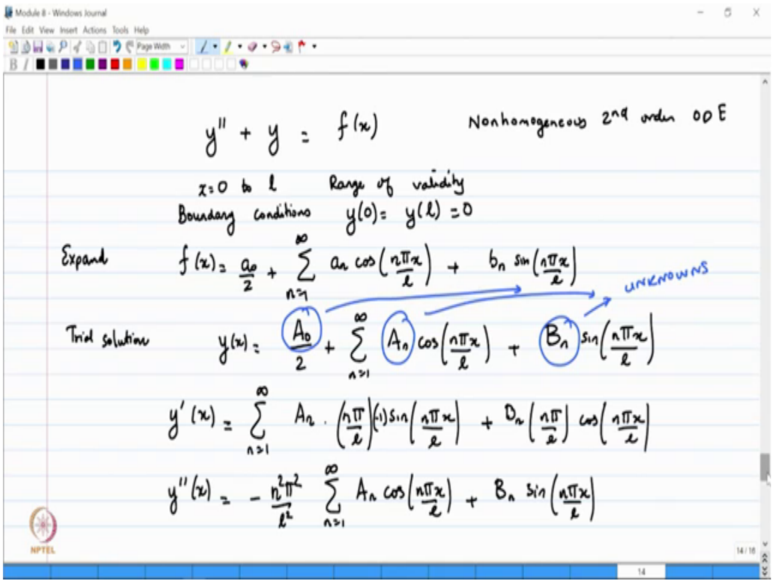

So, let me take a very simple differential equation, let us take y double prime plus y equal to f of x. So, I just took a very simple differential equation. In fact, you can you can do for arbitrary differential equations, but we will illustrate the use of this by taking this simple differential equation.

So, now, what we are going to do is f of x. So, this is a non homogeneous second order ODE, actually you know the solution of the homogenous homogeneous ODE you know the solution , but let us just go ahead and work this out and let us say this is defined for I mean you can choose whichever interval, let us say you choose your interval as x equal to 0 to l, I did not mention this explicitly, but basically we saw when we were discussing earlier when you are discussing periodic functions, that if you go back all the way to the last lecture.

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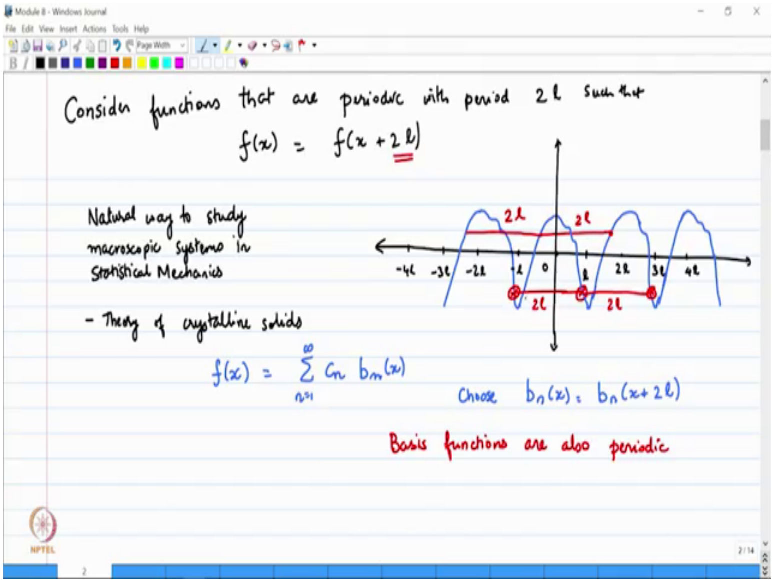

So, basically we chose are interval as minus l to l, but you can choose from 0 to 2 l you can choose from you can choose different intervals. So, we will take from 0 to l and let us let us consider. So, in this case, so for convenience this might not be defined for this particular form of the differential equation it might be valid only from 0 to l, you can take I mean we just consider that case. And further let us take the boundary conditions y of 0 equal to y of l equal to 0. So, we just take this boundary condition.

Now if you want to solve this by Fourier series, what you will say is you will write y of x is equal to A 0 by 2 plus. So, you let plus A n cosine of n pi x by l, plus b n sin of n pi x by l, n equal to 1 to infinity and now. So, what we did was let me write we first write f of x in this form, and then what we will say is if. So, whatever this f the right hand side whatever function we have we expand it in a Fourier series.

Now, further what we will do is write or I should say expand f of x equal to this. So, we wrote a Fourier expansion of this. So, we know how to calculate A 0 A n b n etcetera then what you do is you take a trial solution, y of x is equal to; now what we will do is we will take some other Fourier series I will just call it capital A 0 by 2, plus some more n equal to 1 to infinity, A n cosine of n pi x by l plus and B n sin of n pi x by l.

So, now suppose I have this now what would be y prime of x y prime of x? So, the first term will go to 0 A 0 will not contribute, second term will have and so. So, now, what I will have is sum over n equal to 1 to infinity, I will have A n into n pi by l sin n pi x pi l and there will be a minus. And then I will have plus B n into n pi by l cos n pi x by l and now if I take y double prime of x, I can write it as minus n square pi square by l square and what I will get is, I will get back A n times cosine n pi x by l. So, A n cosine of n pi x by l plus B n sin.

So, I just took 2 derivatives or sins and cosines. So, I will get minus n square pi square by l square into this. So, now, I can substitute back in this equation. So, I go back to the differential equation when I substitute that.

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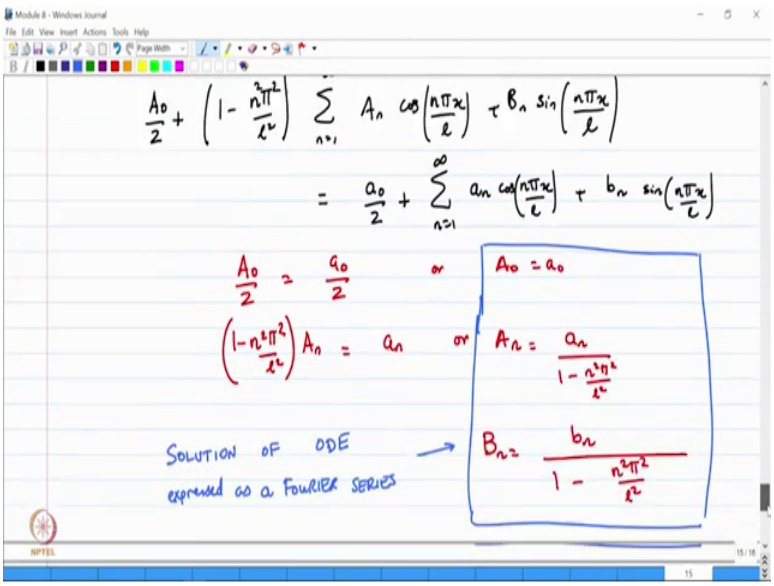

What I will get is I will get A 0 by 2 plus sum over n equal to 1 to infinity, now from the A 0 by 2 I got from the y; now from the y, I will have these terms. From the y double prime I have exactly those terms, but I have multiplied by 1 minus n square pi square by l square.

So, I can just write a factor of 1 minus n square pi square by l square and I can write sum over n equal to 1 to infinity A n cosine n pi x by l plus B n sin n pi x by l . So, this is the left hand side and the right hand side was A 0 by 2 plus sum over n equal to 1 to infinity, A n cos n pi x by l plus B n sin n pi x by l. Now what you get from this is something really nice. If you see the left hand side, left hand side this is a constant term. So, the first term is constant and then after that each term is either proportional to cosine or a sin.

Now, because all these functions are orthogonal functions, we can these are these are like linearly independent functions. So, they form a basis. So, what you can do is you can equate them term by term. You can write A 0 by 2 equal to a 0 by 2 or A 0 equal to a 0 and then you can write 1 minus n square pi square by l square, A n equal to a n or A n is equal to a n divided by 1 minus n square pi square by l square, and similarly you can write for B n also B n is equal to b n divided by 1 minus n square pi square by l square.

So, what we have done is we have actually solve the differential equation, this is the solution of the differential equation. This represents solution of ODE expressed as a Fourier series. Remember what I mean is that your solution we wrote in this form. So, when you write the solution in this form the A 0 is A ns and B ns these are the unknowns. So, your problem of determining the y of x is equivalent to determining the unknowns, if you know the unknowns then you can express it as an infinite series.

So, now, here you got the unknowns in terms of A 0 a n and b n now A 0 the little A 0 little A n little B n are all known because you know f of x see since you know f of x. So, these can be calculated from f of x.

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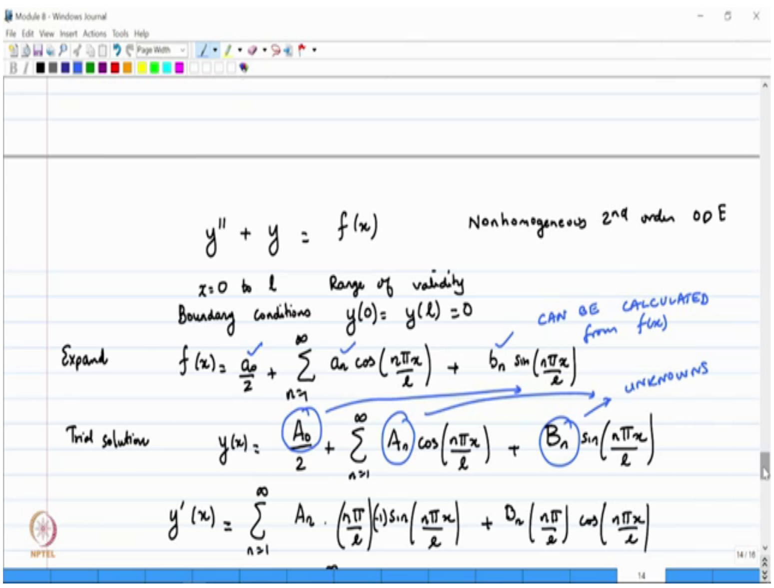

So, can be calculated from f of x using the usual integral formula, so these are all knowns, so, basically by doing this you have actually you have solved it you have solve the equation of course, it is written as an infinite series and that may or may not be convenient depending on what the values of A 0 a n and b n are, but nevertheless you have a solution of the differential equation.

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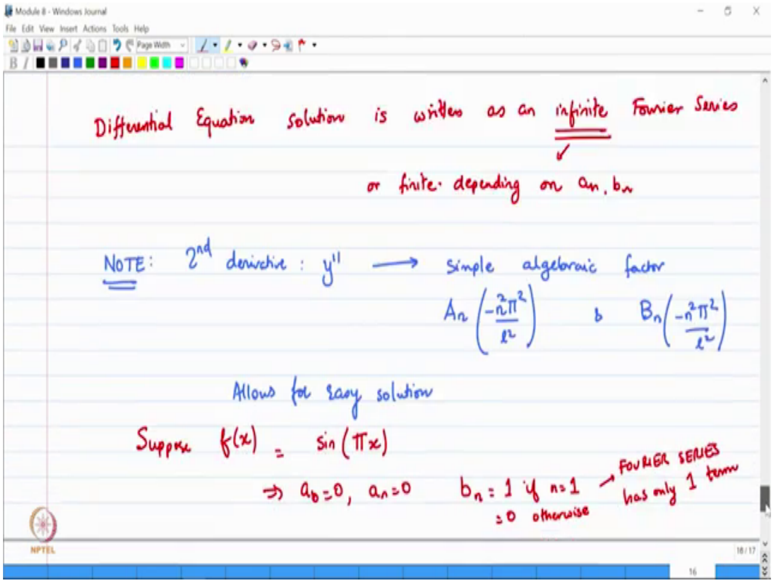

So, differential equation; equation solution is written as an infinite series infinite Fourier series. Well I am writing infinite. So, this can also be finite depending on or finite depending on a n b n. So, this is a general method I am just showing what is what is important. So, the highlight or the most imp most thing important thing to note, second derivative of y double prime this just led to simple algebraic factor.

So, your second derivative of y double prime just led to A n into minus n square pi square by l square. Just this factor of minus n square pi square by l square multiplied by A n and B n was multiplied by minus n square pi square by l square. So, this is the important thing, the second derivative just correspond it to multiplying by this factor. So, where you have to take a second derivative of y of x what you have to do to A n was just to multiplied by minus n square pi square by l square nothing else. So, this is the important lesson.

So when you take y double prime you remove the A 0 term and then each of this whole thing you just multiplied by minus n square pi square by l square. So, this is there the important lesson. So, this is a huge simplification. So, this allows for easy solution. Now incidentally we can also there are there are a lot of other interesting things you can see in this; now suppose f of x is equal to let us say sin omega x or let me let me make things even simpler let me make it as sin pi x.

So, if f of x is sin pi x then what can you say? When you do a Fourier then clearly. So, this implies a 0 equal to 0, a n equal to 0 b n equal to 1, if n equal to 1, b n equal to 0 otherwise if n is not equal to one it is 0. So, you can easily see this just by inspection, you can if you if you want you can actually calculate it by the integral and you will get this. Now if you have something like this if you have only. So, we say that your Fourier series has only one term, if your Fourier series has only one term then what happens. So, what happens to the now what we said is that you are A 0 will be 0 A n will also be 0 B n.

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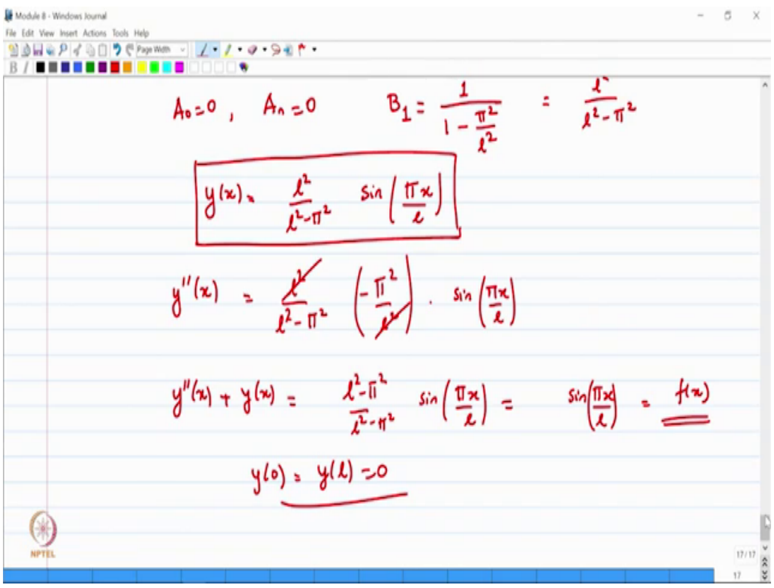

So, now, what you get is A 0 equal to 0, A n equal to 0, B1 is equal to 1 divided by 1 minus now n square n square is 1. So, pi square divided by l square pi x by l let me take it as pi x by l sorry. So, pi square by l square. So, B1 is this or I can write this as l square divided by l square minus pi square. So, then my solution y of x is equal to sin of just l square over l square minus pi square sin pi x by l.

So, this is the solution of the differential equation, you can verify that y double prime of x is equal to. So, I will get l square divided by l square minus pi square into pi square by l square with a minus sign, into sin pi x by l. And you can easily verify that y double prime of x plus y of x is equal to. So, I can just cancel these 2. So, and in y of x will have and l square. So, I will get l square minus pi square divided by l square minus pi square sin pi x by l is equal to sin pi x by l, equal to f of x. So, you can easily verify that this satisfies the differential equation, and y of 0 equal to y of l equal to 0 that is also easy to see.

So, what we have seen is we have solved this differential equation using this Fourier series. In this case are differential equation was really straightforward because your f of x had a very simple form. So, we know how to solve this using I mean you can solve this. So, the left hand side of the differential equation was just constant coefficients, the non homogeneous part was just a simple sin function.

So, the solution will be a sin function and in this case you can show that it is equal to this function. As I said the real power of Fourier series is in solving for you know fairly complicated differential equations, which you cannot solve just in this manner I mean suppose f of x has a very complicated form, you can still write it as a Fourier series and you can still write term by term. And then and then your solution you will get each of the coefficients each of the coefficients of your solution and finally, you can you will get your solution in terms of an infinite series infinite sin and cosine series, and you can write you once you know that the see convergent, you know that taking more and more terms would make it more and more accurate.

So, this is a real power of the Fourier series as a method for solving differential equations. Now in the next lecture what I will try to what I will do is try to step back a little and say this Fourier series we took the advantage of the fact that your sin and cosine are the basis functions, but can there be other basis functions, and why is it that we could use sin and cosine in this case as basis functions for periodic functions. So, these are the problems that we will address in the next lecture, and that will take us to the Sturm Liouville theory of orthogonal Eigen functions.

Thank you.