Advanced Mathematical Methods for Chemistry
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Module - 08
Lecture - 02
Fourier Expansions and Differential Equations
Part A

So in this lecture, I will be looking at Fourier expansions a little more. We look at Fourier expansion of some simple functions just to show you how it works. And then we will show how we use Fourier series to write differential equations in simpler forms and in some cases you can actually solve them. So, first let us you know before we get started, let us write the Fourier series in a slightly different form this is also a form that is very common.

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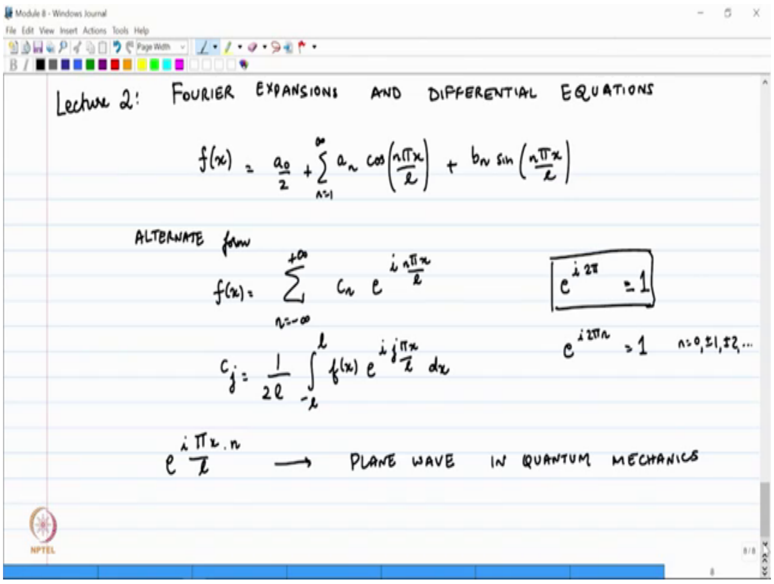

So, we wrote a Fourier series as a 0 by 2 plus sum over n equal to 1 to infinity a n cosine n pi x by l plus b n sin n pi x by l. There is an alternate form of the Fourier series which is to write from is to write it as f of x is equal to sum over n equal to minus infinity to plus infinity c n e to the i times n pi x by l. This is exponential of an imaginary number. So, you know that e to the i times 2 pi is equal to 1.

So, we so, we use this result e to the i times 2 pi is 1. And you take any power of this so is so, if you if you multiply this by any integer then you will get 1. So, this implies that e to the i times 2 pi n is equal to 1, for when I say n equal to minus infinity to plus infinity; this is for any integer n equal to 0 plus minus 1 plus minus 2 and so on. So, this is the alternate form of the Fourier series. And when you write the Fourier series in this form, then our c j and this is you can verify can be shown to be equal to 1 over 2 l integral minus l to l then you have f of x e to the i into j pi x by l.

Now, this j is an integer, j is an integer which is the coefficient, i is the imaginary exponent this times d x. So, this is the alternate form of the Fourier series and very often this is used. In fact, the in quantum mechanics this function e to the i pi x by l times n is referred to as a plane wave in so, this is often referred to as a plane wave. And this writing this f of x in this form is often referred to as a plane wave expansion.

So, this is about Fourier series in a different form. Now a few other things I want to mention about Fourier series. Now let us take some examples.

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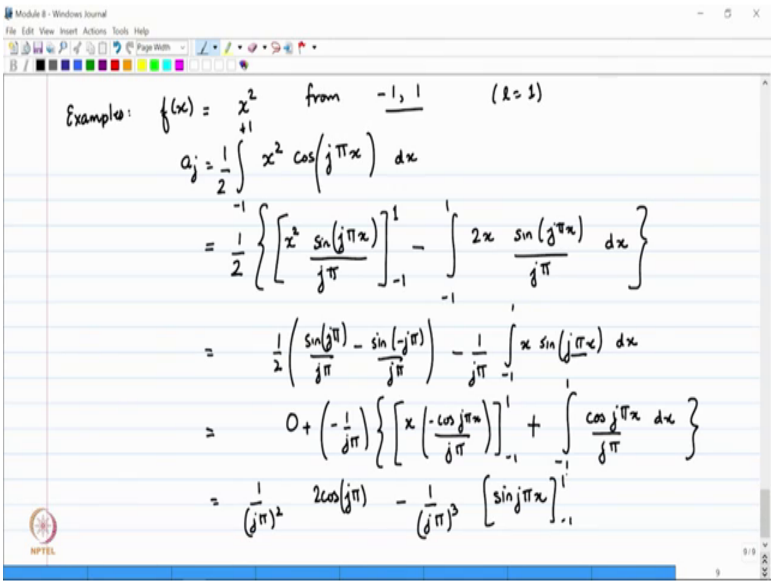

So, f of x is equal to let me write equal to x square. So, suppose f of x is equal to x square. Now obviously, if you have a simple function like x square your Fourier series is not is not really important but nevertheless we will take this function just to illustrate the calculation of your Fourier coefficients, so, then what you will say is that a j is equal to integral 1 over l integral minus l to l.

So, and again; let me take the interval from minus 1 to 1. I am choosing my interval as minus 1 to 1. So, then this becomes 1 over 2 and now I get x square cosine, now I will get j pi x l is 1 d x. So now, what do we; so, can you do this integral. So, the question is can you do this integral? Now can you do this for an arbitrary value of j. Now if you want to do for an arbitrary value of j, what you will say is that you will integrate this by parts.

So, the first term will be x square integral of cosine is sin j pi x divided by j pi. And this is whole thing is from minus 1 to 1. And the other term is minus now what you have is integral of derivative of x square is 2 x times, sin j pi d x from minus 1 to 1. Now when x equal to plus 1 then you have sin j pi. So, x equal to 1 then you have 1 times sin j pi. And when x equal to minus 1 again you have one and you have what you have is plus sin of u rather you have minus sin of minus j pi divided by j pi.

Now sin j pi if j is an integer sin j pi is 0. So, this whole thing is 0. This whole term; so, each of these terms is 0. Now the second term; now you still have; let me cancel the twos. So, I have minus, now I have integral of x. So, I have 1 by j pi I will take it outside and I have integral minus 1 to 1 x sin j pi x j pi x d x. So now so, what I will get is 0 and here I will get minus 1 by j pi.

Now again I will do the; I will do the integration by parts. So, the first term is x integral of sin is minus cosine j pi x divided by j pi. This whole thing is evaluated from minus 1 to 1. Then you have minus integral of now what will have is derivative of x is 1 and I have a cost j pi x 1 d x.

So now, what I can write this as, I can write this as; now let me take j pi and j pi. So, I have a 1 over j pi the whole square and what I have now when x equal to 1 then I have minus cosine of j pi. So, what I have is minus cosine of j pi when x is minus 1 then again I have minus cosine of j pi. So, I and then and then I have a minus sign here. So, I can write this as 2 cosine of j pi.

I will leave it as cosine of j pi for now. We will look at it a little more closely in a bit. Now the other term; so, I have in this case I have minus 1 by j pi square and I have integral of cos j pi. So, what I will write it as I will write it as minus 1 by j pi cube. Now integral of cos cosine I have a sin j pi, pi x from minus 1 to 1. And now what I get is 2 cosine of j pi divided by j pi square minus.

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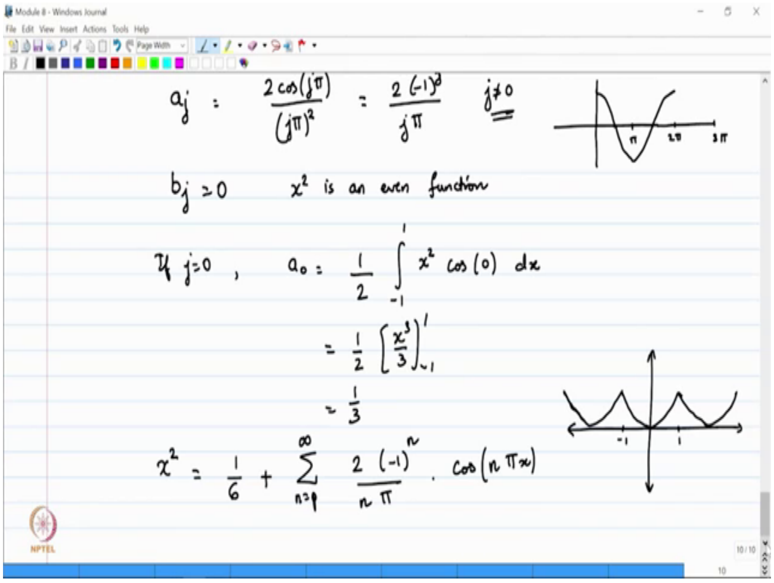

Now sin j pi x of course, will go to 0 sin j pi and sin minus j pi are 0. So, we will just get this.

Now, what is this equal to; so, cosine of j pi cosine of, cosine of pi is minus 1. Cosine of 3; so, if you look at your cosine function this is pi, 2 pi, 3 pi. So, cosine of 0 is so, it goes something like this. So, this is basically you can easily show that this is 2 minus 1 raised to j divided by j pi. So, cosine of j pi is minus 1 raised to j. So, basically you get a j equal to this. And you can easily show that b j has to be 0 because, and why does b j have to be 0 because, because our choice of function x square is an even function. You can easily verify by actually doing the integral. So, therefore, I can write x square is equal to sum over j equal to 0 to ok. What about a 0? So, a 0, a 0 if you put j equal to 0 then you get minus 1 raise to 0 that is 1. In this case you cannot you cannot do this for this is j not equal to 0.

So, this is true for j is not equal to 0. Now if j equal to 0 then, you can see this that if j equal to 0 then a 0 goes to 0. You can see this by looking at by looking at this. So, a 0 is equal to cosine of x square, ok let us let us evaluate a 0 is equal to 1 over 2 integral minus 1 to 1. Now what I have is x square. Now cosine of 0 cosine of 0 d x cosine of 0 is 1. So, this is 1 over 2. Now what you have is x cube by 3 from minus 1 to 1.

So, this is 2 by 3. So, this is equal to 1 by 3. So, a 0 is equal to 1 by 3. So, I can write; I can write x square I can expand it as; now a 0 by 2 is 1 by 6 plus sum over, I can just write it as n equal to 0 n equal to 1 to infinity. Now a j is 2 minus 1 raise to j divided by j pi and then you have cosine of j pi x; n I replace j by n. So, this is the expansion of x square. So, what you did was you are writing x square as a sum of x square in terms of periodic functions. Again we wrote x square from minus 1 to 1; what the implicit assumption is that is that is that what we are doing is, we are we are imposing periodicity.

So, when I would write x square. So, this is minus 1 to 1 x square looks like this. When you impose the periodicity then what we are going to say is that this same function keeps repeating. So, it goes like this. So, what we are really looking at is a function that looks like this. And when you expand this as in terms of in terms of sins and cosines then only the cosine term appears. And it appears in this form. So, this is a very, very nice illustration of the method of Fourier series; another example which I want to emphasize.

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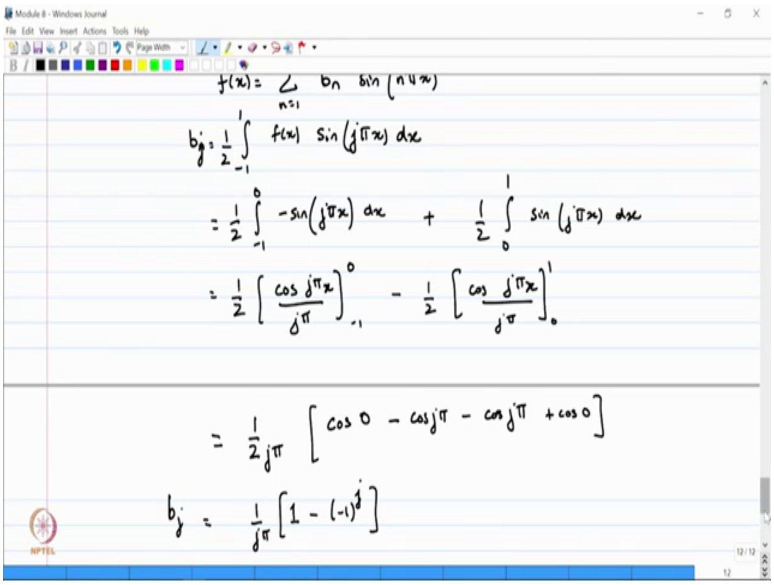

So, suppose you have a discontinuous function; incidentally what I would encourage each of you to do is to actually take the first term. So, put n equal to 1 calculate cos pi x and try to plot, try to plot by taking finite number of terms. So, take n equal to 1; then take n equal to 1 and 2, 1, 2, 3. So, take more and more terms and see and you can actually see how this infinite series will converge to f of 2 will converge to this x square function.

So, that is an interesting exercise that I encourage all of you to do. Now coming back let us take an example of a discontinuous function. So, you can take f of x is equal to 1 for x greater than 0 equal to minus 1 for x less than 0. And l equal to 1. So now, again I can do the Fourier expansion. So, in this case, you can clearly see that f of x is an odd function.

So, an of x a n equal to 0. So, there are no cosine terms. So, f of x is equal to sum over n equal to 1 to infinity b n sin n pi x l is 1. Where b n is equal to integral mine to 1, 1 by 2 and what I have is f of x sin let me say b j sin j pi x d x. And now if I can I can do this integral in 2 ways. So, first I do from minus 1 to 0. So, I get half integral minus 1 to 0 now from minus 1 to 0 f of x is minus 1.

So, I have minus sin j pi x d x, and then plus half integral 0 to 1 sin of j pi x d x. Now what is this integral of minus sin is nothing but plus cosine. So, so I can write half cos j pi x by j pi from minus 1 to 0, plus of write minus half cos j pi x by j pi from 0 to 1. These are the 2 terms and you can easily verify that that when x equal to 0 when x equal to 0 cosine of 0 is 1. So, you get cosine of 0 is 1 by j pi. So, let me take the 1 by 2 j pi outside.

So, I will get cosine of 0 minus, now I have cosine of j pi into minus 1 cosine of minus j pi which is nothing but cosine of j pi. Here I have minus cosine of j pi, the first term will be cosine of j pi I have had a minus sign outside. And I have plus cosine of 0. So, I can write as 1 over j pi cosine of 0 is 1, and cosine of j pi is minus 1 raise to j.

So, this is my Fourier series. So, I know my; so, I know my terms you can check b 1 is equal to 1 by pi 1 minus, minus 1 raised to 1 is minus 1 So, 1 plus 1 that is 2.

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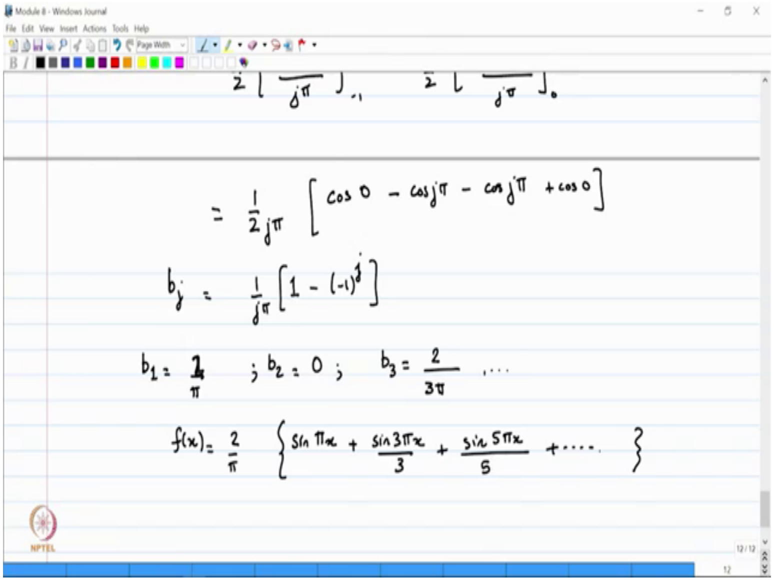

So, b 1 equal to 2 by pi b 2 equal to 0 b 3 is equal to So, again I get 2 divided by 3 pi and so on. So, so basically I can write I can write f of x is equal to 2 by pi sin pi x plus sin 3 pi x by 3 plus sin 5 pi x by 5 yeah plus So on. So, this is my f of x. So, this is how you expand a function that is not continuous.