Advanced Mathematical Methods for Chemistry
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Module - 08
Lecture - 01
Fourier Series, Fourier Expansion of Periodic Functions

In module 8, we will learn about Fourier series, Fourier expansions. And we will also step back and talk in general about Eigen function expansions, and the Sturm Liouville theory. So, Fourier series is one of the most widely used methods in all of engineering and all of science. We regularly use it in to solve differential equations or to express it is or to actually simplify problems, one of the most common uses is in is when we are studying periodic systems like solids, and if you want to do if you want to solve Schrodinger equation for solids, then we expand them in periodic functions, and this is where we use Fourier series.

So, what I am going to do in this module is, talk about Fourier series just as though I mean I mean we will just talked about Fourier series as it is, and then we will step back and try to go back towards the general method of Eigen function expansions. And the theory of Eigen functions expansion which is the Sturm Liouville theory. The advantage of doing of understanding the Sturm Liouville theory is that you can do for several different functions. You do not need to only use Fourier series; you can use other series also. So, let us get started. So, in the first lecture I will be talking about Fourier series and Fourier expansions.

So now before I talk about Fourier series or Fourier expansions, the one thing that you have seen Very often is I mean this from linear algebra.

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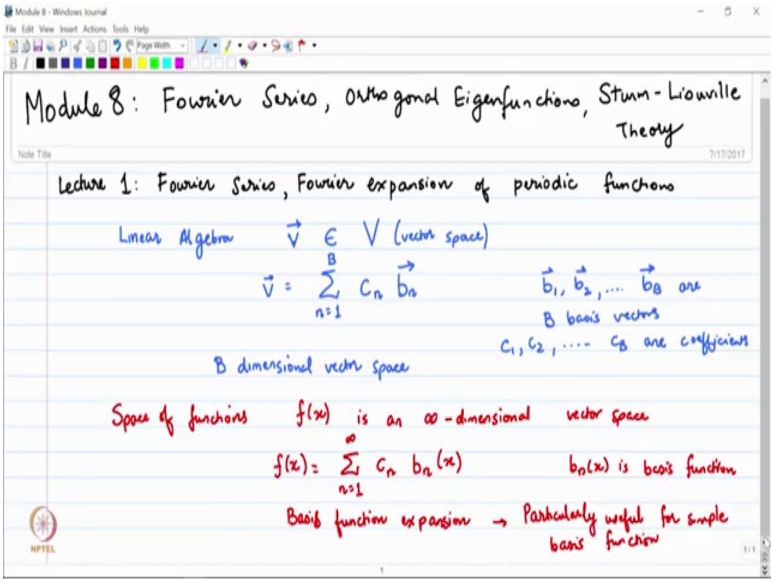

If you have a vector v that belongs to some vector space V capital V. Then we know that we can write v as sum over n equal to; I should write 1 to B. And I will write it as C n where b 1 b 2 up to b B are basis vectors or B basis vectors. And c 1, c 2 I have to c B are coefficients.

So, what I have said is that you can take any vector and expand it as a linear combination of basis vectors there are b basis vectors. So, this is in a b dimensional vector space. So, this is something that you are fairly familiar with you have seen this quite often. Now we also said that recall from your linear algebra that the space of functions is an infinite dimensional vector space. So, the dimensionality is infinite. And So, if you try to do something like this. So, suppose you have So, we might be able to think of something like this f of x is equal to sum over n equal to 1 to infinity, there are infinitely many and you have c n and you have b n this is a basis n of x is basis vector and now this is a vector space of function So, we will call it a basis function. And there are infinitely many of them. So, you have an this series goes all the way to infinity.

So, this is in general you can you can think of this as basis function expansion, what it says is that you can take any function and expand it as a linear combination of basis functions. Now why is this helpful? I mean it this is particularly useful if the basis function has some simple form. So, particularly useful if basis function has some simple form. Now this is the this is the motivation for introducing the Fourier series.

So, what we are going to do is Fourier series, when we talk about Fourier series we are thinking about basis function expansions. And what we want to do is to do this basis function expansion. Now in general you do not know what your basis is; if you have infinitely many if you are the space of all functions, then the your basis set will be infinite, there will be infinitely many basis functions. So, so are there cases when this can become simpler, and the answer is yes. So, we will look at the Fourier series.

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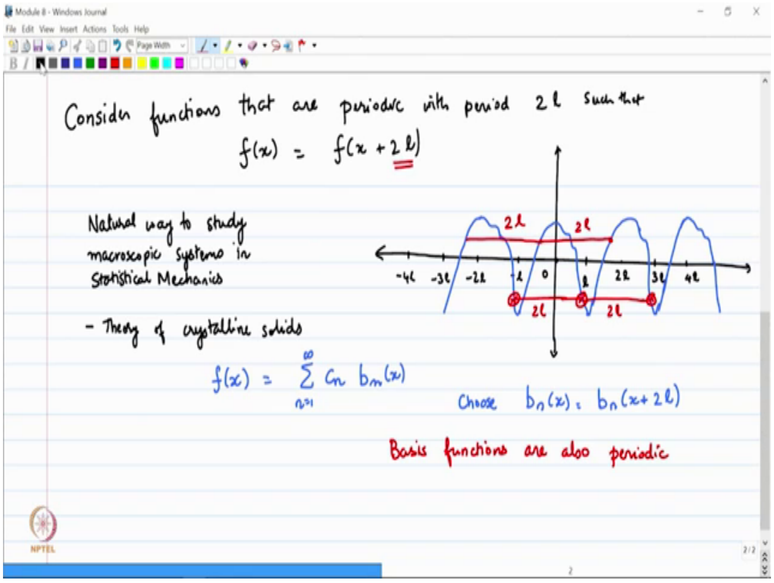

Now consider functions that are periodic with period 2 l such that f of x is equal to f of x plus 2 l.

So, this is the periodic function, the period is 2 l. And what I am going to do is I am going to; so what does of what does a periodic function look like? So, if you if you were to plot this function and I will deliberately show it as a slightly longer in the x direction. So, this is 0 this is 2 l, let me make l, 2 l, 3 l, 4 l. And then I have on the minus side I have minus l minus 2 l. So now, what I can do is I can just to I let us say, I have a function that looks like this.

Now, since it is periodic then the value of the function here and here should be the same. And then it is it has to again do exactly the same thing, I am just exaggerating all these wiggles just to show what a periodic functional look like; so on and then similarly on the other side too. So, so this is what your periodic function will look like. So, basically you take you take the value of the function at any point it will be the same if you if you shift by 2 l, you will get you will get to exactly the same value similarly you shift by 2 l on this side you will get to exactly the same value, you go you can keep going; you go by 2 l oh sorry, I you go by 2 l. you go by 4 l. etcetera, you will basically get the same value.

So, the function just keeps repeating itself. One of the things about this function is that is that you can take any point, you can take this point and you go to 2 l ahead and you will end up with exactly the same point. If you go 2 l forward or you go 2 l backward, you will end up with exactly the same value. So, the value or the function will be exactly the same. So, these periodic functions; they actually they are very they appear very naturally in lot of, very natural way to study; let us say macroscopic systems in statistical mechanics. This is one point that will become clear when you do your statistical mechanics courses that that you know you treat the system as periodic.

But anyway this is just one point, but also they as I said more they might appear in theory of crystalline solids. So, crystalline solid is periodic in space. So, the same pattern keeps repeating. So, in that in that you use periodic functions. But, you know it is much more general than that that is what I want to emphasize. Now suppose I consider a periodic function then I can do I can do the same expansion f of x is equal to sum over n equal to 1 to infinity, and I can use b n or c n b n of x; what I will choose. So, since we have since we have the periodic condition for x so one way to ensure that one way to ensure that f of x is periodic is to choose b n of x equal to b n of x plus l x plus 2 l.

So, the idea is your basis functions are also periodic with the same period 2 l. So now, now what; that means, is if the basis functions are periodic, then any linear combination will be periodic any linear combination of basis functions will be periodic with the same period 2 l. So now, what is the choice of basis? So suppose you choose; b n of x is equal to sin n pi x cosine n pi x by l.

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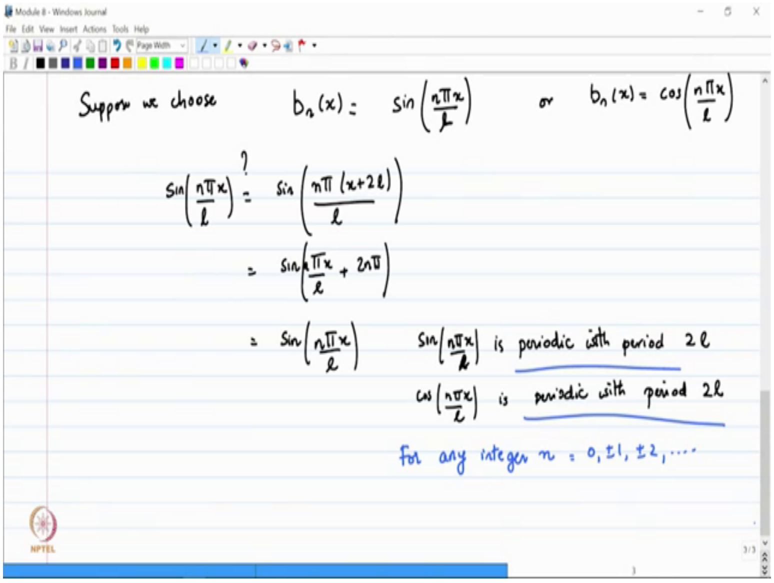

Now notice that that both these are periodic functions. So, sin n pi x by l, is equal to sin or I will put little l here is equal to sin n pi x plus 2 l by l, you can you can verify this you can verify this.

So, this right hand side I can write as sin n pi x by l plus, now sin 2 n pi plus sin n pi x by l this is nothing but sin n pi x by l. So, clearly this is similarly. So, so sin n pi x by l is periodic with period 2 pi, with period 2 l. Similarly cosine of n pi x is also periodic with period 2 l. So, so this is the first thing that both sin and cosine are periodic with period 2 l. So this particular choice where you took it as sin n pi x by l. So, you can take any value of l n.

So, this is true for any integer n, integer means n can be 0 plus minus 1. plus minus 2 and so on. So, now with this, we can either choose sin or cosine, but we notice one thing.

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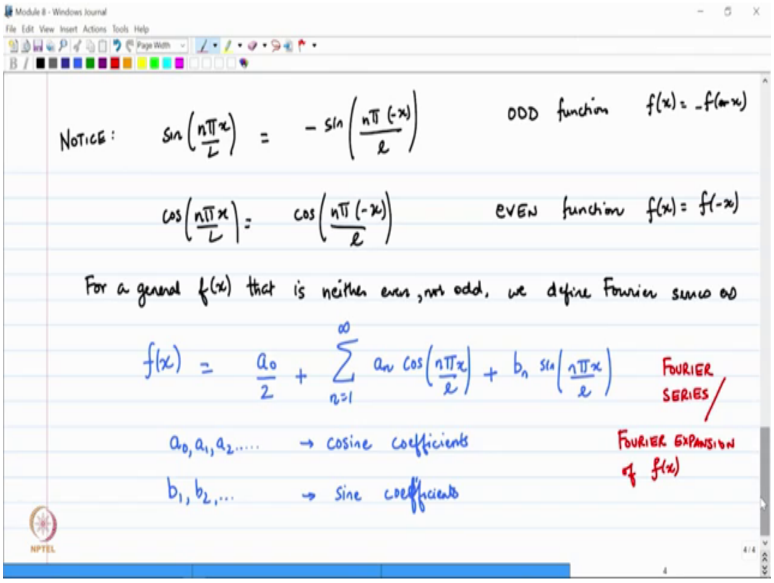

We notice that sin of n pi x by l is equal to minus sin n pi minus x by l. So, sin is an odd function. So, any linear combination of odd functions. So, suppose you take suppose you take a linear combination like this where b n is odd then you will get an odd function. Similarly cosine is equal to plus cosine of n pi minus x by l this is an even function.

So what that means is suppose you just do an expansion where b n as b n is cosine then f will be even function. Even function means it has to have the same signed on both sides. So, odd function means it has to have the say it has to have opposite sin on both sides. Now if you look at this function it is neither even nor odd. So, f of x equal to minus f of minus x and f of x equal to f of minus x that is an even function.

So now so this motivate just so, for a general f of x that is neither even nor odd, we choose or we define Fourier series as. Now also notice that notice that this if n equal to 0 the sin term vanishes sin term goes to 0, if n equal to 0 the cosine term goes to 1.

So, what it is defined as is the following way let me write this in a different color. So, f of x is equal to a 0 by 2 plus sum over n equal to 1 to infinity a n cosine of n pi x by l plus b n sin of n pi x by l. Where an and b n; now a 0 and a 1, a 2 it goes all the way to infinity are called the cosine coefficients. These are scalars and b 1 b 2 up to infinity are call the sin coefficients. Notice that b 0 there is nothing called b 0, because if n equal to 0 there is no sin term.

So, this is the definition of the Fourier expansion or Fourier series or it is called or you use a term Fourier expansion of f of x. So, you are expanding the function in a Fourier series. So, you are writing this function as a linear combination of cosines and sins. There is a constant term. So now any periodic function; so the important thing is any periodic function these 2 words are important.

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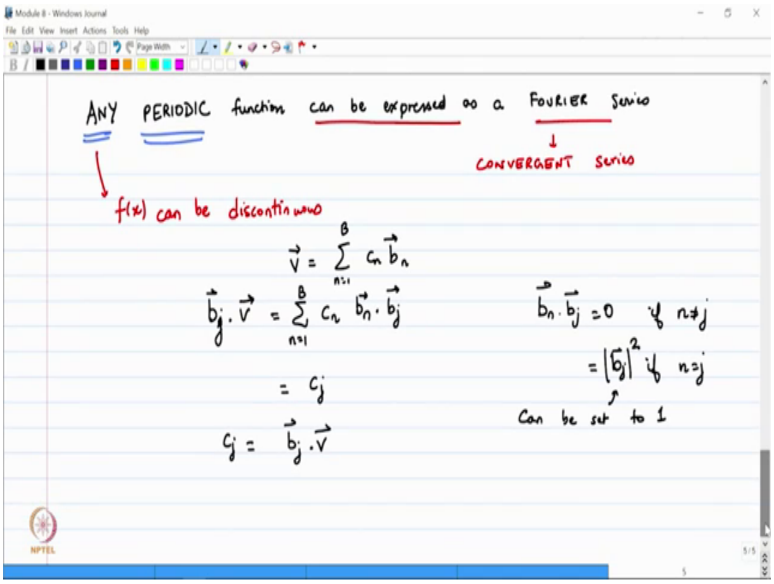

You can take any function and it can be, but it has to be periodic. Any periodic function can be expressed as a Fourier series. Now when I say it can be expressed as a Fourier series; what do I mean it can be expressed.

So, what I mean is that this is convergent; that means the; you take more terms; you get closer to the actual function. Now the other thing is when I say any it f of x can be discontinuous, f of x can be discontinuous also. It need not be continuous. Now a few more things; I want to mention about Fourier series, is the following Now, let us get back to our vector. So, when we write v is equal to sum over n equal to 1 to B c n and b. And then these are these are basis functions. So, suppose I do b j dot v. So, if I dot the vector with one of the basis then, then this will be I can write it as sum over n equal to 1 to b, c n b n dot b j. And usually the basis functions are orthogonal. So, b n dot b j equal to 0 if n is not equal to j. So and is equal to b j square if n equal to j. And you know this can be chosen to be 1. So, can be set to 1; so if you make b j unit vectors, then you then you can you can set to the length of b j equal to 1.

So, b j dot v is nothing but it will just give you c j. So, so what you can do is you can write c j as v j dot v. So, the coefficients of this basis expansion can be got by dotting taking a dot part of the vector of the vector with the basis vector. Now the same thing can be done you can you can do a very, very analogous thing for functions. So, if you have if you have your Fourier series f of x.

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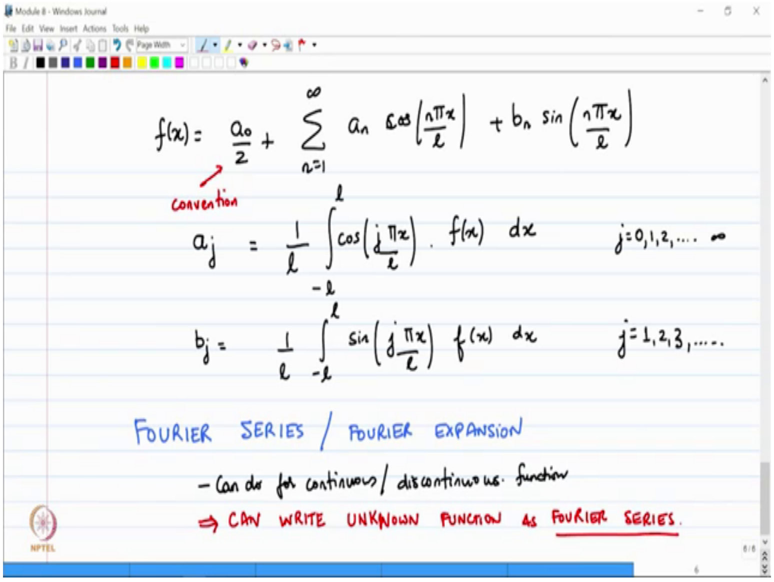

Equal to a 0 by 2 plus sum over n equal to 1 to infinity, a n cos n pi x by l plus b n sin n pi x by l. So, if you have something like this, then I mean; I should emphasize at this factor of 2 is just for convenience. You do not need to take this, but this is d1 by convention. So, this is just a convention, and we will see why it is convention, but it is useful for a; it is done for a particular reason.

So, I can write a n is equal to, now I have to take a dot product of this function with this basis. So or let me write a j is equal to; so I will take now in this case the dot product. So, I have cos j pi x by l. Now I have to take a dot product with f of x. Now in the space of functions a dot product is typically defined in this way. And what is done is that this has a factor of 1 by l this is taken in front. So, this turns out to be a very is very useful way to define a j.

In fact, in fact you can easily verify that something like this is true, by taking by taking various choices of f of x. Now again this 1 by l factor is done actually to it is it is like this normalization constant, it is like, that is what sets b j square to, so this is a j and this is valid for j equal to 0, 1, 2, up to infinity. And b j you can write in very similar way you can just write it as 1 by l minus l to l sin of j pi x by l f of x dx and now j equal to now sin x the 0 term does not exist.

So, you have j equal to 1 to three so on. So, this is the definition of the Fourier series. So, this is what is meant by the Fourier series, Fourier series or Fourier expansion. And as I said you can do this for you can do this for any function can do for both continuous and discontinuous functions; slash discontinuous functions. The other important thing and I will let me emphasize this point; can write unknown function as Fourier series. This is probably the most important application of Fourier series. So, you write an unknown function as a Fourier series and what this does what happens when you write your unknown function as a Fourier series.

So, you had f of x is equal to your, So if this is an unknown function. Now when you write it as a 0 plus some over n equal to 1 to infinity an cosine of n pi x by l plus b n sin n pi x by l.

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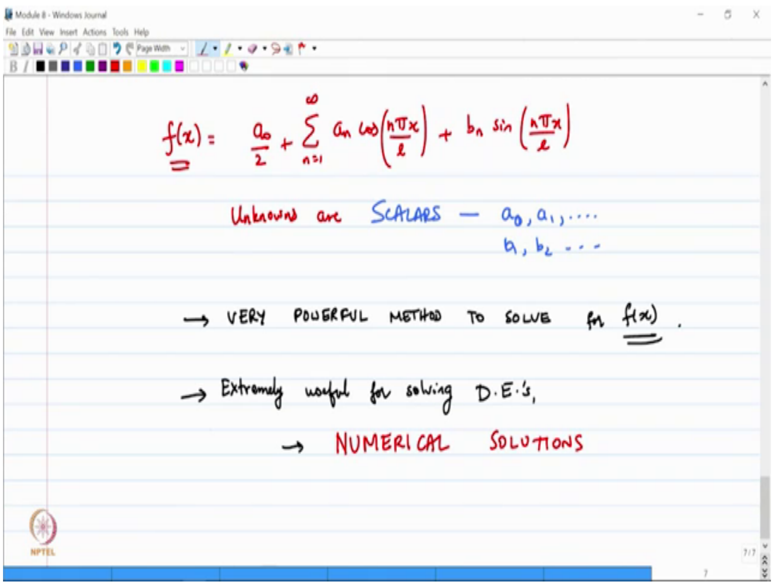

On the right hand side the unknowns scalars a 1 or a 0, a 1, b 1, b 2 and so on. So, the unknowns so now, instead of having an unknown function you just have unknown scalars. And this is a very this turns out to be a very powerful way to solve, very powerful method to solve for f of x.

So now instead of having a function as an unknown, what you have is all these scalars as unknowns. And then and then and then what you will get is we will see that we will see how this can be used to solve differential equations. So, this is extremely useful in solving differential equations, both analytically and numerically. So I should I should emphasize that that numerical solutions are also very; so especially when you are doing especially when you are solving these equations numerically, this expansion is very useful.

So, I will conclude this lecture here. So, in the next lecture, we will actually look at some look at some ways in which Fourier expansion is used. We will see we will look at Fourier series of some simple functions. And then and then we will also see what how you apply it to solve differential equations, and how it transforms the problem of solving differential equations.

Thank you.