Mathematics for Chemistry
Prof. Dr. M. Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture - 22

What we have seen so far is that, if you had a function that was periodic with period 2 L, you could express it as a Fourier series.

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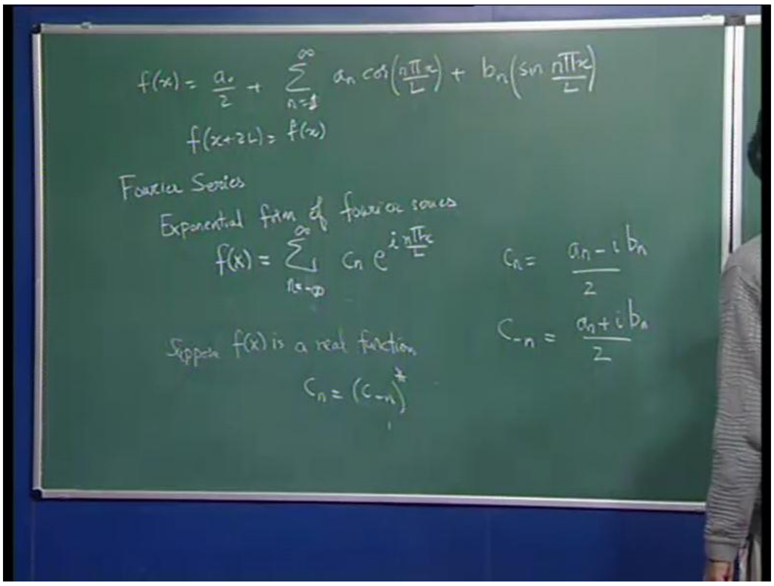

You could write it as a linear combinations of cosins, sins and a constant term. And we saw the expression for each of the a n's and each of the b n's, and so this Fourier series is one of the pillars of modern computational science. So, in almost all fields of engineering and science you will come across the Fourier series, if you have arbitrary functions, you expand them in terms of these Fourier series.

Now, sometimes we use an exponential form of Fourier series, so in this you write f of x is equal to sum over n equal to 0 to infinity or n equal to minus infinity to plus infinity C n e to the i n pi x power L. So, n equal to minus infinity to plus infinity C n times e to the i n pi x by L, so this is the exponential form of the Fourier series and this does one thing, it helps to extended to complex functions and in some cases, it turns out to be easier to work with this.

Now, this series is identical to this series, if you notice that C n is equal to a n minus i b n by 2 and C of minus n, so this goes from minus infinity to plus infinity so C of minus n, this is equal to a n plus i b n by 2. So, you can show this quite easily I mean, by just doing this expansion taking the terms separately, so C 0, you will find that, C 0 is equal to a 0 by 2 because n equal to 0 so C 0 is a 0 minus, b 0 is 0, so a 0 by 2.

And then for C 1, you would have C 1 e to the i pi x by L then you would have C minus 1 e to the minus i pi x by L. So, when you combine those two, you will get something that relates to a 1 so by inverting the relation, you can show that, C n is this and C minus n is this. So, this is the exponential form of the Fourier series and this is also something that is commonly used; now, in this form of the series, we said that we can extended to complex functions.

Now, suppose, f of X is a real function so if f of x is a real function, you can show that, C n is equal to C minus n star so this is something that, you can show quite easily. To show this, what you want to say is that, you have C n times e to the i n pi x by L and you have C minus n e to the minus i n pi x by L.

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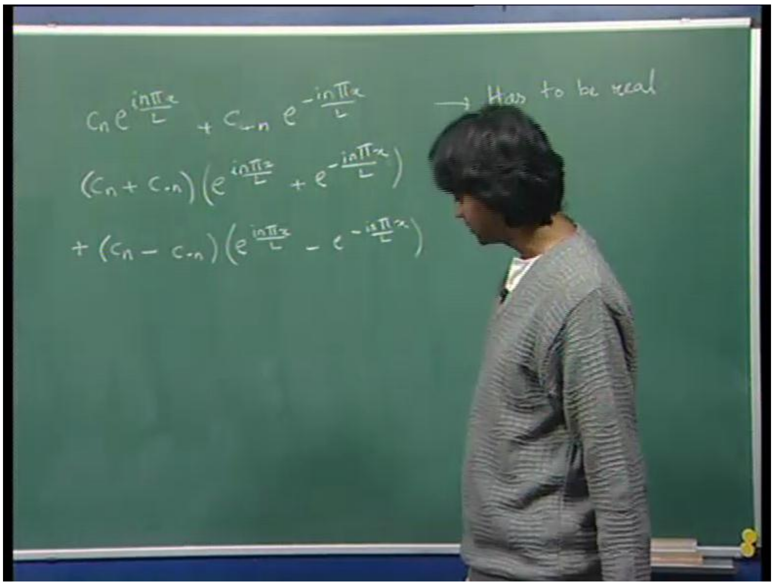

So, you rewrite that as C n plus, to show this you have C n e to the i n pi x by L plus C minus n e to the minus i n pi x by L. So, you will have two terms in this series, that will appear in this form and they should add up to give something, that is real for all values of, for whatever choice of and we want to find the appropriate choice of C's that give them.

So, I can write this as C minus n x by L, so you will have one term, that looks like this and you can write the other term is. So, what I did was, I have added a C n or C minus n e to the i n pi x by L, C n e to the minus i n pi x by L and I should subtract those terms and a factor of 2. So, if you add up these two you will get, this should be a factor of 2 so and this whole thing has to be real.

And what that will imply is that, these combinations have to be real numbers and one way to get that is, if the imaginary parts of C, so what we will say is that, if f of X is a real function then C n, it turns out will have to be equal to C minus n star. And you can see this fairly easily because each of the terms here has to be a real number and this has to be true for all n.

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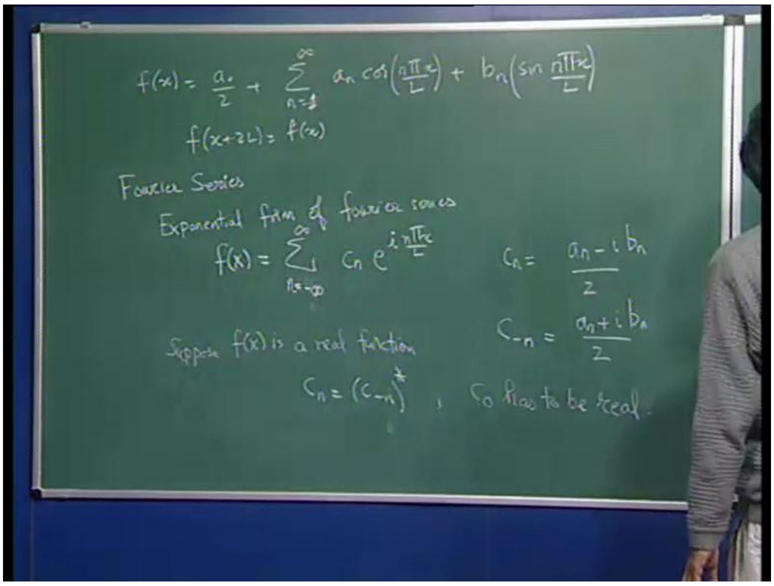

And C 0, in addition C 0 has to be real, so this is the condition so if f of x is a real function then C n has to be equal to C minus n, the complex conjugate of C minus n. So that, what you have is a number plus it is complex conjugate, which has to be a real number.

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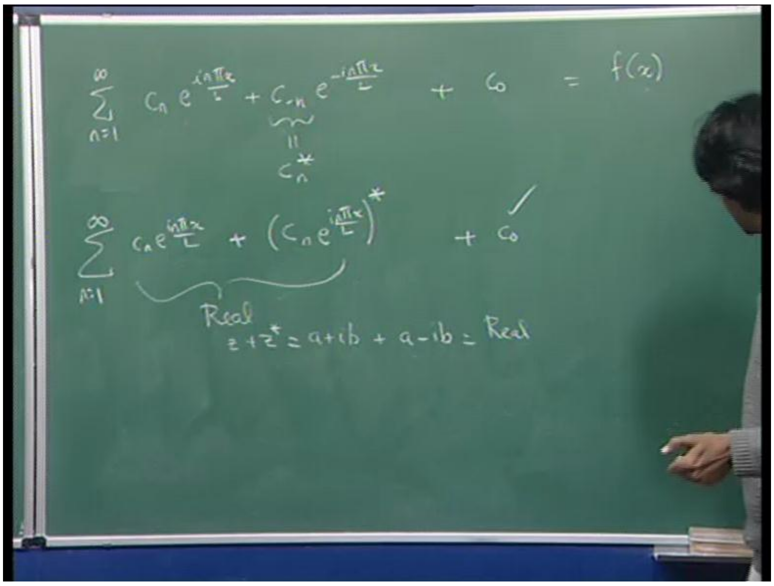

So, if that is true then you have C n by L, we have sum over n equal to 1 to infinity plus C 0 so this series I write in this form and if this is equal to f of X, so if f of X is real, we say that, this has to be real. And then if C n equal to C n star, so if this is c n star then that implies, this is C n e to the i n pi x by L star plus C n e to the i n pi x by L, to infinity plus C 0.

So, this is real now, this is what is that, what appears here is exactly this so a number plus it is complex conjugate, this whole thing has to be a real number. So, if you have a complex number like a plus i b, the complex conjugate of that is a minus i b and so this is real number so it is just 2 a. So, if you have a real function then the Fourier series becomes in the exponential form, has this condition between C n and C minus n.

Now, next what we will do is, we will try to take different limits so here, we chose a boundary condition where, the function was periodic between minus L and L. Now, this L can be anything and very commonly, we take L equal to 2 pi, L equal to pi so 2 L is 2 pi. And this is also very popular in lot of applications so let us write the series when L equal to pi.

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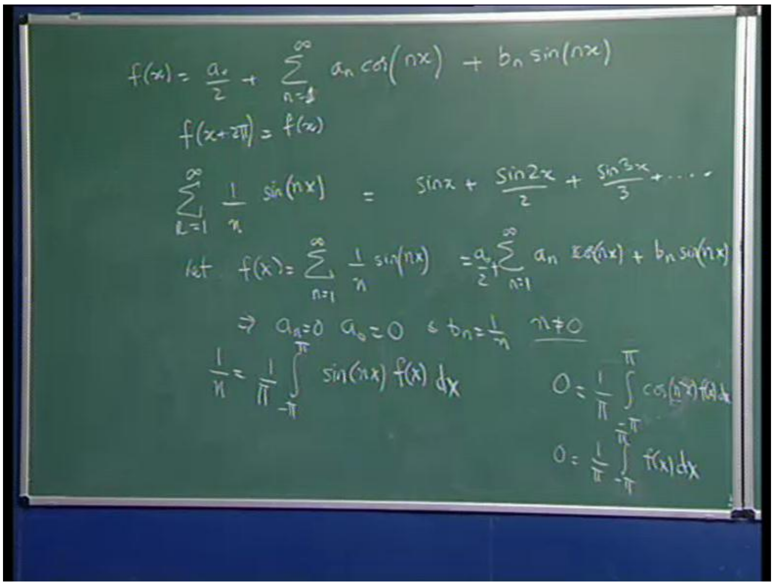

So, if L equal to pi, you can show that, your Fourier series becomes cos now, you have n pi x divided by pi so that is just n x, plus b n sin n x. And in this case, f of X plus 2 pi is equal to f of X and this is also a very common form of Fourier series, that is seen in various applications. Now, you know there are lot of interesting expansions for sins you know, you have the Taylor expansion for sin as an infinite series, involving pi.

Now, there are also lot of interesting inverse relations, for which where, pi can be written as a sum of sin functions and you can often see this, when you do a Fourier series. So, one example is, you can show that, sum over n equal to 1 to infinity, 1 over n sin n x so if somebody asks you, what is the value of this series. So, this is equal to so when n equal to 1 this is sin x, when n equal to 2 is sin 2 x by 2, when n equal to 3 it is sin 3 x by 3 plus so on.

And suppose, somebody ask you, what is the value of this series then it is not very obvious by looking at the series but what you can do, this is quite easily when you see the Fourier representation. So, what you will say is that a n, so we say, let f of X is equal to sum over n equal to 1 to infinity, 1 over n sin n x. So, we just say, let f of X is this now, what we will do is, we will write f of X as a Fourier series so a 0 by 2 plus sum over n equal to 1 to infinity, a n cos n x plus b n sin n x.

Now, since sin n x is a periodic function with period 2 pi, I just wrote it as a periodic function in period 2 pi. Now, this implies a n equal to 0, a 0 equal to 0 and b n equal to 1 by n or n not equal to 0 so for all n not equal to 0, b n is equal to 1 by n. Now, what you want is the following, you want 1 by n is equal to integral 1 over pi, I can do from minus pi to pi and what I will get is, sin n x f of X dx.

So, what you need to have is that, this the value of this integral should just be 1 over n and also you should have 1 over pi, integral minus pi to pi cosine n pi x by L, n x cosine n x f of X dx. And also, the integral under f of X, so when n equal to 0, so also 0 equal to 1 over pi integral minus pi to pi f of X dx so you want the function that is, first of all the function has to be an odd function.

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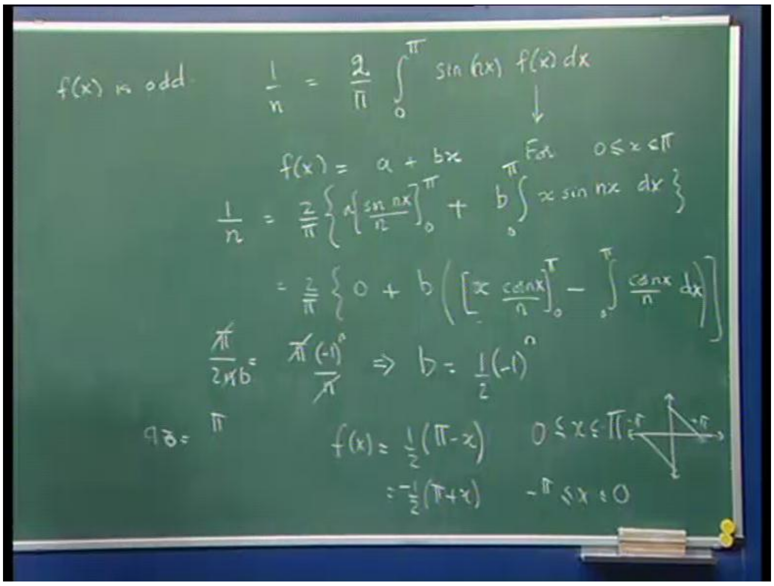

So, implies f of X is odd, if it is an odd function then automatically cosine of not only will this be true but also cosine of n x f of X will be true, for all positive n, it has to be odd. Now, if it is an odd function then sin is also an odd function, f of X is also an odd function, I can write 1 over n is equal to 1 over pi integral 0 to pi or I can write 2 over pi integral 0 to sin n x f of X dx.

Now, you might say that, you still do not have the value of f of X but you can get the value of f of X quite easily just by inspection. You know that suppose, you had f of X was a constant so suppose, f of X was a constant then integral sin n x from 0 to pi will give me 1 over n sin n x. So, then what I am going to demand is that, f of X since it has to be odd, so if for positive x, this was just a constant or just a simple function of x then you would get 1 by n but a constant turns out to be an even function.

So, what we will say is that, let f of X is equal to a plus b x so if it just let f of X equal to a plus b x now, you can immediately see that, 1 over n f of X, this is for 0 less than equal to x less than pi. So, then 1 over n is equal to 2 over pi now, the first term will just give me sin n x divided by n from 0 to pi times a plus b times integral x sin n x from 0 to pi dx. Now, this term goes to 0, so this just becomes over pi 0 plus now, what is b times this integral x sin n x and you can integrate this by parts.

The first term will be x times cos n x by n between 0 and pi, and the second term is minus integral cos n x by n from 0 to pi dx and this whole thing multiplies b. So then you can show this, I will take the pi by 2 n and I will bring the b down, pi by 2 n b now, this is when x equal to pi, you get cos n pi by n. So, you get pi time cos of n pi by n and cos n pi is minus 1 raise to n by n so cos n pi by n and in this case, your integral of cos n x will give me sin n x, sin x from 0 to pi will just give me 0.

So, what you see immediately is that, this is equal to so this implies b is equal to 1 by 2 minus 1 raise to n so b is just 1 by 2 minus 1 raise to n. Now, then what about a, how do you choose the value of a now, you have to choose a such that you get an odd function. And so what we will do is the following, we will choose a so a 0 is pi let us just choose a 0 equal to pi, I will motivate this in a very shortly.

But, what you will finally get is the following that, f of X is equal to half pi minus x, this is for 0 less than equal to x less than equal to pi and f of X equal to half pi plus x, for minus pi less than equal to x less than equal to 0. So, what you will get is that, f of X satisfies this sort of relation and So, what you finally got out of all this is that, this function has Fourier series, that just looks like 1 by n sin n x.

So, this function is also is the same as a saw tooth function so if you plot this, so when x is greater than 0, this looks like pi minus x, when x is less than 0 it looks like pi plus x so it look like this sorry this should be minus. So, this is minus pi, this is plus pi and what you have is, f of X is an odd function, it is an odd function and the Fourier representation is just 1 over n sin n x.

And you can easily verify that, this satisfies this sort of expression now, what is remarkable is the following, there are two things that are remarkable. One is that, your function looks very discontinuous, your function has this sharp discontinuity but if you look at the Fourier representation, it looks perfectly continuous. So, essentially, this is this discontinuous function, a function that looks very discontinuous is represented by this nice looking Fourier series.

So, Fourier series one of the things that is, one of an important application of Fourier series is to convert functions that are very discontinuous into a sum of continuous functions. Now, the next thing is suppose, I take this and I put x equal to pi by 2 so if I put x equal to pi by 2 then what I get is x is greater than 0 so f of pi by 2 is just half pi minus pi by 2 that is, pi by 4. Now, on this side, what I get is the following if x is pi by 2, sin n pi by 2 is equal to 1, if n is odd and it is 0, if n is even.

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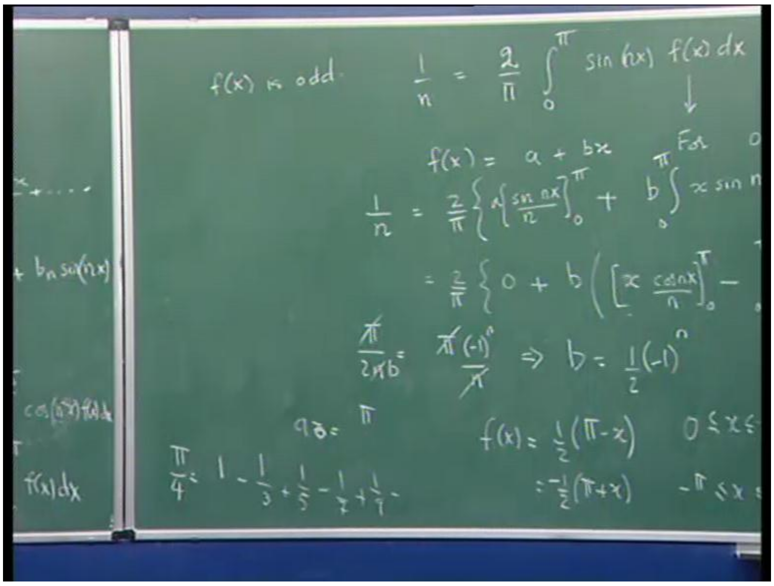

So, what you find is the following, you can write, so pi by 4 is equal to now, I will write the sum explicitly to make things clear. So, when n equal to 1 so you get 1 into pi by 2 that is, sin pi by 2 that is, 1 so this becomes 1. Now, when n equal to 2, this becomes sin 2 n pi by 2 that is, sin n sin pi and sin pi is 0 so you get 0, n is 3, this is sin 3 pi by 2 that is, minus one so you get minus 1 by 3.

Similarly, you can show plus 1 by 5 minus 1 by 7 plus 1 by 9 and so on so this is another representation for pi so pi can be expressed as this infinite series or pi by 4 can be expressed as this series. So, in this way, you can derive lot of series for pi using this method of Fourier transforms. So, the last part I want to do in this lecture on Fourier series is to give the orthogonality relations in this case. In this case, the orthogonality relations will instead of, minus l to l you will have minus pi to pi so that is the only change, I will write those on this side just to complete our discussion.

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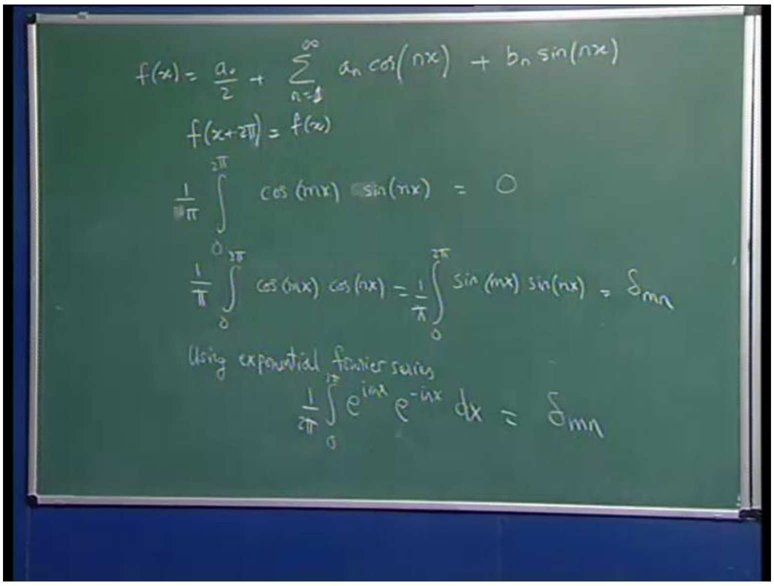

So, I can write this as integral now, I can choose my limits as minus pi to pi or I can also choose it from 0 to 2 pi, there is no difference. The orthogonality relations of cos m x sin n x is equal to 0 and then you have a integral 0 to 2 pi and 1 over pi sorry this is equal to integral sin m x, n x equal to del m n. So, because of the periodicity, I can shift my interval to 0 to 2 pi without any change and I can write my so this is equal to 0, if m is not equal to n and 1, if m is equal to n and this also implies something else, if you do the exponential.

So, using the exponential relation Fourier series, the orthogonality relation becomes integral e to the i m x e to the minus i n x dx, this is equal to delta m n so this is another sorry 1 by 2 pi. Now, this is actually quite an interesting relation now, m and n are distinct so m can either be equal to or may not be equal to, so this means, at integral e to the i m minus n x dx from 0 to 2 pi, that should be equal to 0, if m is not equal to n.

So, next what we want to do is, to go from this Fourier series to something called Fourier integrals and Fourier integrals are used for different class of problems. So, Fourier integrals is the more general version of this Fourier series where, instead of having a discrete set of functions, you have a continuous set of functions so that will be our next topic, that we will do.

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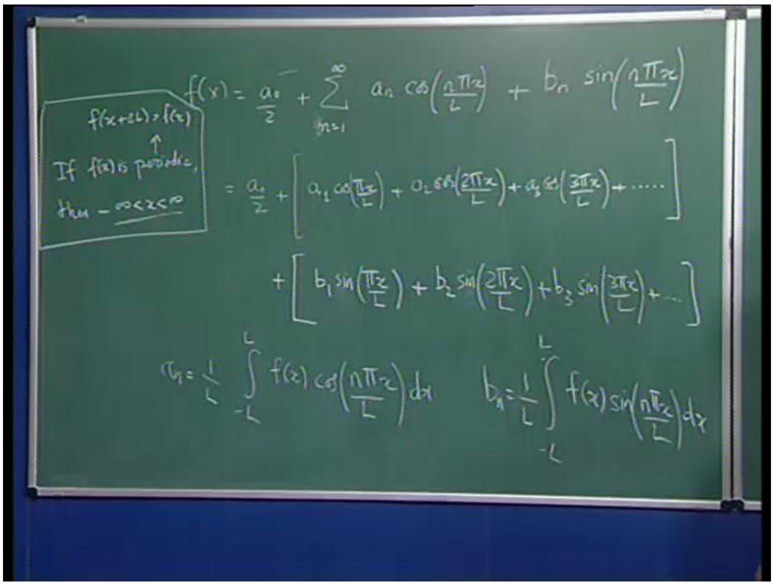

So, we have seen the Fourier integrals and the Fourier integrals in the Fourier series, you represent a function as a 0 by 2 plus sum over n equal to 1 to infinity a n cos n pi x by L plus b n. So, this is the Fourier integral we have been discussing and you should think about this in the following way, you should think about this as a 0 by 2 plus and if I write out a first few terms here, a 1 cos pi x by L plus a 2 cos 2 pi x by L plus a 3 cos 3 pi x by L plus and so on plus similarly for b n. So b 1 cos i x by L plus b 2 sorry it should be sin, it should be b 1 times sin, sin pi x by L plus b 2 times sin 2 pi x by L.

So, this is the Fourier series and if we had this series, you will be said that, a n equal to 1 over L integral minus L to L, f of x cos n pi x by L dx and b n is equal to 1 over L integral minus L to L f of x sin n pi x by L dx. so that is the description of a n and b n and now, what we said, that this the range of x, if f of x is periodic then minus infinity less than x less than infinity so if f of x is a periodic function, this expansion can be done for all x.

So, you should specify periodic, this implies f of x plus 2 L equal to f of x so periodic with period 2 L so 2 L is the period of f, so just put this separately. So, if f of x plus 2 L is f of x then this expansion is valid for minus infinity less than x less than infinity so whenever you have a periodic function, you can always expand it in a Fourier series. Now, there are couple of things, one is we want to extend this to a functions, that are not periodic so that is what, we are going to do in this next class and when you do that, the natural extension becomes something called a Fourier integral.

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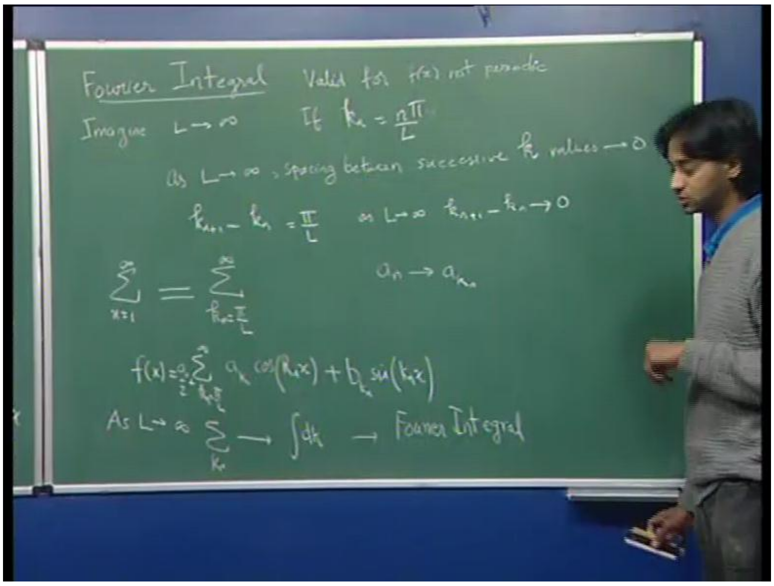

So, that is what, we are going to do now so in the Fourier integral, I will try to motivate the Fourier integral in the following way. So, Fourier integral is valid for f of x not periodic and so how do you do the Fourier integral and the way we will do it is, we will motivate the Fourier integral by the following argument. So, imagine L tending to infinity so you just imagine that, your length is tending to infinity so what was this L, L was the, 2 L was the periodicity of the function.

So, our integral was from minus L to L so 1 over L integral minus L to L now, imagine that L goes to infinity so this seems go to minus infinity to plus infinity. Something else happens, if you look at all these, this is pi x by L, 2 pi x by L, 3 pi x by L and so on so the various terms here, they are of the form n pi x by L. So, if k n equal to n pi by L, so you denote n pi by L by k n then what happens is that, so as L infinity, the spacing between successive k values tends to 0.

So, in other words, if you look at k n plus 1 minus k n that is, the difference between k n plus 1 and k n, this is just pi by L and as L tends to infinity, k n plus 1 minus k n tends to 0. So, what happens is that, in this sum, the successive k values become very closely spaced so now, you can instead of writing this as a sum over n equal to 1 to infinity, I could write this as a sum over k n. So, I can write this as a sum over k n equal to pi by L to infinity.

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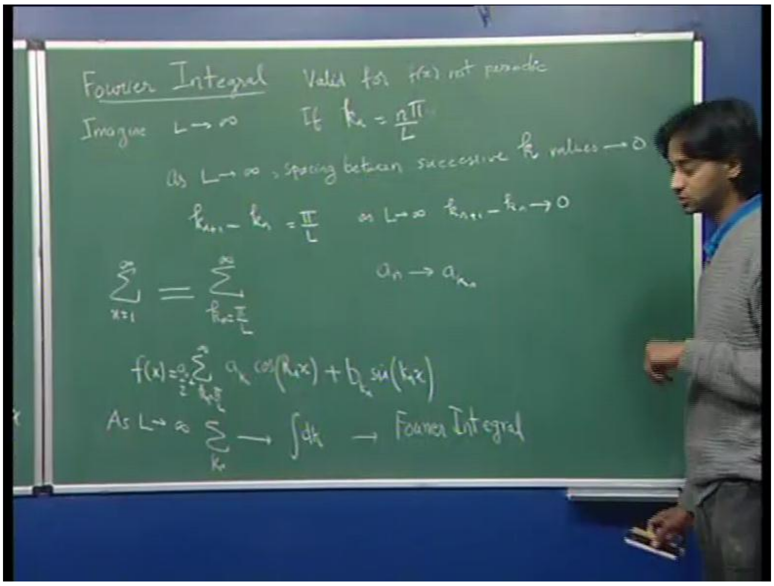

So, this is identical to infinity so that means, it goes from pi over L then in the next function, it is 2 pi over L, 3 pi over L and so on, all the way up to infinity. So, I can write this in this form and instead of a n, I denote by a k, I just call a k instead of, calling it a 1, I will call it a k n. Now, what happens is that, this f of X looks like a sum over a 0 by 2 plus sum over k n equal to pi over L to infinity, a k n cos k n x plus b k n sin k n x.

So, I wrote exactly this but instead of denoting this coefficient as n, I denote it as a k n and the reason for that will become obvious. Now, if you imagine that, L tends to infinity then this sum because the successive values of k are very closely spaced, this sum becomes an integral. So, as infinity sum over k n tends to integral over d k with some appropriate normalization factors or actually more tends to this quantity.

So then what will look like is, you know let us ignore the complex term for now but it will look like some integral and I choose to do this in the sins and cosines but I could also do this with the exponential form. So, this integral will be called the Fourier integral so whatever the integral representation of this, will be called the Fourier integral and since L is tending to infinity, your range of integration will go from minus infinity to infinity.

And you do not need to worry that, the function is periodic because any way L is going to infinity, period is infinity so it is as good as a non-periodic function. So, this is the motivation for using the Fourier integral and seeing how it works now, let us take the specific example of the exponential expansion and we will use that to represent the Fourier integrals.

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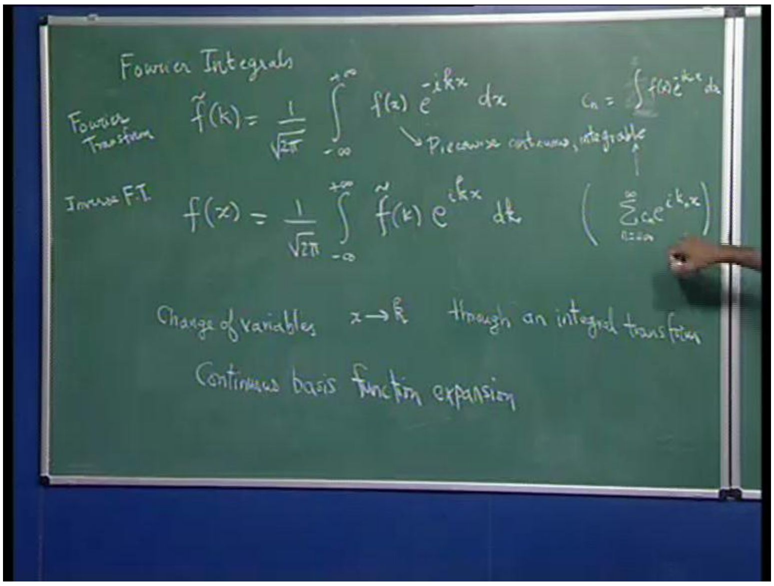

So, the standard definition of the Fourier integral in terms of, you can define it in terms of sins and cosines but we choose to do it in terms of exponentials because that is the most commonly done Fourier integral. So, in that f of k is equal to 1 over root 2 pi integral minus infinity to plus infinity, f of x e to the i k x dx so f of k is written as f of x into e to the i k x so it is written as, it is the minus i k.

So, that your f of x, you can put a tilde on this f of x is, so let us look at this so you write f of x as an integral over d k f of f tilde of k, f tilde of k is like the coefficient of e to the i k x. So, you should compare this with sum over n equal to 0 to infinity, i n equal to minus infinity to infinity C n e to the i k n x, you should compare it with this. So, in the exponential representation of the Fourier series, you had sum over n equal to minus infinity to infinity, C n e to the i k n x.

Now, here instead of that, you have since the k’s are continuous so the sum over n equal to minus infinity to plus infinity becomes integral over d k and e to the i k x so this part is clear and instead of C n, you have f tilde of k. So, f tilde of k should be thought of as the coefficient just like C n is a coefficient here so there is a lot of similarity between this expression and that expression and this is called the Fourier integral. There are some factors of 1 over root 2 pi put here so that, this f of x and f tilde of k have a very symmetric look to them.

Now, this is called the Fourier transform, this is called the inverse Fourier transform now, when you look at this expression, you notice something that, what we have suppose, we started with a function of f of x. When we do the Fourier transform, you get a function of k, this is and I have to use the tilde to say that, this function is in general, a different function.

So, we started with a function of x and you went to a function of k so this is like a change of variables so from x to k. And further thing is that, both f x and f tilde of k, they contain the same information so the same information that is, f of x is there in f tilde of k. So, that means, from f tilde of k I can calculate f of x, from f of x I can calculate f tilde of k. So, it is like a change of a variable but not the typical change of variables that you do, this type of it is a change of variables x to k, through something called an integral transform.

So, this f tilde of k is related to f of x through an integral alternatively, you can also think of this especially, if we look at this connection so this transform looks like a Fourier series. But, instead of having discrete basis where, n went through discrete numbers, you had a continuous basis so this is or you can think of this as a continuous basis function expansion.

So, either of these methods work, so you can think of it as an integral transform, transformation of variables or you can think of expanding the function in a continuous basis. So, that is the other way and notice that in this case, you would say that, your C n is equal to sum over or will be integral f of x e to the minus i k n f x dx with some factors, let us not worry about the factors, but you had something like this. And in this case, what you have is f tilde of k, which is what we associated with C n that looks like integral f of x e to the minus i k x, so there is a lot of similarity between this.

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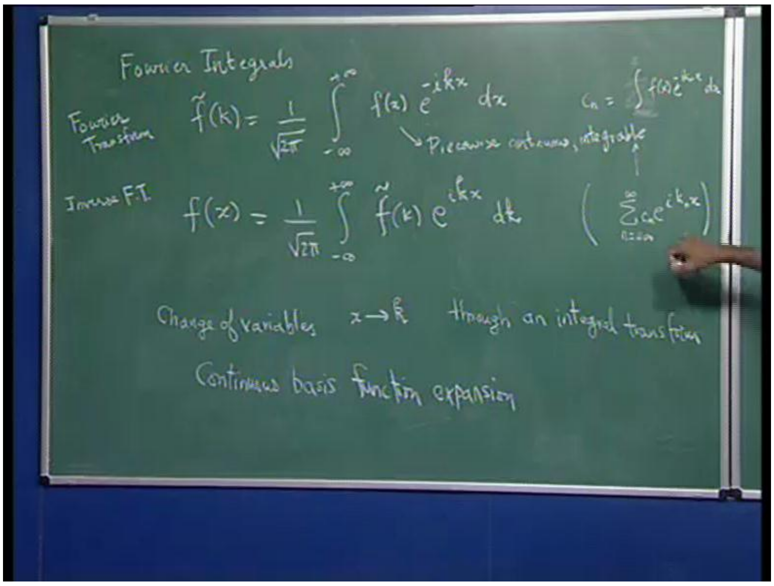

So, in a sense, what you are doing here is just the same thing as this but you are letting your case be continuous. So, couple of more things I want to mention, one is that, this Fourier transform will only defined, if f of x is piecewise continuous so f of x has to be piecewise continuous, it has to be integrable. So, these are certain conditions for the existence of the Fourier transform, so if your function is not piecewise continuous or integrable then it does not have a Fourier transforms. So, now, you come back to something in this case, in this case we said that, the different basis functions were orthogonal.

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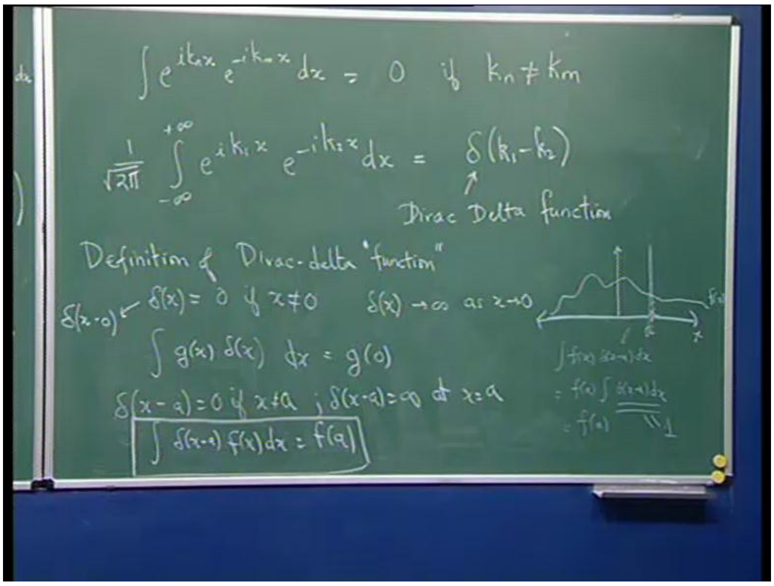

So, we had relations like e to the i k n of x e to the minus i k m of x dx was equal to delta k n k m so we had this orthogonality relation or equal to, let us equal to 0, if k n not equal to k m. So, we had this in the case of discrete now, for Fourier transforms, the orthogonality relation takes a slightly different form. So, in this case, your k is a continuous variable so then it takes this form e to i k 1 x e to the minus i k 2 x dx from minus infinity to plus infinity.

And I will just put a 1 over 2 pi for now 1 over root 2 pi, this is a 0 if k 1 is not equal to k 2, so but since k 1 and k 2 are continuous variables, this goes from a chronicle delta function to something called a dirac delta function. So, this is called a dirac delta function. So, what is this dirac delta function, I have to check whether this is 2 pi or root 2 pi so I am not sure, whether this should be 2 pi or root 2 pi, we will just come to that in a few minutes.

So, we will just leave this as just for now but we will correct it, if necessary so what is the dirac delta function, definition of dirac delta function and some people are not comfortable calling it a function but we will still use the same idea. So, dirac delta function this so we will look at some characteristics so delta of x equal to 0, if x is not equal to 0, delta of x tends to infinity as x tends to 0. And finally the most important part of the definition is that, integral of g of x delta of x 0 d of x, g of x delta of x dx, this is equal to g 0.

So, this is the delta function, this is basically delta of x minus 0 that means, this is equal to 0, if x is not equal to 0 and it is infinity, otherwise. And you can write this as and the more general way write it is, delta of x minus a equal to 0, if x is not equal to a, delta of x minus a equal to infinity, at x equal to a and integral delta of x minus a f of x dx equal to f of a.

So, this is the most important property of the delta function, you multiply a delta function by a function f of x then you get the value of the function at a. So, f of x so you multiply it by f of x and then you integrate over all x, you get the value of the function at a. So, this is the most important property of the delta function and this is what, typically used as a definition of the delta function.

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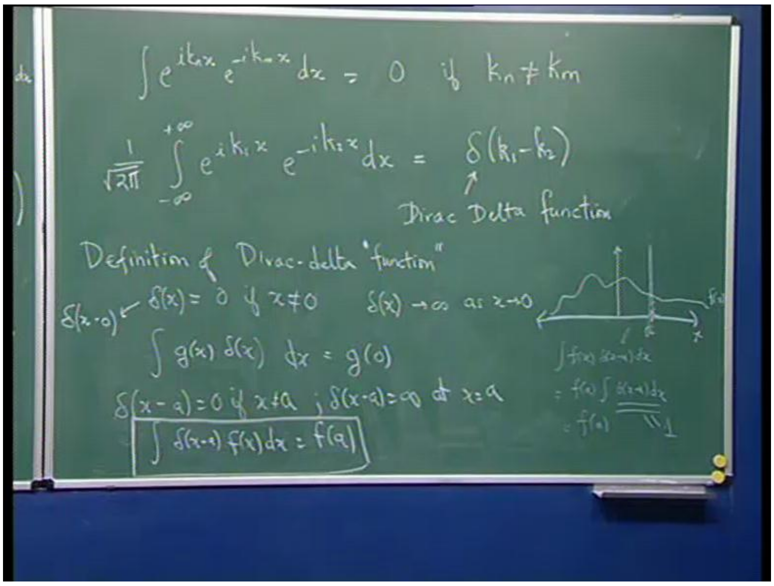

So, let us try to see, what this delta function looks like so suppose, I had suppose, this was my x variable and let us say, this is my x variable now, f of x might have and I show f of x, this is f of x. Now, this delta function delta of x minus a basically, looks like it is 0 whenever, x is not equal to a and right at x equal to a, it goes to infinity. So, it is very, very narrow and looks like this, and it is a very, very narrow function, when it goes to infinity.

Now, you can see, when you multiply f of x by this function, when you multiply these two functions, the function that you will get will be 0 everywhere, except in this region. So, this integrand, so this product is 0 everywhere, except in this small region and in this small region, your f of x is constant at f of a. So, in this region, I can write this as, I can say the following dx is equal to f of a times integral delta x minus a d x and the only function that is non-zero is this small region.

So, and this delta function so the area under the delta function is chosen to be 1, so equal to f of a so this is equal to 1. So, the delta function can be thought of, as this very, very narrow function but it is very, very tall such that, the area under the function is 1 so the integral of the delta function is 1. So, that is how, you should think of the delta function and delta functions are extremely useful in lot of manipulations especially, involving Fourier transforms.

Now, we will discuss an application of delta functions, when we talk about the position and momentum representations or the power spectrums, but what we want to do next is, we want to look at some properties of these Fourier integrals. So, we will look at some properties of Fourier integrals, which makes them extremely useful in lot of engineering and science applications. So, we will use this definition of Fourier transforms and let us look at some properties.

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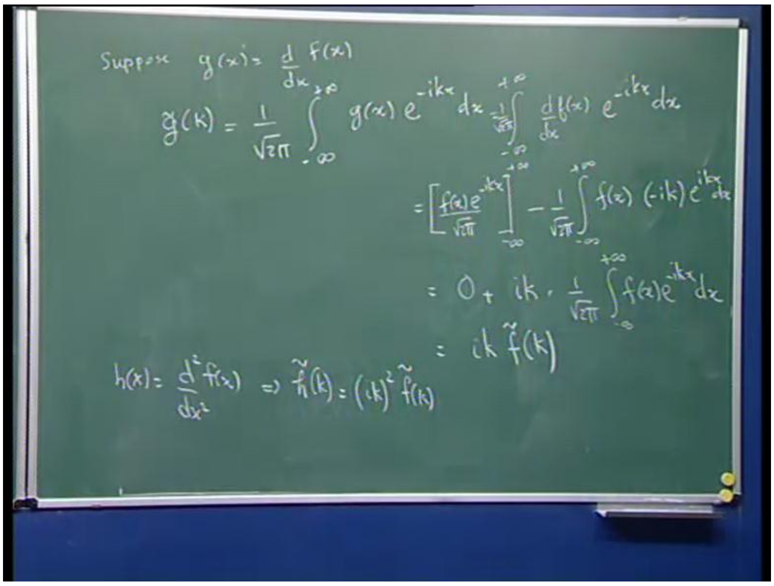

So, suppose g of x equal to d by dx of f of x then what is g tilde of k, is equal to 1 over root 2 pi integral minus infinity to plus infinity g of x e to the minus i k x dx. So, g tilde of k is this so the Fourier transform of g of x is this and so this is equal to dx and then what I will do is, you integrate this by parts. So, if you integrate this by parts, you will get two terms, one is f of x e to the minus i k x at the boundaries, there is 1 by root 2 pi minus an integral f of x times d by d x of this, d by d x of that will give me minus i k e to the i k x.

So, this term now, f of x has to go to 0 at the boundaries because only then the Fourier transform will be well defined also, we assume that, e to the i k x goes to 0 at the boundaries. So then this term is 0 minus 2 pi and I will take this minus i k outside so I will write plus i k times dx. So, this you notice, this is just f tilde of so what it means is that, if g of x is d by dx of f of x then g tilde of k is, i k f tilde of k.

So, the Fourier transform of d by dx of f of x is i k f k f tilde k, this is the first property and you can extend this, so if it is second derivative. If h of x is equal to d square by dx square f of x. Then this implies h tilde of k is equal to i k square f tilde of k and you can go on for all derivatives. So, each time you have a derivative, you get a factor of i k so this is one useful property and this property is, what will be used to so then what we will do is, we will use the Fourier transform to convert differential equations into algebraic equations. So, instead of derivatives, you just have multiplicative factors of i k, the next property that is very useful is the following.

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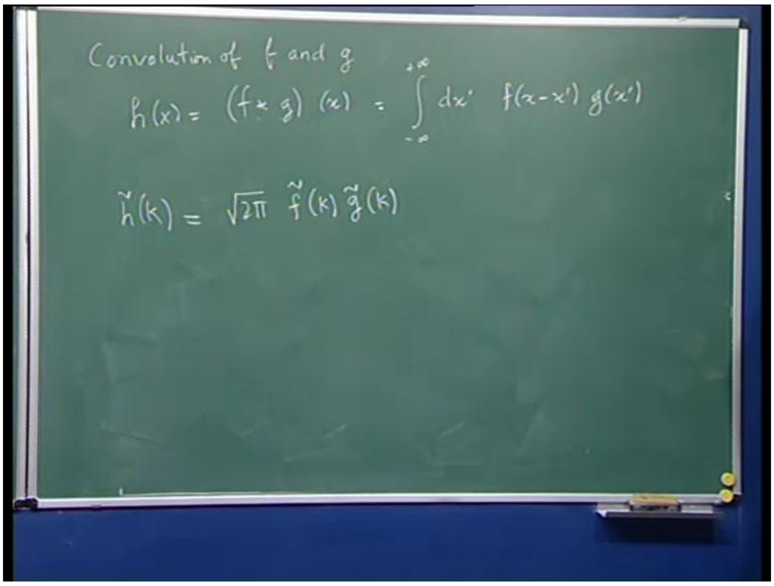

So, let us define the convolution of f and g so this is h of x equal to, it is denoted by f star g and this f star g is a function of x so this is the convolution of f and g and it is a function of x. So, this is equal to integral dx prime f of x minus x prime, g of x prime so you take f of x minus x prime g of x prime such that, they add up to give x and you integrate this over the usual range and this is called the convolution.

So, now, h tilde of k so if you calculate h tilde of k, you can show that, this is nothing but square root of 2 pi f tilde of k g tilde of k. So, the Fourier transform of a convolution is nothing but the product of the Fourier transforms with some factor of 1 by root 2 pi so this is called the convolution theorem and this is very useful, when you want to invert Fourier transforms.

So, when you have a Fourier transform of this kind and you want to calculate, what is the function of which, this is the Fourier transform, you can use this convolution theorem. So, what we will do next time, is to use these theorems, use Fourier transforms to solve certain differential equations.