Advanced Mathematical Methods for Chemistry
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Module - 09
Lecture - 01
Fourier Transforms, Fourier Transform Pairs, Dirac Delta function

In module 9 we are going to discuss various integral transforms. And by integral transforms I mean Fourier transforms and primarily Fourier transforms. But all but there are also other transforms like Laplace transforms, and there are actually several other transforms. But we will primarily be focusing on Fourier transforms, because that is one part of mathematics that is very useful in solving various differential equations. And In fact, we will also show that the Fourier transforms is a way to understand some of the foundations of quantum mechanics like the uncertainty principle.

So, we will discuss all these in this module and I will start the first lecture by introducing the Fourier transform. So, a good way to understand Fourier transforms is to think of them as extensions of the Fourier series for a function that whose period is actually going to infinity. So, when we did the Fourier series, we said that we wrote the Fourier series as in the following way.

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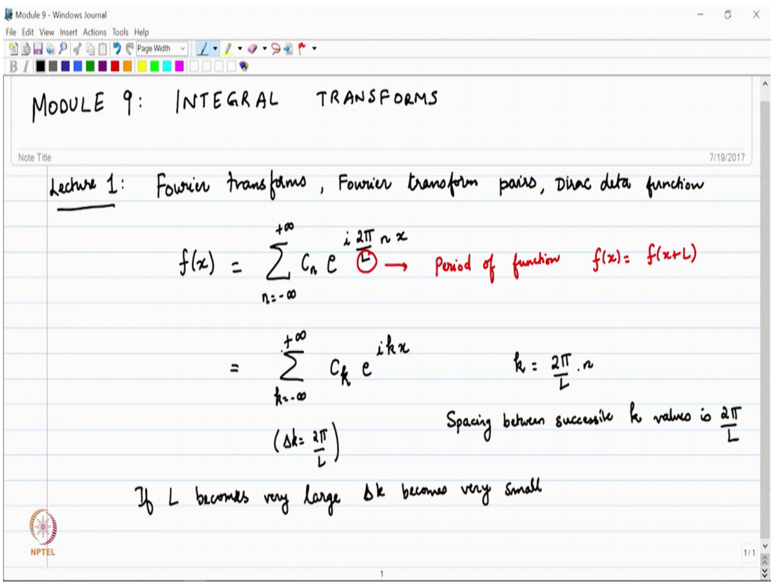

So, we wrote f of x I will use the complex form, and you set sum from n equal to minus infinity to plus infinity, and we said it is e to the i into 2 pi by l n x. And this times C n we had a coefficient C n. Let me put the coefficient before the exponent.

Now let us highlight a few things, first is l this represents the period of function. So, the period of function is l, I alternatively used 2 l as the period, but in this case I am using l as the period of the function. So, what you have is f of x equal to f of x plus l. Now you can ask the question what happens if we let l go to infinity if we imagine that that l is going to infinity what will happen. So, that is the that is the idea of the Fourier transforms now, now let me write this in a slightly different way I will write this as sum over, now I will call this factor of 2 pi 2, 2 pi n by l, I will call it as k. And instead of C n I will you I will use ck e to the i k x. Where k is equal to 2 pi by l into n ok.

And as n goes from minus infinity to plus infinity, k will also go from minus infinity to plus infinity. So, k equal to minus infinity to plus infinity. However, k is not you know k the spacing in k spacing between successive k values is 2 pi by l. So, that, that means, if n equal to 1 then you will have 2 pi by l if n equal to 2 then you will have 4 pi by l, and the difference between 2 pi by l and 4 pi by l, l is 2 pi by l. So, between any 2 successive values of n the spacing is 2 pi by l, the spacing in k is 2 pi by l ok.

So, we so will just make a note we will say delta k equal to 2 pi by l. Now this already motivates are motivates us to think about, what happens if l becomes very large. So, if l becomes la becomes very large delta k becomes very small. And if delta k is very small; that means, you have k values that are very close to each other. So, the success of k values are very close to each other. So, this sum will be related to an integral I am not saying it is equal to an integral. So, what you can see is that if the successive k values are very close to each other, then this will look like an integral with this factor of delta k ok.

So, what so, this motivates us to the definition of the Fourier transforms. So now, we will write the definition of transform.

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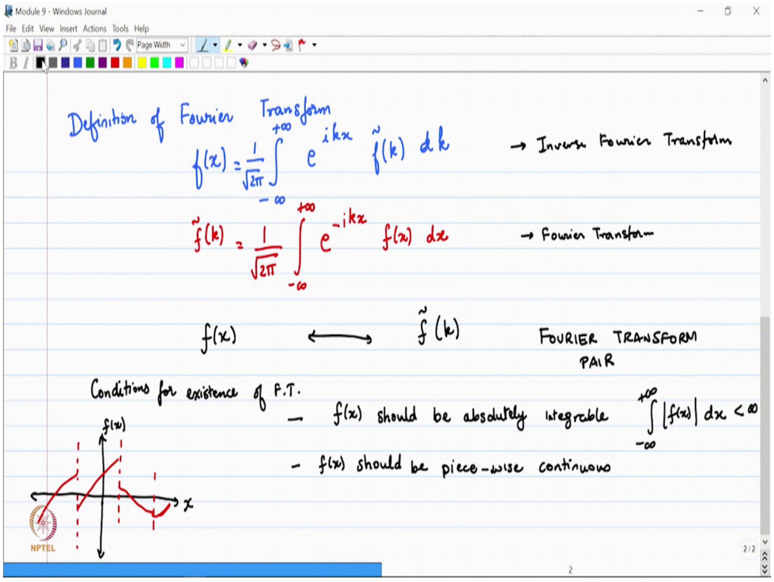

So, when you have when you have k being very closely spaced, then what you do is you write f of x is equal to integral from minus infinity to plus infinity, and we take a factor of 1 over root 2 pi, it will become clear why the why we put this factor. You have e to the i k x f of x d k. So, you are integrating over the variable k and you have you have e to the ikx f of x e to the e to the ikx f of k dk ok.

Now, just notice the notice a similarity between this expression and what we had here. So, instead of a sum you have an integral you have this factor of 1 by 2 square root of 2 pi. Now instead of ck i am calling it as f tilde of k then the reason for that will become clear and you have e to the ikx. So, basically you can see that the Fourier transform is like an extension of Fourier series for when the period goes to infinity ok. Now I call this as f tilde of k instead of calling it as ck i just called it f tilde I wrote it as a function of k because k is a continuous variable ok.

Now when you when you write a Fourier series, when you when we write a Fourier series one of the things that we that we that we note is that you can write C n as sum over, I can write C n as integral f of x e to the minus I 2 pi x n by l dx. So, I can I can I can write I can write C n in this form and x goes from 0 to l and 1 by l. So, this is what I can write your C n as, when you write a Fourier series. Now the same way same way now notice C n is written as an integral over f of x and you have this, now by the same by the same argument I should be able to write f tilde of k, you can show this as 1 by root 2 pi, integral minus infinity to plus infinity e to the minus i k x f of x dx.

Now, actually you can see why the factor of 1 by root 2 pi is there that is here, because now it makes both these Fourier transform and the inverse Fourier transform look very symmetric. So, the only difference between the 2 expressions in one case you had e to the plus ikx in the other case you have e to the minus ikx. And you integrate in one case over k and the other case you integrate over x. So, this f of x and f tilde of k, tilde of k they constitute a Fourier transform pair. That is f of x is the Fourier transform of f, f tilde of k and f tilde of k is a Fourier transform of f of x. Sometimes this second expression is called the Fourier transform and this is called the inverse Fourier transform. So, this might be called the s Fourier transform and this is called the inverse Fourier transform, but actually there is I should I should emphasize that it is best to think of these 2 as a Fourier transform pair.

So, if you call one the Fourier transform then the other will be the inverse Fourier transform. So, this process where you convert a function of x to a function of k is called Fourier transform. So, you write fk f tilde of k. So, you start with a function of x convert it to a function of k and that is called the Fourier transform, then you take the function of k and convert it back to a function of x that is called the inverse Fourier transform. Now there are a few conditions. So, conditions for existence of Fourier transform ok.

So, condition for a So, this integral exists now if you take the absolute value of this integrand absolute value of e to the ikx is just 1. So, the conditions for existence is that f of x should be absolutely integrable. So, that means, integral f of x absolute value of x dx from minus infinity to plus infinity should be less than infinity. That is a condition and in other words f of x should be piecewise continuous. This is an important condition. It need not be continuous it can be discontinuous, but it should be piecewise continuous. So, what that means, is that you can have a function if I if I just plot it right here a piecewise continuous function might look. So, if I put x and f of x a piecewise continuous function might look something like this it might look something like this.

So, it is not continuous there are points of discontinuities, but the points of discontinuities there are only finite number of these discontinuous points. So, that would be a piecewise continuous function. So, if you can do this integral if this integral is less than infinity then here you are just multiplying it by some quantity whose absolute value is less than on less than or equal to 1 or it is equal to 1. So, that integral we will also exist. So, this is the condition for existence of Fourier transform and so, in general you know the Fourier transform is something that we assume exists for various functions and we and we try to calculate.

So, let us look at some examples let us look at Fourier transform of some functions.

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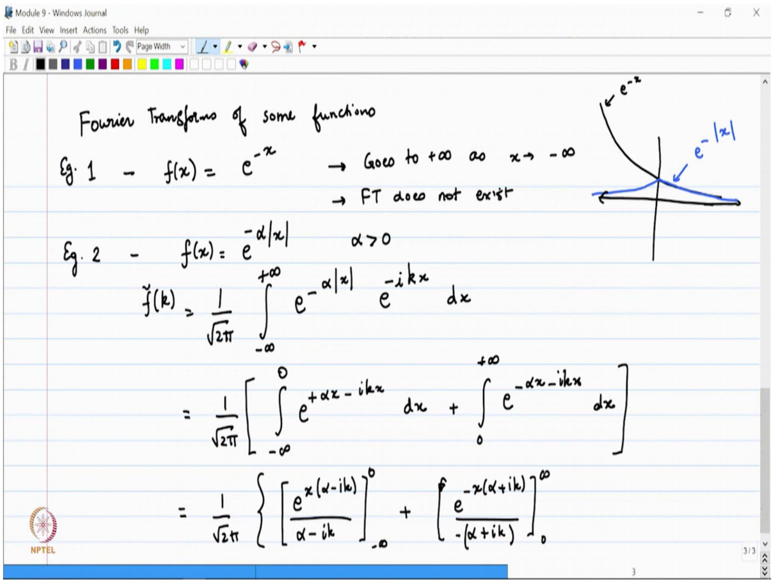

So, suppose I have f of x equal to, now if I have e to the minus x. So, this you can see that e to the so, this function goes to infinity has x tends to minus infinity. So, when x goes to minus infinity this function goes to infinity. So, Fourier transform does not exist. This is a this is the first thing. So, you cannot take Fourier transform of e to the minus x. So, what about so now, is So, this is the first example.

Now let us look at let us look at a slightly modified function f of x is equal to e to the minus absolute value of x. And let me put a constant k here. So, just to just to say that you know you have some factor k times absolutely not k let me put alpha, alpha times absolute value of x. So now, it is let us if you if you just had e to the minus x your function look like your e to the minus x looks something like this. This is e to the minus x. Now on the other hand if you take e to the minus absolute value of x then it looks like this yeah. So, and now and now so this so, if you put a factor of alpha it would look it will essentially look like this. And you can clearly see that this integral is finite where this integral goes the integral under this function goes to infinity ok.

So, suppose you take this now let us evaluate the Fourier transform. So, f tilde of k is equal to 1 over square root of 2 pi integral from minus infinity to plus infinity e to the minus alpha absolute value of x times e to the i k x d x, e to the minus ikx. So, the assumption here is that alpha is greater than 0. So, 1 over root 2 pi of now alpha is greater than 0. So, I can split this integral into 2 integrals. So, I ntegrate from minus infinity to 0 and from minus infinity to 0 x is negative. So, absolute value of x is minus x.

So, you will have e to the plus alpha x minus ikx dx and then you have plus integral from 0 to plus infinity. And now you have e to the minus alpha x minus ikx dx. So now, now you can do this integral by treating this alpha So, I will do this integral we will just. So, e to the x alpha minus i k divided by alpha minus i k. This I will just write this integral in this form. So, I just did the integral of an exponential I just treat it like a regular exponential and I do this integral. And now the limit is here are from minus infinity to 0 plus the same thing e to the minus x alpha plus i k alpha plus ik minus of alpha plus i k and this integral is from 0 to infinity.

So now, we can put the limit is and we can we can go ahead and calculate.

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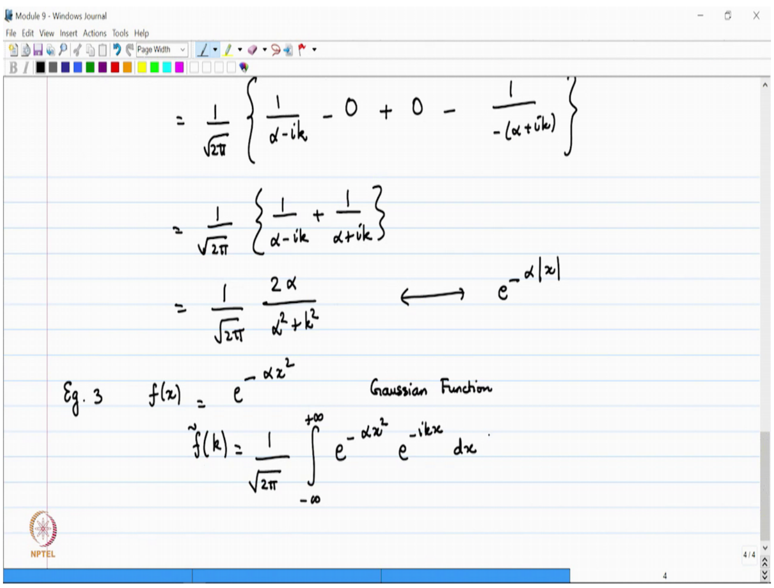

So, when x equal to 0 this becomes 1. So, I just get 1 over alpha minus i k. So now, when x goes to minus infinity this is e to the minus infinity. So, e to the minus infinity is 0. So, e to the minus infinity is 0. So, that the you will just have a minus 0 plus 0 minus 1 over minus of alpha plus i k. So, these are these other terms. So, I can write this as 1 over square root of 2 pi and I have 1 over alpha minus i k plus 1 over alpha plus i k and I can write this as 1 over square root of 2 pi ok.

Now I get if I just multiply it out I will get 2 alpha divided by alpha square plus k square. So, this is the Fourier transform of this is Fourier transform of e to the minus alpha absolute value of x. So, this illustrates a how to how to take Fourier transform of a function. I will take one more example again this is very commonly used Fourier transform. So, here I take f of x as I take e to the minus alpha x square this is a Gaussian function, and in this case I can go by the same argument.

So, f tilde of k is equal to 1 over square root of 2 pi integral from minus infinity to plus infinity e to the minus alpha x square e to the minus i k x dx and if you can you can you can work this out exactly the same way.

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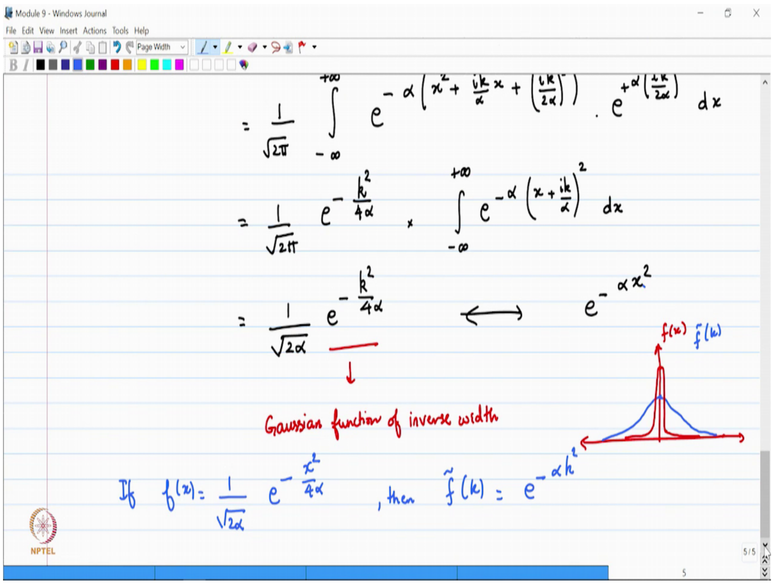

So, we write 1 over root 2 pi, and what will do is a very we use a very popular method in solving these Gaussian integrals. So, we this is called completing the squares. So, we will write it as e to the I will e to the minus alpha x square plus i k by alpha x and. So now, if you complete the squares if you want to write this as a perfect square then you will write i k by 2 alpha whole square. And what you have to do is since you since you added this term you have to subtract the same term.

So, what you will do is multiplied by e to the now we will write plus alpha times ik by 2 alpha whole square dk, dx. Sorry, now you notice that this last term is independent of x. So, I can take it outside the integral. So, I get 1 over square root of 2 pi. And So, I get e to the minus alpha k square by 4 alpha. So, I get e to the minus k square by 4 alpha. And what I am left with here is minus in to infinity to plus infinity, e to the minus alpha times I have x plus i k by alpha whole square.

So now this is nothing, but a Gaussian integral, but it is Gaussian shifted by some quantity shifted by some distance. And we and we treat this as though it were a real number and we just used a usual formula for Gaussian integral. So, this integral will be square root of pi divided by alpha. So, the square root of pi will cancel and you will get square root of alpha divided by 2 or sorry 1 over square root of 2 alpha e to the minus k square by 4 alpha. So, this is f tilde of k and this is the Fourier transform of e to the minus alpha x square. So, this is a Gaussian function and here actually the this involves 1 over 4 alpha whereas, here you had alpha that is the difference. So, in other words if this was a narrow of width of inverse width I will just say inverse width ok.

So, so what that means, is that if your initial function is a is a Gaussian with So, if my if my f of x is a very narrow Gaussian. So, very, very narrow Gaussian then f tilde of k will look like a very wide Gaussian. And of course, the if I had chosen if I chosen this as my as my Gaussian function then this would be the Fourier transform. So, just to emphasize what we mean by these Fourier transform pairs is that is that if f of x is equal to 1 over square root of 2 alpha e to the minus x square by 4 alpha. Then f tilde of k is equal to e to the minus alpha k square. So, that is this is what you mean by your Fourier transform pair.

So, the Fourier transform of this function is given by this function. Now if I had an x here then the Fourier transform would be given by a k here. So, that is what you mean by Fourier transform pairs. So, I will conclude this lecture by giving a table of a few Fourier transform pairs. So, what we said is that if you had a very narrow Gaussian function then it is Fourier transform very, very wide. So, similarly if you have a very wide Gaussian function it is Fourier transform will be very narrow. And this is generally true that if you have a if you have a function which is very broad then the Fourier transform will be very narrow. You can ask the question what happens if function is very broad very as in very broad.

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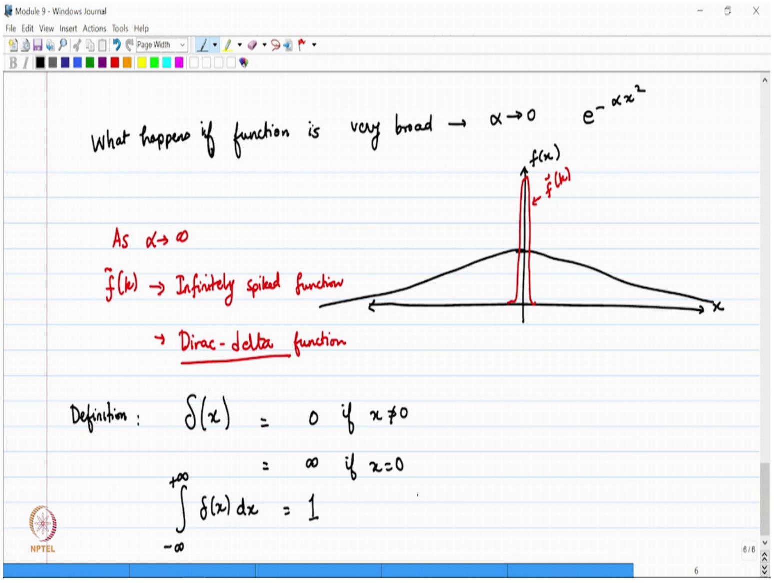

So, what I will say is that your alpha tends to 0. So, if we take e to the minus I alpha x where alpha tends to 0. So, what you would expect is that is that as alpha tends to 0 your Gaussian function will look like this. So, it will look like this that is what it is going to look like. And now you can you can show that the Fourier transform of this we look will also look like a Gaussian and it looked like this. So, as alpha tends to infinity f, f tilde of k tends to infinity spiked function. And this is such an infinitely spiked function is referred to as a Dirac delta function. So, it is related to a Dirac delta function ok.

Now So let me define the Dirac delta function. Delta x equal to 0 if x not equal to 0 equal to well we will say equal to infinity if x equal to 0. So, that is an infinitely spiked function, but there is another condition. So, it goes to infinity now it is it is still treated as though it is a continuous function and integral delta of x dx from minus infinity to plus infinity this is equal to 1. So, area equal to 1. So, this is the definition of the Dirac delta function. You can also have a Dirac delta function Centered away from x equal to 0.

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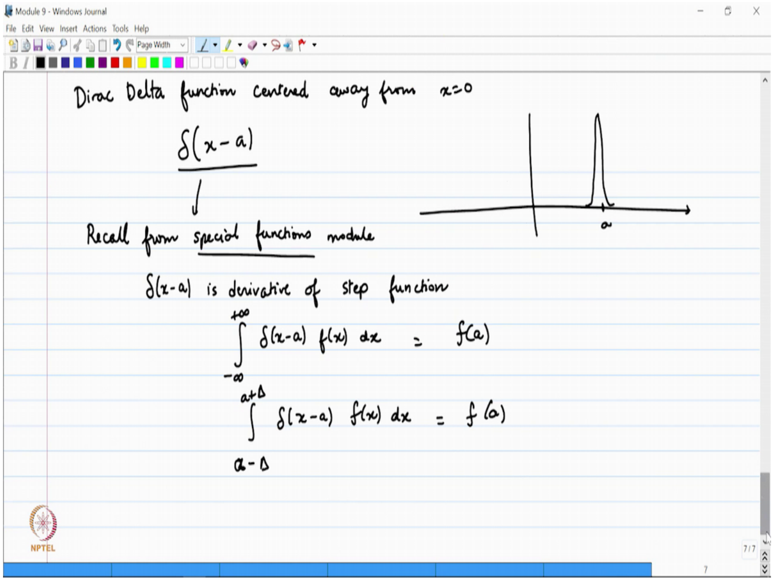

So, for example, you can have delta x minus a ok.

So, delta x minus a. So, if this is my a then the function will look like this. It will be it will be it will be spiked at x equal to a. So, Dirac delta function we have already seen this in when we were doing special functions. So, we have already seen the Dirac delta function as a derivative of the so, recall from special functions. So, when we did special functions module we did Dirac delta function as derivative is derivative of step function. And we also said that it is defined under the integral. So, delta x minus a f of x dx from minus infinity to plus infinity is equal to f of a. And we also said that you only need to do this integral from integer I mean because when x is not equal to a this will be exactly 0. So, the only contribution will be from a region a minus delta to a plus some small interval delta in that in that small interval then you will get f of a ok.

So, so the Dirac delta function actually appears very naturally when you do dealing with Fourier transforms. And what is done is you since the Dirac delta function is only defined under the integral what is done is suppose you have f of x equal to constant equal to a constant.

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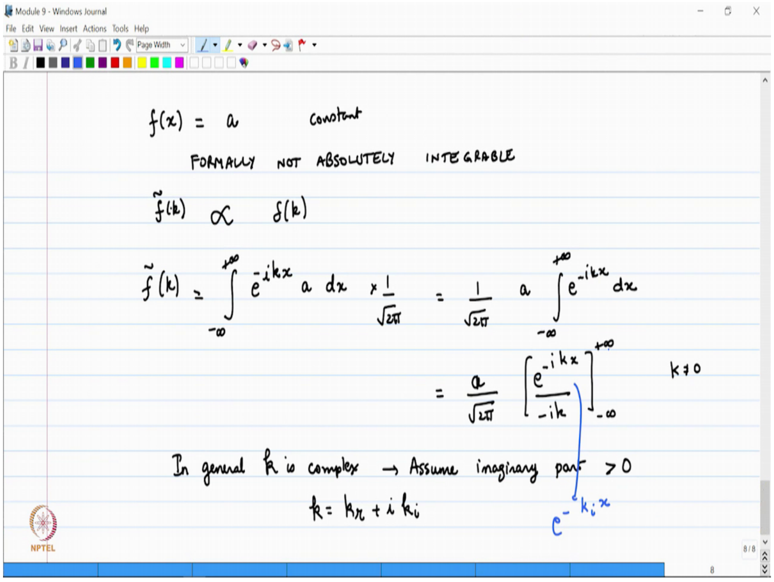

Now formally this is not this is not absolutely integrable. So, formally not absolutely integrable, but nevertheless we define f tilde of k equal to delta of k. So, if I if I choose this now you can see that you can see that integral e to the I will ok.

So, let us let us work this out. So, f tilde of k is equal to integral e to the i k minus ikx into a dx from minus infinity to plus infinity with a factor of 1 over square root of 2 pi there should be I think. So now, this is equal to 1 over square root of 2 pi let me let me just write this is proportional to this. So, it will turn out to be proportional to this. Now if you just write it in this way then what you have is a integral e to the minus i k x dx from minus infinity to plus infinity. So, this is equal to a by square root of 2 pi.

Now what you have what you have here is you have an integral. Now if you just think if k is not equal to 0, if k is not equal to 0 then this looks like e to the minus i k x divided by minus i k. This is for k not equal to 0. Now if we now in general k is complex. So, we assume assumed imaginary part greater than 0 yes. So, if you just assume that the imaginary part of k is greater than 0. Then what happens is this will have e to the e to the minus. So, imaginary part So, if I write k is equal to kr plus I ki. Then what you will have is you will have a you will have a term here that looks like that looks like e to the minus k i x where k and k is greater than 0. So, what will happen is that as this goes to infinity this will go to this will go to 0.

Now, this is a So, if you if you go with this assumption then basically you can show that this is equal to 0 if k is not equal to 0. So, this integral goes to 0 if k is not equal to 0. So, formally can be shown that so, integral Goes to so I will I will write f tilde of k equal to 0 if k is not equal to 0.

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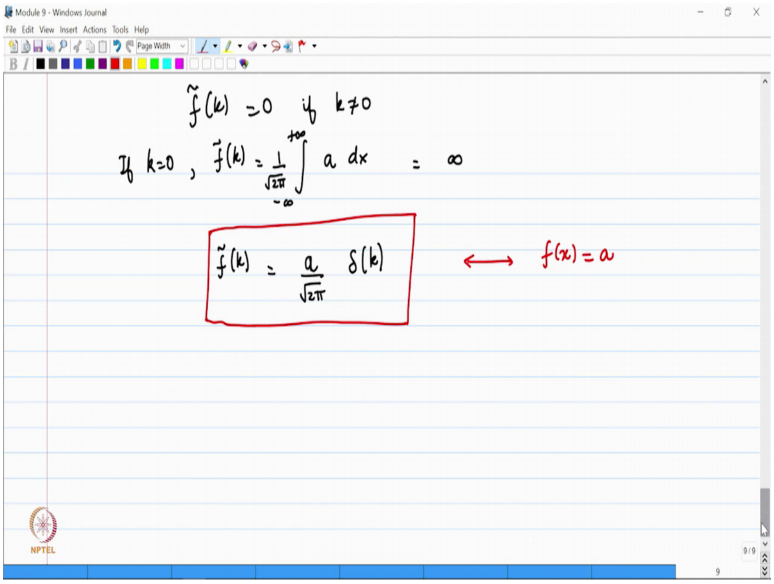

If k equal to 0 then f tilde of k is equal to integral a dx from minus infinity to plus infinity equal to infinity 1 by root 2 pi. So, formally what we do is that we can we can also verify what the integral of f tilde of k is. So, what will write is that we will write tilde of k as 1 by root 2 pi delta of k. So, this is a function that that I should I should put an a here a by a by root a by root 2 pi delta of k ok.

So, this is Fourier transform of Fourier transform of a constant function. So, this is how delta function the Dirac delta function appears naturally when you are dealing with Fourier transforms. So, we have seen a few Fourier transform pairs. So now, in the next lecture we look at we look at other properties of Fourier transforms. And when they when we when will study them in some more detail we learn a few theorems about Fourier transforms.

Thank you.