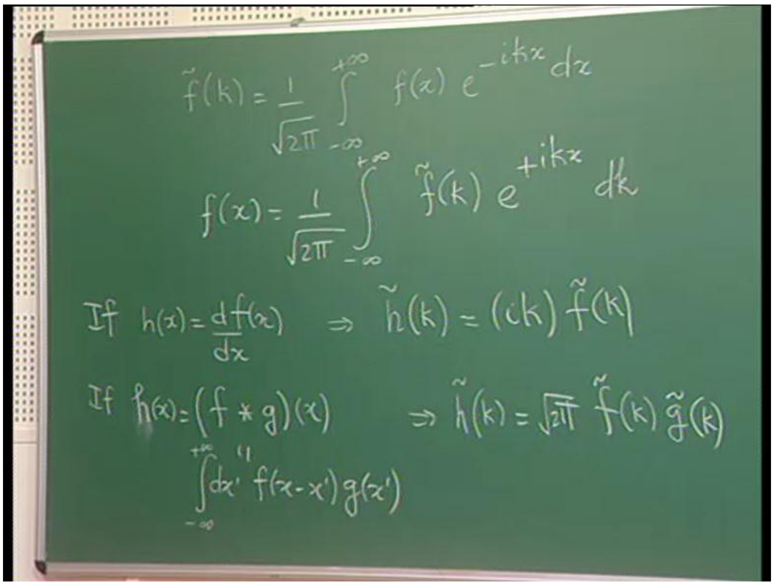
Mathematics for Chemistry
Prof. Dr. M. Ranganathan
Department of Chemistry
Indian Institute of Technology, Kanpur

Lecture - 23

(Refer Slide Time: 00:26)



Let us remind ourselves again that what we have learnt about the Fourier transform. So, the Fourier transform was defined as f tilde of k is equal to 1 over root 2 pi integral minus infinity to plus infinity f of x e to the minus i k x d x. If, you have this sought of expression, you could also write f of x is equal to 1 over root 2 pi integral minus infinity to plus infinity f tilde of k e to the plus i k x d x. So, we naturally like to think of this as an expansion, so we are expanding the function in terms of e to the i k x, it should be d k where k is a continuous variable, that goes from minus infinity to plus infinity.

Now, this sort of expansion right now, it just looks like a mathematical trick, but we will see real application of this shortly. Before that I want to mention a couple of things; one is that if you look in different books, they might use different definitions of Fourier transforms. So, some books might use a plus sign here, might use a minus sign here, instead of plus some books will not have the factor of 1 over root 2 pi.

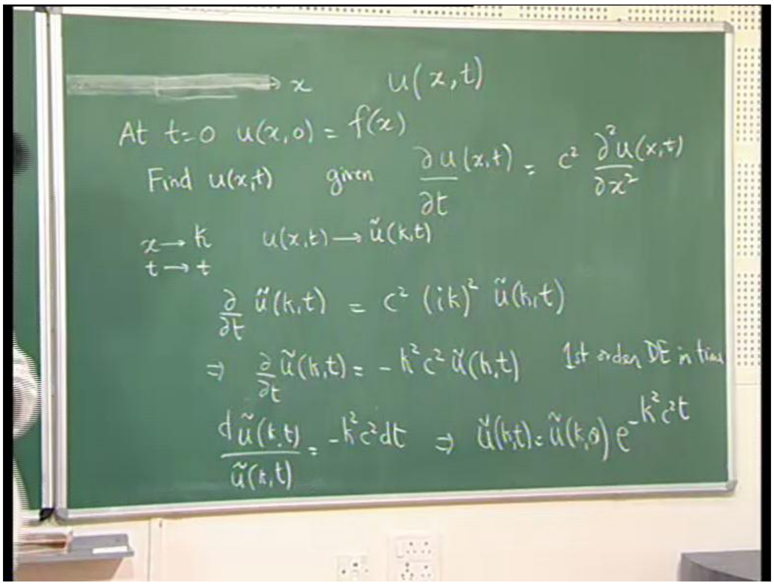
So, will have just this term and then they will take the 1 over 2 pi here, but these will just cause small changes in the numerical factors, but the method is fairly general and you can still apply it. So, the lesson I want to mention is that there is no unique definition of

Fourier transform, each book or each author chooses to definite in a way convenient for them. The other thing is should mention is that in order for this to be well defined especially, when k equal to 0, you can see that integral f of x d x should be well defined, so f should be piece wise continuous in order for this to be define.

So this is like a transformation of variables you have go from a function of x to a function of k so you are changing from x to k, so you are transforming a variables of a problem from x to k. So, it is similar to that and in this is what we will use in order to solve differential equations.

The other thing which, I mentioned was that suppose, h of x equal to if h of x is d f by d x of x then h tilde of k is equal to i k f tilde of k, this is the property that if the Fourier transform of derivative is nothing but i k times Fourier transform of the function. The other property that, we saw is that if g of x is equal to the convolution of f and g, f star g is a function of x and this function we wrote is as integral f of x minus x prime g of x prime we call this h of x. Then h tilde of k is equal to square root of 2 pi times, f tilde of k g tilde of k and this is the convolution theorem. Now, let us look at an example of how we use Fourier transforms to solve various problems.

(Refer Slide Time: 04:52)



The problem that I will take is a problem in conduction of heat so in this problem you consider that this be the x direction and you imagine that, you have a very long bar, a bar of some material, that is very long and this bar extends infinitely long and this direction.

So, it is a 1 dimensional bar and the temperature of this bar is not the same everywhere, so the temperature is same everywhere.

So, this the temperature is different here, it is different here so u is a function of x and then the other thing that happens is that suppose, you initially you program the bar with a certain temperature. Let us say initially, you keep the bar at constant temperature, but you could make it very hot on one side then over time the temperature will changed. So, the temperature is not only a function of x but it also a function of time.

So, the temperature is both a function of x and time so that means, at any point the temperature of the bar keeps changing with time. So, suppose you go to a point x and you look at a time t, the temperature of the bar is function of both x and t. Now, let us consider the problem is we want to start with some condition. So, at t equal to 0 u of x 0 is equal to f of x that means, it is some function of x that means, you could choose f of x to be any form that is it is 0, it is at you could choose f of x to be a constant for example, or you could choose f of x to be oscillating function. So, it is some function which describes what the initial temperature of this bar is so this is at t equal to 0 and now, we want to find u of x t.

So, in order to do this, you should know how u of x t varies and you told that the equation of motion says at the rate of rate at which heat flows out if, at any point this is given by c square dou square u by dou x square. So, this is the Fourier's law of heat conduction which says the rate of flow of heat is related to the gradient of temperature or the second derivative of temperature.

So, what you have to do is to solve this differential equation. So, you need to find the u that satisfies, this differential equation and this boundary conditions, so mathematically what you need to do is to solve, this differential equation with this boundary conditions. Now, if you want to solve it. If you try to solve it you have a partial differential equation in both x and t, if you there is not much, you can do it if you try to separate variables then you will get that both of them have to be 0, both of them have to be constant.

So, we will just get a trivial solution, when u is constant everywhere but you want a solution where that can never satisfy this boundary conditions unless f itself is a constant but if you have an arbitrary function f then you cannot solve this equation by simple separation of variables. So, what do is you transform x to k.

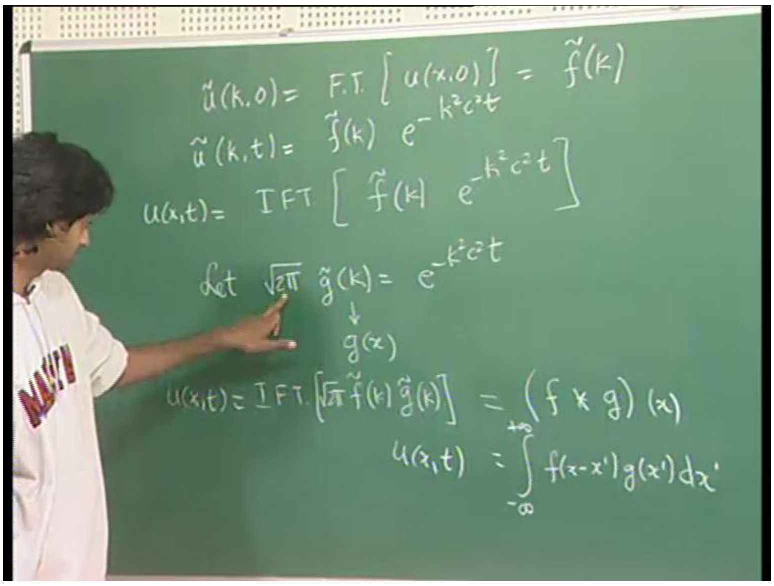
So when you transform x to k u of x t goes to u tilde of k t so x to t and when you do this you keep t, the same you do not do anything to t. So, what we shall do is take the Fourier transforms on both sides and what we will get let see what we get. So, we have d by d t of u of x t, when you take the Fourier transform of that the transformation only acts on x so it goes within this t so what you will get on left hand side is d by d t of u tilde of k t. So, that is a left hand side, the right hand side you get c square times Fourier transform of this derivative and this is where you use this theorem that Fourier transform of the first derivative of function is i k times f of k.

So, Fourier transform of the second derivative will be nothing but i k square u tilde of k t so you can show this now where equation becomes is equal to minus k square c square u tilde of k t. So, that is what happens to so your partial differential equation, now became a much simpler looking equation, now this you can solve this for u of k t since this is a just first order differential equation in time.

So, I can just integrate it out and I can so if i integrate it out I will get u. So, let us do it explicitly d u tilde of k t by u tilde of k t is equal to minus k square c square t b t b t and this simply implies u tilde of k t equal to u tilde of k 0 e to the minus k square c square t. So, u tilde at k of k at time t time 0 times e to the minus k square c square t. So, in that is what you get when you integrate this…

So, this is good you got u tilde of k t in terms of u tilde of k 0. Now what is u tilde of k 0 u tilde of k 0 is nothing but the Fourier transform this is nothing but the Fourier transform of u of k 0 of u of x 0, so the Fourier transform of this is equal to this.

(Refer Slide Time: 12:12)

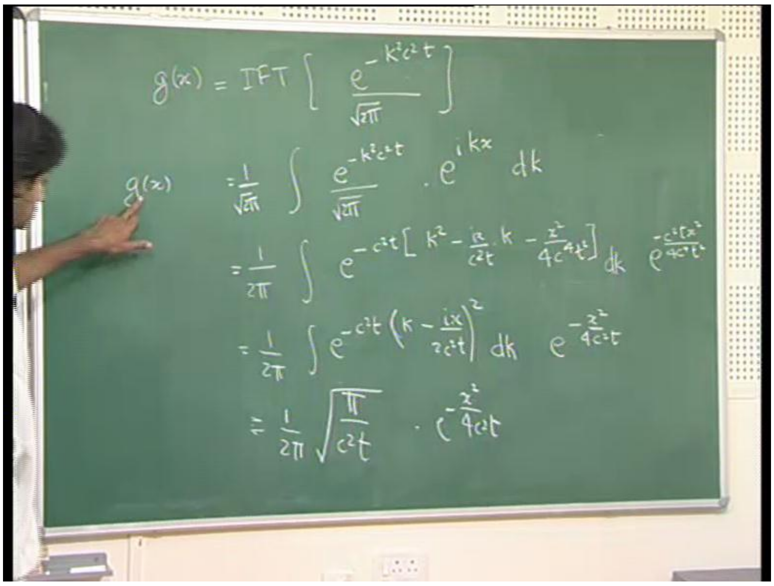


So, what we have is that u tilde of k 0 equal to Fourier Transform of u of x 0 is equal to f tilde of k. So, is the Fourier transform of this f of x so whatever f of f of x I am given whatever your problem specifies the f of x you take the Fourier transform of that. So then you get the equation u tilde of k t is equal to f tilde of k e to the minus k square c square t so this is the expression. Now, what you wanted was u of x t but what you got is u tilde of k t and then from to go from u tilde of k t you just take an inverse Fourier transform to get u of x t. So, this procedure is an inverse Fourier transform, so what you are do is the inverse transform of this. So, what you will say is that u of x t is equal to just the inverse Fourier transform of this quantity.

Now, you have to take the inverse Fourier transform of product of 2 functions. Now we will use a convolution theorem so let square root of 2 pi times g tilde of k is equal to e to the minus k square c square t. So, then the inverse Fourier transform of this is g of x so the inverse Fourier transform of this is g of x then this is just then u of x t is equal to inverse Fourier transform of f tilde of k square root of 2 pi f tilde of k g tilde of k is equal and the inverse Fourier transform of this from convolution theorem is just f star g of x so from the convolution theorem this is just this.

So, what you have to do is to is you need to know. So, f star g of x f star g of x is integral f of x minus x prime g of x prime d x prime of minus infinity to plus infinity, now f is known so what you have to do is to determine g, if you know g then you have the solution. So, u of x t is equal to this, so the last step is to determine g of x, so g of x is the inverse Fourier transform of this of function divided by square root of 2 pi.

(Refer Slide Time: 15:35)



So, what you have is that g of x is equal to inverse Fourier transform of e to minus k square c square t divided by square root of 2 pi and what is the inverse Fourier transform of this you can show this. So, this is equal to integral e to the minus k square c square t 1 by root 2 pi and then you have another 1 by root 2 pi, so this is this function times e to the i k x d k so this is the of g of x.

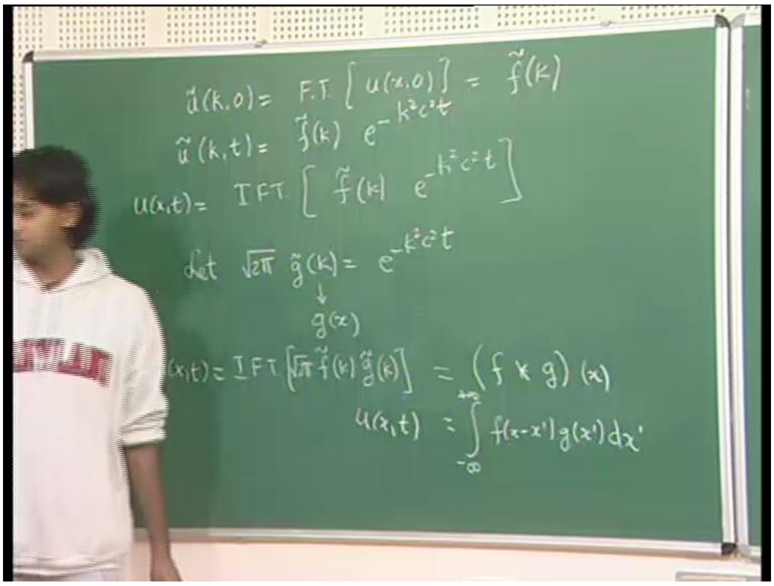
Now, you can actually calculate this it is not hard to it not hard to calculate this so and your answer will come out to the following before I calculate that, I will just mention how we do it. So, you have 1 over 2 pi integral e to the I will write this in the following form minus c square t k square k square and then I had what I will have here is minus i x by c square t into k.

So, when I am multiply this 2, I will get plus i k x and so I have this and just to carry out this Fourier transform, I will complete the square. So, if I complete the square then the remaining term will be minus x square by 4 c 4 t square and then what I have to do is so this times d k and then since I multiplied by e to the minus since, I added this extra term, I have to do e to the I have to put the opposite of that so that will be c square t minus c square t x square divided by 4 c 4 t square.

So, what you can see is that I multiplied this term and then I multiplied by the inverse of that so this is the simple trip to evaluate the Fourier transforms. So, then this just becomes 1 over 2 pi integral e to the minus c square t times k minus i by 2 c square t i x by 2 square t 2 c square t whole squared k into e to the. Now, I will just simplify this minus x square by 4 c square t the now this integral can be done fairly easily, this is just simple Gaussian integral instead of having e to the minus a x square, this is just c square is the c square it is the constant.

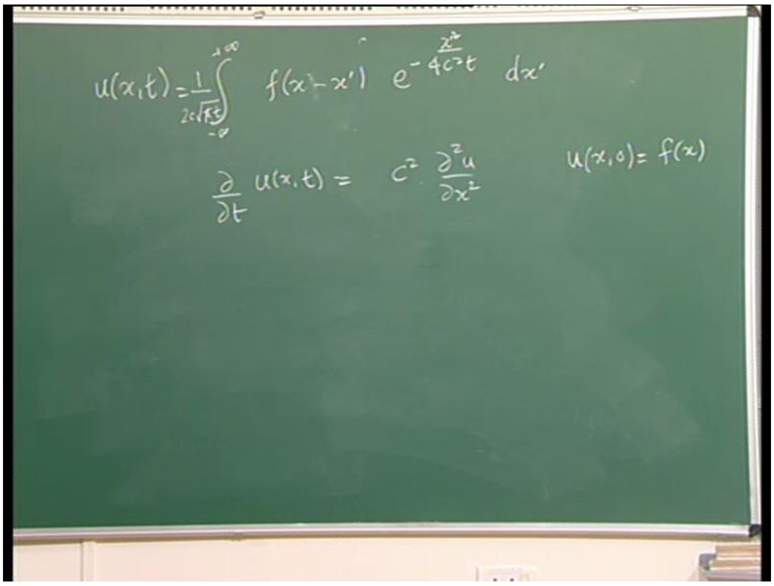
So, I can just write this integral 1 over 2 pi root pi divided by c square t so this all integral from minus infinity to infinity just root pi by the coefficient of the Gaussian term, that is this root pi by c square t and this multiplies e to the minus x square by 4 c square t. So, this is the answer that we that we were looking for and this is the final answer that you will get using this calculations, so g of x has this form.

(Refer Slide Time: 20:16)



Now, you can take this and you can substitute here and you will get the form of u of x so what we saw was that starting from very complicated looking partial differential equation, we could use we could use Fourier transform method and we could very quickly arrive at the solution. So, when you put all of it together what, you will say is that you put g of x here, you know the form of we are given the form of f of x whatever form of f of x, you are given you can do this integral.

(Refer Slide Time: 20:51)

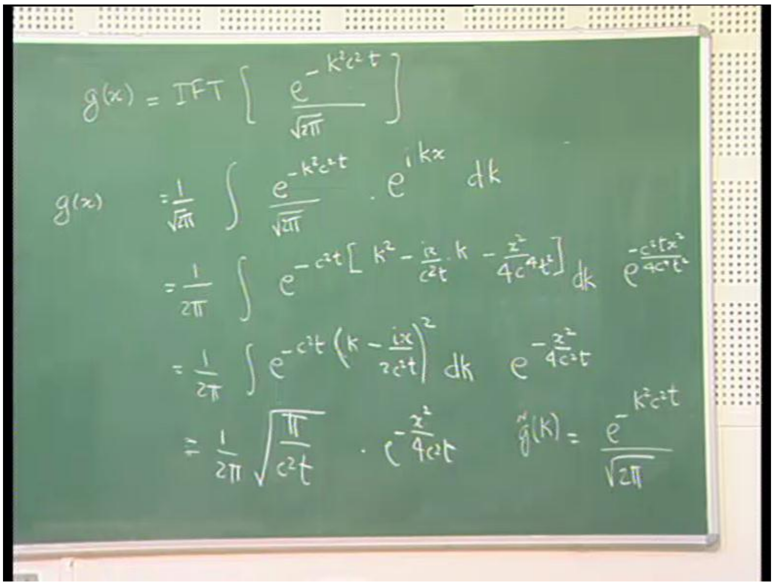


So, the final solution u of x t integral f of f of x prime into 1 over root 2 pi so I had a 1 over root 2 2 pi. So, if I take that with that root 2 pi, so I will get 1 over 2 c root pi t so this is I will take the c outside and an I have 1 root 2 pi will cancel. So, I have been left with a root pi t f of x minus x prime e to the minus x square by 4 c square t d x prime x prime square x minus square. So, this is my final answer.

So, this is the very powerful result that we got because I do not need to specify, what my function is and still I can solve the differential equation so I solve the differential equation, even though I did not tell you what f of x was. So, if you remember the differential equation was dou u by dou t of u of x t is equal to c square dou square u by dou x square with the that u of x 0 is equal to f of x.

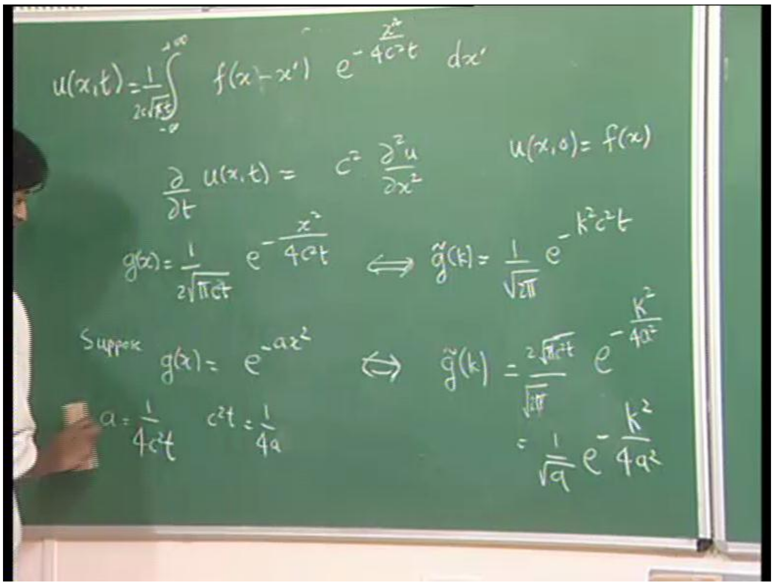
So, given any form of f of x you can go ahead and you can and you can say that this is the form of the solution so we solve. This differential equation using this method of Fourier transforms and in fact, Fourier transforms is 1 of the most commonly use method to solve differential equations.

(Refer Slide Time: 22:56)



The other thing I would, I wanted to notice was that g of x was this where g of g tilde of k, if you remember. So, g tilde of k was e to the minus k square c square t divided by root 2 pi, so g tilde of k is nothing but this quantity. Now this is another interesting feature you notice that g of x is a Gaussian function so it is it is some constant multiplied by you know it is e to the minus x square into some constant and the Fourier transform is also a Gaussian function e to the minus k square into some constant so this what we see is that Fourier transform of a Gaussian is also an Gaussian.

(Refer Slide Time: 23:49)



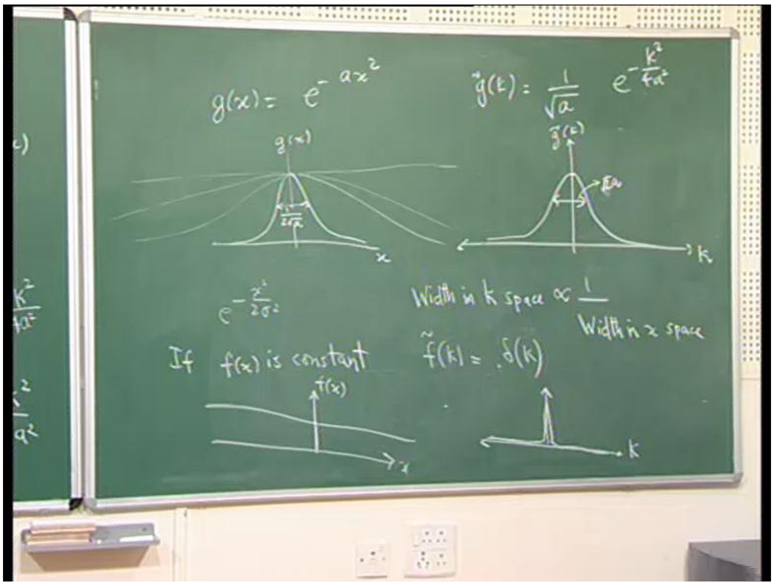
So, this is so we also noticed I will just write it down again. So, if g of x is equal to 1 over 2 pi, I can take this pi inside 1 over 2 root c t e to the minus x square by 4 c square t then this gives you g tilde of k is equal to 1 over root 2 pi e to the minus k square c square t. So, g tilde is a function of k is also this.

So, suppose e g of x is equal to e to the minus a x square, then you can immediately see you can just compare the terms and you can say that g tilde of k so instead of 1 over 4 c square t, I had a so wherever I have c square t i replace it by 4 over a so you can just go ahead and do this and what I am get is the following, let see and then they have to put the constants properly 2 pi c square t so let us 2 root pi so with some constant of proportionality this will just be e to the minus k square by a square 4 a square so let us check that is correct.

So a can be compared with c square t therefore, c square t is equal to 1 over 4 a square so c square t is 1 over a square so you get this and then c square t 1 over 4 a square. So, what I have to do is to multiplied this out it is 2 root pi c square t divided by root 2 pi so that is what I will get so I can this I get root 2 c square t and this is c square t is just a is 1 over 4 c square t.

So, this is c square t is 1 over 4 a square. So, square root of that is 1 over 2 a. So, will just get 1 over a e to the minus k square by 4 a square 1 over c square t is 4 a square 4 a sorry a. So, 1 over root a, I got that right. So, what you got is the following the final result you got is that, if g of x is e to the minus a x square, then g tilde of k is 1 over root a e to the minus k square by 4 a square so that is the result that we have shown. So, let us look at this a little more.

(Refer Slide Time: 27:39)



So, I will just write it again here g of x is equal to e to the minus a x square g tilde of k is equal to e to the minus k square by 4 a square multiplied by in this constant 1 over root a. So, lets this function is called a Gaussian function, so this a Gaussian function. So, it is look like this. So, it is maximum is at x at x equal to 0. So, as a function of x g of x looks like this now, the width at half maximum so this is if you can you can calculate this.

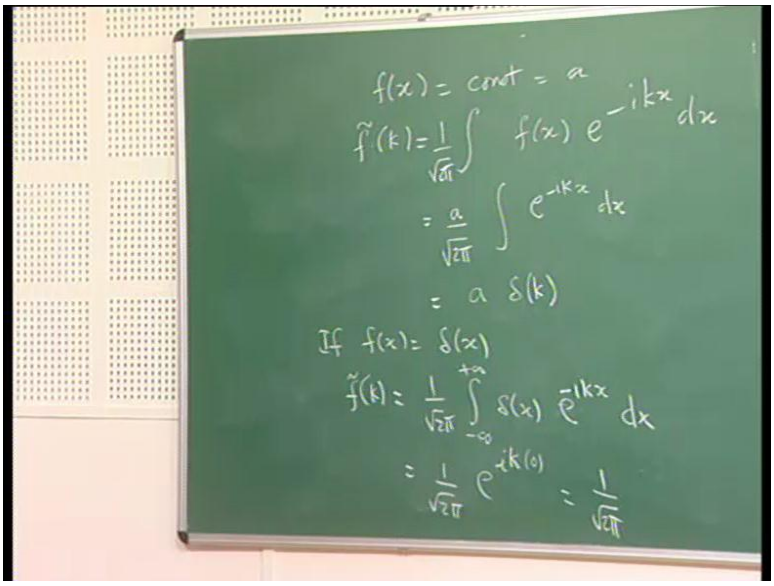
So, when width is nothing but 1 by 2 root a now so the width is inversely proportional to square root of a and in this case, what you have is the following k and let us not bother about, the constant but if you ignore the constant what will see is that this is also a Gaussian and now the width is 2 a sorry, width is just a sorry, root 2 a. So, the way to find the width of a Gaussian and Gaussian is a basically Gaussian function the is represented by e to the minus x square by 2 sigma square, where sigma is the standard deviation of the width at half maximum so in this case this width is 1 over 2 root a and in this case width is root 2 a.

So, what we are shown is the following that if, a is very large then that means, you have a very non narrow Gaussian in x space it is very narrow this width is very small if, this width is very small on x space, then this width becomes very large in k space, so that means width in k space is inversely proportional to width in x space.

So, if you have a very narrow function in x space, it becomes a very wide function in k space and vice versa is we have a very wide function in x space and it will becomes very narrow function in k space and extreme example of this is suppose, you have a constant function if f of x is constant. So, f of x is just constant can be thought of as a Gaussian of infinite width you can think of it as Gaussian function, where the width of the function is infinite.

So, as you make this wider and wider you will go finally, to Something that is almost a constant the f tilde of k equal to delta of k it is proportional to delta of k so if you have a very wide function on x space then you get delta function. So, in this case you have f of x is some constant then f tilde of k becomes a delta function so becomes a delta so very wide function becomes a narrow function and this is a usual property of Fourier of this Fourier transforms function now, how do you show that f tilde of k is constant, how know how do you show f tilde of k is delta of k to do this, you just use the definition of f tilde of k.

(Refer Slide Time: 32:32)

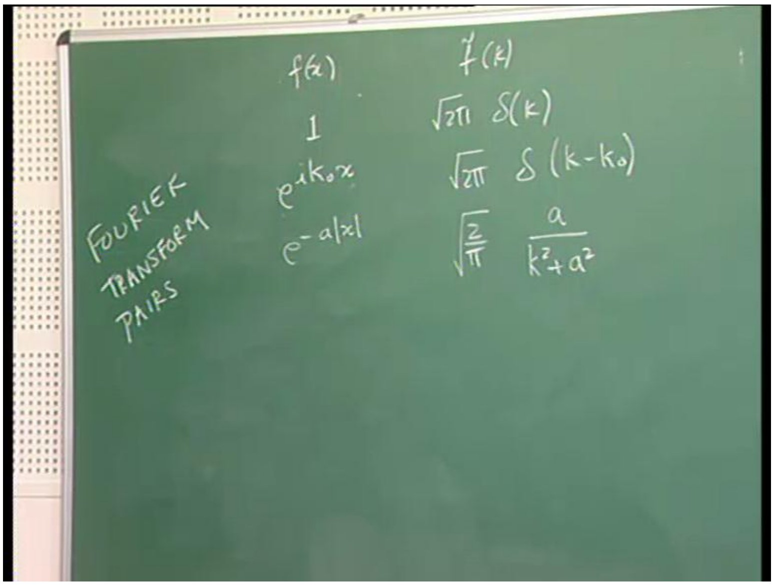


So, what you say is that f of x equal to constant equal to a say it is a then f tilde of k is equal to integral f of x e to the minus i k x d x 1 over root 2 pi. So that is just I can have this is constant a that I take it outside. So, a times a by root 2 pi integral e to the minus i k x d x then this we already said is this is nothing but delta function in k so this is equal to with some constant. So, we get the some constant right, so this quantity with the 1 over root pi so this a times delta of k, so therefore if you have constant function then you it is Fourier transform is a delta function.

So, this is a property of Fourier transforms that if you have a function that is very narrow and 1 is similarly, the Fourier transform of delta function, if you have a delta function is Fourier transform would be a constants of x equal to delta of x then f tilde of k is equal to 1 over root 2 pi integral delta of x e to the i k x d x e to the minus i k x.

So, and you can immediately see that this is equal to so that means, if I want to do this integral then I just I can do this integral by just writing this as 1 over root 2 pi then e to the i k and instead of x i put 0 because I have delta x minus 0. So, i k is 0 so I will just put the value of function at x is equal to 0 and this is just 1 over root 2 pi. So, f tilde of k is just a constant so this is the property of this Fourier transforms.

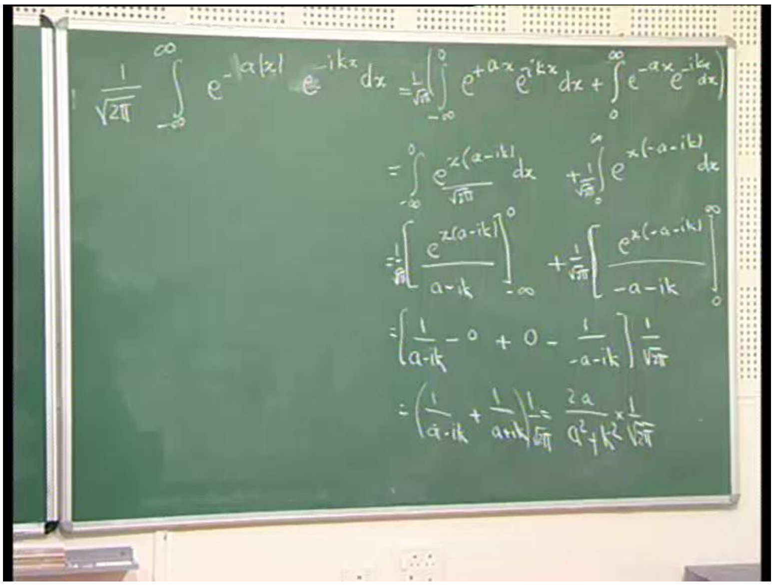
(Refer Slide Time: 35:03)



So, next will look at some pairs of Fourier transforms, now will lists some Fourier transform pairs. So, these are all what are called as Fourier transform pairs delta of k but the term I have taken f of x as square root of 2 pi times delta of x f tilde of k would, have just been 1.

So, they always have this inversion relation then if f of x was e to the i times a constant times x then the Fourier transform that you can easily show this is square root of 2 pi times delta instead of k, you have k minus k 0, this is fairly easy to show then will show this in a minute, if you had f of x is e to the minus a absolute value of x. Then the Fourier transform is root 2 by pi a over k square plus a square just to show this, I will show it to you really quickly.

(Refer Slide Time: 36:00)



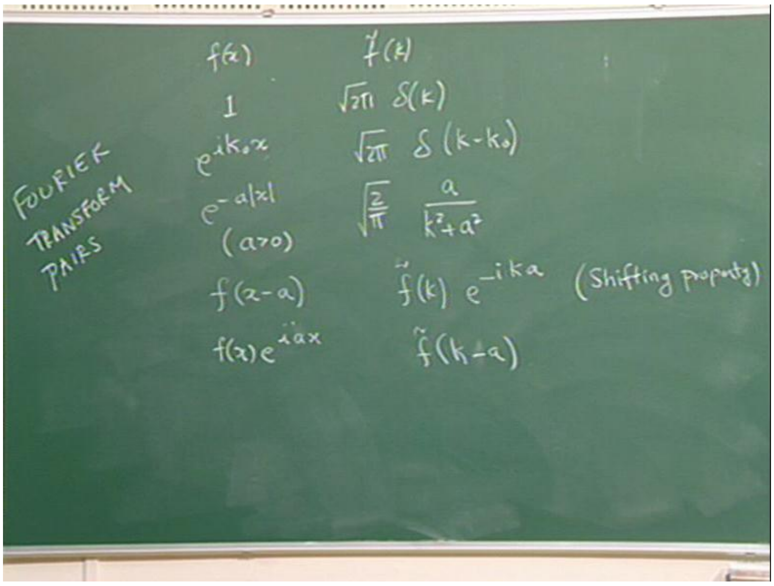
So, f of x is so the Fourier transforms is e to the minus a times absolute value of x d x from minus infinity to infinity into e to the minus i k x d x, so the Fourier transform is this and this is equal to a with a 1 over root 2 pi. So, this is equal to now, we can write this as integral minus infinity to 0 e to the minus a times, now absolute value of x, when x goes from minus infinity into 0. So, x is negative.

So, absolute value of x is minus of x. So, you have plus a x e to the i k x d x then plus integral from 0 to infinity e to the minus a x. So, when x goes from 0 to infinity then absolute value of x is just x so will get this e to the minus i k x d x and each of these can be evaluated so this is integral minus infinity to 0 e to the x a minus i k d x plus integral 0 to infinity e to the x minus a minus i k d x and each of these is an exponential function so you can just integrate this out.

So, this is will be e to the x a minus i k divided by a minus i k from minus infinity to 0 plus e to the x minus a minus i k divided by minus a minus i k from 0 to infinity, now the upper limit corresponding to x equal to 0 will give me 1 over a minus i k then lower limit corresponding to x equal to minus infinity. So, when x becomes minus infinity you get e to the minus infinity into a is the I should mentioned. So, is a greater than 0 so in this case a assumed to be greater than 0 so since a is greater than 0 then e into minus infinity into some positive number that gives me e to the minus infinity and we do not need to worry about the e to the i k x at the lower limit, I will just get 0 similarly, in this case at the upper limit I will get 0, because e to the infinity into minus x.

So, that is the e to the minus infinity at the lower limit I will get 1 over minus a minus i k. So, what I will get is 1 over a minus i k plus 1 over a plus i k. So, I can take all these minus signs together, so I have 1 over a minus i k plus 1 over a plus i k and this is just you can multiply out so i k plus a minus i k so that is 2 a divided by a square minus k square a square plus k square sorry, a square k square. So that is what you will get with this so 1 over root 2 pi 1 over root 2 pi angle around everywhere because this whole thing is divided by root 2 pi 1 over root 2 pi and 2 pi here also we have 1 over root 2 pi we have root 2 pi.

(Refer Slide Time: 40:35)



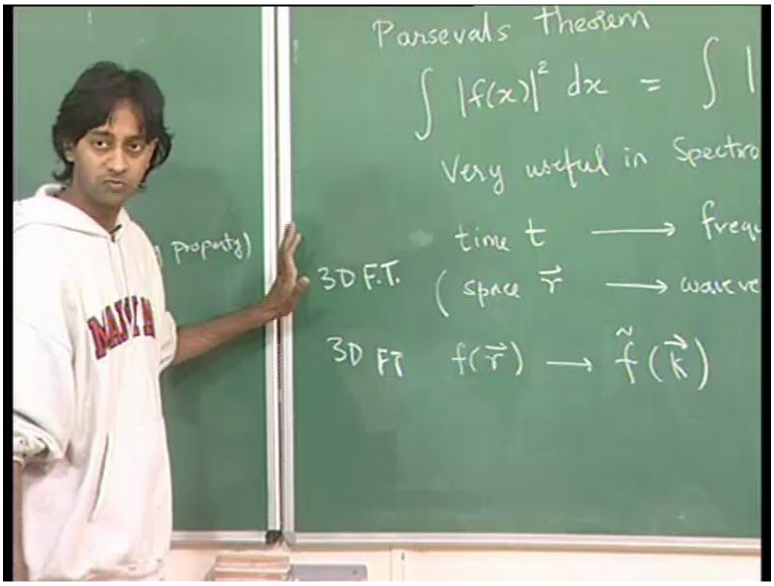
And that is just this answer so we take 1 over root 2 pi into a divided by a square plus k square. So, will get exactly this answer, we showed. So, we have shown this relation, there are few more Fourier transform pairs, which you can also find out I will just write a general shifting property very interesting property for a shifting property. So, f of x minus a so the Fourier transform of f of x minus a is related to it Fourier transform of f tilde of k but this relation is this is the following, so f tilde of k into e to the minus i k a.

So, if you shift here so this is just f of x instead of x my argument is x minus a then my Fourier transform will just be a f tilde of k multiplied by e to the minus i k a. So, this is called the shifting property and it works other way also. So, if I had f of x into e to the i a x sorry e to the i a x yes then i would, just get f tilde of k plus a or k minus a sorry minus a. So, it was works both ways so this is the property of this Fourier transform and that is what we use right here so this is 1 into e to the i k 0 x.

So, the Fourier transform of this is the same as the Fourier transform but not at k but at k minus k 0 so that is this shifting property of Fourier transforms. So, the Fourier transforms the way we defined them, there is a nice symmetric to the relations and you can do many more such Fourier transforms pairs, the last thing I will mentioned is the following, will look at some applications of Fourier transforms in the real chemistry problems, I will just mention one another interesting property of Fourier transform, which is called the Parsevals theorem, this is the theorem that makes Fourier transform very useful For in spectroscopic.

So, many of you might of you heard things like f t i r or f t n m r. So, Fourier transform of i r or Fourier transform of n m r so this makes use of very powerful theorem of Fourier transforms that is called Parsevals theorem. So, I will just stated for now and then and then will close the discussion on Fourier transform will look at some specific examples in the next class.

(Refer Slide Time: 43:43)



So, this called the Parsevals theorem, and this basically states that integral f of x square d x is equal to integral f tilde of k square d k, so this theorem states that the area under square of Fourier transform is square f of x is same under the area of the square of f tilde of k under k. And this means, that if f of x let us say some electric field, that is being applied, so when you do spectroscopic you shining light. So, light has some electric field component then the square of the amplitude of the electric field is related to the intensity.

So, what you are saying is that the total intensity is and the Fourier transform of the intensity what is called the power spectrum, so this connection between power spectrum and intensity is what allows you to use Fourier transforms to do spectroscopy.

So, this is something that is very useful in spectroscopy and so this is something that used a lot infact in spectroscopy to do your variable x instead of your variable x is your time so in spectroscopy typically you have time t and you transform to frequency omega so the angle of frequency omega. So, this is what is typically done and in some cases in some. So, this is done in spectroscopy, now in x-ray diffraction you use space r to Fourier space k, so wave vector k.

So, this is the three dimensional Fourier transform form where instead of just having a 1 dimensional scalar variable x you have a vector r with 3 components and you take this Fourier transform. So, in that case typically what you do is you have f of r to f tilde k vector so this is the 3 d Fourier transform and this is a very important component of x-ray diffraction, we were talking much about the about 3 dimensional of Fourier transform but in the next class I want to give an example of how we use of where this Fourier transforms appear very naturally.