Statistical Mechanics
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Lecture – 13
Mathematical Preliminaries 1

Good afternoon students, today I will discuss some Mathematical Preliminaries required to do the problems that, you have encountered that you will encounter in this course. So, I will be giving couple of lectures on some important mathematical results, which are handy, if you are dealing with numerical problems.

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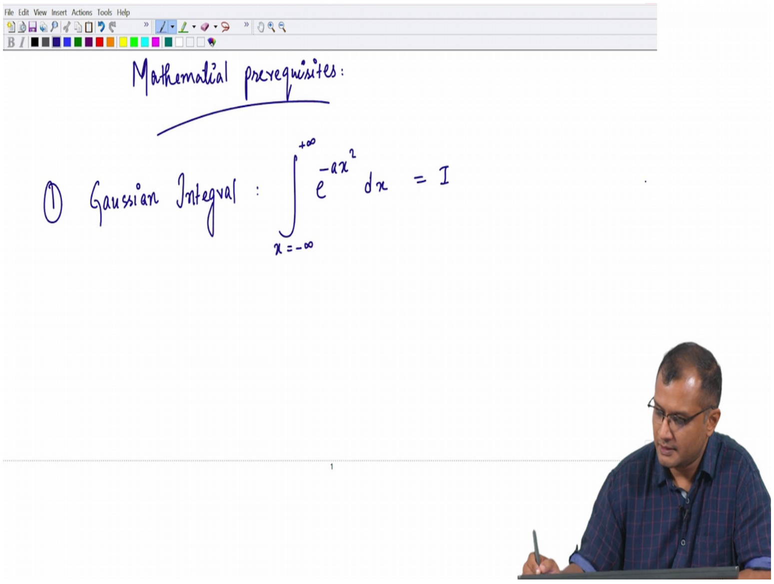

So, very simple so, I am going to title this lecture as mathematical pre requisites, you can skip these pre requisites if you are already familiar with them but, just in case you are not familiar this might turn out to be useful ok.

So, couple of things that I will discuss, I am going to write them down. So, one is to compute how you know, compute the Gaussian integral. So, basically we are looking to integrate function, from minus infinity to plus infinity and the function here is the Gaussian function. Let us say this is I fine.

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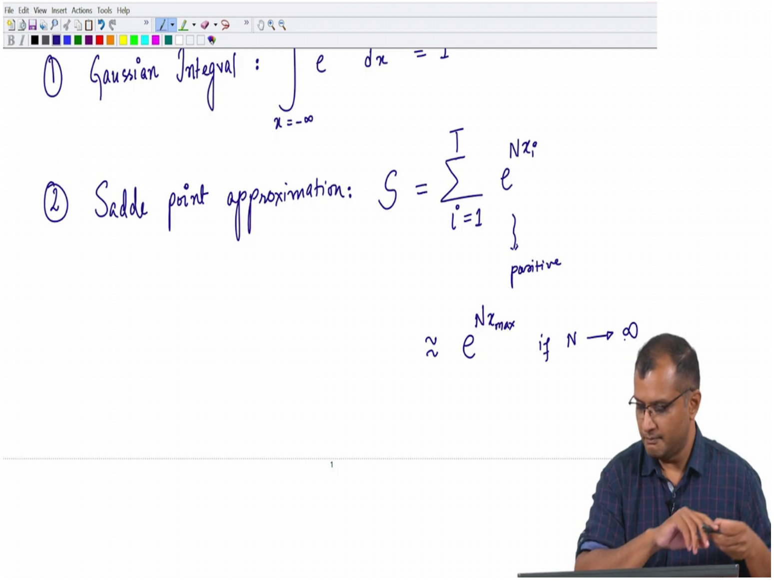

So, this is the first problem on the agenda, second I will discuss an important technique which is the saddle point approximation that, we have let we will using in, the second chapter of statistical mechanics is basically a very important approximation method and if you want to approximate the sum of exponentials.

So, suppose I have exponentials, I going from 1 to some T number of terms and I have these exponentials of the type e raised to N times some x of i ok. So, these all these terms here are positive because, they are be exponents they cannot be negative. So, they are all positive in nature, each term is positive in nature and exponent is some N times x i ok. So, I will show that, saddle point approximation says that, I can approximate this sum, as is the maximum of the terms.

So, suppose the maximum term in this expression is e to the power N x max then, I can approximate the entire sum with the maximum of the terms, if N goes to infinity ok. So, if you encounter a sum of exponentials, where each exponent, where each exponential term as a power N times x or N times some function of x. Then as you take N to infinity, you can approximate this sum as e raised to N x max ok. So, this is the very important approximation that I will be discussing today.

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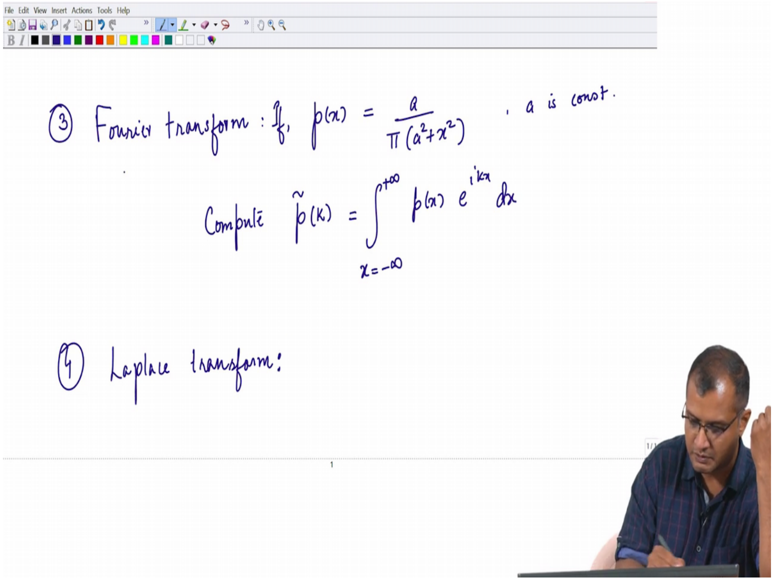

The third thing that I want to discuss is that of Fourier transform. So, some important Fourier transforms that you have encountered in chapter 1, you will be encountering Fourier transforms everywhere in theoretical physics. So, I am not sure how much of the background you already carry in the context of Fourier transfers but, we will take some simple Fourier transform examples and for example, I will take a function that you are encountered in this course, which is the Laurence distribution or a Cauchy distribution. So, we have taken this as a distribution, after proper normalization it came out to be some a by pi into 1 by a square plus x square.

So, here a is constant. So, I will take the Fourier transform this function. So, let us say our function is defined as p of x. So, we will compute the Fourier transform of this function, which defined as x going from minus infinity to plus infinity, p of x e to the power i k x dx. And the last topic of this lecture would be to compute some important Laplace transforms, I have discussed Fourier transform I will take one example of Laplace transform and show how it is very important to construct important results ok. So, Laplace transform is defined.

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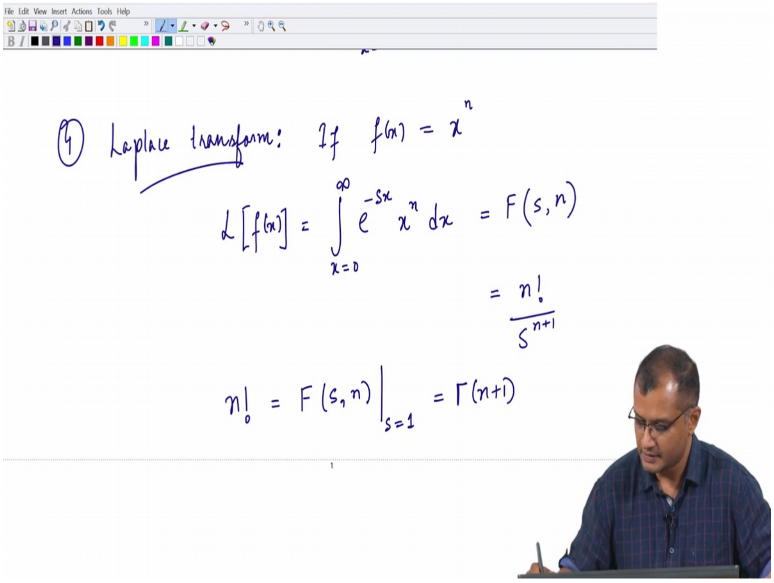

So, if you take a function, let us see you take a power law, x to the power n, then the Laplace transform of this function is defined as an integral x going from 0 to infinity, e to the power minus s x, x to the power n dx. A naturally this is a integration on x, a definite integration on x, this result is nothing, but a function of s and with the parameter n and we will show that, this is equal to n factorial, over S to the power n plus 1 and derive an important result that your n factorial is nothing but, this function at n equal to 0, at s equal to 0 ok. Our Laplace transform.

So, this function would be at f s n, taken at s equals to 1, which we also call sometimes as the gamma function. So, that is the definition ok, it is gamma n plus 1 is called as n factorial.

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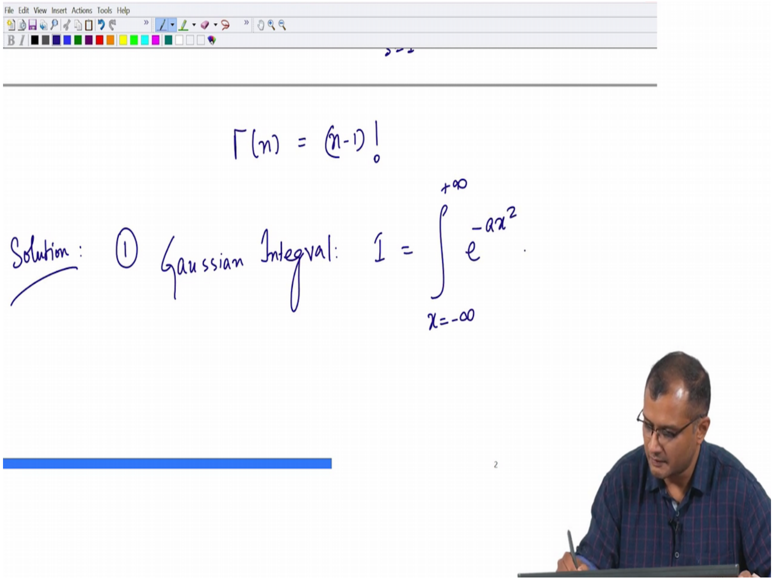

Which means, if I want gamma n, this would be just n minus 1 factorial or we can use with whichever definition you want to choose so, let us start with the Gaussian integral ok, the first topic on our agenda so, we will first start with Gaussian integral because, you are encountered this many places. So, we have the integral, which is basically x going from minus infinity to plus infinity, e to the power minus a x square ok.

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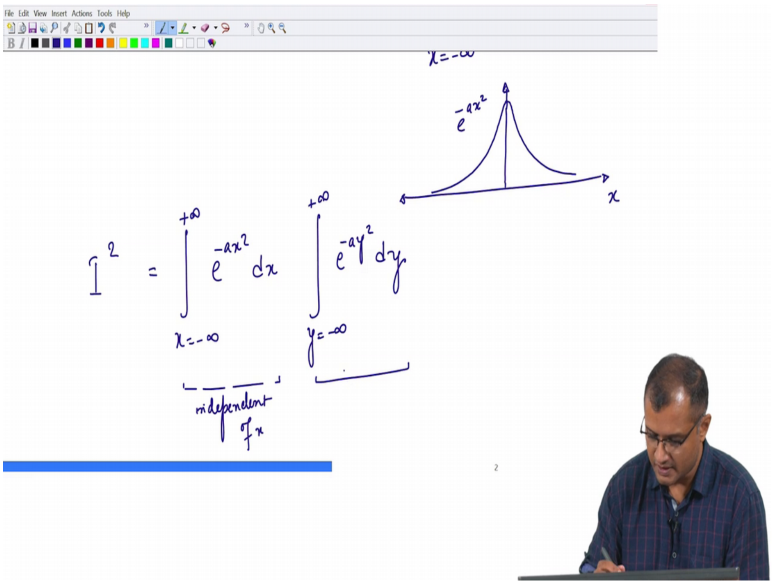

So, if you want to understand what is the Gaussian function? Well, this is a bell function. So, the way I have written my function, it peaks at the origin and it has a if you understand this as a probability distribution function then, it is mean value is 0. So, this is the bell curve or the Gaussian function and the integration of this Gaussian function is the agenda of our discussion.

So, I am going to make a small trick here that, if I want to compute I, I can instead calculate I square ok. So, I am going to write down, I square as a the integral x going from minus infinity to plus infinity, e to the power minus a x square, dx and square it up which means, I can write it as some y going from minus infinity to plus infinity, e raised to minus a y square dy. The reason being x and y are independent coordinates, they are the coordinator that are integrated over.

So, they are being, they serving the purpose of dummy variable ok. So, neither is this integral function of x, neither is this integral function of y, which means I can keep the integration variable as x y z or anything. So, is this just a function of a.

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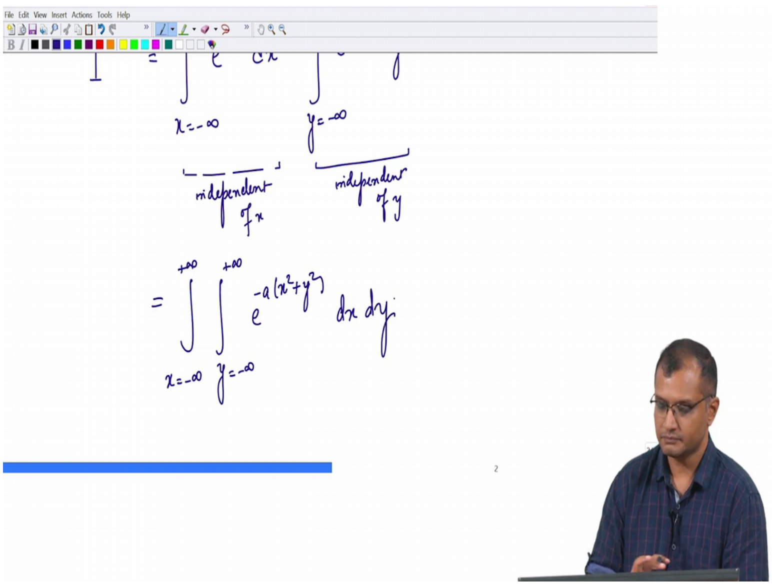

And this is also function of ok, just a function of a and this is also function of a. So, this allows me to write down the square as two separate definite integrals and now again combine these two definite integrals and use a double integral, one for x and one for y and I can take the integrand and combine it has call as a e raise to minus a, x square plus y square, dx dy and then actually I can you know pause here, instead of proceeding further and notice that this is nothing but, in area integral ok.

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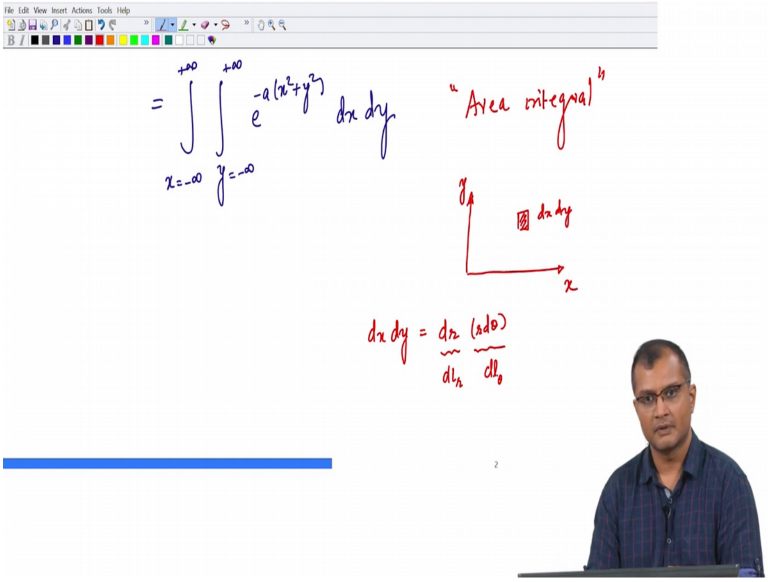

So, I have taken a function e raise to minus a, x square plus y square and I am doing area integral of this function. So, I can make some substitutions already. So, I know in two dimensions and this is a two dimensional integration. So, if I take this is my x axis and if I take that is my y axis, then any small area element that I can consider here, some small area element would be just you know, dx dy and I can simply integrate over the entire space, that would be my total area. So, I can write down my area element dx dy, in polar representation, as simply dr into r d theta ok.

So, if you want you can think of this as my small increment in the direction of unit vector r and this is a small increment in the direction of unit vector theta. So, whether I use the Cartesian components or if I use the r theta components, the displacement components dr and rd theta, if I go into the polar components.

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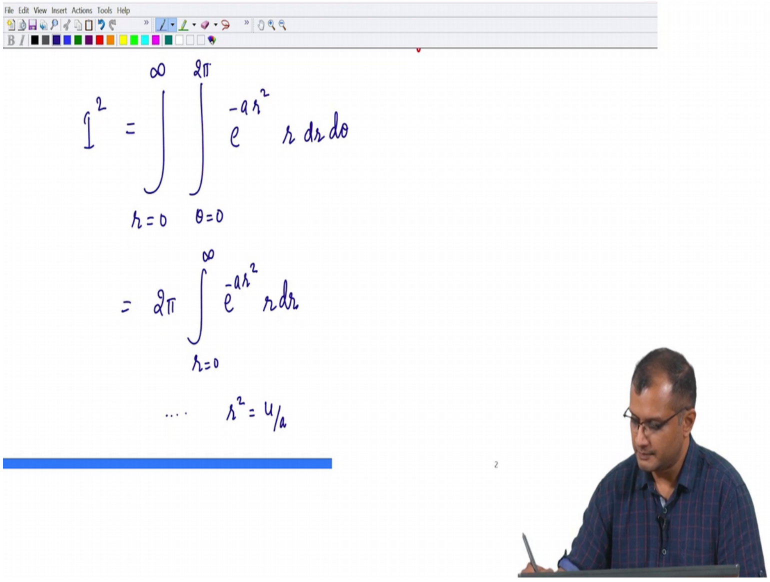

And hence I can write down my x square plus y square, as the length r square and similarly the limits on integration will now become. So, my integration, which is I square. Now, becomes this double integral that I have written, is now our integral r, that is going from 0 to infinity because, if I look into this figure.

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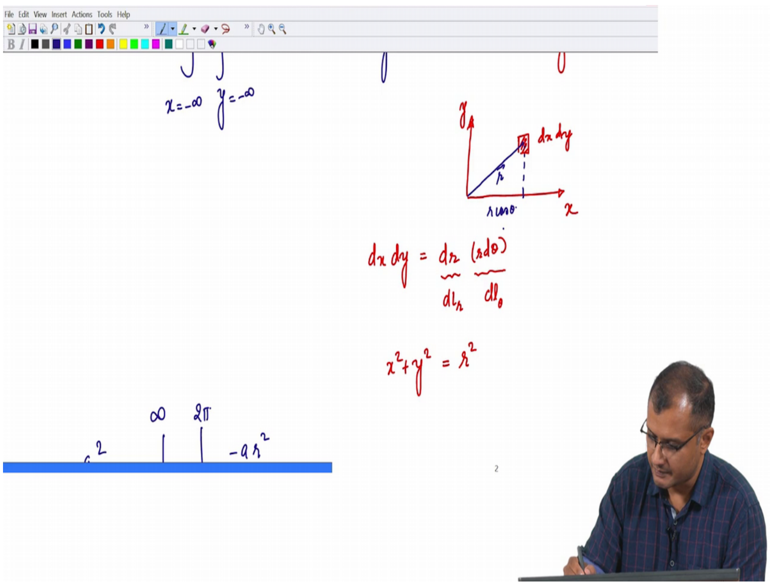

To compute an area integral, at location r, you know what I need to do is basically, take my aerial vector, aerial displacement ok. At various points in my surface and at each point this would be nothing but, a aerial element located at coordinates r comma theta.

So, theta here will go from 0 to 2 pi and the location would be just specified at a distance r from the center ok.

So, then I can simply write down my theta to go from 0 to 2 pi and this particular integrand, is just e raise to minus a, r square and I can write down this element dx dy, as what I have written here ok, r into dr d theta fine. And then, simply take the theta integration first. So, that would simply give me 2 pi and the integration and r would become just e to the power minus a r square, into rdr and by substituting r square as just u by a ok.

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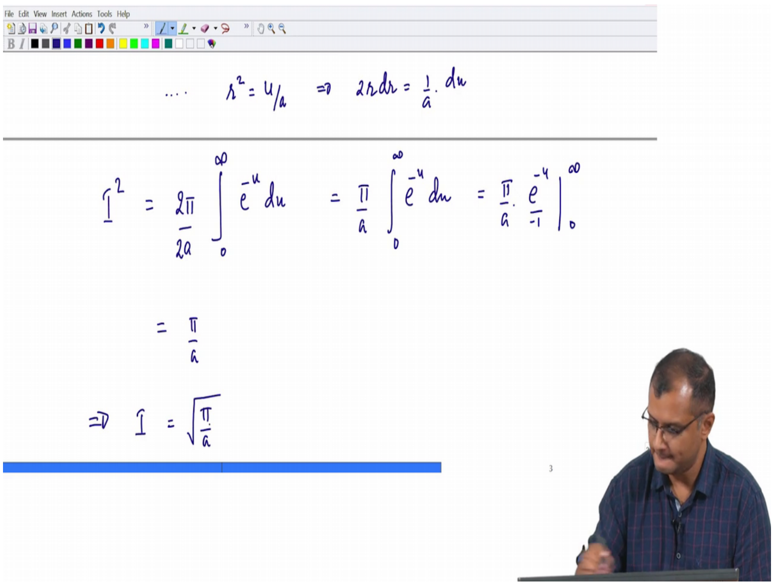

I can write down twice rdr, as just 1 upon a into du. So, this will give my I square as 2 pi, into integration 0 to infinity because, the limits on r are the same as limits on u and I get e to the power minus u into 1 upon 2 a du.

So, this will give me just pi by a, integration 0 to infinity, e raise to minus u d u and that is nothing but, pi by a, this will give me just pi by a and then I can write down, I as square root of pi by a ok.

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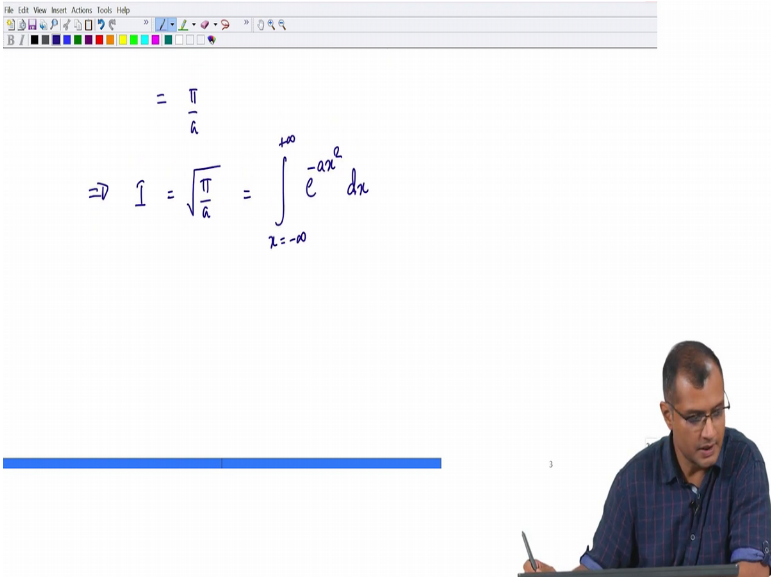

So this is the Gaussian integral that we were chasing. That is the result of Gaussian integral. So, our next problem in the agenda is to use a saddle point approximation.

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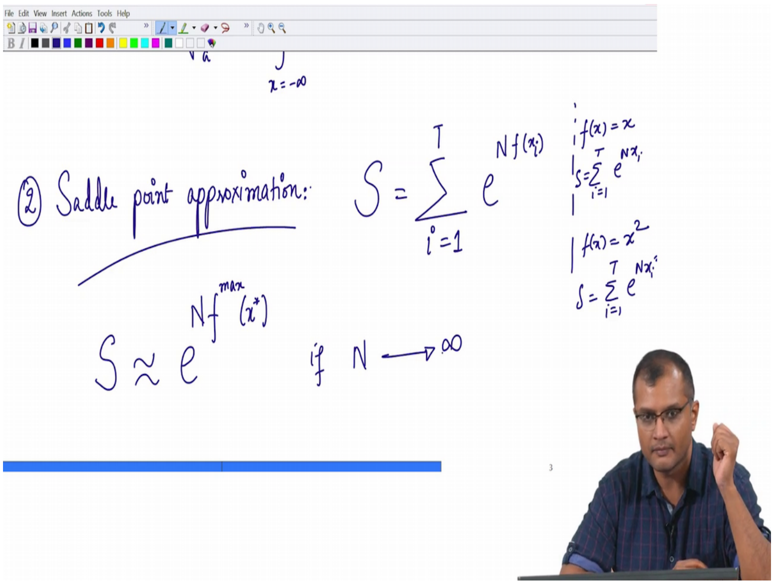

And we can do this. So, these were important topic that, we deferred for a separate lecture and you have to recall some of the concepts that we discussed in second chapter, where we have used saddle point approximation especially, in the computation of entropy for an ideal gas system.

So, I will describe this as just approximation for a sum, over a large number of exponentials. So, if I have T exponentials and if I summed them up and here each exponential is of this form, e the power some N times of function of x, let me take this as the function of x. Simplest function of x is x itself, you can take any function of x here and the index i here is just f of x i ok. So, you can take f of x as simply x, then this becomes just a summation over then, my s simply become summation over i going from 1 to T, e to the power N x i ok.

You can take f of x as x square then, your summation becomes i going from 1 to T, e to the power N x i square, you can take any function basically. So, what I am going to do is take any function f of x and simply over simply some over various values of x and take T such terms and add them up. The argument is I can approximate S, by the largest term in the sum and the largest term would be the term which is at you know, the maximum of f coming at sum x star.

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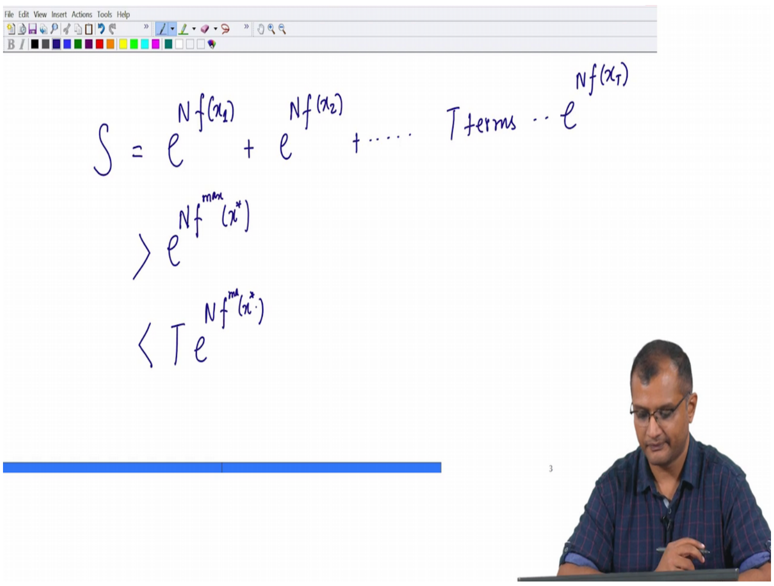

If N tends to infinity so, we can do this very simply by saying that, look my sum was composed of a large number of terms. So, I am going to write it as, if I going to, if I am writing my original sum as a sum over all these exponentials, as f at x 1, plus e to the power N f x 2 ok. In the last term being so, I can definitely say that my summation would be less than, e to the power N f max, at sum x star. Let us say one of these terms is the maximum, at occurs at x star ok.

So, I definitely know that my sum is less than that and I can definitely say that my summation. So, this is very clear and it is also I have to say that this. In fact, I have made a small error here, it has to be definitely greater than and it has to be definitely less than, if I replace each term in the summation by the maximum, then what I would get it just N times just sorry, if I reach replace each term by the maximum then, I would get T times T maximum ok.

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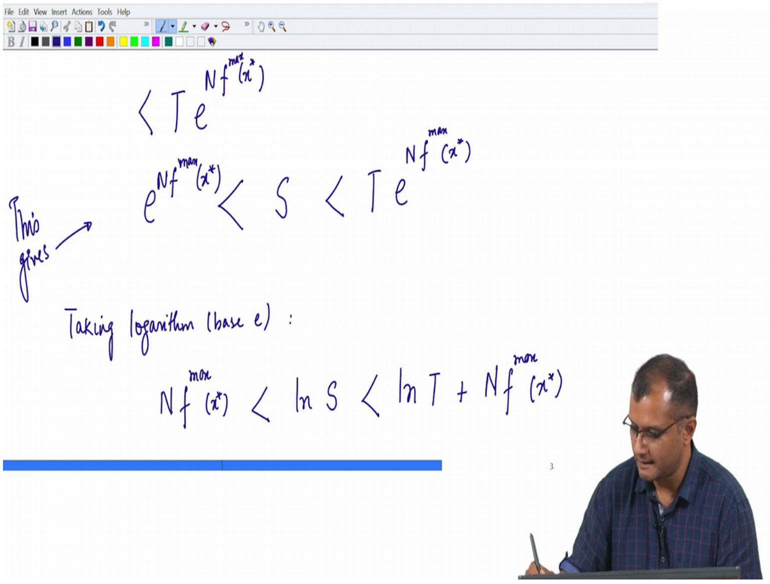

So, then I can say that, my S is less than it is definitely less than, T times, T being the total number of terms, if I replace each term with the maximum then, definitely it is over counting my sum and if I just take the largests in the sum, the definitely my x is greater than that.

So, this gives us, this very nice in equality. Now, you can do a couple of things here, you can take a logarithm on entire inequality. So, taking logarithm, natural logarithm so, taking natural logarithm, you would get N times f maximum, at sum x star ok, which should be less than natural log of S, which should be less than natural log of T, plus N times f max, at sum x star fine. You have taken natural log throughout and natural log to the base e of e is 1.

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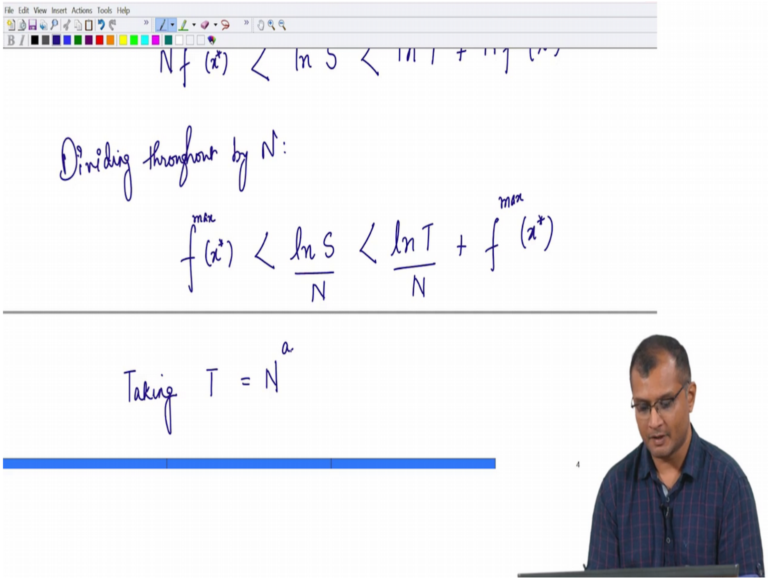

Now, you can divide throughout by N ok. So, if you divide throughout by N, what you get is nothing but, the maximum of the function, at the at one of the values of x. Let us say that is x star, is less than lon S over N, is less than lon T over N, plus f max at sum x star. Now, this is very gets interesting, if you take and which is always possible or I will say taking not if but, I will say taking our T, the total number of terms, as sum power of N ok, which is always possible.

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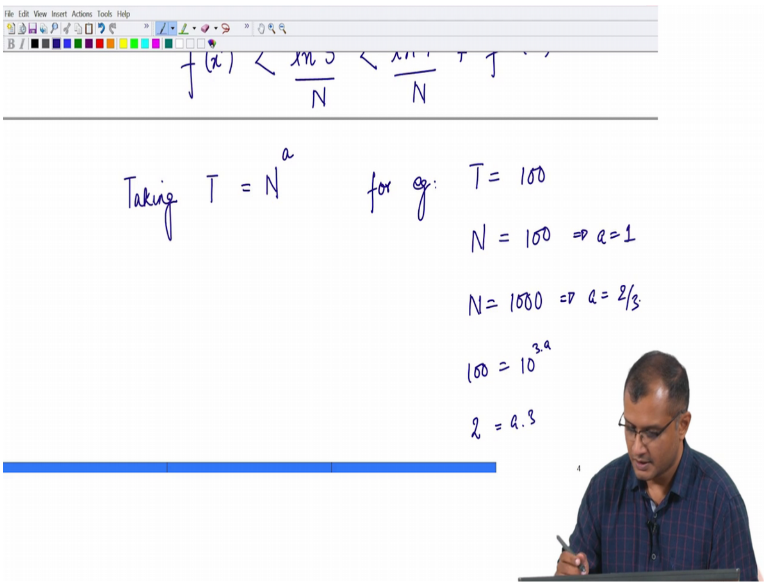

Suppose you take for example, you have total 100 terms and your number of you can say your big N is 100 then, I know a is equal to 1 because, 100 to the power 1 is 100 ok. So, that is one case but, if I take let us say you now. So, this would give me a as 1 but, if I take N as 1000 ok. So, here I can get my a to be. So, I can compute my a as simply, 100 equals to 10 to the power 3, times raise to the power a. So, if I take a lon on both sides this would be roughly 2 and this would be just a into 3. So, I can say that a should be 2 by 3 because, 1000 to the part 2 by 3 is 100.

So, this may you can take any N and always find that, you can rise into a sum power and get the number of terms that are required, toughly to an order ok. So, then I can always write down my inequality that is written above. So, in this in equality is now re casted as, by know with the substitution T as N the power a.

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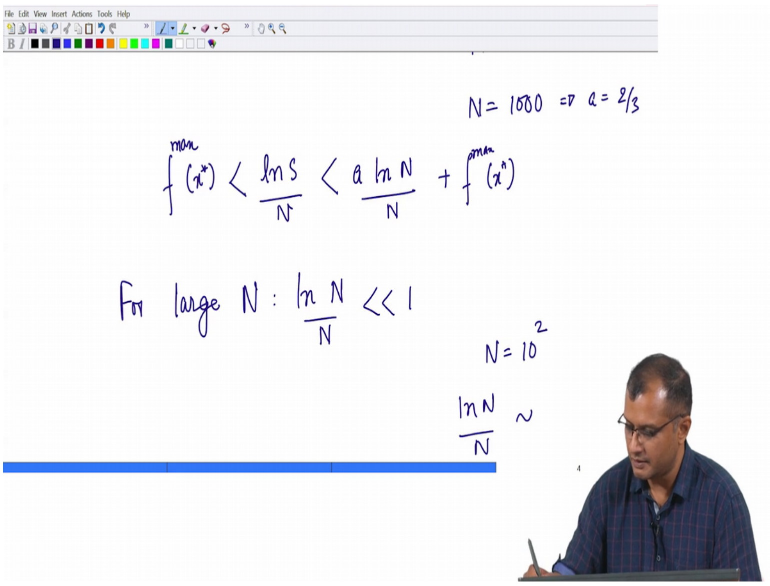

You can write it as, f maximum, it is sum x star, this will be less than, lon S by N, which should be less than a lon N by N, plus f maximum, at x star ok. Now, you can see that, for large N, which is the case that we are chasing, I can ignore lon N by N, simply being suppose you take N as 100.

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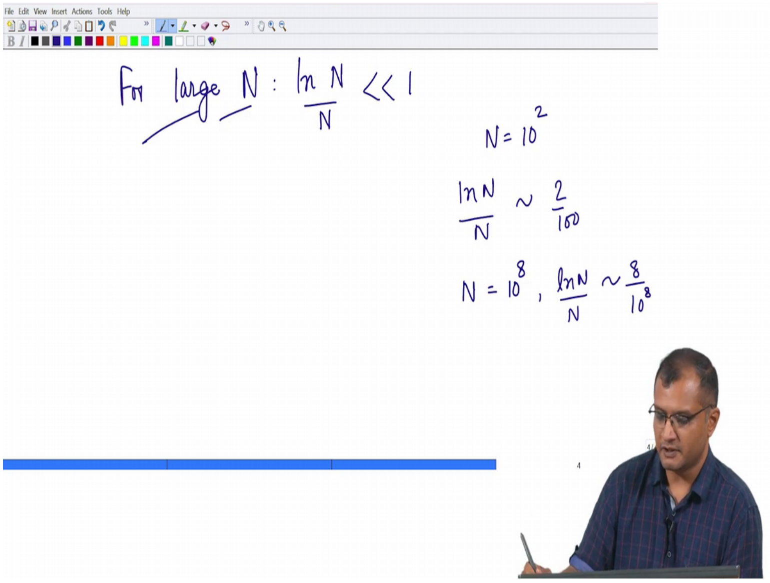

Then lon N by, is roughly 2 by 100 and if you take N as, let us say even larger 10 to the power 6 or 8, some larger number then, you know you can say that lon N by N, is an even smaller number, this would be just 8 by 10 to the power 8.

So, as you take N to be very large, it is typically the number of particles that you would have in a system and then in the limit of such large Ns, you can always drop lon N by N because, that is going to be a number of vanishing magnitude. So, I can then recast my inequality here as simply.

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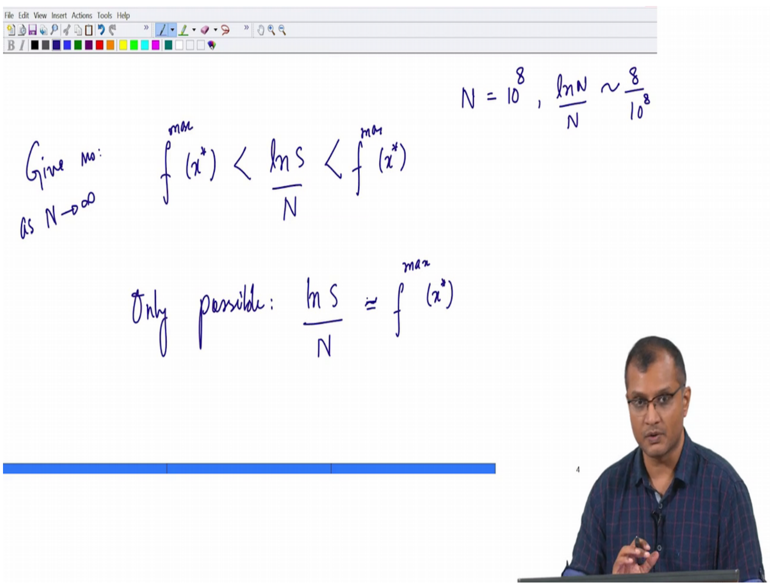

So, this gives us as N goes to infinity ok, f star f max, at x star less than lon S by N, which is I am going to drop my a lon N by N, as simply write this as f max, at x star. Now, you can see that lon S by N is now bounded from above and below, by the same number, which is f max and this is only possible, if I write down lon S as it takes the value, one of them ok. It is bounded forwarded and below by this same number. So, we will say that lon S by N is equal to f max, at x star ok. I am going to use an approximation here because; you have drug lon N by N in the approximation that N goes to infinity.

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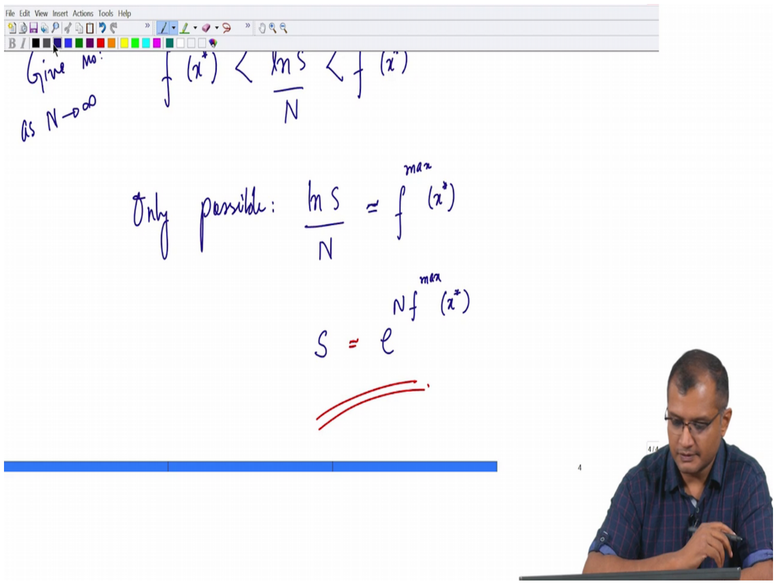

So, then we can write down our S, as simply e to power N times f max, at x star. So, that completes our saddle point discussion ok. So, this is very important equality or approximation that, we can use in the limit of large N right. So, we will go to the next topic which is, if you recall, this is like taking Fourier transform of function and as an example I have taken Lorentzian function. So, let me take it is Fourier transform right.

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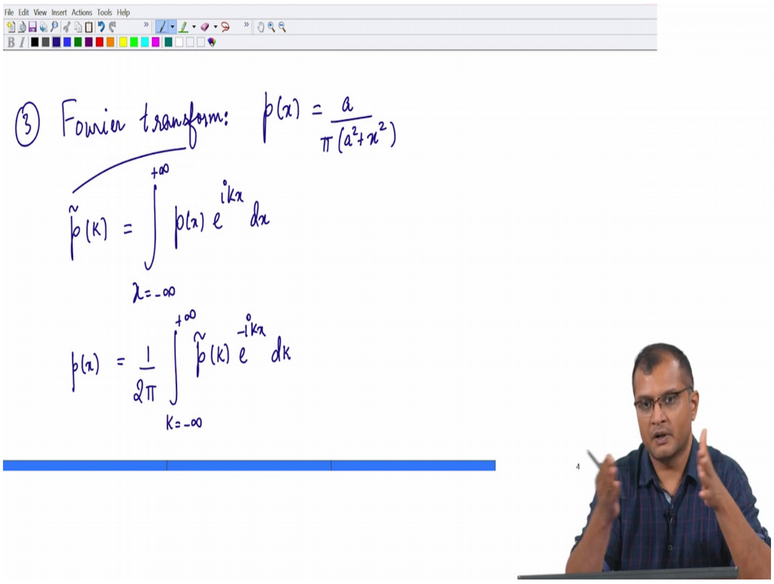

So, one of the important mathematical techniques is the technique of Fourier transform. So, we will take our function, in such a way I am given a function with the motivation that is follows, you know this function will require you to compute the Fourier transform by the method of contour integrations. So, it is like hitting 2 birds with 1 both 1 arrow. So, we will also learn something about contour integrations here. So, the Fourier transform of this distribution function, which is also called as the characteristic function of the distribution and that you will see in the chapter 1, is nothing but, the limits x going from minus infinity to plus infinity, p of x e to the power i k x, dx.

Now, you must have taken some course in Fourier transform, if you are not then the take home messages that, you have a function that is required at each points in the direct space, in this case p of x and the Fourier transform will then give me the function, in the Fourier space at 1 value of k. So, as you can see, a function p of s is taken at all values of x, from minus infinity plus infinity, to generate one value of the Fourier amplitude at mode k. The inverse transform, would mean that I will get my function, at one value of the direct space, by simply taking inverse Fourier transform; that means, my Fourier amplitudes have to be known everywhere in the k space ok.

So, if I know the Fourier amplitude everywhere in the k space then, I can compute the inverse Fourier transform recover the function. So, all x give me 1 k and all k giving me 1 x, is the logic here and usually the function that we are usually in fact, almost always the function that we take, for Fourier transforms are a periodic functions because, Fourier transformers are derived from Fourier series in the limit, when the functions seizes to become periodic or fails to complete one cycle ok. So, in distinction to Fourier series, which applies to periodic functions in box of size l, Fourier transforms are useful for functions which are a periodic ok. So, let us compute the Fourier transform here.

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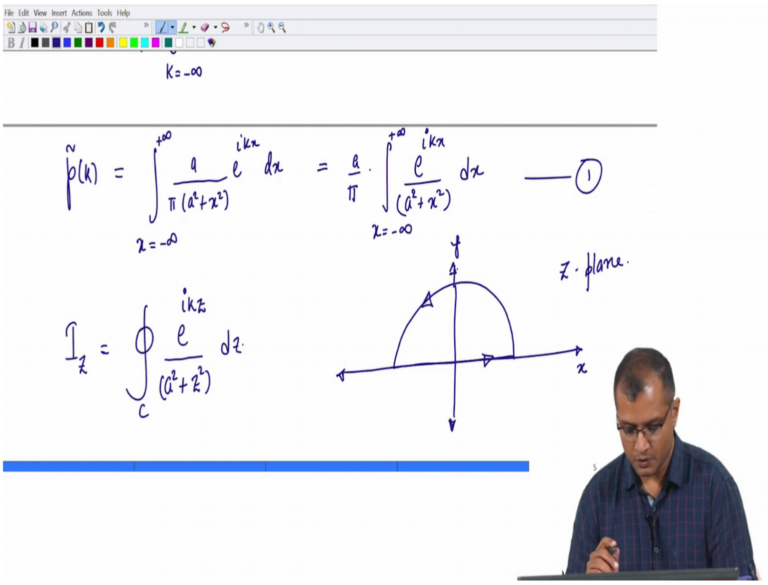

So, you can I will take the Fourier transform and leave the inverse to you, so this should be just integral x going from here computing the Fourier transform. So, x going from minus infinity to plus infinity, our function is a by pi into a square plus x square, into e raise to i k x, dx ok. So, this can be written as, a by pi into integration of minus infinity to plus infinity, e to the power i k x, over a square plus x square.

Now, expect that you have taken some course on complex variables and because I will be using complex integration to compute this integral. So, I am going to call this integral 1 and say that instead of computing this integral, I will compute some integral in the complex plane which is nothing but, the contour integral, of e to the power i k z, over a square plus z square, dz.

So, I must indicate my contour here. So, the contour that I am using is basically, so this is my complex plane and I am using semicircle contour and this the direction of my contour integration, this is my x axis, this is y axis and there are 2 poles of this function.

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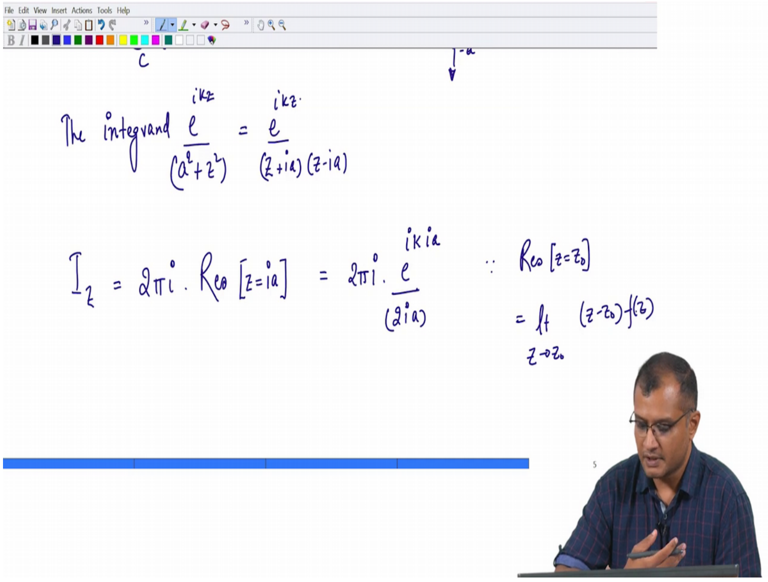

So, the function has the integrand, you know it has, I can rewrite this integrand, to show that it to basically expose it is poles, it can be written as e raise to i k z upon z plus i a, into z minus i a. So, there are 2 poles, I am going to use only one of them, which is at a and there are another pole at minus a, that I am going to drop.

So, as you can see ok. So, then I can easily write down my contour integral, this would be nothing but, 2 pi i, into the residue at z equals to i a ok, only the contour in the only the residue in inside the contour that is drawn. So, this would be nothing but, the residue at z equals to i a, would be nothing but; would be nothing but, if I just substitute z equals to i a, it is a simple pole. So, all I have to do is just substitute z equal to i a there, so it will give me e to the power i k into i a, divided by 2 i a, just substituting z equals to i a in my function. So, the residue here is, at any z naught is nothing but, limit z tending to z naught, into a function ok.

So, you multiply z minus z naught which is, z minus i a and that would be just e to the power ikz upon z plus i a, in that you substitute i a, that would give you your residue.

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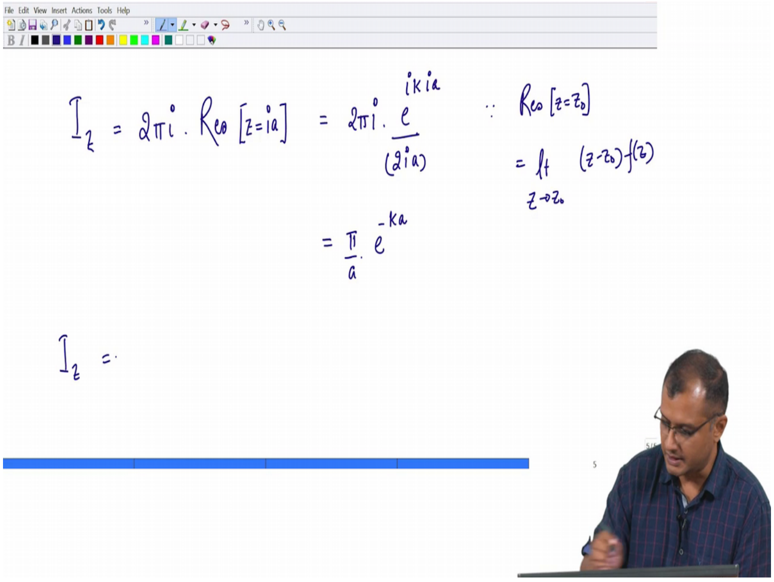

So, this would be nothing but, pi by a, into e to the power minus ka fine. Now, there is something that I would like to mentioned here, my contour integral e raise to I mean the integral of e raise to i k z upon a square plus z square, can also be written as a sum of 2 integrals.

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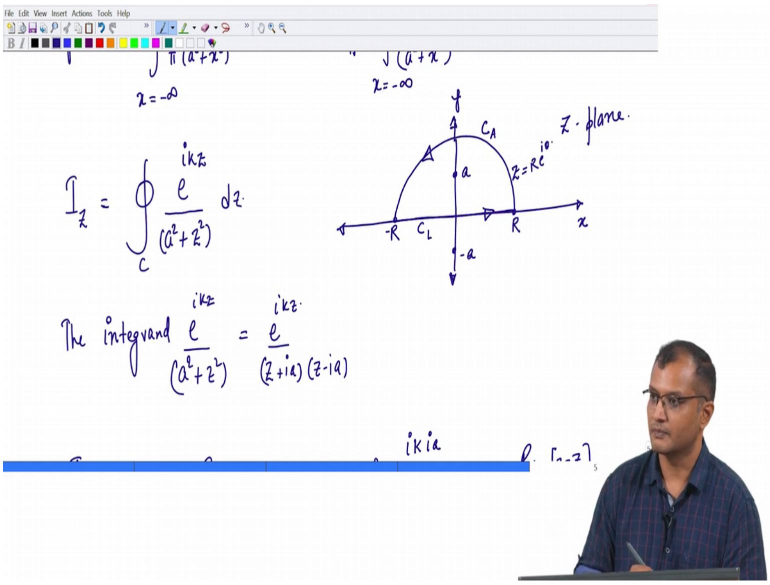

So, I can write down there is a line integral here and there is a contour integral here, I will call it as CA and I am going to call this as CL, the straight line part ok.

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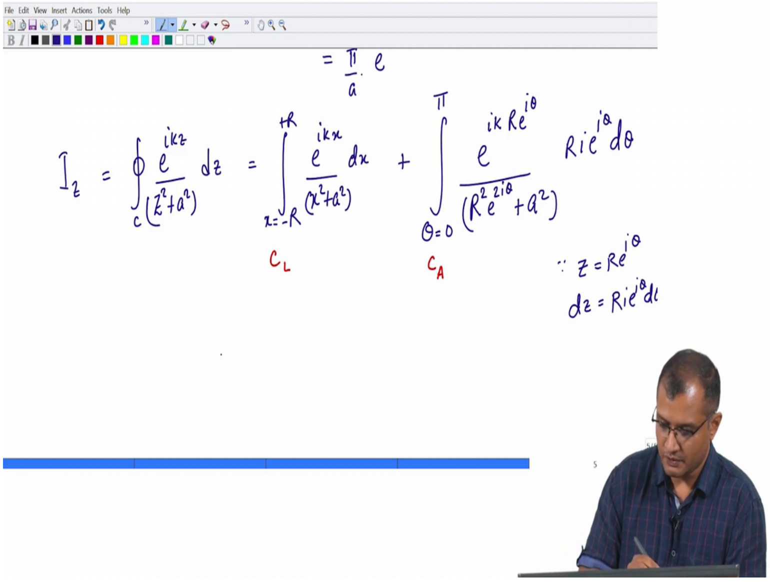

So, I can write my contour integral, which is e to the power i k z, over z square plus a square d z ok, as simply the straight line component, which is going from if I call this point as plus R and this point as minus R, this is a circle of radius R, semicircle of radius R. Then this the straight line part goes from x equals to minus R to plus R ok, that is my CL. And here my function is e to the power i k x, dx over because, z is just x here ok. Plus I will have a part where, if you look at the contour here, the only degree of freedom is theta because, R is fixed here. So, I can call my complex variable z, on this contour as simply R, each point on the surface is just on the circle is just R e to the power i theta ok, that is my complex variable.

So, here theta goes from 0 to pi and this is my contour CA the arc, the pi arc and here my function is nothing but, e to the power i k and the complex variable is R raise to, R into e raise to i theta, divided by z square is nothing but, R square, e to the power 2 i theta, plus a square and d z would be nothing but, R i, e to the power i theta, d theta ok. Since, I have taken z as R e raise to i theta, d z would be R i e to the power i theta d theta because, R is not constant, R is constant, only theta varies on that semicircle.

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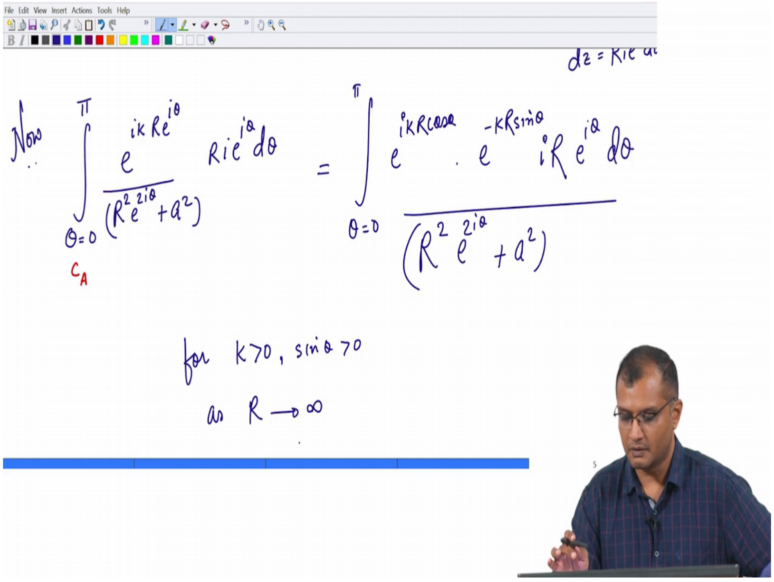

So, now you can see that, the this contour integral, if I going if I am going to just consider this one, you can see that; you can see that, it can be written as, theta going from 0 to pi, I can split up the numerator as, e to the power i k R cos theta into e to the power minus k R cos sin theta because, e raised to i theta is cos theta plus i sin theta, i into i because, you have minus sin, into R, i e to the power i theta and d theta divided by R square, e to the power 2 i theta plus a square fine. So, as you can see as, for k greater than 0, I know in the quadrant that I am doing my integral, the first quadrant the second quadrant, sin theta is always positive.

So, if k is greater than 0 and sin theta is always positive because, I am in the first and second quadrant and as R goes to infinity, I can see that my numerator goes to 0 because, it is going as e to the power minus R into R and the denominator is going as R square ok. So, the denominator will become larger and larger the numerator will go towards 0.

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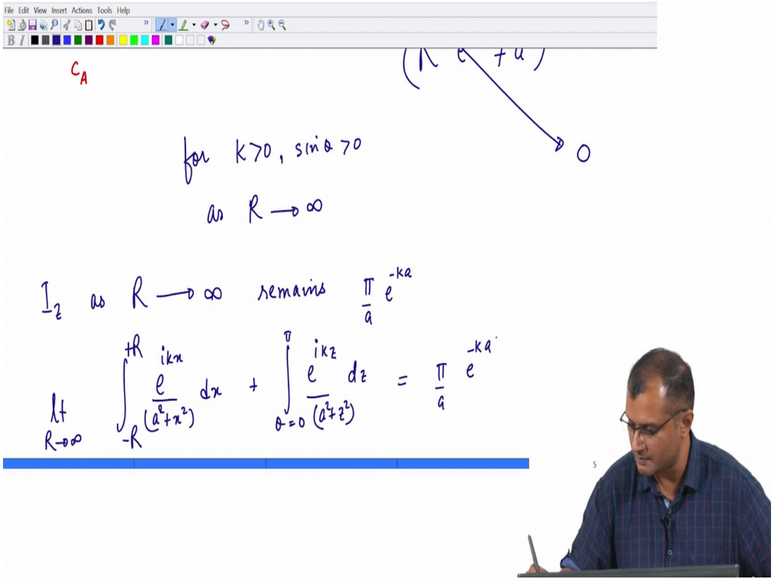

This means my overall integral here, will only go towards 0, it is magnitude will go towards 0 ok. So, the numerator is going as e raise to minus k R into R that will go to 0, the denominator is going much faster towards, you know denominator is going as quadratic in R but, towards infinity. So, the ratio of numerator of a denominator, we will definitely go toward 0. And so, if I take a bigger circle and even a bigger circle eventually, if I take my semicircle at infinity, my function remains analytic, e raise to i k z remains analytic because, that is going towards 0 but, it is integral on their contour on the arc becomes 0, which means I can say that the residue does not change the residue is unmoved.

So, the integral I z as R goes to infinity, remains if the same. So, it remains pi by a, e to the power minus k a and I can write down for a fact that, the integral on the arc goes to 0, as long as k is positive which means, I can write down my integral, this part the CL part that. So, I can now write down the entire thing as, limit R tending to infinity, minus R to plus R, e to the power i k x over a square plus x square dx, plus theta goes from 0 to pi, e to the power i k z and d z over a square plus z square and I have just shown that and this integral is basically pi by a, into e to the power minus k a.

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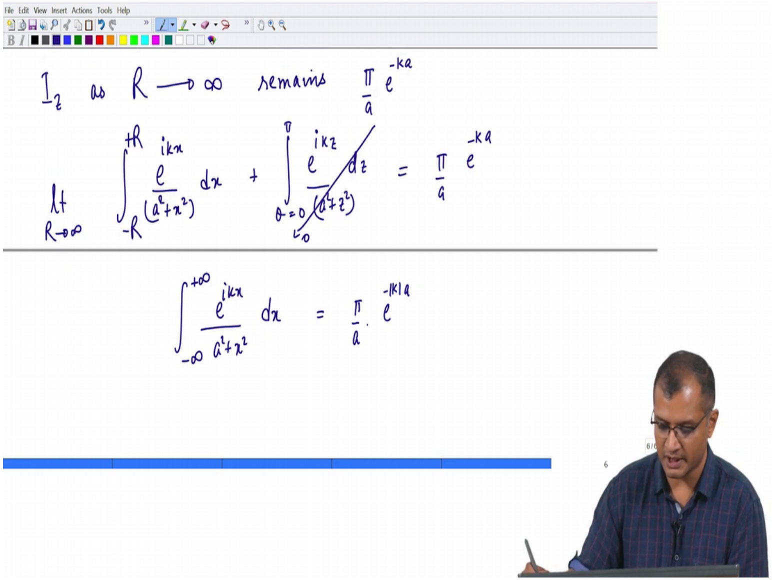

So, as R goes to infinity, if I want to drop this term then, I have to change my k to positive. So, I have to write down 2 things happened; one is that the straight line integral becomes a minus infinity to plus infinity, e to the power i k x, upon a square plus x square dx and what we does to my right hand side is that is makes my k always positive.

So, I have to take it as minus of mod k into a because, only then I can put the semicircular contribution to 0. Now, combining this with what I wanted. So, what I wanted is basically a factor of a by pi outside in equation 1.

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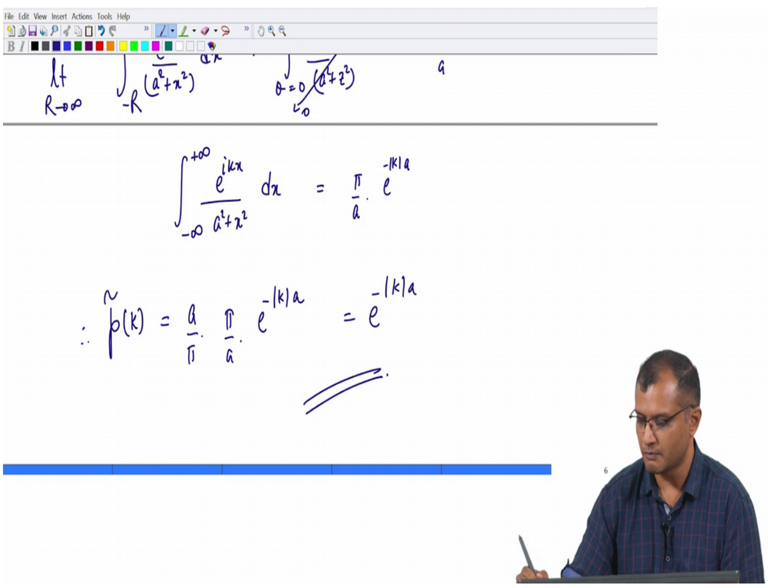

So, my Fourier transform, is basically a by pi into pi by a, e to the power minus mod k to a which is nothing but, e to the power minus mod k into a, that is the answer ok. You could have taken the bottom circular contour also but, that would have given your integration from infinity to minus infinity with the negative sign. So, it gives you the same answer, whatever contour you take fine. And this brings us to the last topic in the discussion which is a gamma function.

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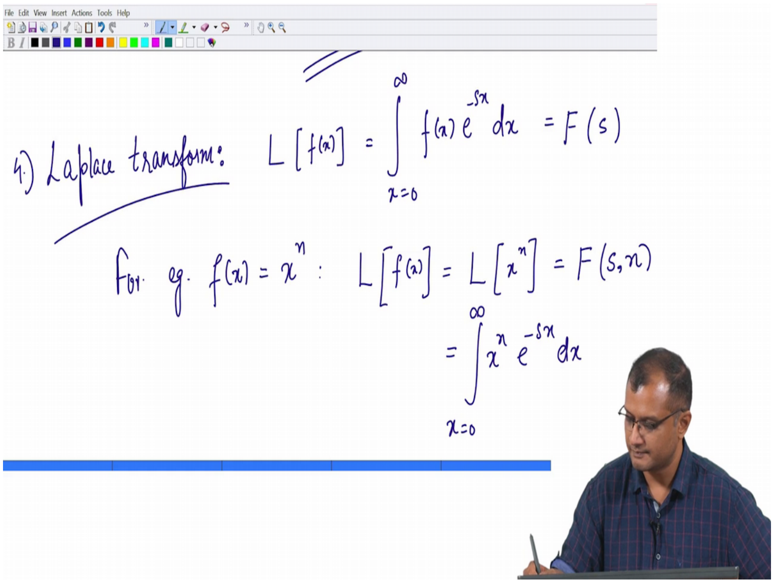

So, I will introduce the gamma function from Laplace transforms. Since, I have already taken Fourier transform and example in Fourier transform I will take one example in the Laplace transform. So, Laplace transforms and Fourier transforms are connected in the sense that, if you are unable to take a Fourier transfer of a function that diverges in the limits then, you can pat this function only on the positive side and take a Laplace transform for the imagery frequencies.

So, they are related to each other, I will skip the background of Laplace transform, except that I will tell you what Laplace transform mathematically means. So, if you want to take Laplace transform of some function then, it basically amounts to taking this integral, 0 to infinity, fx e to the power minus sx dx. Now, since this is a definite integral on x, the answer is a function only of the s, which is basically your frequency imaginary frequency or imaginary wave vector, depending upon whether you take x as displacement or time ok.

So, it is just a function of s ok. So, now, if I take you know for example, if I take our function as some x to the power n then, the Laplace transform of my function is nothing but, Laplace transform of x to the power N and this will be nothing but, a function of both my variable s and the parameter n because, it is defined as an integral x going from 0 to infinity, x to the power n e raise to minus sx dx ok. So, this is very simple we have computed Laplace transforms in the grand canonical ensemble, I think the Gibbs canonical ensemble and so, this is basically going to help you, if you are not aware of how to take Laplace transform. So, here this is I will take simple example, which is x to the power n.

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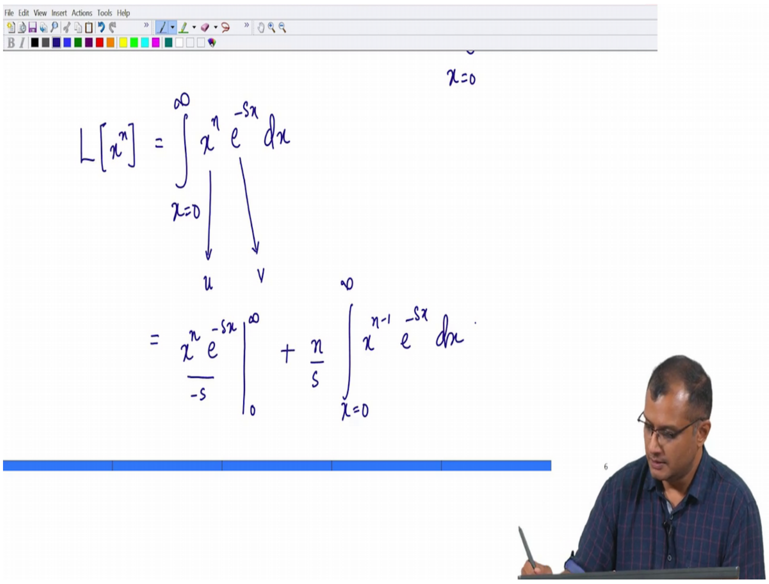

So, you can write down this as a, in the form of a recursion relation. So, this is just x going from 0 to infinity, x to the power n e raise to minus sx dx. Now, to solve this you have to do integration by parts and our encourage you to take this as the first function, x to the power n as the first function and e to the power minus sx is the second function but, the reasons are simple, each successive derivation of x to the power n reduces it is order, order of derivative, that is the encouragement to take this as the first function.

So, you take this and perform the integration by parts, what you get in the first term is x raise to n, e raise to minus sx, over minus s, and you apply the integration limits, plus n by s into the integration x to the power n minus1, e raise to minus sx dx ok. Now, look at the first term, at x equals to infinity, e raise to minus sx will go to 0. Of course, x is to n will go to infinity but, you can easily show by L Hospital's rule, that x raise to n, e raise to minus sx will go to 0 and for x equals to 0 which is the lower limit, the exponent becomes 1, but x raise to n become 0.

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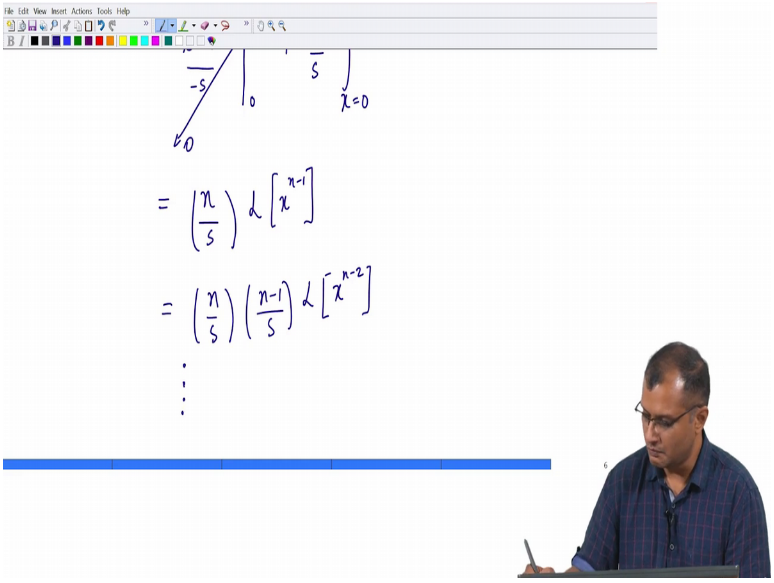

So, this is overall 0 at both the limits, first limit you can show by L 'Hospital's rule, second limit you can just show directly but, what is left over now is interesting, it is n by s multiplied to the Laplace transform of x raise to n minus 1 ok. So, this way if you continue so, if you take one more Laplace transform, it would be n by s, into n minus 1 by s, into Laplace transform of x raise to n minus 2, I will keep continuing, what you will get at the end of the overall steps.

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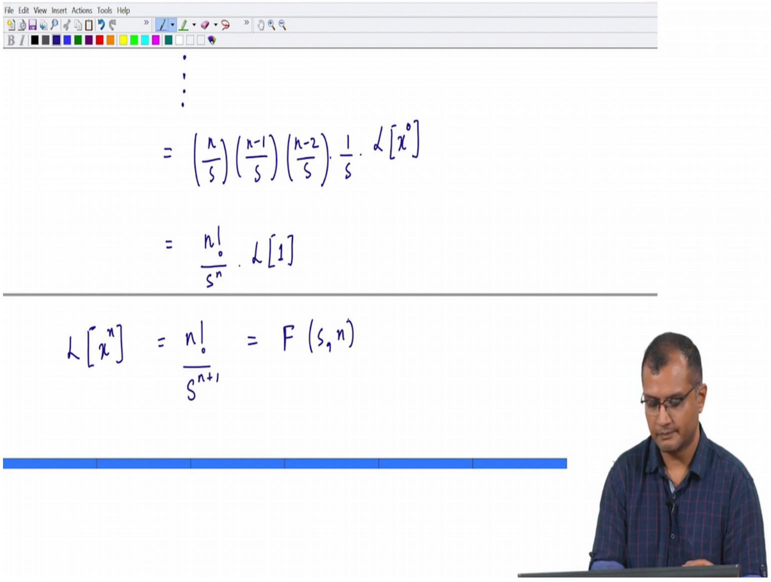

Would be n by s into n minus 1 by s, all the way to n minus 2 by s and the last term would be 1 by s, into Laplace transform of x raise to 0 or 1 ok. So, basically what you have here is nothing but, n factorial over s to the power n, into Laplace transform of 1, which is nothing but, Laplace transform of 1, if you look at the definition, just put n equals to 1 here, you will get just 1 upon s ok. So, this will be n factorial over s to the power n plus 1 and that is the Laplace transform of x raise to n and this is the function of s and n ok.

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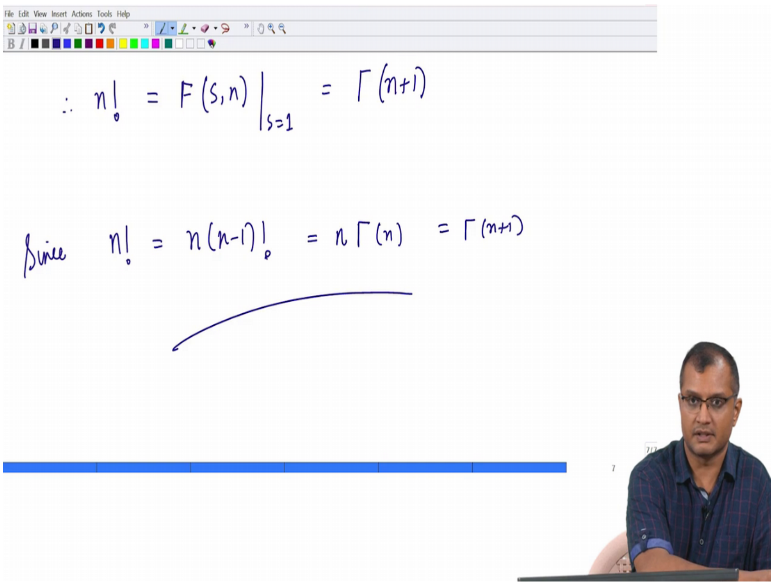

So, the definition of n factorial is also the value of this function, the Laplace transform, taken at s equals to 1 and this can be also define mathematically to be as gamma function. In such a way that gamma n plus 1 is always n factorial; it is just definition, nothing more than that ok.

So, you can always, since n factorial is equal to n into n minus 1 factorial, I can call this as n into gamma n and this is nothing but, gamma n plus 1. So, that is how you form a recursion of gamma function. So, n gamma minus gamma n plus 1 right so, this is how we compute gamma functions or n factorials, all right. So, this is where we end and when we meet in the next class will, you will have one more mathematical preliminaries, where I will discuss some more important useful integrals and we will take it from here.