Welcome back to the lectures in quantum chemistry introductory and also molecular spectroscopy this lecture continues the review of elementary mathematical functions and their properties as I have started in the previous lecture, with some description of exponential and Gaussian functions. Now today we shall look at some of the other functions that we need for the purpose of this course and we will start with one of the most elementary functions, trigonometric namely, let us start with F1 of X is a constant A1 x ray sin another constant A1 of X. This is periodic and the period is between 0 and A1 X is equal to 2 Pi or X is equal to 2 Pi by A1, okay, that's the value.

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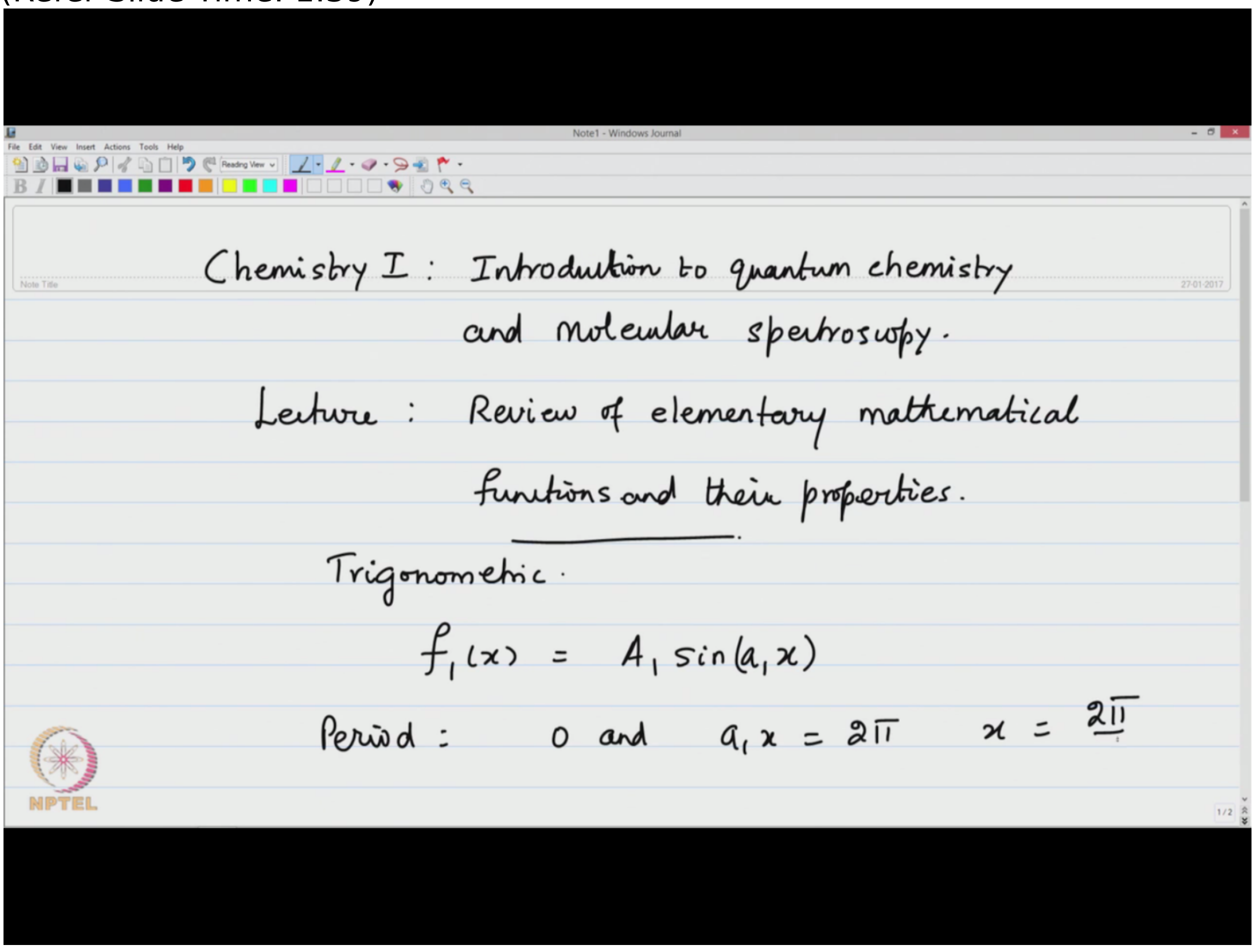

So this function repeats after that value of X and all of us know that this function can be plotted in a very simple manner. If this is F1 of X and this is X then what we have is the function starts at 0 and reaches again 0 at half the interval and you know the sin function goes until it reaches 0 again. So this if you call it as 0, this is the maximum that you have and this maximum is, if you recall the function as a1 sin A1 of X ray, A1 sin A1 of X ray, the maximum is A1 and it happens for the value X is equal to Pi by 2 A1, so that this becomes sin Pi by 2, okay. The 0 happens for X is equal to Pi by A1 and the minimum, which if you draw this axis, the minimum is minus A1... is minus A1 and this happens for the value 3 Pi by 2 A1 and this one is the last

one namely 2 Pi by A1. So this is the simple oscillatory function. And the function is important in quantum mechanics, in that it satisfies the differential equation D square F by DX square plus A1 square F is equal to 0.
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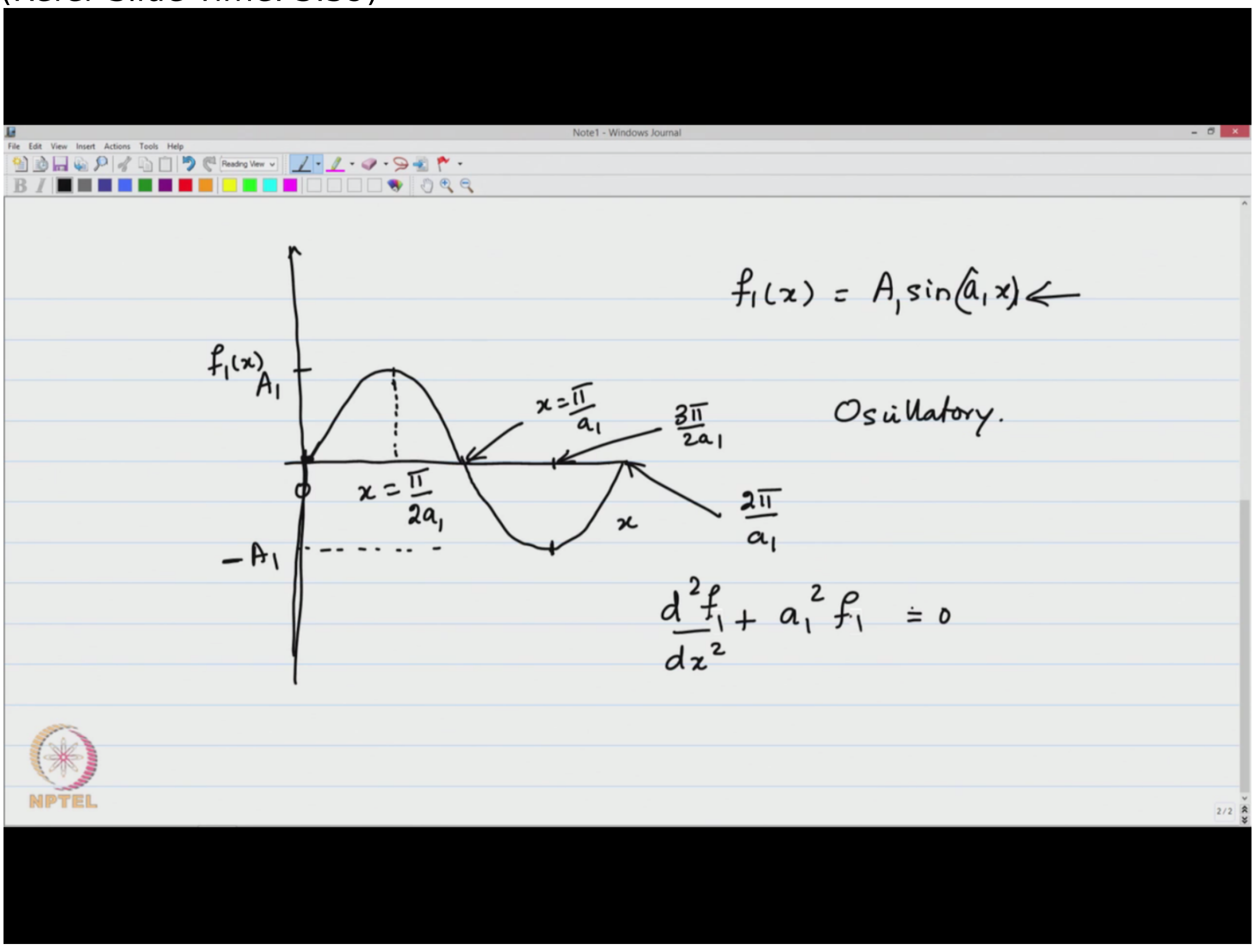

It's a very elementary differential... second order differential equation A1 square of F is equal to 0. That's easy to derive because you know DF by DX is little A1... A1 cos A1 of X and the second derivative D square F by DX square is the derivative of cos S minus sin and therefore you have a minus DA 1 square and this is A1 sin, A1 X, that’s A1, which is that equation, okay. Cos sin A1 X, if we have to write that is different from the sin only by a phase factor of Pi by 2. it's an independent function, trigonometric function, but the relation between cos sin and sin is that it is A1 sin A1 X plus Pi by 2, okay it's just an argument of Pi by 2, that differentiates between cos sin and sin. What's the integral of sin A1 X, the integral if you leave it with the constant A1 outside simply gives you minus A1 by A1 cos sin A1 of X and if you don't have the limits of integration, you normally have a constant which is undetermined and the constant is determined if you do the integration between specific limits.
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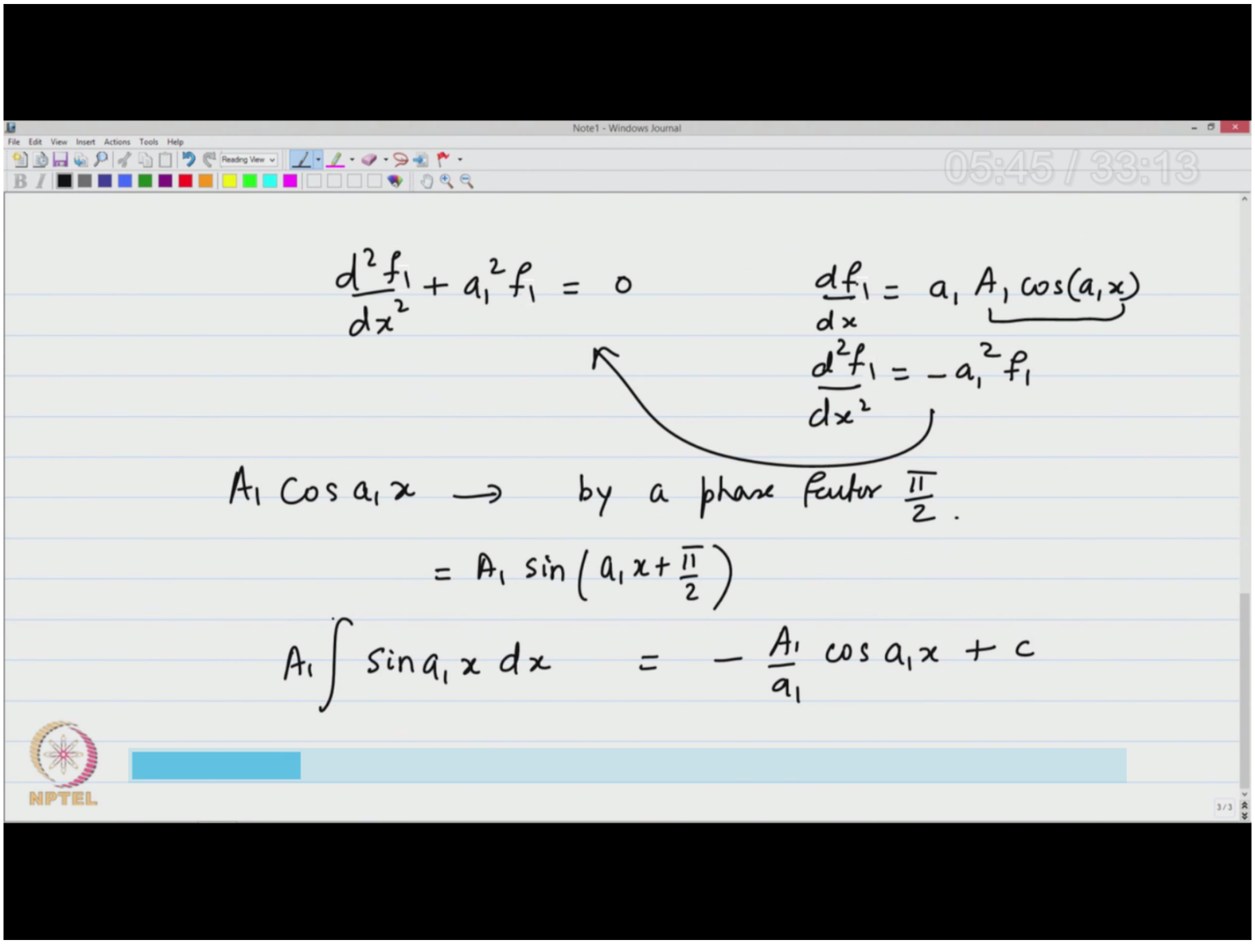

And the limits that we often will use is a function, something like 0 to 2 Pi by A1, A1 sin A1 of X square A1 of X DX, this is one function we will see and another function that we will normally use in this whole course is a product of two of these functions 2 Pi by A1 sin N1 A1 of X sin N2 of A1 of X DX where N1 and N2 are integers and here of course we may as well do the integral sin square M1 A1 of X DX between 0 & 2 Pi by A1 sorry this is A1 square and this is A1 square. So different types of these integrals and functions will be used in the course and it's very easy to see that the integral of the function itself 2Pi by A1 A1 sin A1 of X DX, the integral itself is 0, that you can verify from the the figure here.

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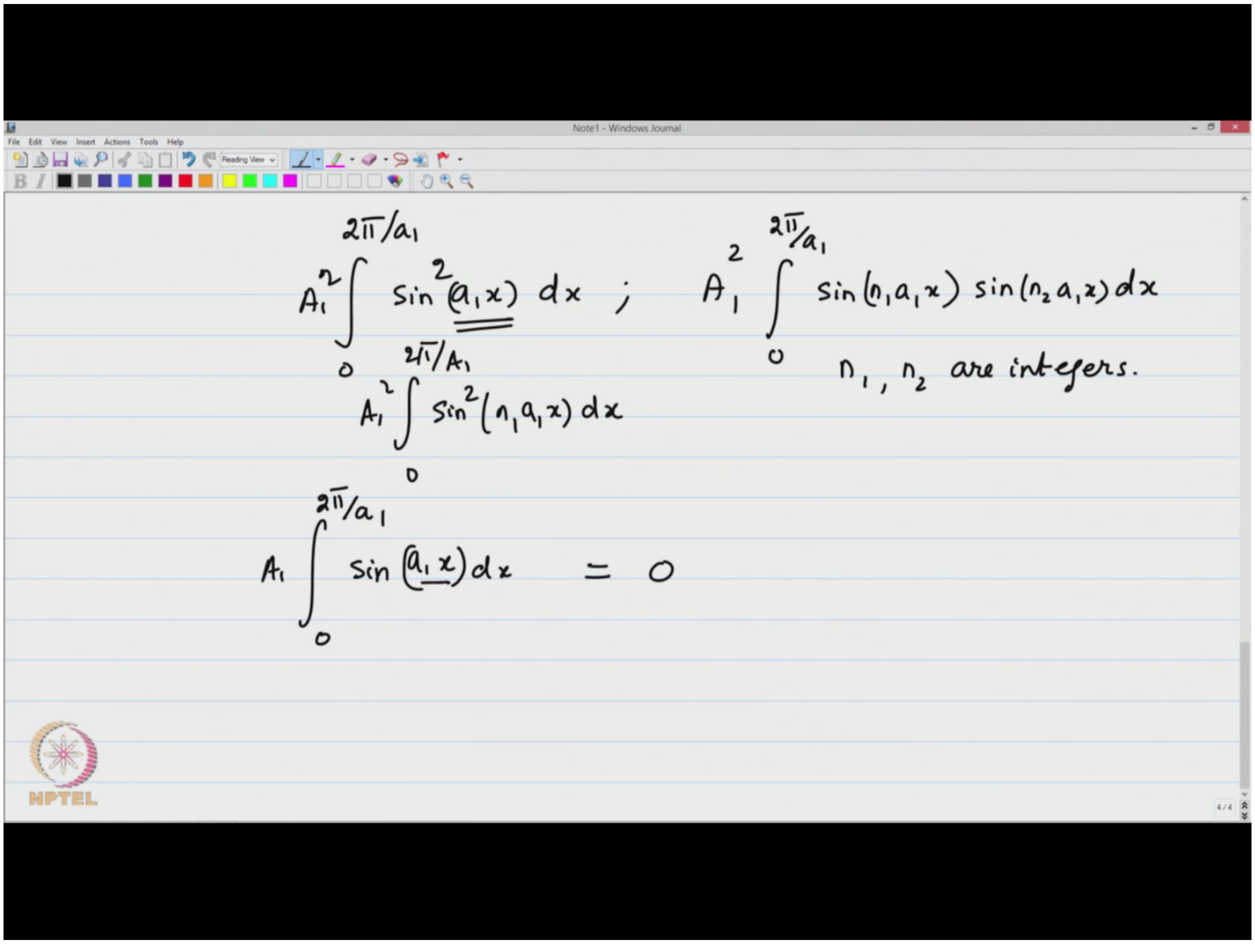

See that the integral is the, if this is the function the integral is the area of this function and you can see that the area under the first half of the interval 0 to Pi by A1 is positive and the integral in the second half of the area is negative, therefore a full cycle, the integral is 0. On the other hand the square of the functions are not like that, so if you plot the square of the function for example F1 of X square, if you do that, that's A1 square sin squared A1 of X and you know that the sin square function doesn't have any negative component and also it has a slowly increasing in the beginning and reaching to a maximum value and reaches 0 again and then it continues that again. So this is A1 square, this value this is F1 of X squared, this function is plotted on this axis and this is the X axis and you know that this is the zero that you had earlier namely Pi by A1 and this is 2 Pi by A1. The sin squared integral, if you have to do that A1 square sin square integral A1 of X DX is again between 0 and 2 Pi by A1, this integral is not 0 because both the components of the area are positive.

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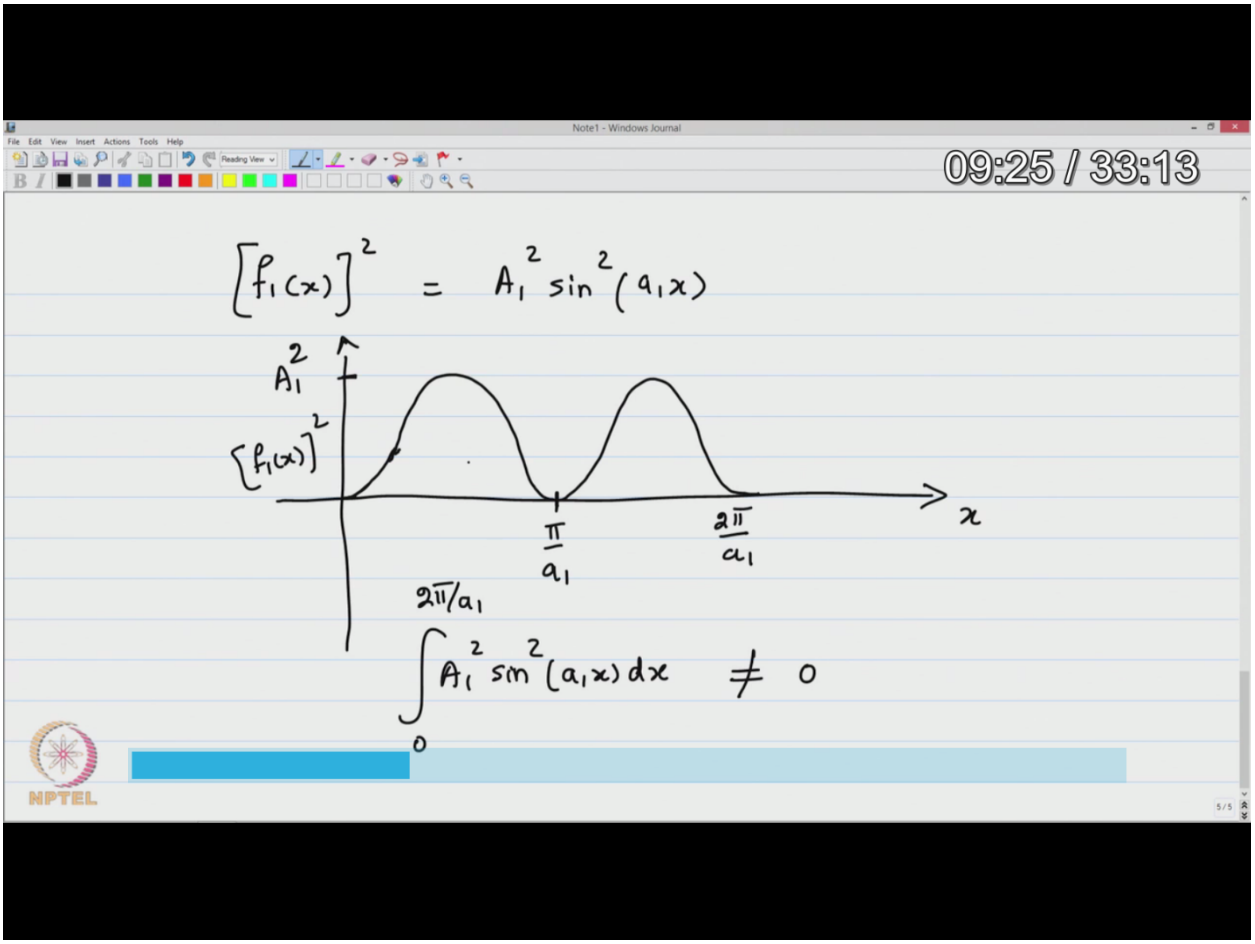

And therefore it's easy to do this integral by simply using the formula that A1 square by 2 between 0 and 2 Pi by A1, 1 plus cos 2 A1 of X ray, sorry 1 minus 1 by 2… 1 minus 1 by 2 DX and thus you can see immediately that the cos sin integral, the integral 0 to 2 Pi by A1, cos sin 2 A1 of X is also two complete cycles of the cos sin functions and that will be 0. So what is left over is simply A1 square by 2 0 to 2Pi by A1 and you have DX, which will give you X and therefore it gives you A1 square by 2 times 2Pi by A1 or it's A1 square Pi by A1. This is the value of the square of the function and these are important when we talk about wave functions, which are normalizable, or how to normalize a wave function etc and the normalization will involve Psi star Psi as we had discussed in the beginning of one of these lectures that the wave function times its complex conjugate and if the wave function here is the real function the complex conjugate is the same as the function itself therefore Psi star Psi is equal to Psi square and the Psi square integral will be a finite value and if we use that to define what are called the normalized wave functions for interpretation using probabilities okay, so this is about the Psi function.

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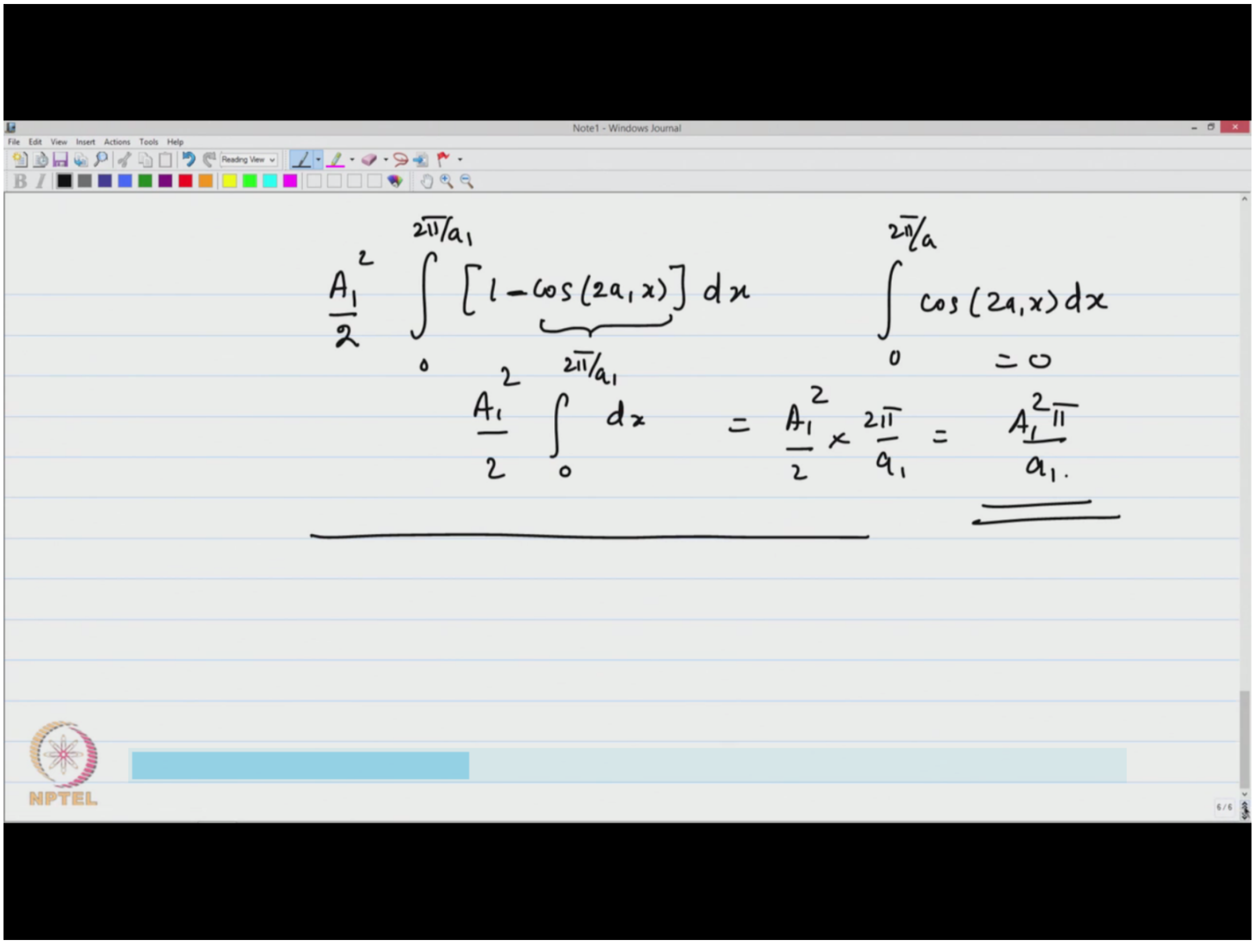

Now another function, which is actually not very much used by us, but which is something that you can see in quantum mechanics, is going to cause a lot of trouble is tan X, let me get rid of the A1, we will not worry about that, let's put A1 is equal to 1 and so let this be another function F2 of X, which is sin X by cos X and you can see immediately that this function is troublesome for us to do any quantum mechanics, as if you have locked this function, this is 0 and you know when X is Pi by 2 sin X is 1 and cos x is 0 therefore if I do X is equal to Pi by 2 I have a problem that this function increases forever... this function increases forever. It goes very steep and it goes to infinity at the value of Pi by 2. So let me get this Pi by 2 here, this is Pi by 2. What happens immediately after Pi by 2, so this is between 0 less than X less than Pi by 2. Now what happens after Pi by 2, so let's just change the color Pi by 2 less than X less than Pi, what happens, so you see that sin x is positive sin Pi by 2 is 1 and then from Pi by 2 to sin Pi the function decreases, but cos X increases from 0 in the negative direction because cos X is minus 1, when you go to, X is equal to Pi therefore cos is negative in the second quadrant, therefore the whole function is negative, but it's growing from very large negative values, please remember, cos X is very close to 0, when X is very close to Pi by 2, therefore this is a very large negative function and therefore if I mark Pi here, let's see it grows very large values to... from... large negative values to 0 at Pi by… at Pi and then up to 3 Pi by 2, both sin and cos sin are negative Pi X 3Pi by 2, you can see that the function both of this are negative and sin X goes to minus 1 cos x goes again to 0 and therefore this function continues to increase because it's, the ratio is positive and this is 3Pi by 2, so this one is Pi, this one is 3 Pi by 2. And what happens on this side quite obviously function goes like that okay. They are all exactly the same curve in the interval in… in the half intervals. The problem is this function goes to infinity and minus infinity very quickly and the number of such infinities that this has in… in a very large segment, you know, it increases. Therefore such functions are not very useful, but you have to be very careful dealing with functions like these. it's important to have a visual picture or a representation of the simple one dimensional and two dimensional functions before or as you go along the course, because they help you in understanding what are areas, what are volumes and things like that, okay. So this is for that so important. Lets let's go to the next one, we have already done the exponential KX and the exponential minus KX and exponential X square.

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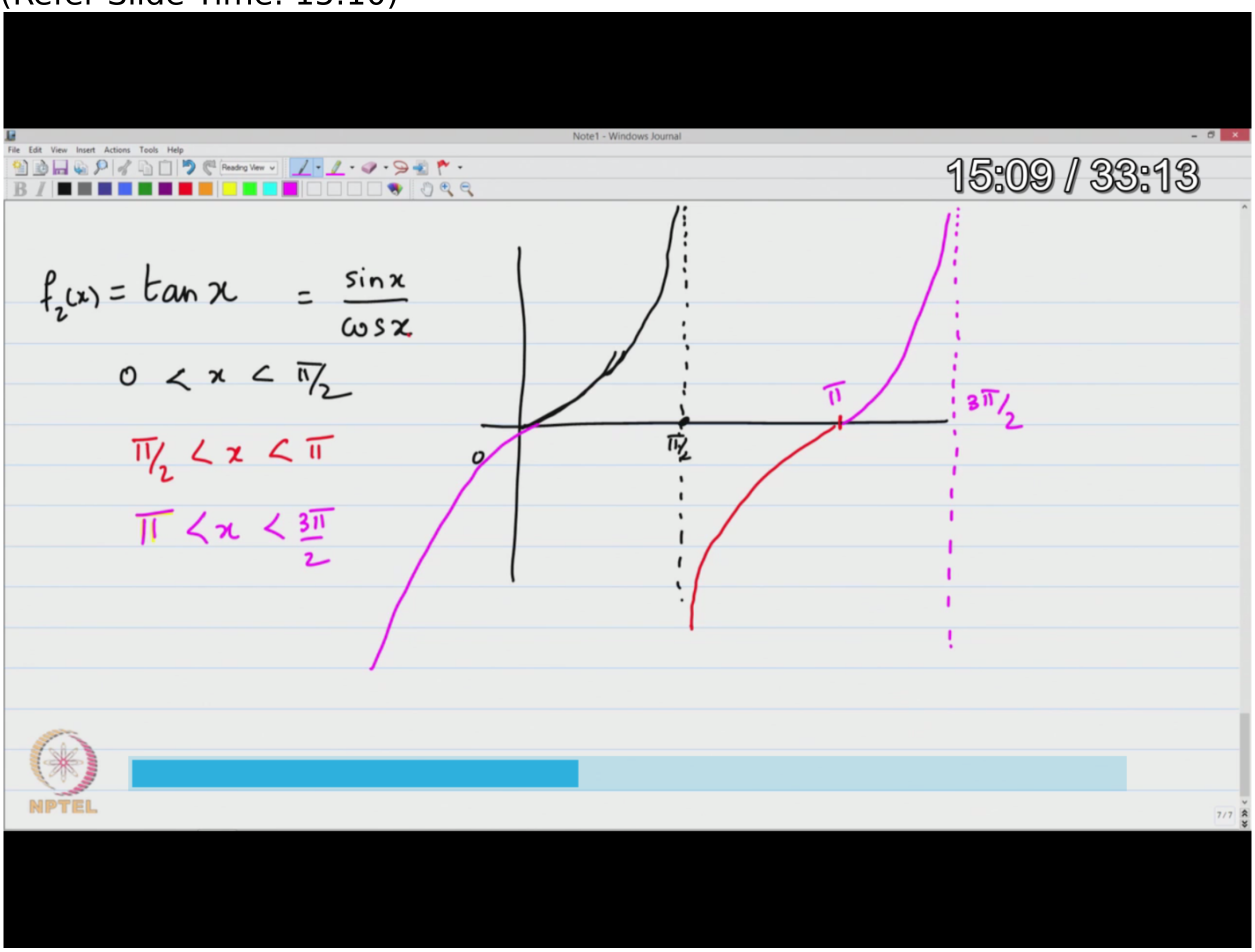

So let's start with the complex variable, which all of you know is defined as X plus IY, I is square root of minus 1, I square is minus 1, I into minus I is 1, minus I whole square is also minus 1, okay those are the properties and you also know that this is usually written as Re to the I theta and R therefore is square root of X squared plus Y square and theta is Tan inverse Y by X, and that comes from the representation that X is equal to cos theta and Y is equal to sin theta, and therefore you can see that square root of x square plus Y square, it should be R cos theta R cos theta, okay. Therefore the square root of X square plus Y square will be equal to R and the tan inverse comes from that, okay this is the exponential function and we need such functions when we study particle in the ring and also on the hydrogen atom, the angular functions of the hydrogen atom and so on. The complex conjugate of Z is X minus IY and in the polar representation, it is Re to the minus I theta. Therefore Z, Z star is X plus IY into X minus IY, which gives you X square plus Y square and that's exactly what you will get from Re to the I theta times Re to the minus I theta giving you R squared, that's what the definition was earlier. So this is the elementary level.

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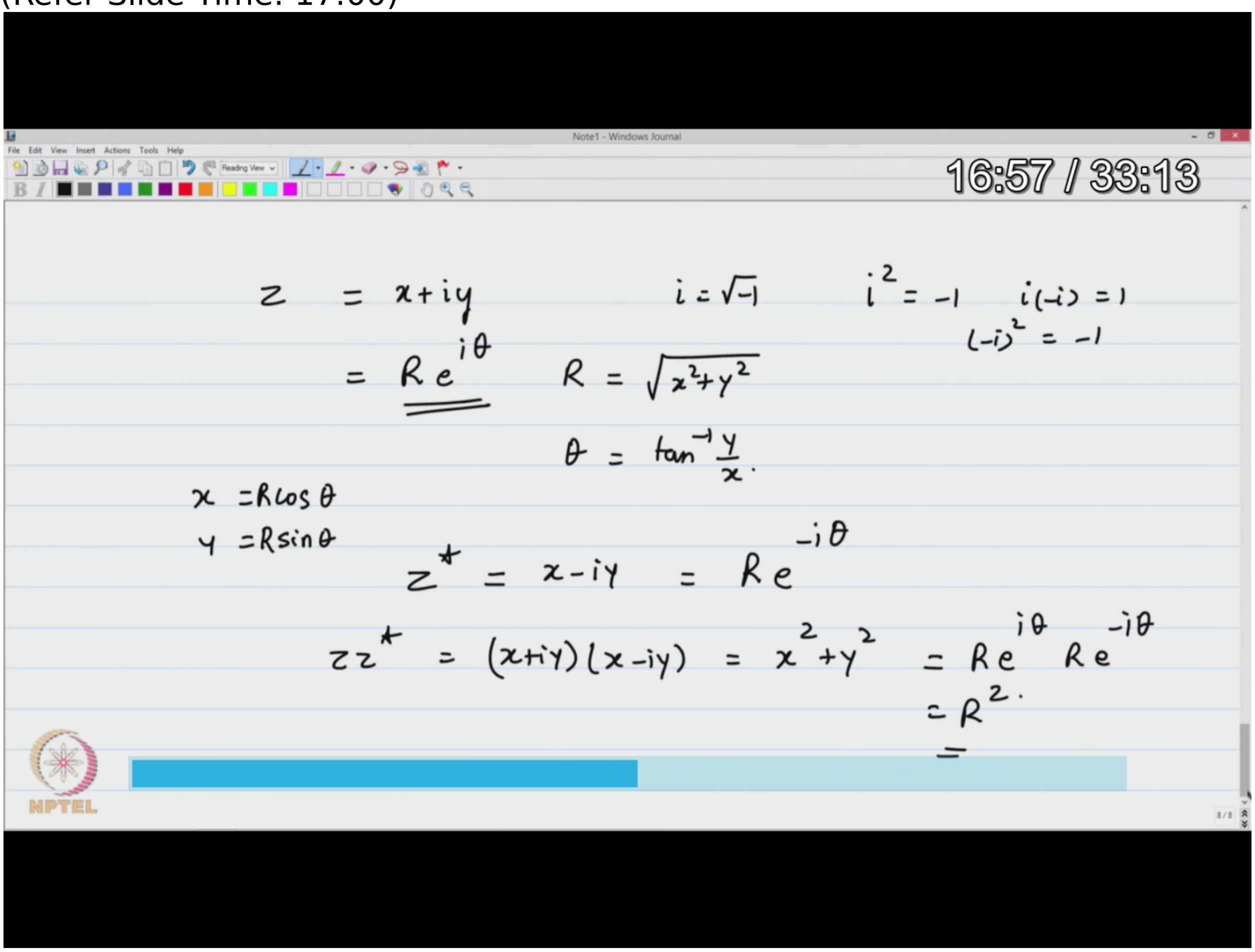

What about the integral of exponential IN theta 0 to 2 Pi where N is an integer, okay. Okay now D theta, of course. You must remember the Euler formula, namely exponential I theta is cos theta plus I sin theta, you have already used that in this part okay R cos theta plus R sin theta so when the R is there, exponential I theta is of course cos theta plus I sin theta. What about E to the 2I theta, this is E to the I theta whole square and exactly the same thing, cos theta plus I sin theta whole square which gives you cos square theta, I square is minus 1 minus sin square theta, so that's the real part, plus I into cos theta sin theta plus sin theta cos theta, so you have 2 sin theta cos theta and that you know is the double angle formula, it is cos 2 theta and this is sin 2 theta. So that's also very easy to see because that's nothing other than E to the 2Y theta.

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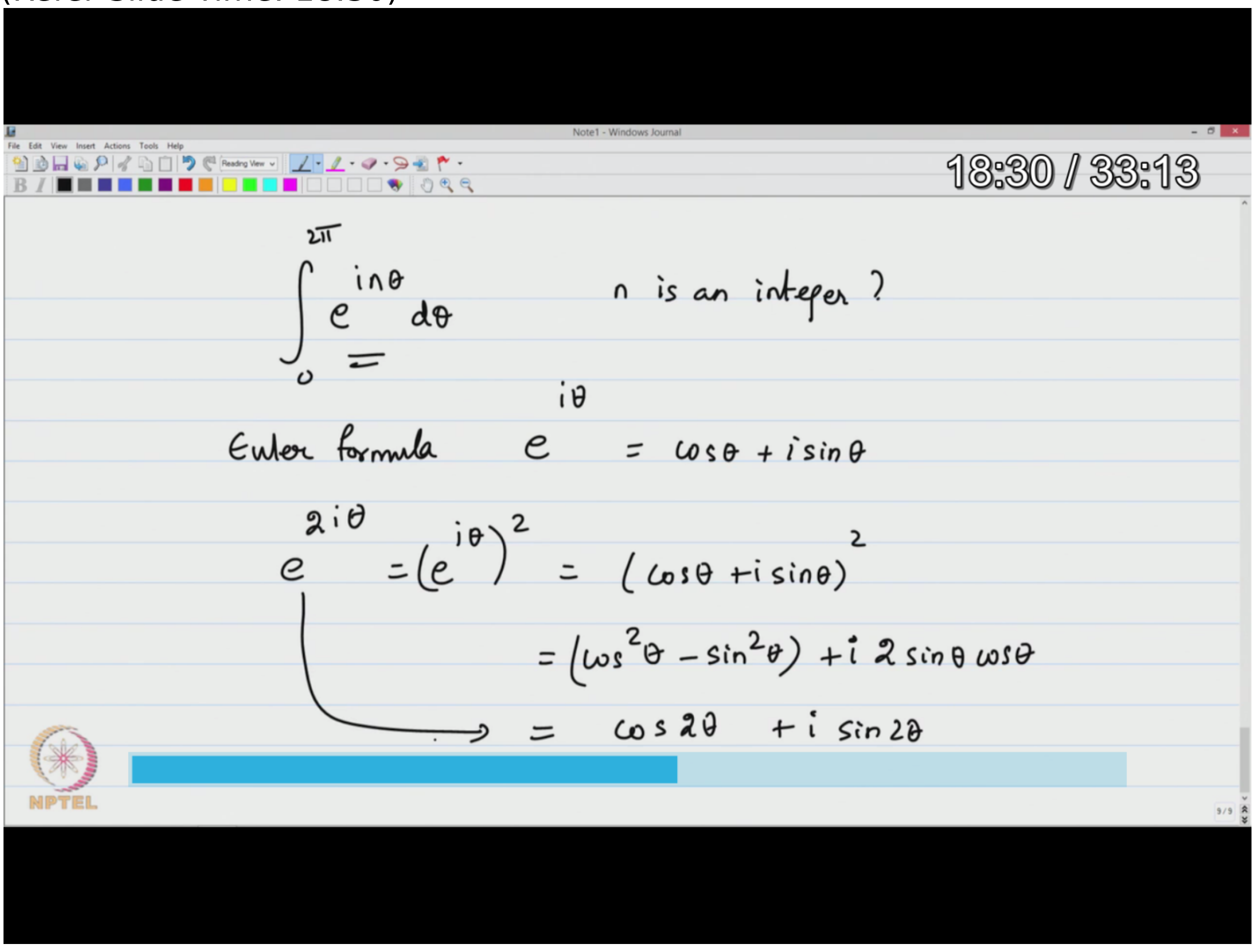

Therefore what is the integral of E to the IN theta D theta between the limits 0 to 2Pi, it's quite obviously 0, because you can see that it is the integral of cos N theta, where N is an integer D theta plus I 0 to 2Pi sin N theta, D theta. Each one is a complete cycle N times within the interval 0 to 2Pi, therefore the areas cancel each other 0 0, okay, therefore this integral is 0. What about the integral Psi, suppose you call the Psi theta as E to the IN theta, what is, is Psi Star Psi, you know that it's nothing other than E to the IN theta times E to the minus In N theta, and that's one, okay. Therefore what is the integral Psi star Psi D theta between 0 and 2Pi, that you know is nothing other than 0 to 2 Pi 1 D theta, therefore it gives you 2 Pi. So these things are important.

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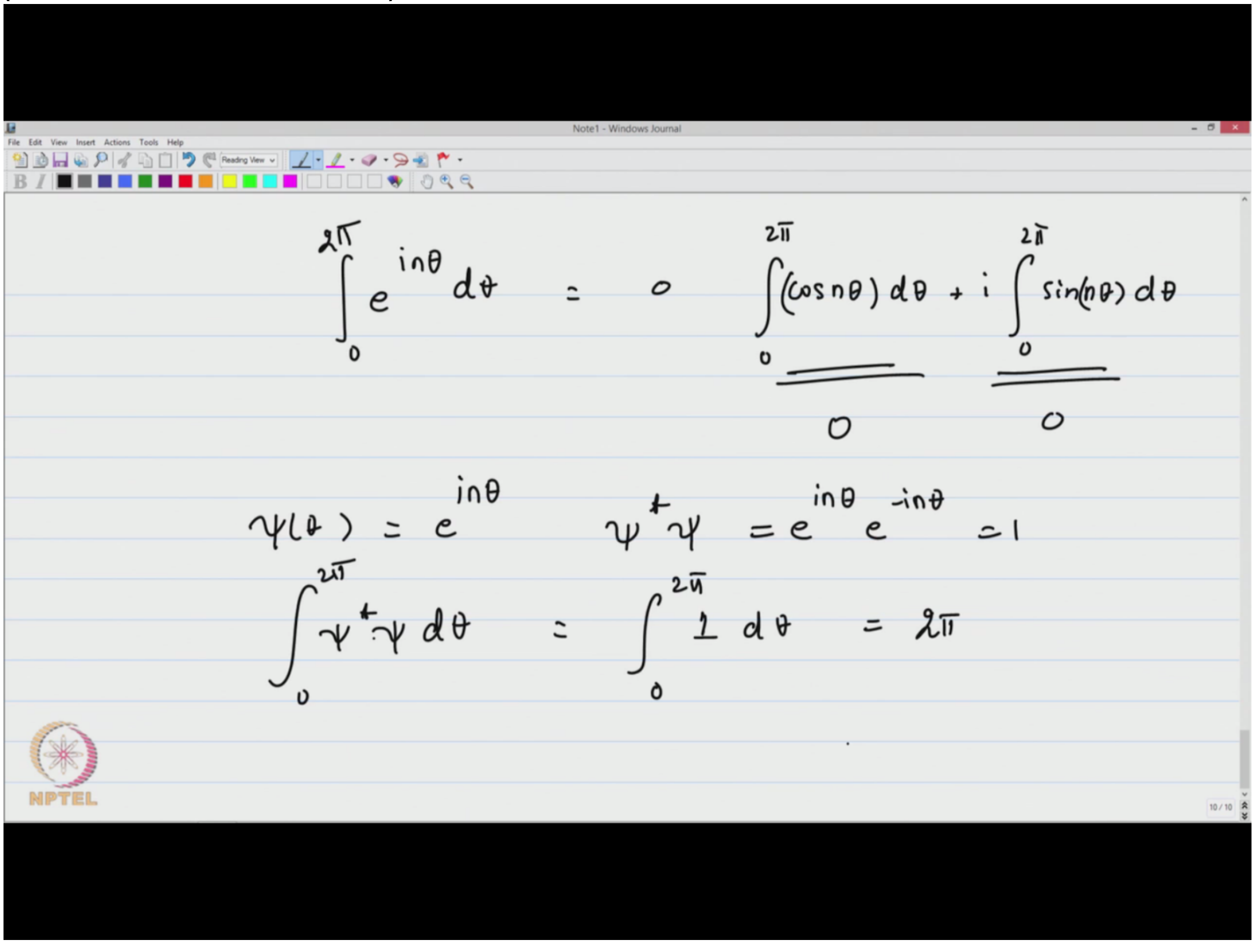

And one last one with respect to our course requirement is the integral E to the IN theta E to the minus IM theta, D theta, where N M are integers, and N is not equal to M. So it's between 0 and 2Pi. You can see right away, that this is nothing other than another integer E to the I, N minus M theta, D theta, whatever, number that is, since the N and M are both integers the difference is also an integer plus or minus does not matter, therefore this is also 0. Therefore we say Psi N theta, which is E to the IN theta and we say Psi M theta, if it is another function which is E to the IN theta, then these two functions are orthogonal Psi N and Psi M or orthogonal to each other and we will use this idea later.

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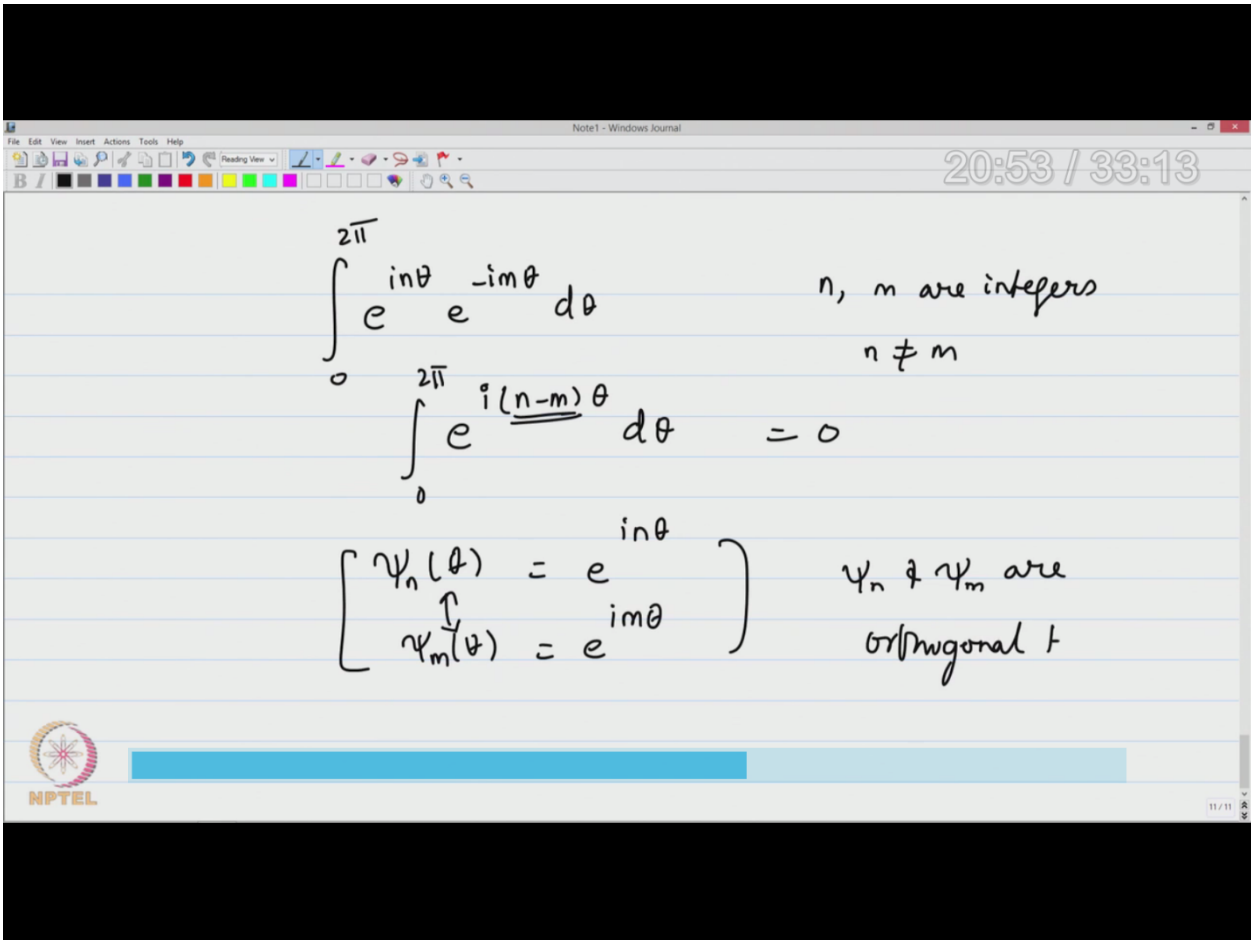

Integral generally of E to the IN theta D-theta, if you don't have the limits it is 1 by IN, E to the IN theta, plus a constant okay. So you can manipulate and multiply these, and you remember E to the I theta itself is given by the organ diagram from 0, It's an proximate circle, proximate circle, let's see if I can make it slightly better. Yeah perhaps this is slightly better, okay. Theta is 0 Pi by 2 plus Pi, Pi by 2 Pi, 3 Pi by 2 and this is coinciding also with the 2 Pi, therefore E to the IN theta, this has the same value between the ranges theta 0 and 2 Pi and whatever this is, is faithfully reproduced 0 between less than or equal to 2 Pi less than or equal to theta, less than or equal to 4 Pi and so on. Therefore it's... it has, for different values of theta the function has the same value in the domain 0 to 2 Pi, 2 Pi to 4 Pi, 4 Pi to 6 Pi and so on and so forth, keep that in mind.

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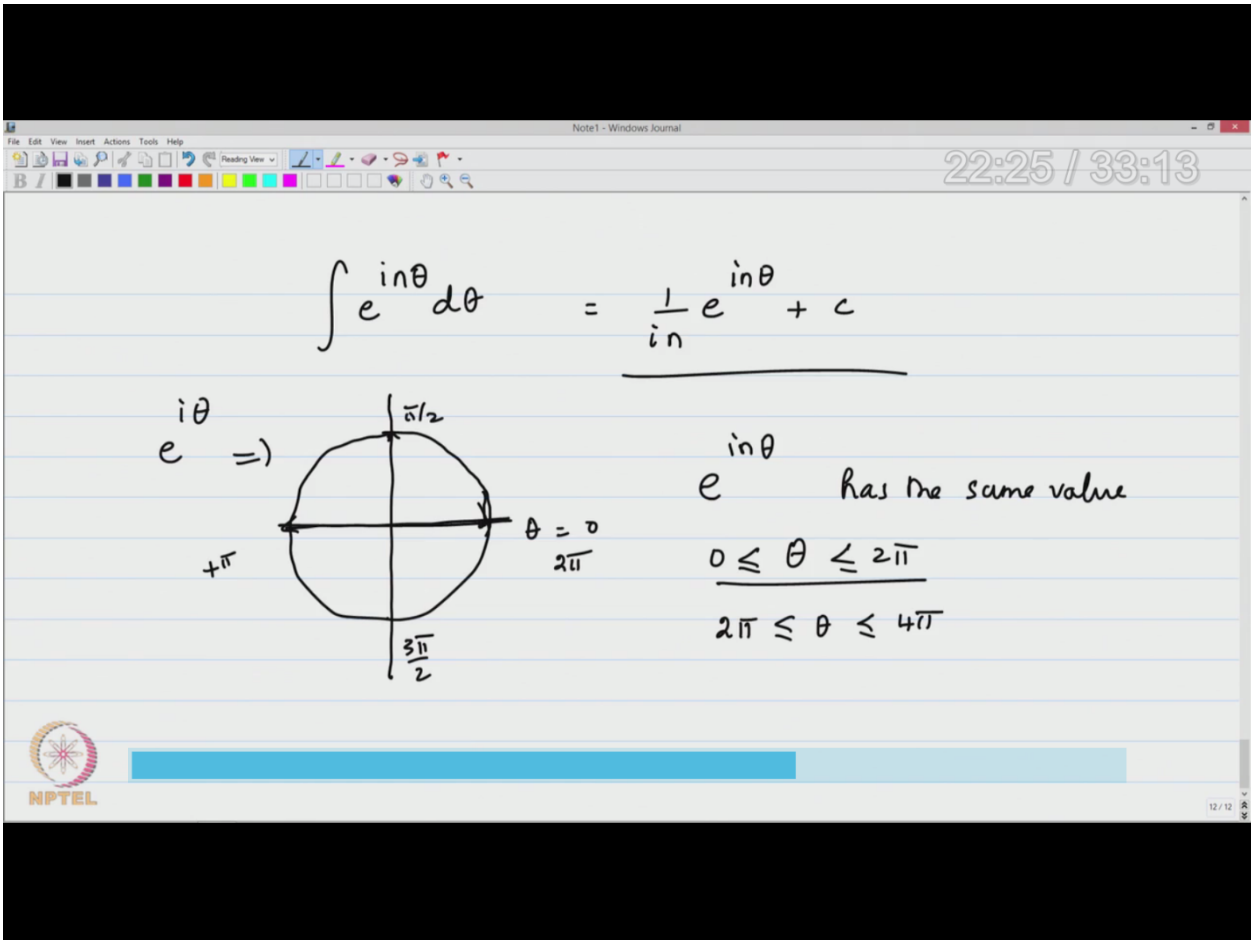

So one last function that we have to worry about, or two is that exponential minus KX, X between 0 and infinity okay, actually you can include both. The integral all of you know 0 to infinity, exponential of minus KX DX is 1 by K, okay. Now what is the exponential when you have a power of X ray N of X multiplying E to the minus KX DX 0 to infinity. I think I have mentioned this in the last lecture and one can calculate this by an iterative very simple process, with the N equal to 1 and N equal to 2 and then generally for any value of And, okay and you know that it has to be N factorial Pi, K to the M plus 1, okay. Yeah it has to be K to the N plus 1. What about this integral exponential minus AX square DX between minus infinity to plus infinity, all of us know that the answer given is root Pi by A, but there's nothing here which tells you how to get the root Pi, you can see that this integral contains N and K and the solutions contain N and K, there is no Pi here. And how do you get Pi. It’s a very beautiful story of this function by a very famous physicist called Wigner on the unreasonable effectiveness of mathematics in physical sciences, where he tells a funny story about the integral, but let's not worry about that, let's worry about how to get the answer.

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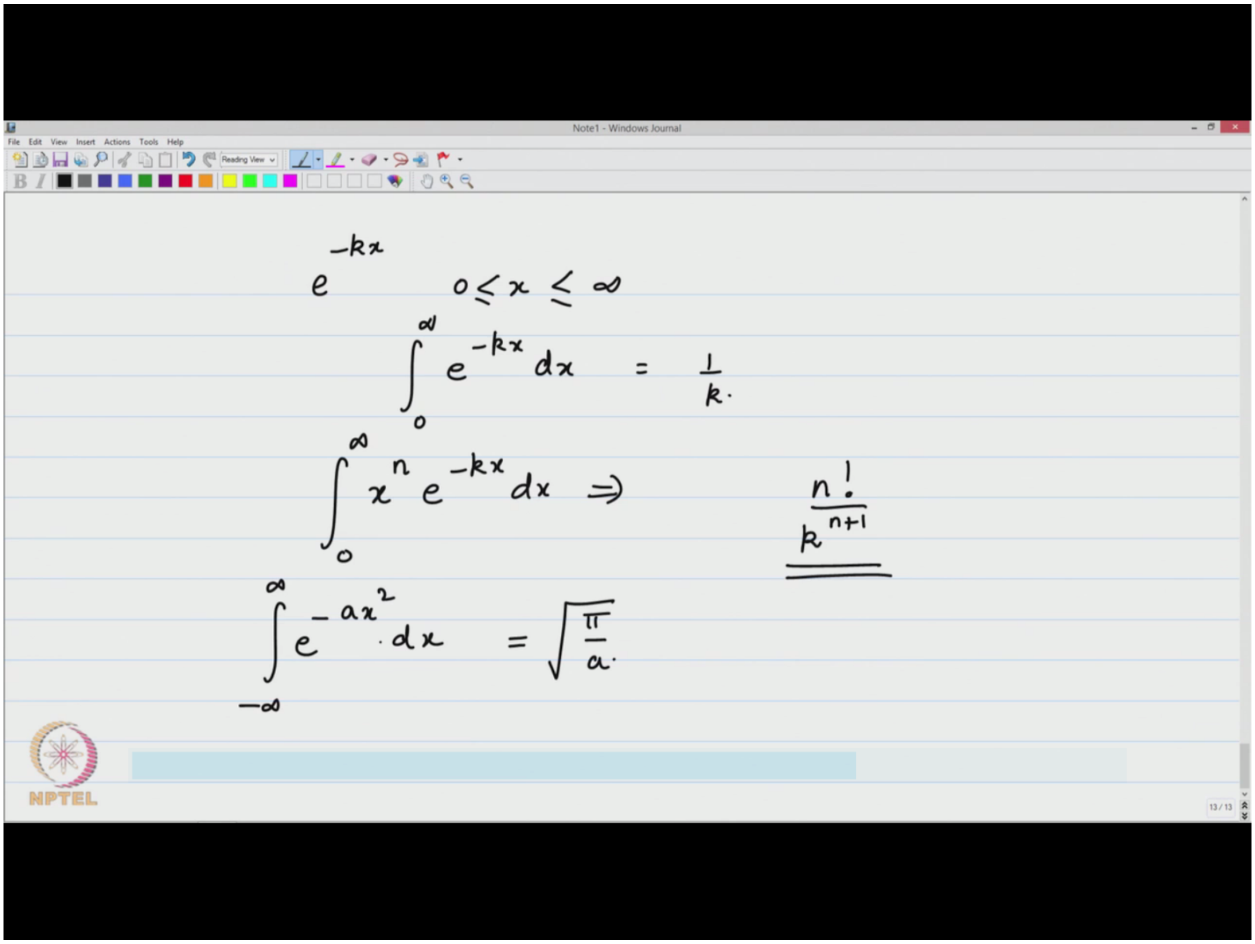

So if we write the integral I from minus infinity to plus infinity, E to the minus AX square DX, then you can write I squared is two such integrals minus infinity to plus infinity to the minus AX squared DX and a different variable minus infinity to plus infinity E to the minus A Y square DY, because both X and Y are dummy variables, they are variables inside and the integrals are independent, therefore we can write this as a double integral between minus infinity to plus infinity E to the minus A X square plus Y square DX DY. Now what does this do, the integration is done over DX and Y for all values from 0 minus infinity to plus infinity.

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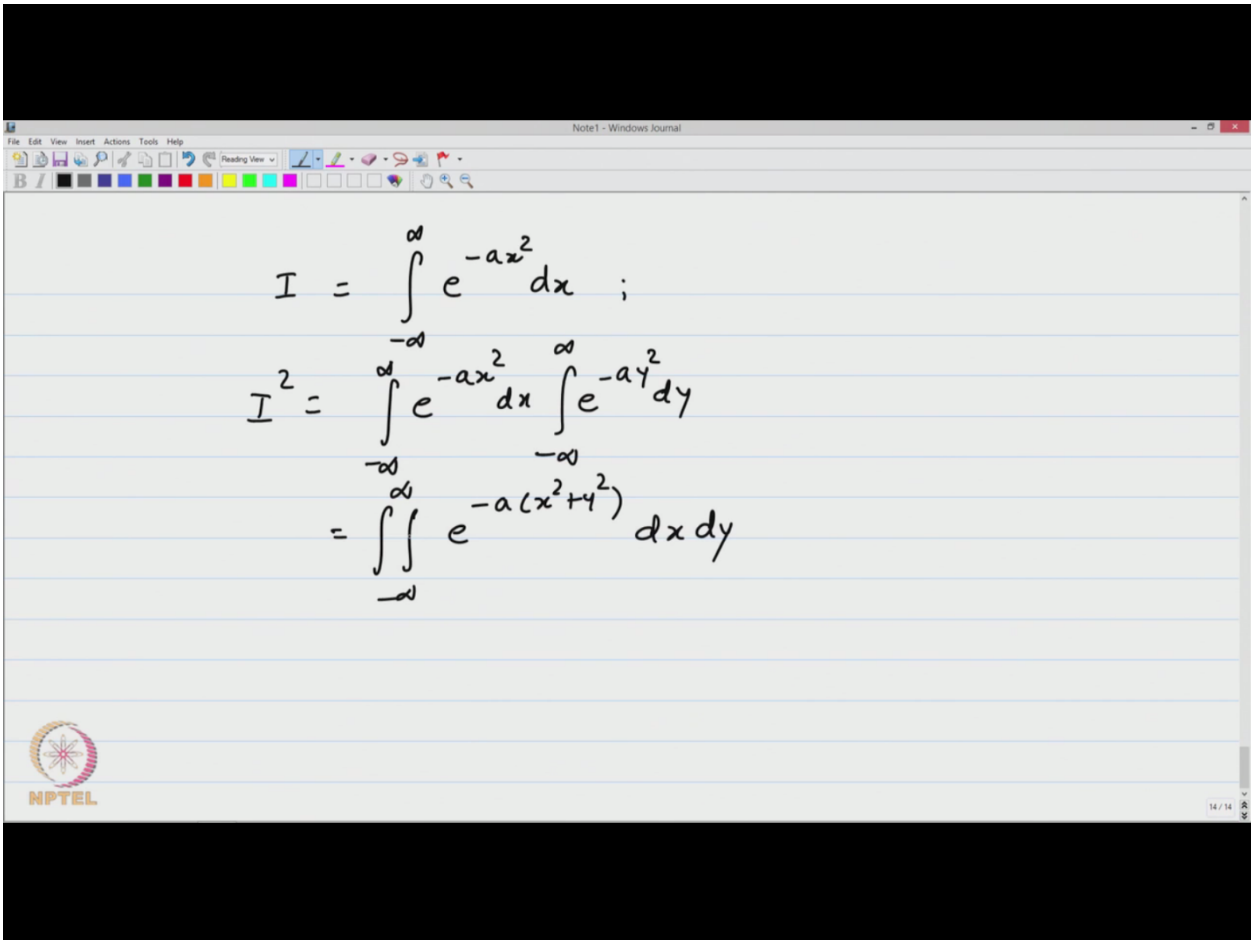

So let's assume that X is something like this then for all values, all the way from minus infinity to plus infinity and for a given value of Y Y is equal to some value Y1. Now again you do this integration for another value of Y and therefore you do the double integration so that you cover, you cover the entire XY plane... the entire XY plane, therefore this integral is a double integral covering the whole plane, infinite to infinite, infinite to extent.

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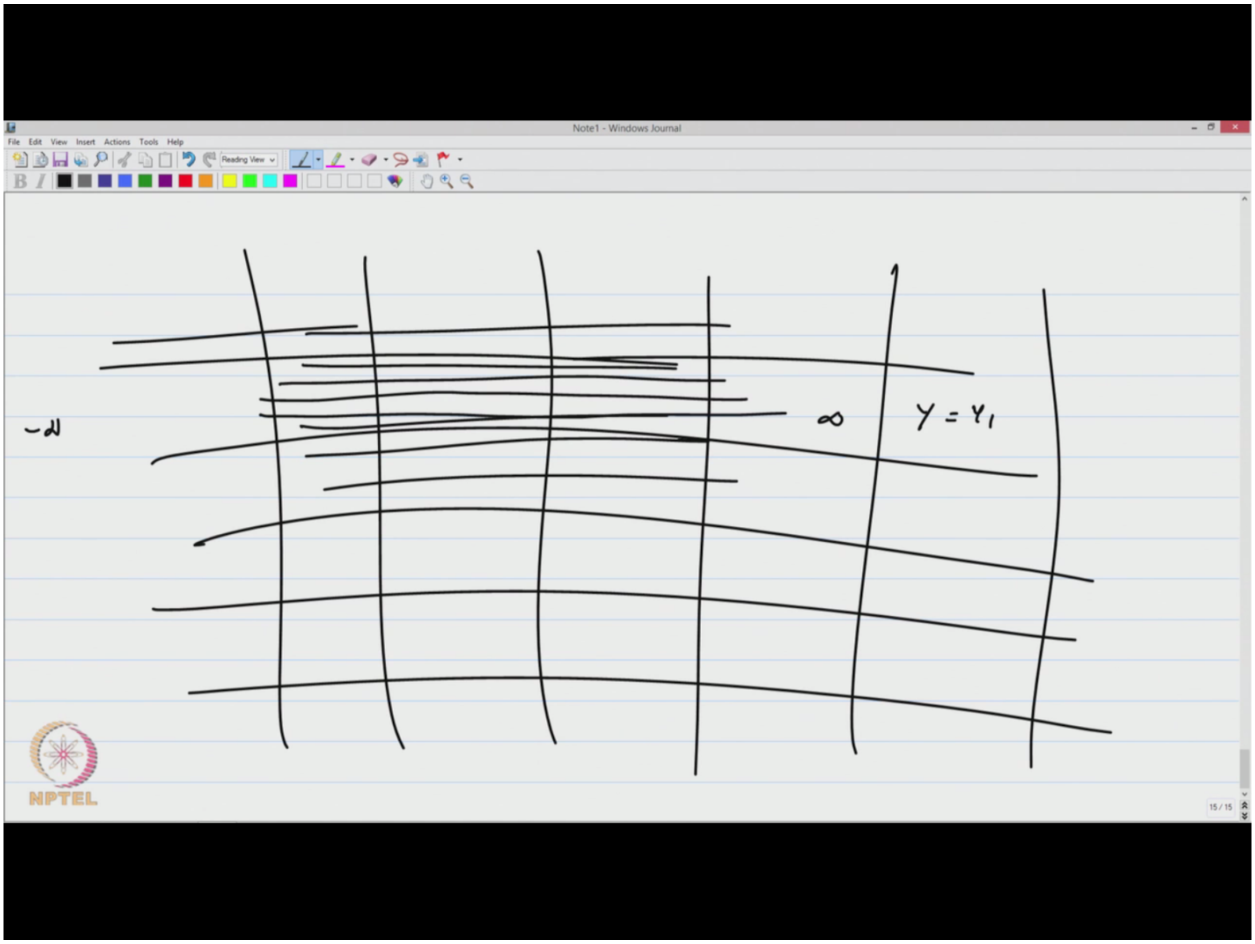

How do you do this integral, you can also do the same by defining a new variable X is equal to sum R cos theta, I think we used the capital R earlier, so we will use the same thing, X is equal to R cos theta and Y is equal to R sin theta okay, and then we can see that the integrant DX DY in terms of the variable DR and D theta, can be seen this way or is basically the… is the radial part. So if you have to plot this as a, sort of a simple way, X is X and Y, the DX DY is equivalent to doing integration for different values of R, but for all values of 0 to 2Pi, theta is equal to 0 to 2 Pi for all values of R going from 0 to infinity okay, then you have everything, all of them. There for the integration using polar coordinates is equivalent to the integration using Cartesian coordinates.

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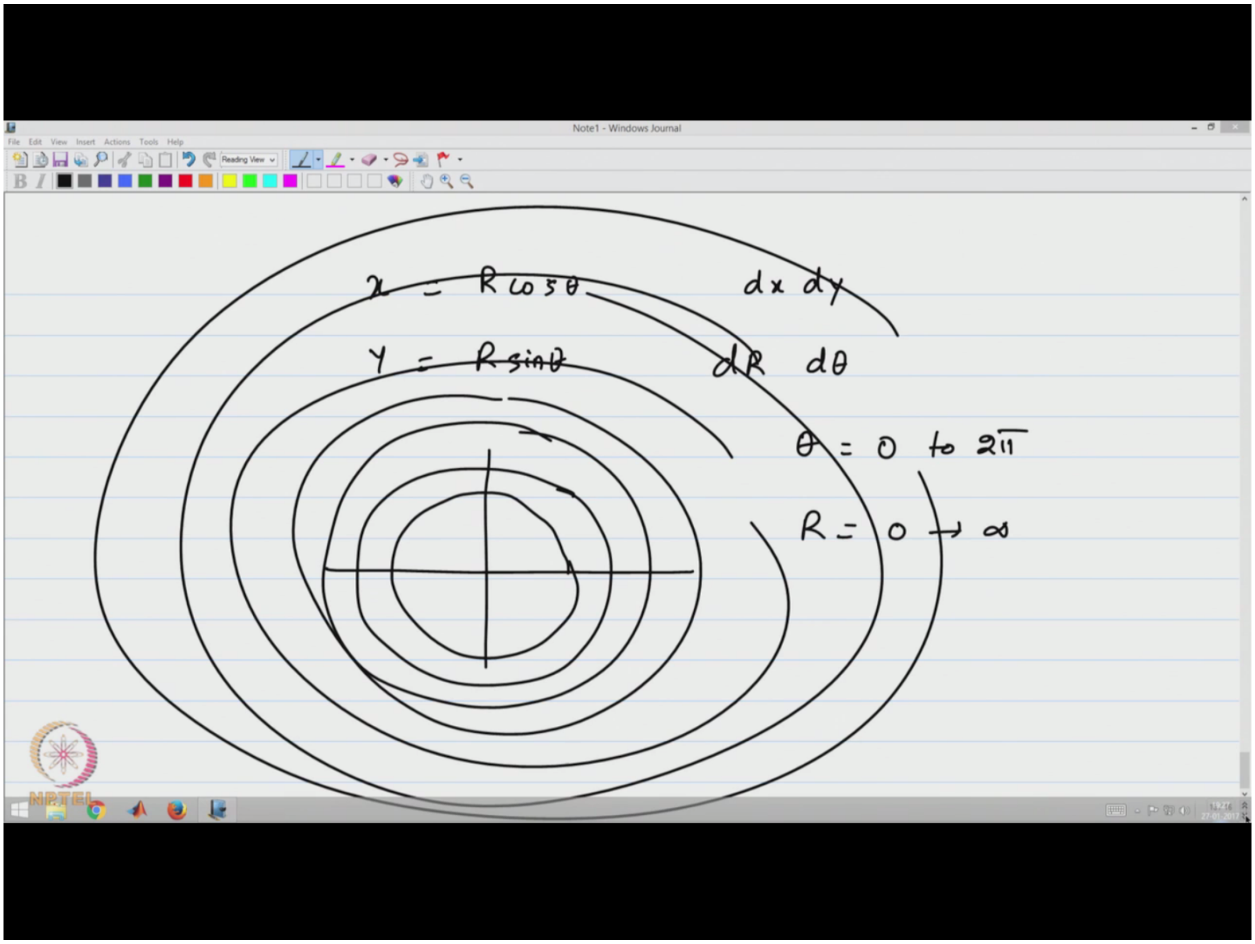

So DX DY is replaced by the R D theta, except that there is a small element here called the Jacobian, which tells you how to weight these small elements, carefully here the weighting is uniform for each of these variable and that is given by the simple partial derivative Dou X by Dou R, Dou X by Dou theta, Dou Y by Dou R, Dou Y by Dou theta, that's the equivalence, and in the lecture notes I have shown you that this is nothing R DR D theta and the limits minus infinity to plus infinity, minus infinity to plus infinity for DX and DY are now replaced by the... the limits 0 to infinity 4 R DR and 0 to 2Pi RD theta. Therefore what is I squared now, I square is this integral minus infinity to plus infinity DX minus infinity to plus infinity DY E to the minus A X squared plus Y squared and that now becomes, the cause of X square plus Y squared giving you R square, the integral becomes R 0 to infinity, D R E to the minus A R square and then 0 to 2 Pi D theta, there is no theta dependence here therefore this gives you 2 Pi, this is the origin of the Pi that comes into the I square is proportional to 2 Pi and this integral if you calculate you will get the answer 1 by 2 E okay.

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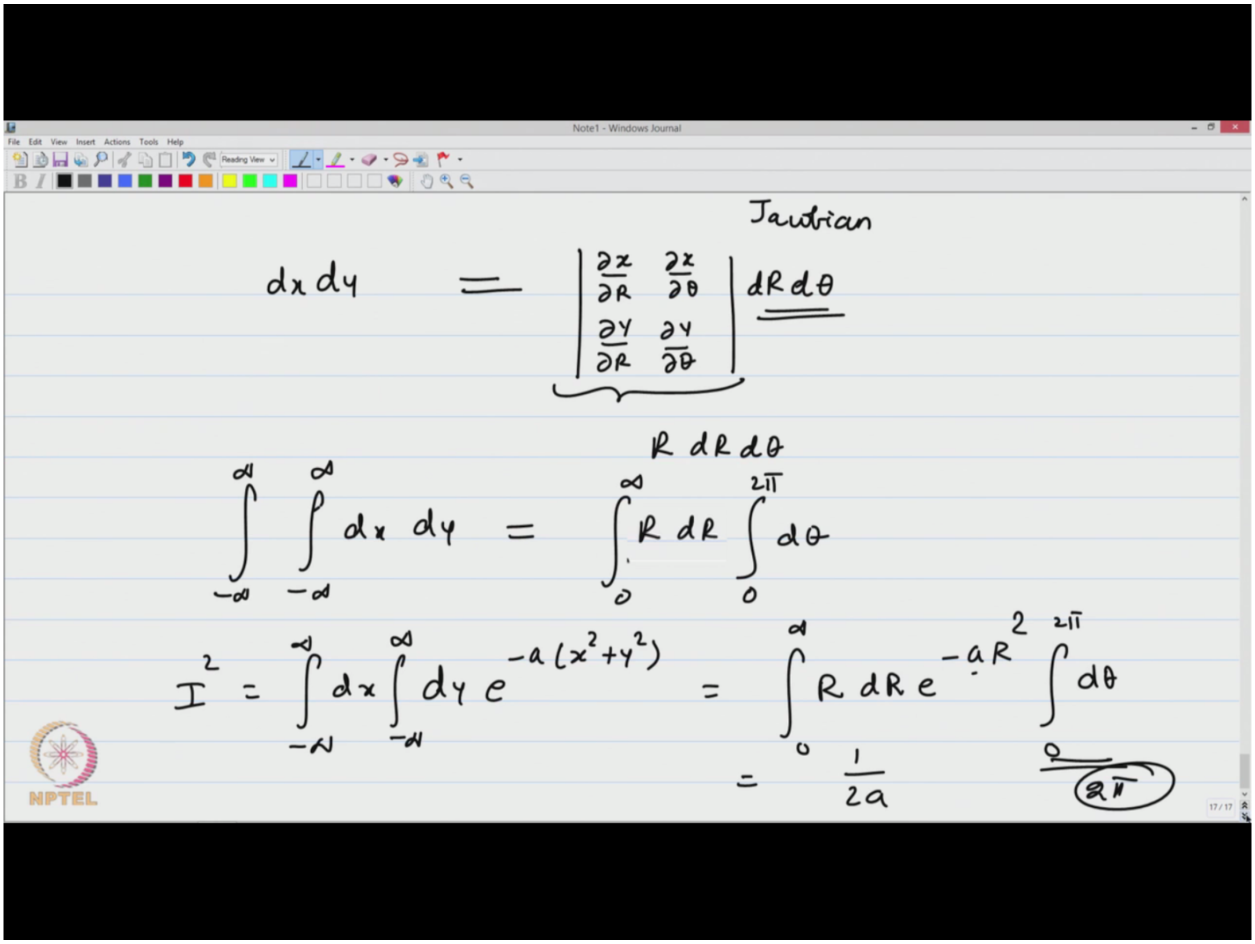

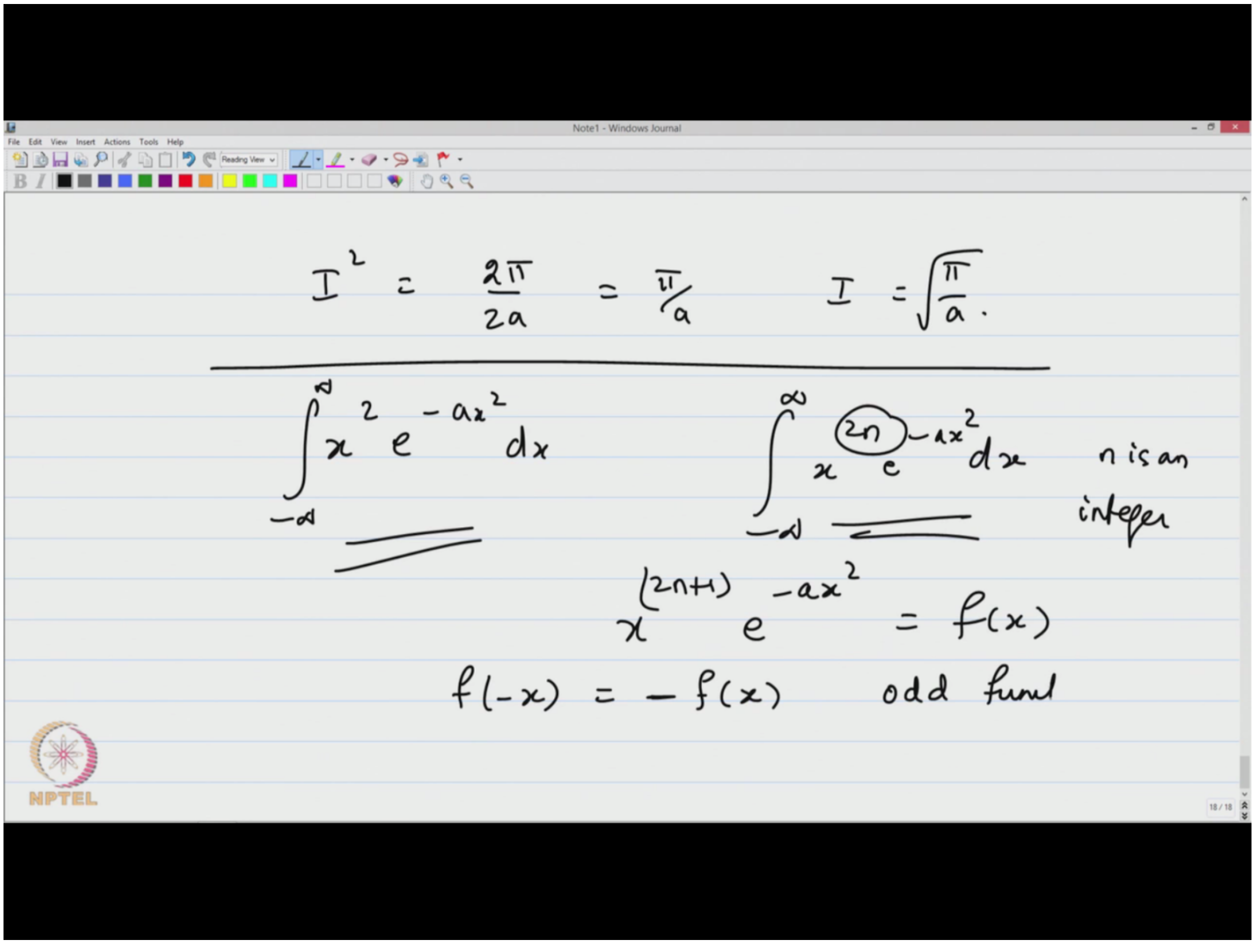

And odd functions have this beautiful property namely between symmetric intervals minus A to plus A, F of X and odd function of X is DX, is 0minus A to plus A, F of X an even function of X, in function of X, F of X is an even function, DX is 2 times 0 to A F of X DX. So these integrals involving powers and, of polynomials of X multiplied by the Gaussian functions are also important in the study of harmonic oscillator and later in spectroscopy, therefore some of these mathematical exercises, you may please go through and refresh, please refresh some elementary integrals. I shall give you in the lecture notes a small collection of formulas that you might need, there's no need to remember any of them, if you need them in the examination or in the assignment, you can look up to it, examination will contain that, but elementary integrals and differentials, differentiation are important for you in order to follow a course on quantum mechanics and spectroscopy.

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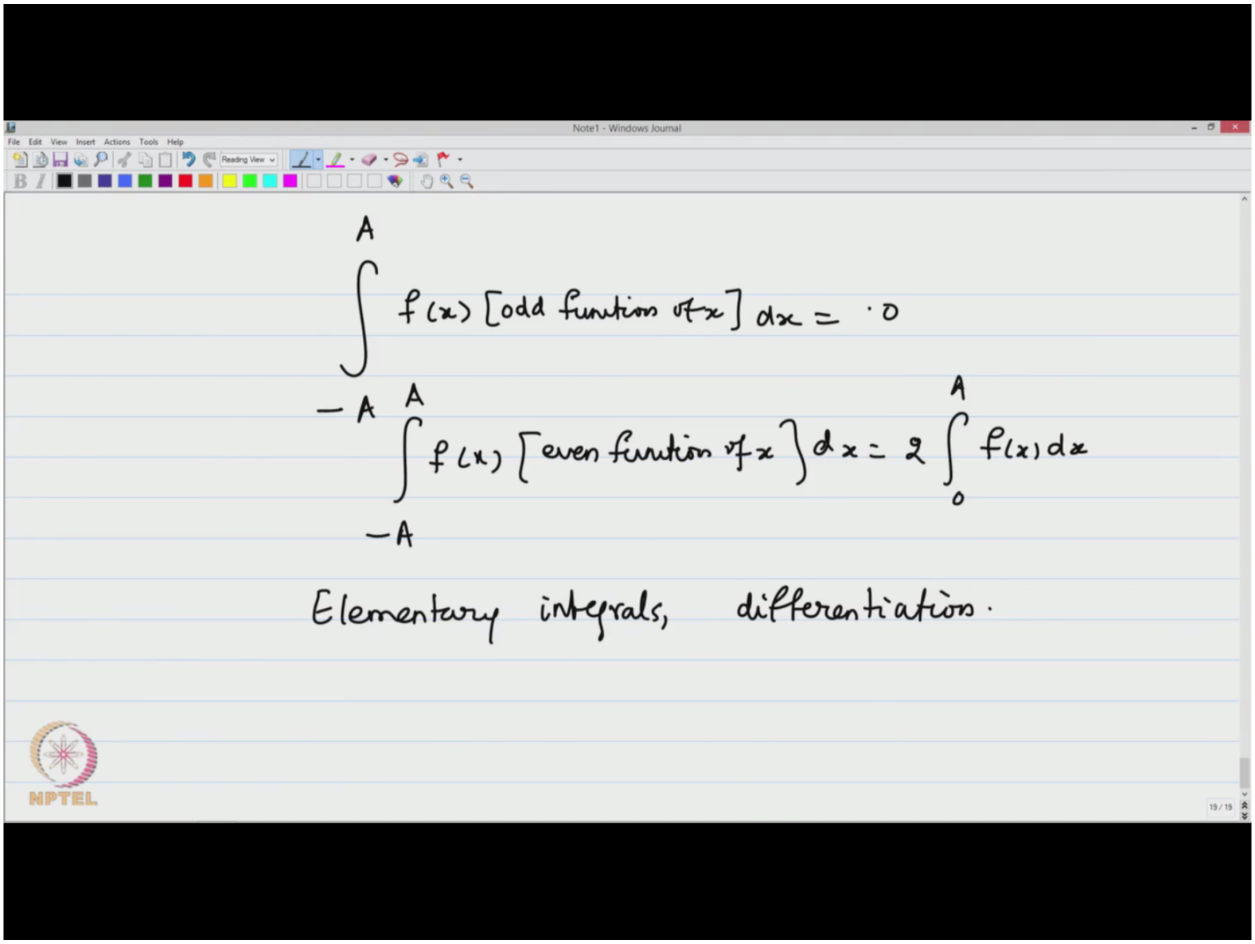

We shall not continue this any further. We will see the mathematics as and when we need them and depending on the model problem we will discuss that at that point. But a preliminary review like this would hopefully help you when you see the same thing again and at that time when this is being described you will recall. I hope this is a very elementary, but it's an important exercise for you to remember and we will continue with the particle and the box model in the coming lectures and they'll start solving the model problems, until then thank you very much.