Chemistry I – CY1001
Introductory Quantum Mechanics and Spectroscopy
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Lecture – 02
Elementary Mathematical Functions Used in our Course

Welcome back to the lectures, the purpose of today's or this lecture is to introduce Elementary Mathematical Functions. A few of them that you will need time and again during this course, either as solutions for the quantum problems that you study or a functions which you will need in order to understand the behaviour the mathematical and the spectroscopic outcomes of experiments and so on.

So, let me start with something very very elementary and this lecture is titled Elementary Mathematical Functions used in our course, it is not exhaustive in 20 minutes, I cannot say too many things.

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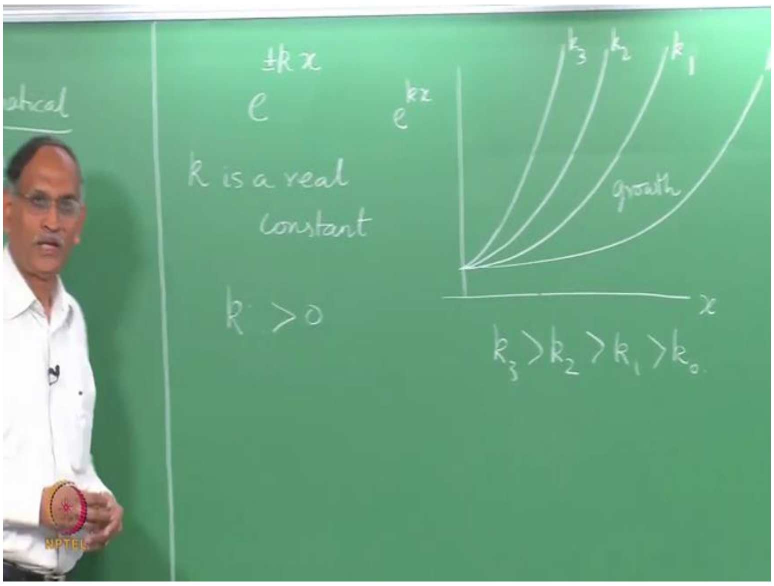

The first function that we will look at or the two sets of functions exponential e to the plus or minus kx; k is a real constant, if k is imaginary or complex it has its own different set of properties, k is real constant. Let us look at what the exponential actually means, I think most of you remember the plot when we picture the exponential as a function of the variable x and you write this the y axis as a exponential k of x. For a given value of k, if you plot this function obviously, at x is equal to 0, this function has a value 1. We will start from somewhere here, some scale and then you can see that if k is positive, k is greater than 0 then this is a growth function; growth meaning that the function increases its value as x increases.

Now, that is for one value of k; now let me call that k as k 0 some constant. Now suppose I have a different value of k, the function may again start from 1, but it may go something like this or it may be slower for another value of k or it may be really fast. So, let us do it by making this as k naught, k 1, k 2, k 3 as some different values of k. What is the relation between these; it is quite obvious that this grows much faster for a given value of x than any other function; obviously, k 3 is larger than later than k 2 than k 1 than k naught.

That is a pictorial representation of the function; that is not the understanding of the function. Understanding of the function is slightly different. I mean if you know that the constants are in this order, the function when it is plotted it looks like that what is the understanding of the exponential growth.

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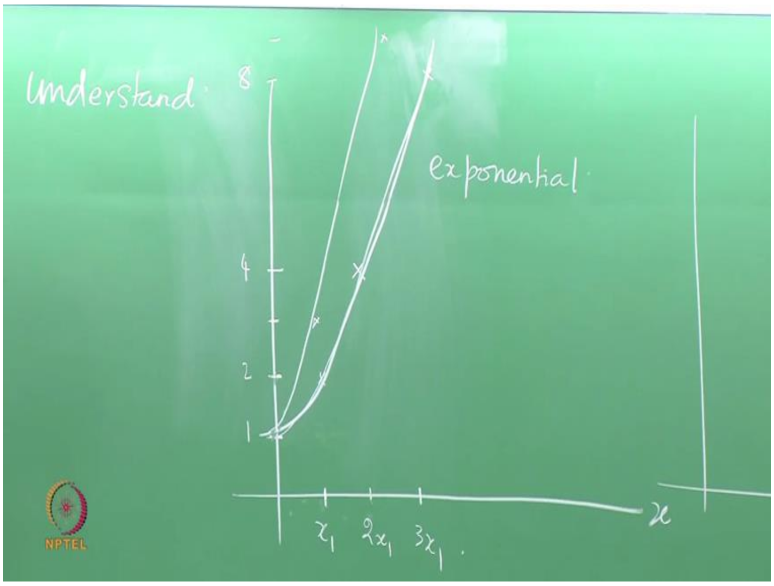

Let us try and understand this function, now the way to see this is to consider this particular case; namely for x. We start with 1 when x is 0 at a particular value of x, the function reaches some value here, when x becomes this is x 1, 2 x 1; 1, 2, 4. At 2 x 1, so at x 1 we have here and at 2 x 1 the function has the value 4 for example, some units and at 3 x 1 it reaches a value 8, that is every increment, identical increment, if the value of the function doubles its previous value such a behaviour is an exponential growth.

There is nothing special about being doubling; being a double or doubling. The function may start with some value in the first interval, whatever value that it becomes from one it may become 3, but in the next same amount of interval, the function 3 becomes 3 square, in the next interval 3 square becomes 3 cube; such growths are called exponential growths. If you do it for 3 quite obviously, it is even steeper or in this picture itself if you do it for 3, you are somewhere here and then 9 you were somewhere here. So, the point is you have here and then for 2 x 1 you are here and you see that the function grows even steeper, this is what is meant by k, this is what is implied by k; k tells how fast in what ratio that the function grows with respect to the variable x; this is for exponential growth.

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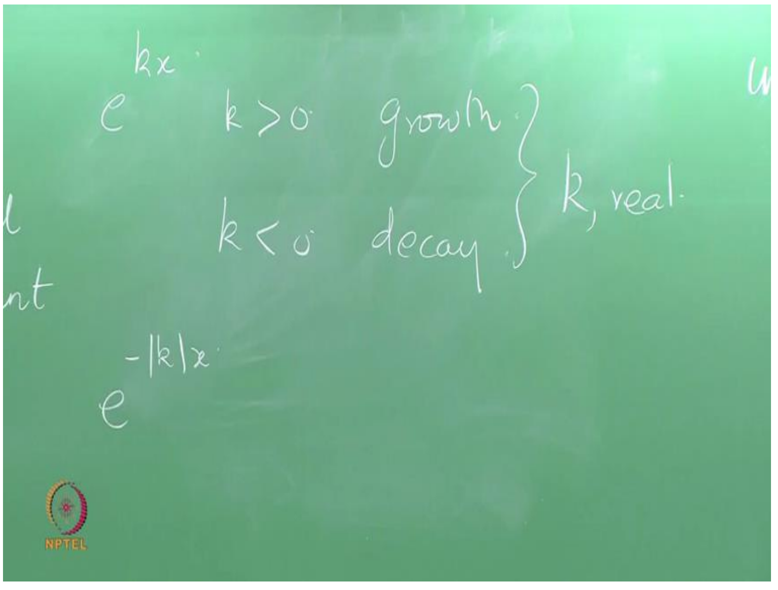

Now what about k less than 0; that is negative which we call as exponential decay; e to the kx, k greater than 0 growth, k less than 0 it is decay; of course, in both cases k real. So, you have e to the minus some value of k whatever is the number of x, so if you plot this it has exactly similar, but an image kind of a picture.

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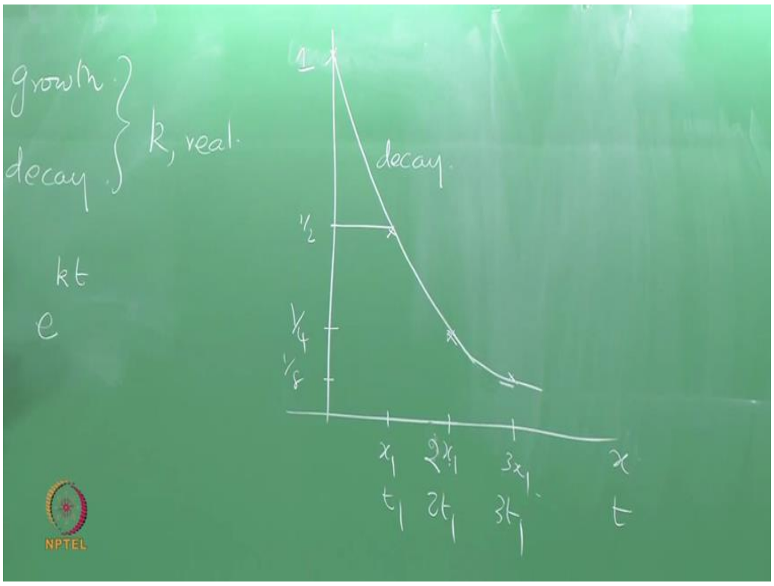

We will start with x and e to the kx is 0 that is it is 1 and suppose for a value x 1, the function becomes one-half; 1 by 2 then that is the value. For the same interval x 1 that is 2 x 1, the function decreases by the same fraction one-half becomes one-fourth. One-fourth in the next interval identical it will 3 x 1 becomes one-eighth. Such a behaviour if you connect is exponential decay, that is also exponential that is the nature of the exponential function.

The ratio of the function for any given period, the ratio is the same from that is the ratio of the value before, the value after if you take that value; that ratio remains for one particular interval ratio. So, here this is what is called the half life if you are interested in decay processes and the number becomes one-half, at a particular time t 1 if you write the function exponential k t, where t is time if you do that; instead of x, you use t; then you have t 1, 2 t 1, 3 t 1 and so the exponential is an extremely important function having this specific characteristics.

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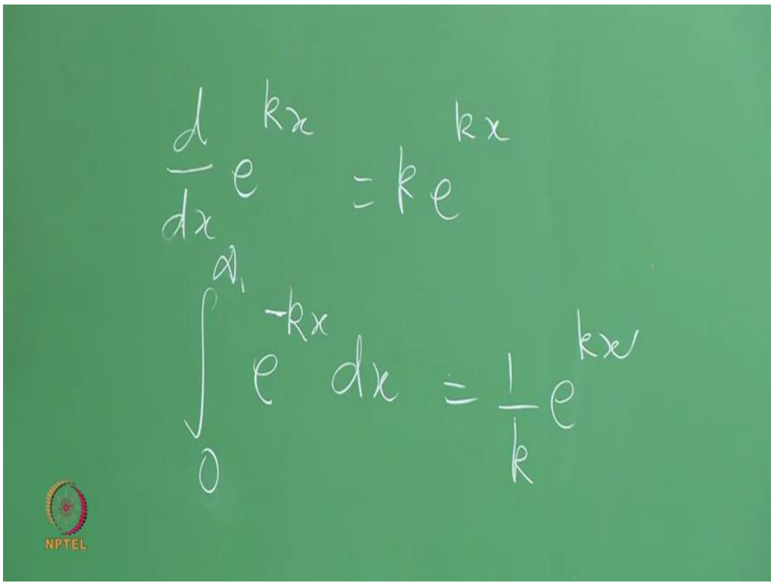

And the derivative of an exponential d by dx of e to the kx is k e to the kx that you should know and the integral of 0 to some constants t 1; finite value of an exponential kx dx is obviously you can calculate that. If you do not put the limits, you know that is going to be 1 by k times e to the kx. Therefore, you have to be careful that this integral is for a finite limit and if k is positive if we go from 0 to infinity; this is infinite the function is unbound the integral is infinite. If it is negative you know that 0 to infinity if you have exponential minus kx, you know what the answer is. So the properties of integration, the properties on differentiation and the simple nature of exponential is one extremely important function for you.

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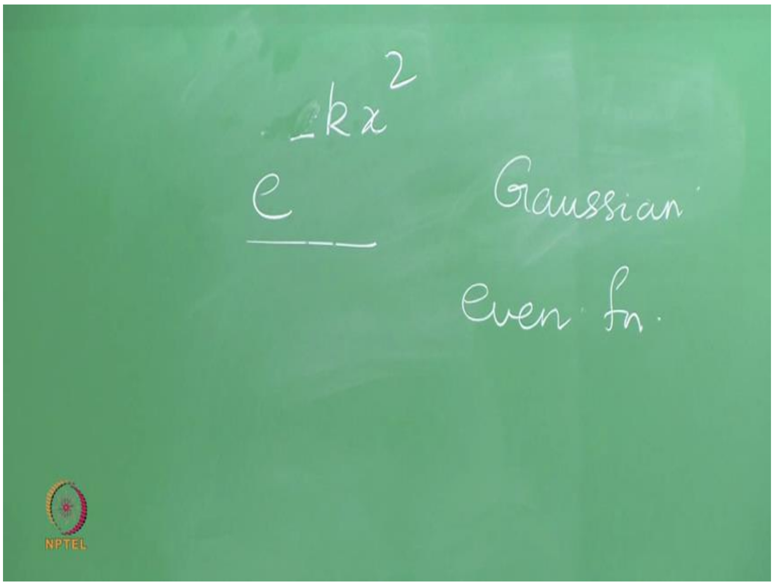

The second function that you need to worry about is also an exponential, but it is not called the exponential. It is called Gaussian, if it is minus we usually call it a Gaussian function. This is again important in all the quantum and spectroscopy studies that you have, what is the nature of this function. Unlike what you saw here, it is not increasing forever it is in fact is decreasing forever because if k is real and positive; this whole thing is decreasing as x either increases from 0 to infinity or x decreases from 0 to minus infinity because the function is dependent on the square of x, this is also known as an even function.

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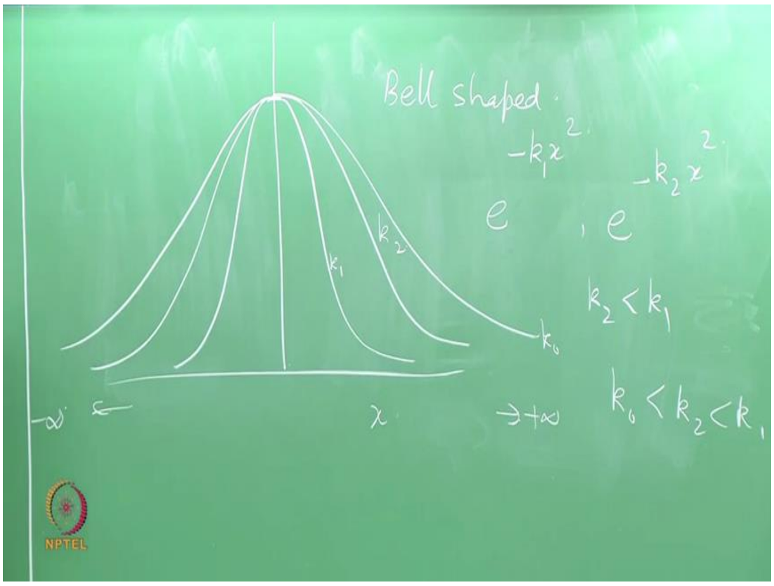

And the shape of this function when you plot it or x this is plus infinity and this is minus infinity, if you do that at x is equal to 0, this whole thing is exponentially 0, it is 1 and for all other values of x positive and for the value of x positive and negative; it is symmetric above to the line and this is obviously a bell shaped even function.

Now, again e to the minus kx square for one value k 1, suppose I want to plot this for another value k 2, where k 2 is less than k 1, it is quite clear that for any given x this will be smaller because k 1 is more than k 2, this one is smaller, this one is slightly larger and therefore, you can see that the function that if k 2 is less than k 1 we will have a more elaborate, a wider function; this is k 2. If you have k 0 sorry; you have k 2 is less than k 1 and you have k 0 now less than k 2 less than k 1, if you do that then the function is even that k 0.

So, the smaller the value of the exponent, the wider the more extended the function is or the opposite; the larger the value of these case, the more narrow; the narrower the function is you go in the reverse direction. This is another function which is extremely important for your calculations in spectroscopy and quantum mechanics.

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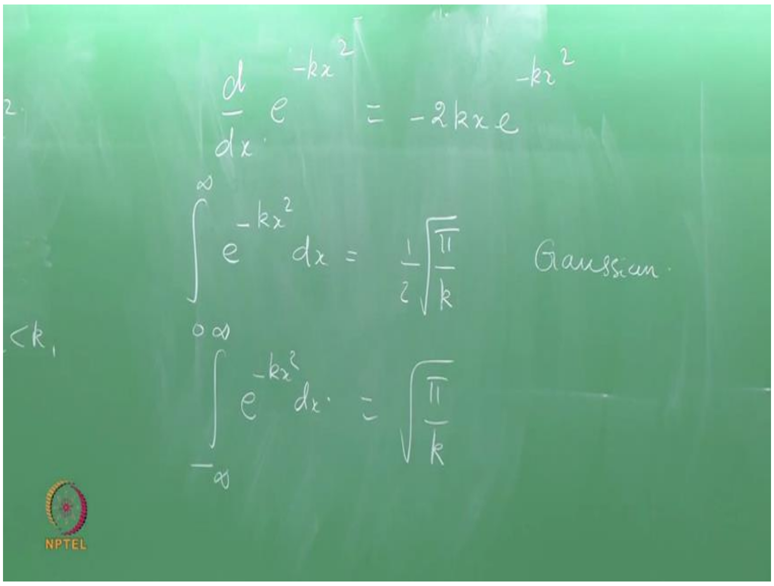

And again you must know that the derivative of this function e to the minus kx square minus 2 kx; e to the minus kx square and the integral of this function from 0 to infinity, e to the minus kx square dx is given by 1 by 2 root pi by k. This is the property and this being an even function, you can also do the integral of the same function between the entire x coordinate e to the minus kx square dx and that is exactly twice this integral root pi over k. So, these are standard integrals known as Gaussian integral.

This is another function that you would need in studying the properties of harmonic oscillators and quite a lot in understanding spectroscopic line shapes and so on, so basic properties you should be familiar with throughout.

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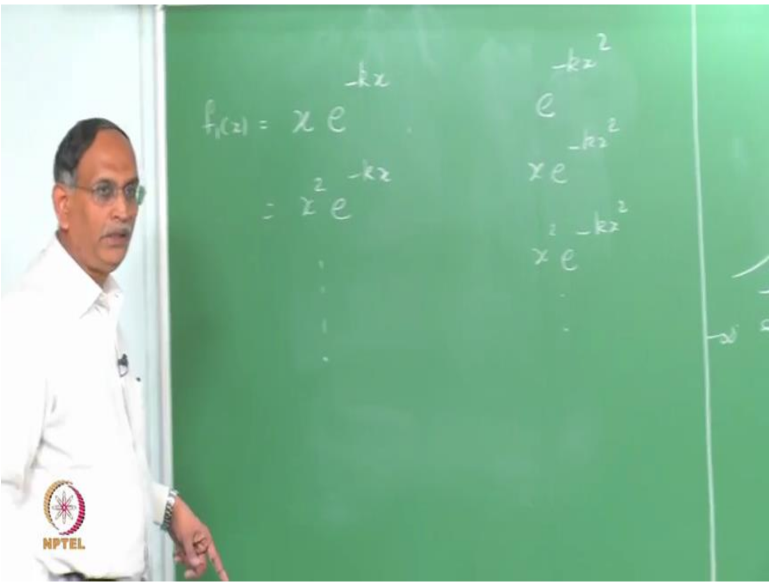

Similar functions that we will see which are slightly modified from these functions; namely multiplied by a polynomial instead of e to the minus kx, we may have and x multiplying e to the minus kx; f 1 of x some function. We may have x square e to the minus kx and so on, many many such functions. And also for the Gaussian, we will have e to the minus kx square and we will have x; e to the minus kx square, we will have x square; e to the minus kx square so on. These are functions which we will see time and again in the limited 6 to 8 weeks course and the properties and the shapes of these things should be known to you, go back and draw some of these things. Let me draw two of them before I conclude this small introduction to the mathematical ideas.

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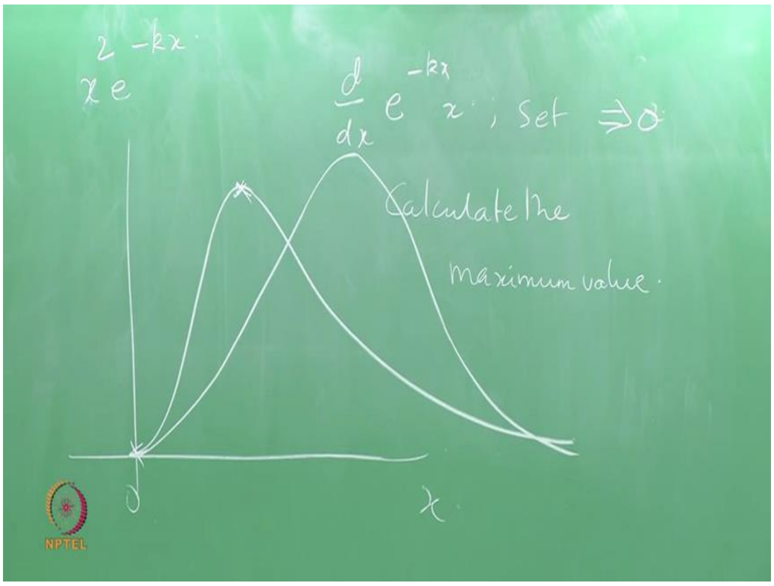

Suppose we want to plot x e to the minus kx for some value of k and we will do that for the positive segment. Please remember, we cannot try to do this in the negative segment that is for the negative values of x, you see that the exponent, this whole thing becomes positive and therefore, e to the positive number keeps on increasing; therefore, on the negative side this function increases beyond limit for very large values. Therefore, we will stay from 0 to some positive values and you can see that at x is equal to 0, this is 1, this is 0; therefore the function is 0.

And for any other x; as x increases, this increases e to the minus kx decreases and therefore, there is a competition between x and e to the minus kx up to a point and that point is obviously called the maximum of that function and after that point, the exponential minus kx drops off so much more quickly than x increasing that the competition is lost, the function decreases forever. And therefore there is a maximum and then the function goes to 0 and how do we determine this maximum? We take the derivative of this function e to the minus kx; x and then set that equal to 0.

Then you will find out that the function has some maximum, the derivative of this is clearly it is a u, v. So, you can do that and when you set the derivative to be 0, you will get your value for the maximum, so that is the maximum here that is an exercise; calculate the maximum.

Similarly when you go to x square, you would see that x square increases again and exponential minus kx decreases. Since x square increases for larger values of x; much more than x itself, the competition is taken over for a little longer or a little larger value of x and after that again the exponential wins over. In fact, the exponential wins over for all powers of the polynomials of x; if you go sufficiently far enough on the x, eventually it is the exponential that will kill the whole thing, it is very very important. Therefore, if you think about x square e to the minus kx, I can only say that it would be somewhere else, the maximum will be somewhere else; further away maximum and the value of this will also be different.

So, these polynomials multiplied by the exponentials are extremely important in understanding the wave functions and the properties of the wave functions for hydrogen atom. The polynomials involving the Gaussian and the polynomials in front of them x and x square and so on are important in understanding the harmonic oscillator and other elementary models in quantum mechanics. Therefore, please keep this is mind and please attempt to some of the exercises given at the end of this lecture, until we meet next time.

Thank you.