Chemistry Atomic Structure and Chemical Bonding

Prof. K. Mangala Sunder
Department of Chemistry
Indian Institute of Technology, Madras

Lecture - 02
Elementary Mathematical Functions Used in Our Course

Welcome back to the lectures the purpose of 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 functions which you will need in order to understand the behavior the mathematical and the spectroscopic out 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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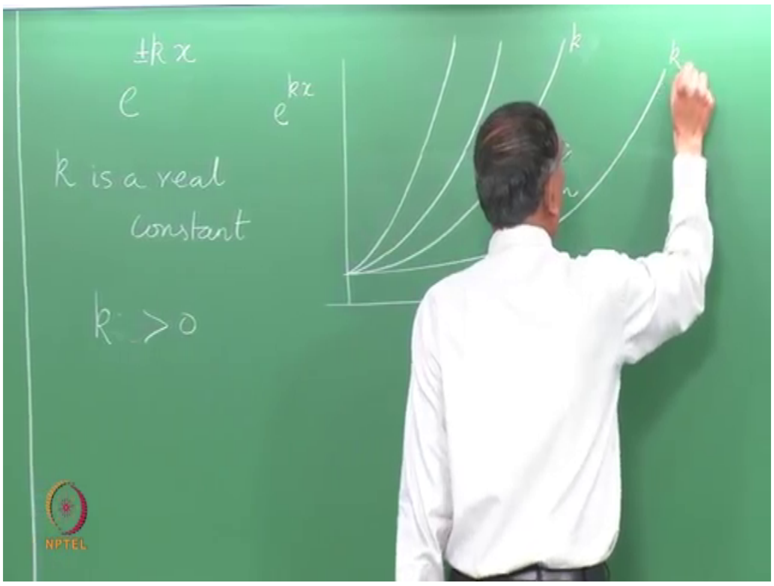

The first function not we will look at are the two sets of function exponential e to the plus or minus k x; k is a real constant. If k is imaginary or complex it has its own different set of properties k is real constant. Let us look at what the exponential actually means I think most of you remember the plot, when we write when we picture the exponential as a function of the variable x and you write this the y axis as 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. So, we will starts from where 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 in its value as x increases.

Now that is for 1 value of k. Now let me call that k as k 0 sum constant. Now suppose I have a different value of k the function may again start from 1, but it may grow something like this or it may be slower for another value of k or it may be really fast ok.

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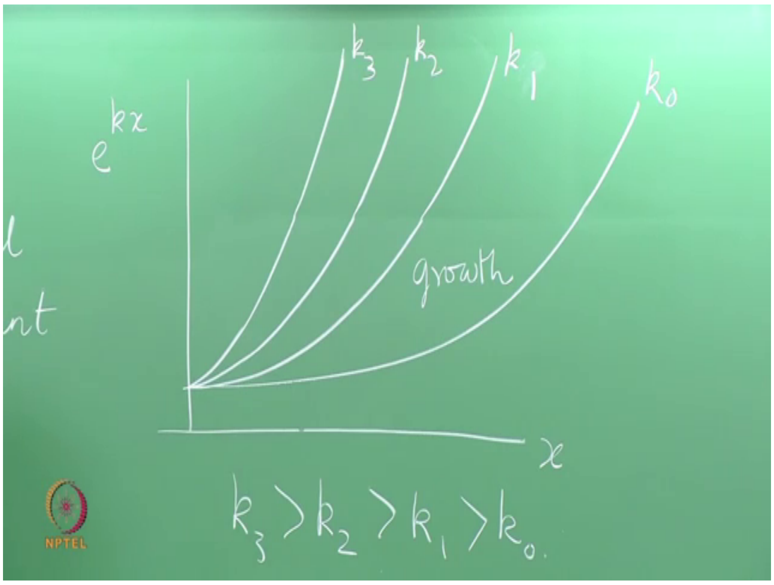

So, let us do it by making this as k naught k 1 k 2 k 3 as some different values of k, what is the relation between these? It is quite obvious that this grows much faster for a given value of x than any other function; obviously, k 3 is larger than k 2 then k 1 then k naught. That is a pictorial representation of the function that is not the understanding of the function. Understanding of the function is slightly different.

I mean if we know that the constants are in this order the function when it is plotted looks like that, what is the understanding of the exponential growth? Let us try and understand this function ok.

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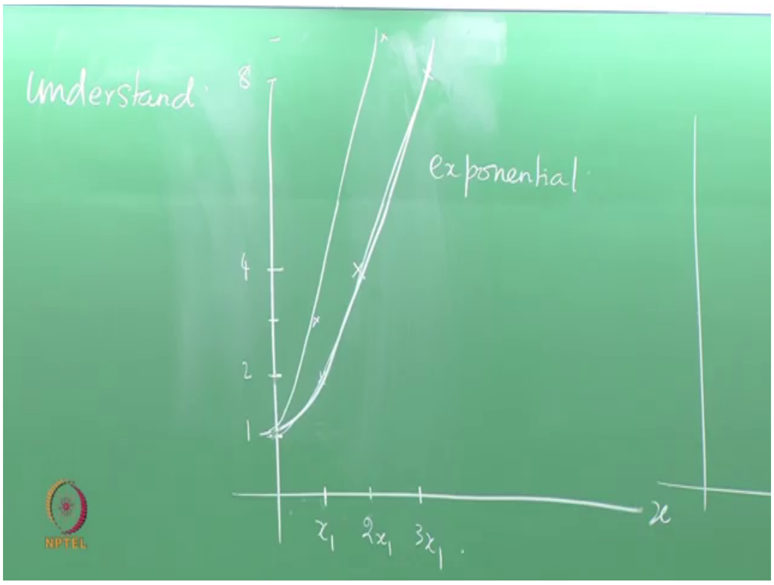

Now, the way to see this is to consider this particular case, namely for x we start with 1 when x is 0. At a time sorry at a particular value of x the function reaches some value here, when x becomes this is x 1 2 x 1 1 2 4 2 1 at 2 x 1. So, at x 1 we have here and at 2 x 1 the function has the value 4 for example, some units and at 3 x 1. It reaches a value it that is every increment identical increment if the value of the function doubles its previous value such a behavior is an exponential growth such a behavior exponential.

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 1 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 q, such growths are called exponential growths ok. 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 are somewhere here. So, the point is you have here and then what 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 ok, this is for exponential growth now what about k less than 0 that is negative.

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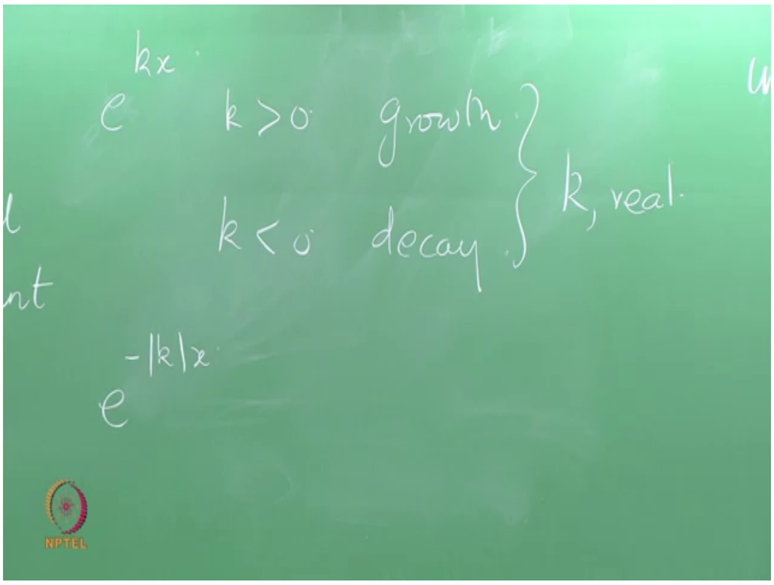

Which we call as exponential decay e to the k x k greater than 0 growth k less than 0 its decay of course, in both cases k real. So, you have e to the minus some value of k what other reason number of x ok. So, if you plot this it has exactly similar, but in an image kind of a picture ok.

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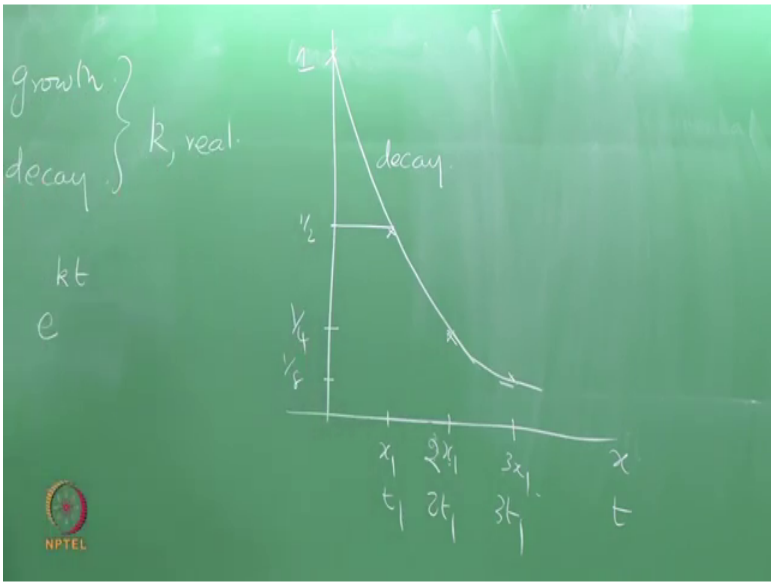

Let us start with x and e to the k x is 0 that is its 1 ok, and suppose for a value x 1. The function becomes one-half 1 by 2, then that is a value for the same interval x 1 that is 2 x 1. The function decreases by the same fraction one-half becomes one-forth, start one-forth in the next interval identical interval 3 x 1, becomes one-eighth such a behavior if you connect is exponential decay.

That is also exponential that is the nature of the exponential function, the ratio for 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 well that ratio that ratio remains for 1 particular interval ratio ok. 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 on. So, the exponential is an extremely important function having this specific characteristic ok.

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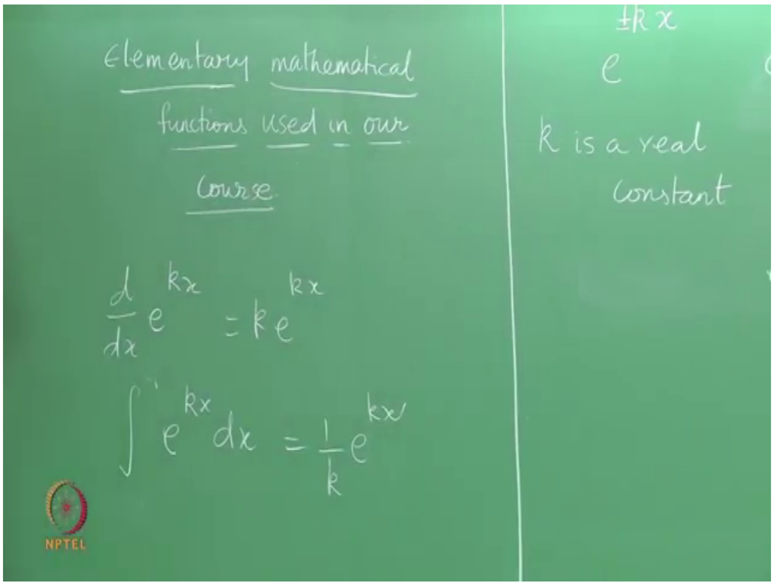

And the derivative of an exponential d by d x of e to the k x is k e to the k x that you should know and the integral of 0 to some constant c 1 finite value of an exponential k x d x is; obviously, you can calculate that. If you do not put the limits you know that it is going to be 1 by k times e to the k x. Therefore, you have to be careful that this integral is for a finite limit. If you go from and if k is positive if you go from 0 to infinity this is infinite the function is unbounded the integral is in finite.

If it is negative you know that 0 to infinity if you have exponential minus k x you know what the answer is 1 by k ok. So, the properties of integration the property is on differentiation and the simple nature of exponential is 1 extremely important function for you, the second function that you need to worry about is also an exponential, but it is not called an exponential.

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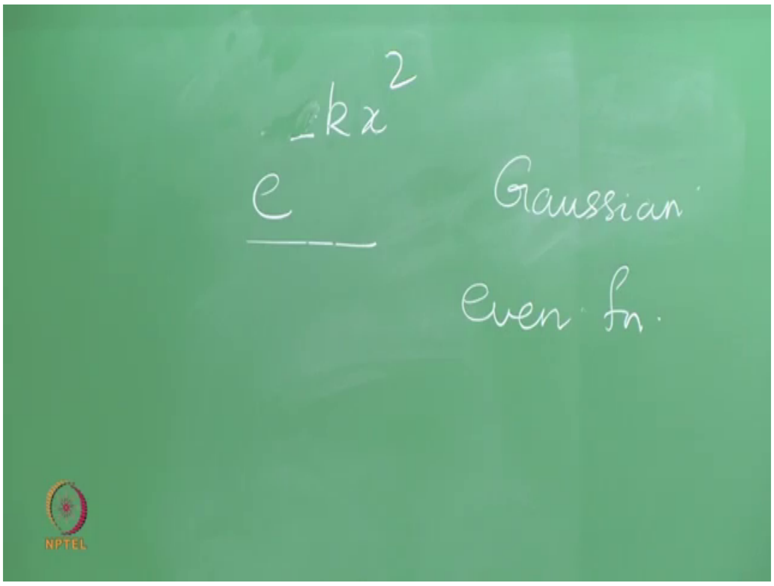

It is called a it is called Gaussian, if it is minus we usually call it a Gaussian function this is again important in all the quantum and spectroscopy studies that you have what is the nature of this function, unlike what you saw here it is not increasing forever its. In fact, its decreasing forever, 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 this square of x this is also known as an even function, ok.

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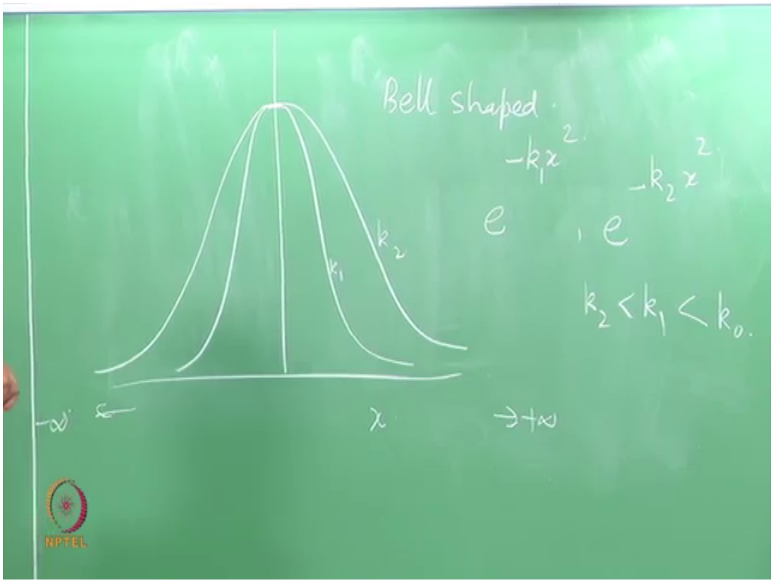

And the shape of this function, when you plot it or x this is plus infinity and this minus infinity. If you do that at x is equal to 0 this whole thing is exponential 0 it is 1 and for all other values of x positive and x negative it is symmetric about to the line and this is obviously bell shaped even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

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

So, the smaller the value of the exponent the wider the more extended the function is are the opposite the larger the value of this ks the more narrow the narrower the function is you go from in the reverse direction this is another function, which is extremely important for your calculations in spectroscopy and quantum mechanics and again.

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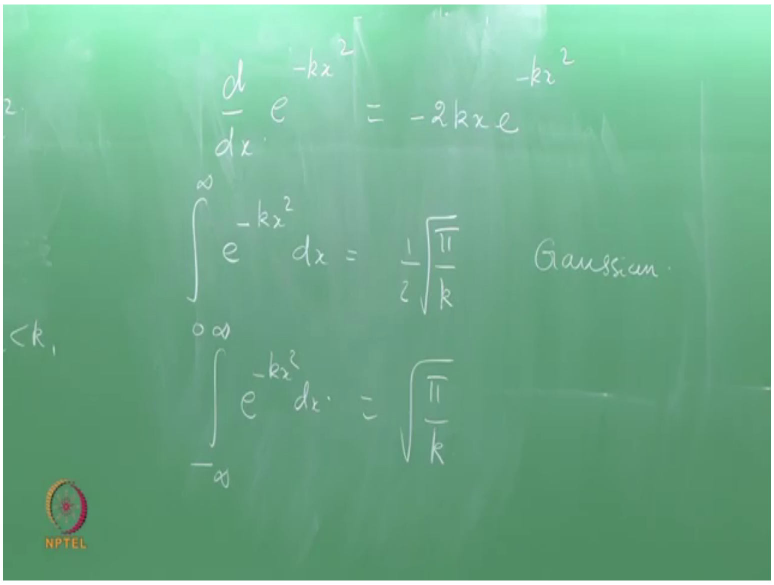

You must know that the derivative of this function e to the minus k x square is minus 2 k x e to the minus k x square ok. And the integral of this function from 0 to infinity e to the minus k x square d x is given by 1 by 2 root pi over k.

This is a 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 k x squared d x and that is exactly twice this integral its root pi over k. So, these are standard integrals known as Gaussian integral ok. This is another function that you would need in studying the properties of harmonic oscillators and quite a lot in the in understanding spectroscopic line shapes and so on. So, basic properties you should be familiar with there are similar functions that we will see which are slightly modified from these functions namely multiplied by a polynomial.

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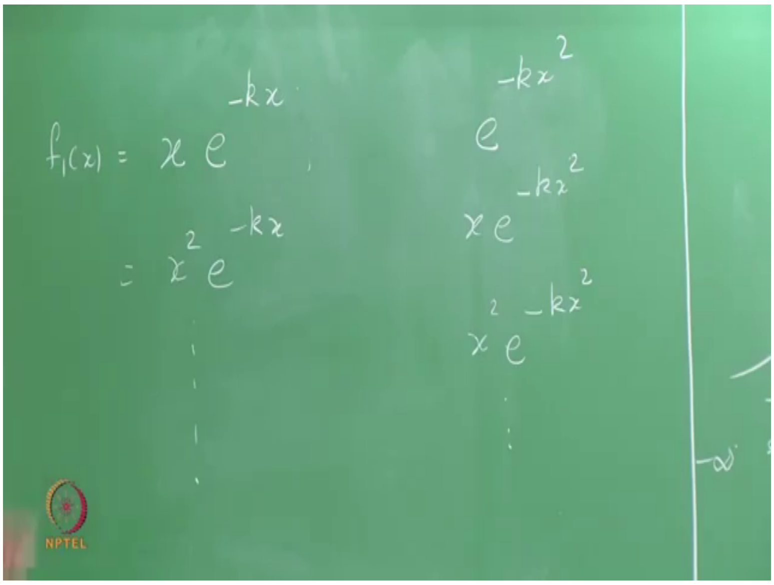

Instead of e to the minus k x we may have an x multiplying e to the minus k x f 1 of x some function, we may have x square e to the minus k x and so on. Many, many such functions and also for the Gaussian we will have e to the minus k x square and we will have x e to the minus k x square. We will have x square e to the minus k x square and so on. These are functions which would which we will see time and again 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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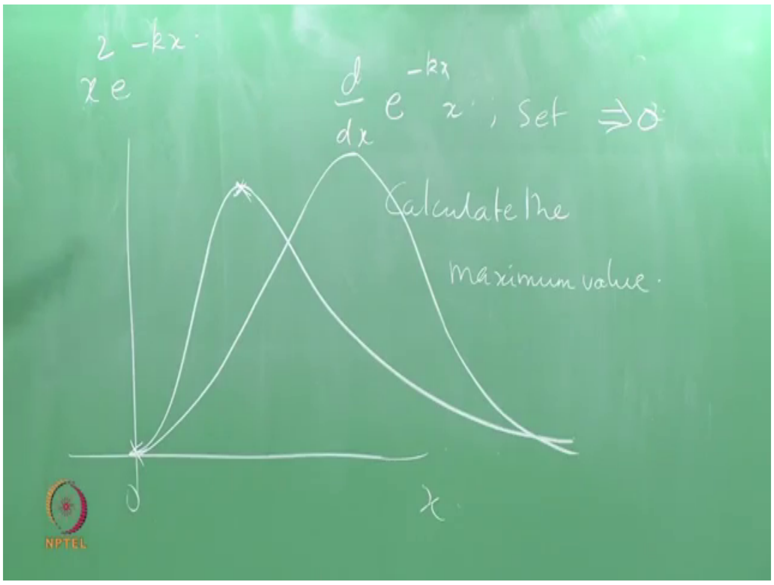

Suppose we want to plot x e to the minus k x for some value of k, and we will do that for the positive segment please remember we cannot try to do this in the negative segment that is for the negative values of x you see that the exponent this whole thing becomes positive. And therefore, e to the positive 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 for any other x as x increases this increases e to the minus k x decreases.

And therefore, there is a competition between x and e to the minus k x up to your point and that point is; obviously, called the maximum of that function and after that point the exponential minus k x 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 ok. And how do we determine this maximum we take the derivative of this function e to the minus k x x and then set that equal to 0. Then you will find out that the function has a 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 a value for the maximum ok.

So, that is a maximum here that is an exercise calculate the maximum value. And similarly, when you go to x square you would see that x square increases again and exponential minus k x decreases a since x squared 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 its very very important. Therefore, if you think about x square e to the minus k x I can only say that it would be somewhere else the maximum would be somewhere else ok, farther away maximum and the value of this will also be different ok.

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 or important in understanding the harmonic oscillator and other elementary models in quantum mechanics.

Therefore, please keep this in mind and the please attempt to some of the exercises given at the end of this lecture until we meet next time.

Thank you.