Advanced Mathematical Methods for Chemistry
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Module - 03
Lecture - 01
Lecture 1 - Step Function, Delta Function

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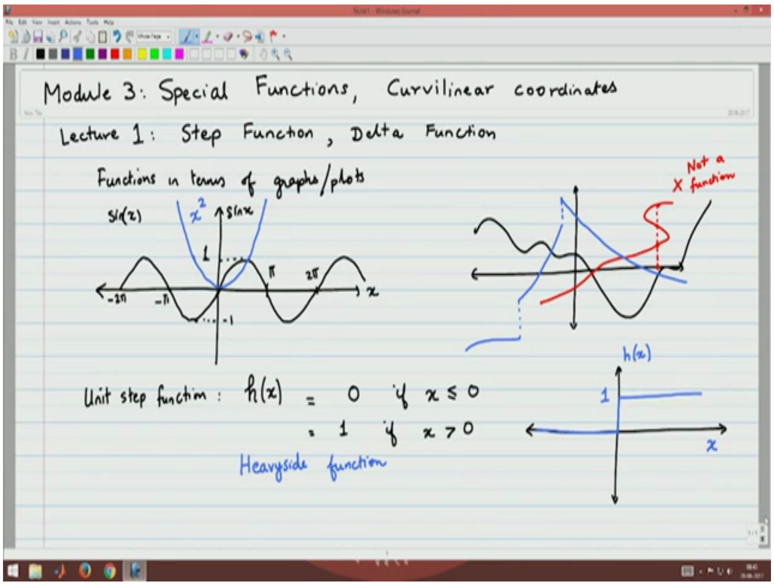

So in this module we will be discussing special functions and curvilinear coordinates. So, there are several functions which we use during various applications which fall in the category of what are called as special functions and there are different reasons why these are special. We will be looking at some of these special functions during this module. The first special function that I want to talk about and which will be discussed in this lecture is the step function and its derivative which is a delta function.

So, before I get into the step function in the delta function, let me introduce you to a way of thinking about functions. So, whenever you have a function it is very useful to think of the graph of the function. So, think of the functions in terms of graphs, in terms of, graphs or plots or plots and this idea is extremely important and it will really help you understand the behavior of functions lot more. So, whenever you see any function it is a good idea to plot the function. So, suppose you have for example, if you have sin x then when you plot it you know that it will look as a function of x, you will plot your, you will plot sin x and you immediately know that it will have this sort of behavior will level be periodic and it will be oscillating and you know that the peak period is 2 pi. So, it will go and then and then it is an odd function. So, you will see that it goes the other way on the other side.

So, this is minus pi minus 2 pi and also you know that the amplitude, the amplitude is equal to 1 its maximum value is 1 and its minimum value is minus 1. So, you think of the function in terms of the graph. Now suppose on the other hand you had a function like let us say x square, x square. So, x square you know that what will happen is that x square will start at 0 it will always be positive and it will go it will keep increasing higher and higher. So, unlike sin x which is oscillating x square is something that will be that will just keep increasing. So, that is what x square looks like the graph and blue and sin x looks like this.

Now these are, it is always very useful to plot functions and what I will be doing during this course is to say that if you have some arbitrary function if you have some arbitrary function then it will have some graph, will have some graph and you know you can just show it as some graph. Now what is important about the graph is that for each value of x there should be only 1 value of the function. So, you cannot have a graph that looks like this, this is not possible because for this value of x this is not a function because it does not have a single value. So, suppose you ask what is the value of the function here it can be either this or this or this.

So, it is becomes multi valued here and in general we do not talk of this as a function. So, the other thing is now you can have a graph and what mode you can have functions where the graph is not continuous. So, you could have a function that looks like this and then goes like this and then he goes like this. So, you could have a function that looks like this. So, it is discontinuous in this point. So, all these are examples. So, it is very important that just by that you should get a sense of what the function does just by looking at the graph. And arbitrary functions will have some graph and which will have some features which we can analyze.

So, now, let us come to the step function. So, I will call it the unit step function and I will call this h of x and h of x is defined it is equal to 0 if x is less than equal to 0 and is equal to 1 if x is greater than 0. So, what you notice just from the definition of the function, you notice that that at x equal to 0 there is a discontinuity and now we can make a plot of this function. So, the plot of this function will look like this. So, let me show it in blue. So, the plot of the function will be 0 for all values of x less than 0. So, it is 0 on this axis then it at x equal to 0 it goes to 1 then it stays at 1, this value is 1.

So, this is what your function looks like, this is x, this is h of x incidentally this function is also called the heavy side function the heavy side was a mathematician. So, it is named after him. So, the heavy side function is has this feature that it is 0 for x less than 0 and is equal to 1 if x is greater than 0. Now you could also have step functions which are slightly modified versions of step functions.

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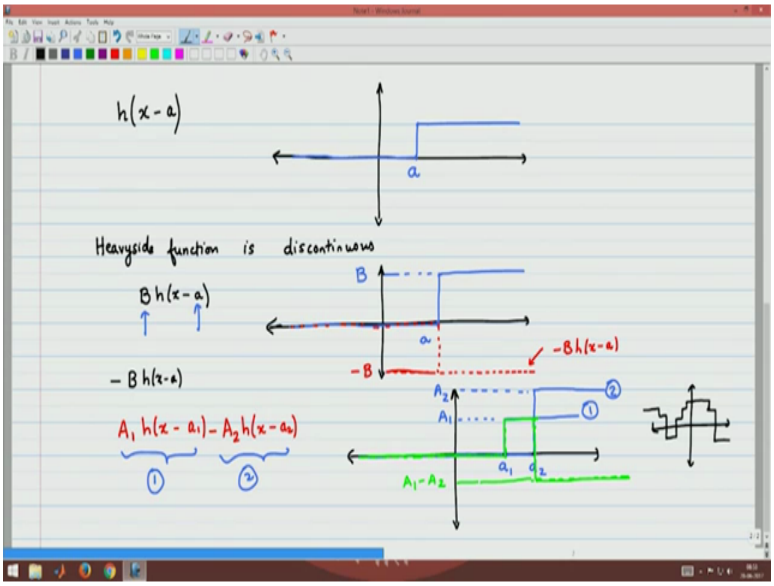

For example instead of you could have h of let us say x minus a. So, what will h of x minus a look like? So, it is a heavy side function of x minus a. So, what this will look like is the following. So, it will be 0 when x minus a is less than 0 that is x is less than a and let us say a is this value this is x equal to a and it is 1 when x is greater than a. So, this is heavy side function of x minus a.

So, this heavy; heavy side function is actually the is, so heavy side function or unit step function is discontinuous. Now you can construct several different versions of this heavy side function. Now suppose you want a function, suppose you want a function that is whose which whose amplitude is not 1, but it is something else. So, what you can do is you can; if you can multiply by h a B - capital B h of x minus a. So, this will look like a heavy side function whose amplitude which is 0 all the way until x equal to a and whose amplitude is b. So, this amplitude equal to b.

So, you can actually manipulate heavy side functions to get various kinds of heavy side functions, you need not have just amplitude 1 and you need not have only the discontinuity at x equal to 0. So, you can change the location of the discontinuity and you can change the amplitude. You will get different functions which are also step functions which are not unit step functions, but they are sort of you know slightly modified step functions. Now you could also have a heavy side function which is suppose you take minus you take minus of; I will just say B times h of x minus a. So, suppose I take minus of B times h minus a, h of x minus a and I will show this in red. So, that will look it will be 0 and then it will go to minus and this value is minus B. So, I could have this is minus B h of x minus a.

Now I could do lot of other things I could let us say if I add these 2 functions of course, I will get 0, but I can do things like let us say I take I consider a function that is has this form. So, let us say I say A 1 h of x minus a 1 plus or let me make and put a minus sign here just to minus A 2 h of x minus a 2.

So, what will this function look like? So, so if you take this function and. So, let me I will draw each of the functions. So, I want explicitly told you the values of small a 1 and capital A 1 and small a 2 and capital A 2, but you know whatever their values are will plot the functions based on their value. So, let us say this is let me, let us assume this is a 1 then what you have is you have it coming up you have it 0 all the way to A 1 the first function. So, this is first function and this is the second function. So, the first function will be 0 up to here then it will go all the way to a 1, A 1.

The second function let us say let us let me say it goes. So, this is the first function the second function let us say it goes 0 all the way up to A 2 and then it goes in up all the way to A 2 this is the second function. Now if you take the difference of these 2 if you take the difference of these 2 then you can see what will happen is that in this region [vocalized- they both are 0. So, their difference is 0 in this region you will just have a 1 because the second function is still 0.

So, all the way up to here you will have the same. So, so let me show this in green just to show you what the difference is looks like. So, it follows this graph then it goes here then it goes along this. Now what happens at this value? At this point you have the value becomes equal to A 1 minus A 2. So, it goes A 1 minus A 2 and I will have shown A 2 greater than A 1. So, A 1 minus A 2 will actually be negative. So, it will go to something like this and it will go it will stay at this value of. So, this values A 1 minus A 2, A 1 minus A 2 is less than 0 and that is what the value will be.

So, what we got what we got through this exercise we got a function and I will make it in dark now yes. So, we got a function that looks like this. So, by basically adding and subtracting heavy side functions we can get functions that look like you know it that that are nonzero for some value you can get all kinds of functions by this. So, essentially I will just conclude the discussion of step functions right here. So, you can get functions that look like you know you might get something like this, might have a function that looks like this. You can get a function that looks like this by combining step functions. So, suitable combinations of step functions you can give you all kinds of shapes and some of those are fairly useful in various calculations.

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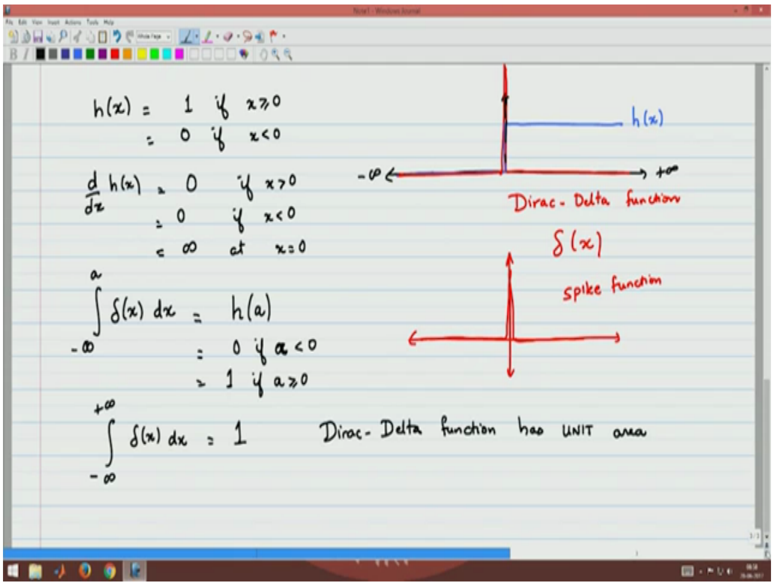

Now, the next, now, we set that the that the step function. So, h of x equal to equal to 1 if x is greater than equal to 0, equal to 0 if x is less than 0, now the exact value at 0 is cube a table, you can it jumps from 0 to 1. Now suppose I take, suppose I take d by d x of h of x. So, clearly if x is greater than 0 the derivative is 0 because the function is constant, if x is greater than 0 equal to 0 if x is less than 0. So, now again you go to a graph and you see you see what happens. So, what you have is you had your step function, your unit step function. So, this is h of x and now you are taking the derivative of this, now if you take the derivative clearly it is 0 here because the graph since derivative is nothing, but the slope of this curve. So, since the curve is flat your derivative is 0 here your derivative is 0 here.

Now what about write at x equal to 0? At x equal to 0 your change of the function, your function changes by 1 unit over essentially no interval. So, over an infinitesimally small interval it jumps from 0 to 1. So, the derivative has to be equal to infinity here. So, write here your derivative becomes infinity because it is changing very very rapidly and have exaggerated, but basically your derivative, if you made a small mistake here. So, the derivative is actually 0 here. So, your step function the derivative is 0, here it is 0 on the right, the function has value 1, your function has value 1, but the derivative is actually 0. So, function has value 1 the derivative is 0 on this side. So, your derivative looks like this. So, it is 0 here, it is 0 here and it has a big jump here. So, equal to infinity at x equal to 0.

Now let me call this function, this function in red I will call it as a it is known as a Dirac-Delta function or simply a delta function sometimes and it is denoted by the symbol delta of x. So, what the delta of x look like? Delta of x if I plot it then it just looks it is 0 everywhere and it has a spike here and again it is 0. So, it is sometimes called the spike function. Now what is the feature of this delta function? So, suppose you integrate over the delta function integration is the opposite of differentiation. So, if you integrate over delta of x d x from let us say 0 to a, what you will get is exactly h of a. So, that is equal to 0 if x is - if a is less than 0 equal to 1, if a is greater than equal to 0.

So, the integral will be 0 all the way here because your function is 0 everywhere, then just when you cross this your integral go to 1 and then once it goes fastest your integral will always be 1. So, what that means? So, if you look at integral from I should say minus infinity, from minus infinity. So, this is minus infinity to plus infinity. So, integral from minus infinity to plus infinity delta of x d x. Now a is greater than 1 a is greater than 0, so it is equal to 1. So, the delta function has this feature that it is integral as 1. So, Dirac-Delta function has unit area. There is one more feature of the Dirac-Delta function which makes it really useful is the following.

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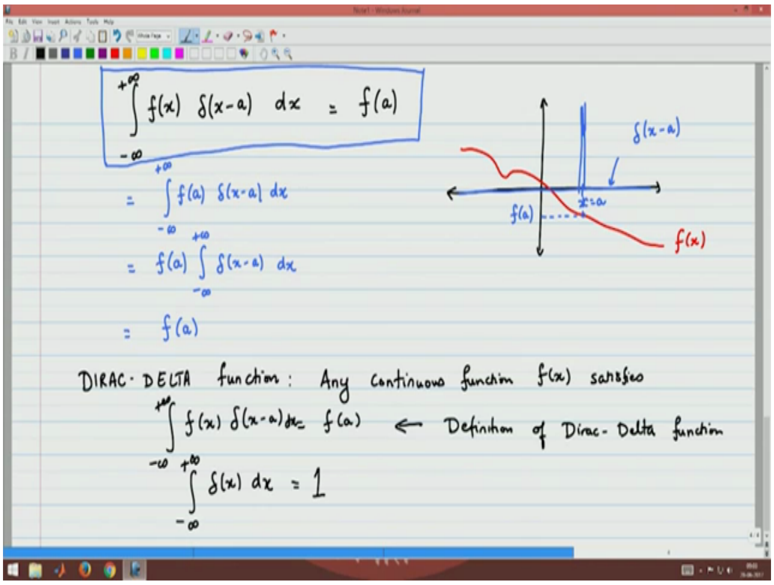

Suppose I take f of x multiplied by delta of and let me say, let me say x minus a d x and I integrated from minus infinity to plus infinity, this will give me exactly f of a. So, what did I do here? So, I have, I can show this pictorially. So, you have you have let me show it in red. So, let us say I have f of x this is f of x and I multiplied it by a delta function delta function delta of x minus a. So, now, delta of x minus a will give me a spike at x equal to a. So, this is delta of x minus a. Incidentally I did not go through this detail, but basically delta of x gives the spike at x equal to 0, delta of x minus a will give me the spike exactly at x equal to a.

So, the infinite spike that you get will be at x equal to a. And now and now when you when you multiply these 2 then what you will get is essentially this value, this value of the function, this is f of a. So, what you will get is this will be 0 unless x equal to a and at x equal to a you can replace f of x by f of a, so you just get f of a. So, just to work this out you can do it, you can think of this the following way. So, this is integral minus infinity to plus infinity f of a times delta of x minus a d x and since f of a, is because this is this is 0 unless x equal to a. So, this product is 0 unless x equal to a. So, I just take f of a outside so I can write f of a and what I am left with is integral of a Dirac-Delta function which is equal to 1. So, I just get equal to f of a. And this is sometimes used as the definition of the Dirac-Delta function.

So, basically in, so the Dirac-Delta function you can think of as having 2 features. So, the Dirac-Delta functions, so what we. So, if you take any continuous function f of x satisfies integral f of x delta of x minus a equal to f of a from minus infinity to plus infinity d x. So, any continuous function will satisfy this.

Further you have integral minus infinity to plus infinity, delta of x. So, if I just put a 1 you can think of this as just putting a 1, instead you can just think of f of x equal to one. So, f of a will also be 1, so this is equal to 1. So, you can use this as a definition of the delta function, so any function that satisfies this for any arbitrary f. So, if you have that will be called the Dirac-Delta function. So, this is sometimes used as a definition of Dirac-Delta function.

So, a Dirac-Delta function is essentially always defined only under the integral. So, this is a function that is only defined under the integral, you do not you do not write Dirac-Delta functions without the integral. So, you cannot evaluate you if you asks what is the value at x equal to a of the Dirac-Delta function you cannot say it, but it is perfectly well defined under the integral.

So, I will conclude this lecture here. So, in the next lecture we look at other special functions.