Advanced Mathematical Methods for Chemistry
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Module - 03
Lecture - 02
Lecture 2 - Gamma Function, Error Function

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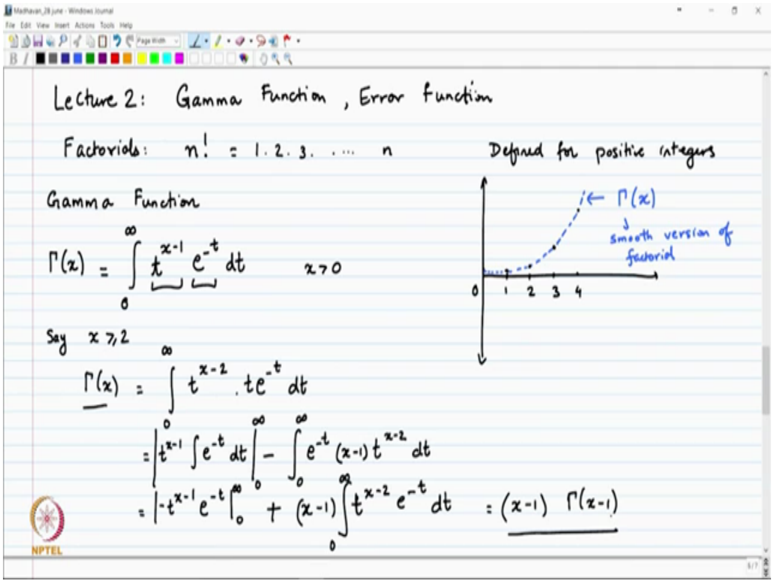

In the current lecture we are going to be talking about more special functions here we will talk about 2 special functions that you will see very often both quantum mechanics and statistical mechanics. These are the gamma function and the error function. There are many different special functions that you will see in various applications in chemistry and I will not be discussing each of them individually, but you know once you see how one special function works you will be able to do various different special functions.

So, let us talk about the gamma function. Now to motivate the gamma function let us look at a very familiar concept that is factorials. You know that suppose I write n factorial. So, this is 1 into 2 into 3 a product up to n, this is defined for, this is defined for positive integers and you know that the factorial function will have this form where basically as you can think of it this way. So, if this is 1 2 you can see that 1 factorial is 1, 2 factorial is 2, 3 factorial is 6, 4 factorial is 24 and soon 5 factorial is 120. So, essentially it will have this kind of behavior. So, it will keep going and then and then it will go very high very quickly.

Now, if you imagine if you imagine that you have a function which is essentially a smooth function now I should add that you usually define 0 factorial as 1, usually 0 factorial is also defined as 1, 0 factorial is also 1. Now if you imagine having a having a function which essentially passes through all these points some sort of smooth function that passes through all these points. So, if you imagine such a function that would be an example of what is called, this is what we will call the gamma function. So, gamma function of x is the smooth version of factorial, see the factorial is defined only for positive integers now if you have a smooth function that whose value at the integers is equal to that of the factorial that would; that is what is. So, the gamma function is related to this function.

So, now, let us write the definition of the gamma function. Gamma of x, so x is the variable of the function this is a defined as an integral 0 to infinity and let the variable of integration be t, t raised to x minus 1, e raised to minus t d t this is the definition for x greater than 0. So, this is the definition strictly for x greater than 0. If you see this function it does not appear to it does not appear to be related to a factorial, but you can easily show that this is related to the factorial by a small trick. So, let us say x is greater than or equal to 2, if x is greater than or equal to 2 then you will have t raised to some power which is greater than or equal to 1.

So, then what I can do is I can write gamma of x I can do an integration by parts. So, I can write this as integral 0 to infinity t raised to x, x minus 2 into t e raised to minus t d t. So, basically I am writing it as x minus 2 plus 1, let me just to make the story short. So, so if you integrate this by parts then what you will get is the following. So, let me take this as the first function and this as the second function. So, then my first term will be will be integral 0 to infinity I will have t raised to x minus 1, e raised to minus t d t and then you will have minus integral. Now you will have e raised to minus t into derivative of this derivative of that is x minus 1 t raised to x minus 2 d t. Now actually should be a little more careful you should you should not put the limits here the limits should be put here from 0 to infinity.

Now, so we have to evaluate this whole thing from 0 to infinity. Now what this will give me is the following. So, I will get t raised to x minus 1, e raised to minus t and with a minus sign from 0 to infinity minus integral this integral is from 0 to infinity. Now this integral I will write as x minus 1 times t raised to x minus 2 e to the (Refer Time: 07:03) this will become a plus sign because integral of e raised to minus t is minus e raised to minus t. So, t raised to minus t d t or if you look at this quantity when x; when t equal to 0 since x is greater than or equal to 2 this goes to 0, the first term goes to 0 and when t equal to infinity the e raised to minus t will make this 0. So, this integral is exactly equal to 0 or this value at 0 and infinity is both equal to 0. So, basically you just get, so you only have the second term.

Now the second term I can write as I can write as x minus 1 and this is exactly like this only thing instead of x I have x minus 1. So, so this is gamma of x minus 1 this is this integral is exactly the gamma function, but the argument is not x, but it is x minus 1. So, basically you get gamma of x equal to x minus 1 times gamma of x minus 1.

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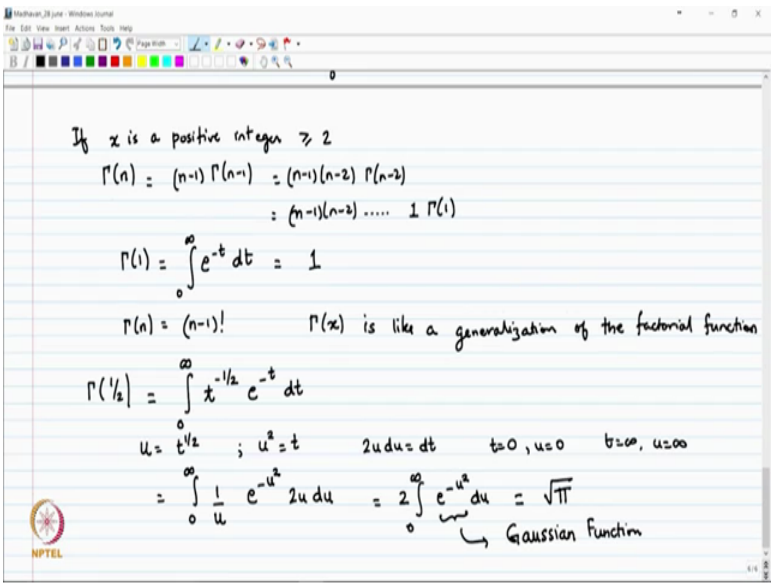

Now you can immediately see that if x is a positive integer greater than equal to 2 then you can see that gamma of n, so n will be n minus 1 times n minus 1 times gamma of n minus 1 is equal to n minus 1 times n minus 2 times gamma of n minus 2 and you can so basically you can go all the way up to 1 all the way up to 1 and you will be left with gamma of 1. Now we need to calculate gamma of 1. So, gamma of 1 is integral e to the minus t d t from 0 to infinity and this is equal to 1, you can easily show that this integer if this is equal to 1. So, basically what you will get is gamma of n is equal to n minus 1 factorial. So, this is how you can show that the gamma function is related to the factorial function. So, the gamma function f for integer values takes the value of the factorial function. So, gamma of n is n minus 1 factorial.

So, gamma of x is like a generalization of the factorial function. Now what is the other I mean, the reason why we decided to generalize this factorial function is that this integral is something that appears a lot in applications. So, now, let us look at gamma of half. So, half integer is also something that appears very often. So, I can write this as integral 0 to infinity t raised to minus half, e to the minus t d t and what you can do is that you define, we will do this integral explicitly. So, that you see how we can do this integral and in doing this we will also see how these how these half integers are related to Gaussian functions.

So, in order to do this integral you set u, set u is equal to t raised to half or u square equal to t, then what we will get is 2 u d u equal to d t and the limits t equal to 0 then u equal to 0, t equal to infinity, u equal to infinity. So, what we will get is that integral this will becomes integral 0 to infinity and what t raised to minus half will be u raised to minus 1. So, it will be 1 over u, e to the minus t will be e to the minus u square and d t will be 2 u d u. So, the this u will cancel and what you will get is integral 2 e to the minus u square d u from 0 to infinity.

So, so this function is what is called a Gaussian function. So, e to the minus e to the minus u square is a Gaussian function. So, this is integral of the Gaussian function from 0 to infinity. Now how do you do this integral? Now it turns out that you can you can do this integral by something called by changing to plain polar coordinates, but I want to explicitly do that I will just tell you the final answer. So, this will give me root pi. So, twice this integral from 0 to infinity will give me exactly root pi. So, what is important is that your, if the gamma function of half is equal to root pi.

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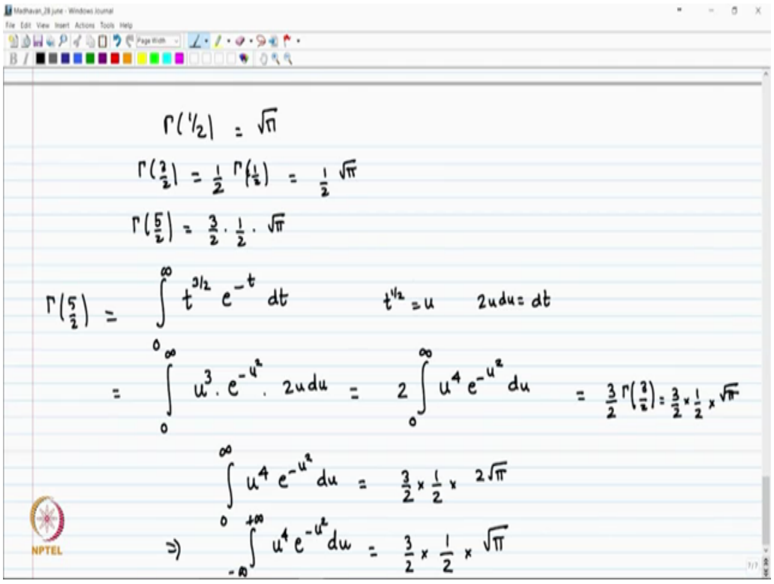

Now, gamma function of 3 by 2 is equal to half gamma function of half this is from the last expression that we saw we saw that gamma function of x is x minus 1 times gamma function of x minus 1. So, gamma function of 3 halfs will be half times gamma function of half and so this is half root pi. Similarly you can do gamma function of 5 by 2 is equal to 3 by 2 into 1 by 2 into root pi.

So, you can do this gamma we can calculate gamma function for all half integers using this method. Now let us just look back at this at this procedure. So, what we did in the substitution we replaced t raised to minus half by u and so that converted this to an integral over the over a Gaussian function now since you had t raised to minus half this u cancel this with this u. Now suppose you had; suppose you had let us say you had integral t raised to let us consider gamma function of 5 by 2 let us just take an example of a gamma function of 5 by 2. So, this is t raised to 3 by 2 e to the minus t d t. Now if I do the same substitution if I make the same substitution that is t raised to half equal to u. So, then you will have 2 u d u equal to d t just as before and now if you go through the same exercise what we will get is 0 to infinity now instead of t raised to half I have u cube e to the minus u square and what we have is 2 u d u. So, this is twice integral u raised to 4 e to the minus u square d u.

Now what I wanted to emphasize through this we know the value of gamma of 5 half. So, what you get is that, what you will get from this is the following. So, this is equal to gamma of 5 half if you write it you can write it as 3 by 2 gamma of 3 of gamma of 3 by 2 this is equal to 3 by 2 into half into gamma of half is root pi. So, what you can write? You have the following expression integral 0 to infinity u raised to 4, e raised to minus u square d u this is equal to 3 by 2 into 1 by 2 into 2 root pi. So, this is a very nice expression because you will often find such integrals appearing.

And also what this implies if you look at this function u raised to 4 is an even function e raised to minus u square is an even function. So, this whole thing is an even function. So, so what I can do is I can change the range of integration from minus infinity to plus infinity u raised to 4, e raised to minus u square d u I could do this only because the integrand was an even function. So, integral from 0 to infinity is same as integral from 0 to minus infinity. So, if I make it from minus infinity to plus infinity. So, that will just be half of the right hand side. So, that will just give me 3 by 2 into 1 by 2 into root pi.

Now, such integrals where you have a Gaussian function multiplied by a power are though are appear very commonly in both quantum mechanics and statistical mechanics and so through this gamma function we have an efficient way of evaluating these integrals. Now as I said you can do for odd also.

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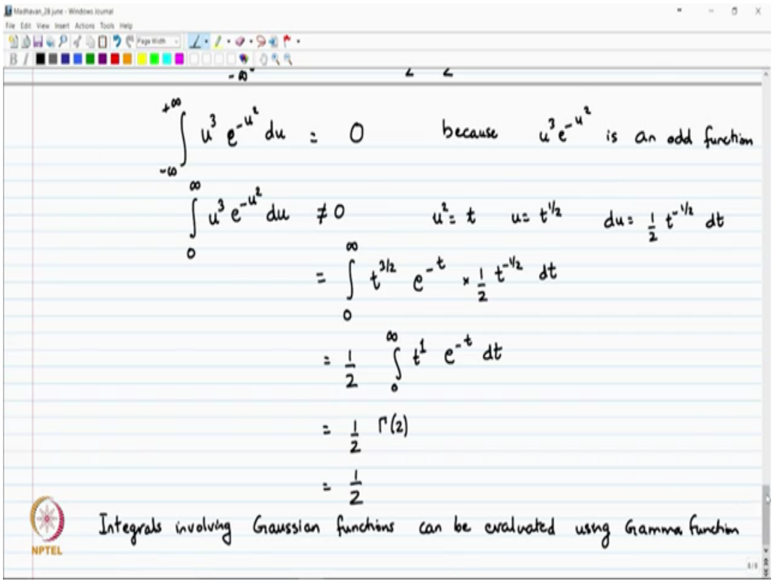

So, if you have an odd function if you have let us say integral u cube e to the minus u square d u from minus infinity to plus infinity, now this equal to 0 because u cube e raised to minus u square is an odd function in the range of integral is from minus infinity to plus infinity. However, if you take integral 0 to infinity u cube e raised to minus u square d u this is not equal to 0, this is equal to; you can use the same, you can use the same method in terms of gamma functions. So, what you will do is you go backwards. So, when we wanted what we did here was go from a gamma function to a integral of a Gaussian. So, here we will do exactly the same thing, but in the in the opposite order.

So, you put u square equal to t and u equal to t raised to half, d u equal to half t raised to minus half d t and again the limits will be the same. So, I can write this as integral 0 to infinity. Now u cube will be replaced by t raised to 3 by 2, e raised to minus t and what I have here is d u is replaced by half t raised to minus half. So, I will have half t raised to minus half d t.

So, what I will get is 1 by 2 into integral 0 to infinity, t raised to 1. So, 3 by 2 minus half is 1 or t raised to 1, e raised to minus t d t, this is half gamma function of 2 and gamma function of 2 is just 1 factorial and so this is equal to half. So, gamma function of 2 is 1 factorial which is 1, so this gives half. So, through this gamma function we efficiently evaluated these kind of integrals. So, integrals involving Gaussian functions can be evaluated using gamma functions.

Now, the last thing that I want to mention is the following. So, let us just get back to this. So, what we saw right here is that integral e to the minus u square d u from 0 to infinity is basically equal to root pi by 2.

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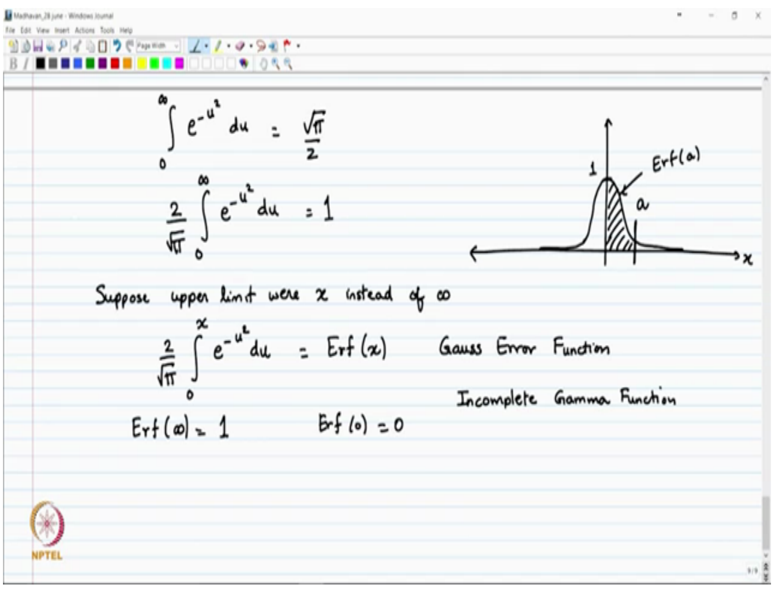

So, what we have is that integral from 0 to infinity, e to the minus u square d u is equal to root pi by 2 or in other words if you say 2 by root pi integral e to the minus u square d u from 0 to infinity this is equal to 1. Now suppose upper limit were x instead of infinity, suppose you have 2 by root pi integral 0 to x, e to the minus u square d u, this is a function of x, this is called the error function. So, Erf of x error function this is called the gauss error function or simply the error function. So, what do you know about the error function? You know that, therefore, we know that Erf of infinity is equal to 1, Erf of 0 equal to 0 that is what we know about the error function and what does it measure. So, what does it measure; and you can see this again using the integral x using a graphical representation.

So, suppose you take a Gaussian function. So, this is x, now a Gaussian function e to the minus u square will look e to the minus u square is 1 when u equal to 0. So, this is 1 when u when u equal to 0, now as a function it looks like this. So, a Gaussian function has slope 0 and then it comes on very rapidly and then it goes to and then it goes to 0.

So, unlike an exponential, an exponential function has a cusp I mean it comes sharply from 0, but a Gaussian function is flat at x equal to 0. So, this is this path e to the minus u square. Now if you integrate it, so if you imagine that you integrate it so the area under this area under this is basically this area will be root pi by 2. So, suppose you integrated it over all space and then you will get root pi by 2, but suppose you integrate it only up to a point up to some point. So, let me call this a suppose you integrate instead of integrating from 0 to infinity you integrate from 0 to a, what you will get is this area is what is the error function of a.

So, the error function is the area under the function. So, error function is also sometimes called the incomplete gamma function because the gamma function has integrals from 0 to infinity error function has integral from 0 to a. So, it is also referred to as an incomplete gamma function and error function is also something that appears very very much in both quantum mechanics and statistical mechanics. So, for example, if you are doing a harmonic oscillator problem then if you want to calculate the probability that the particle is in some region. So, the harmonic oscillator wave functions have this Gaussian form and when you evaluate integrals involving them you often encounter these error functions.

So, I just wanted to show you some of these, this I just wanted to show you this Gaussian function and this incomplete gamma function, but as we go on and we work out examples during the course you will see these functions appearing again and again. So, I will conclude this discussion on special functions here.

Thank you.