Advanced Mathematical Methods for Chemistry
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Module - 03
Lecture - 04
Cylindrical Polar Coordiates, Integrals

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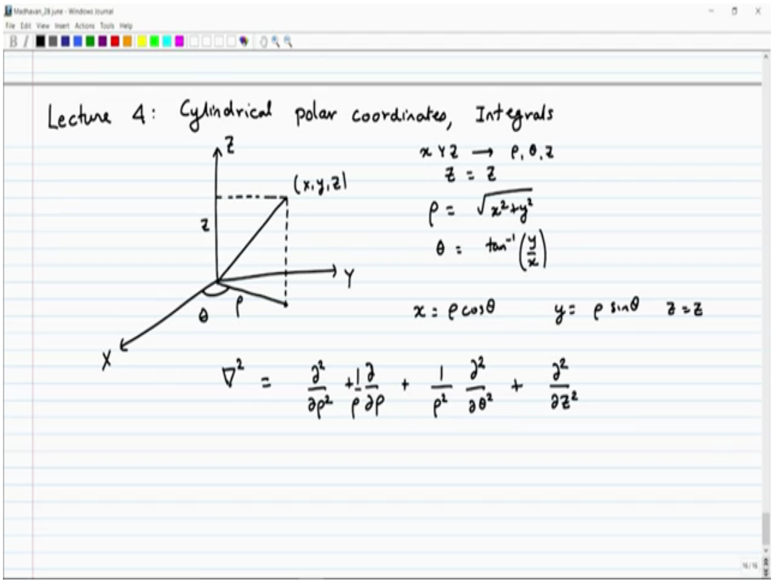

So, in this lecture I am going to discus about cylindrical coordinates and also show how you can use polar coordinates to evaluate certain integrals. So, let us start with, let us start the discussion on cylindrical coordinates. This is another coordinate system that is fairly widely used and you will see some of these in your quantum mechanics and statistical mechanics courses, but in general it is a very useful thing to know I will just briefly mention I will not do all the derivations like how we did in the case of spherical polar coordinates.

So, cylindrical coordinates are often used when you have cylindrical symmetry in your system. So, what do cylindrical coordinates look like? So, here you go. So, if this is my x y z coordinates and if I have a point whose coordinates are x y z then the in the cylindrical coordinate system the z coordinate is kept as it is, what is done is just like in the spherical polar coordinates you drop a perpendicular and this coordinate is called as rho, rho or r I mean. So, I am using rho to distinguish it from the coordinates from the r in spherical polar coordinates. So, it is a distance of the projection on to the x y plane of this point and then this is theta, this is a planer angle.

So, what do you have? So, z equal to z. So, you go from r theta phi sorry, you go from x y z to rho theta z the z is the same z is on changed rho is square root of x square plus y square and theta is tan inverse y by x. So, it is like using plane polar coordinates in the x y plane and using z as it is. So, that is where the, it is like using the circular coordinates in the x y plane and the z axis as it is. So, I can also write this as I can write x equal to rho cos theta y equal to rho sin theta and z equal to z. So, I can write this as my cylindrical polar coordinates.

And now you can write expressions for the Laplacian, the Laplacian in cylindrical polar coordinates looks like dou square by dou rho square plus dou by dou rho 1 by rho plus 1 by rho square dou square by dou theta square plus dou square by dou z square. Now thing to keep in mind is that rho is a distance. So, it has it has dimensions of length similarly it has the same dimension as x y z. So, when you are taking a second derivative with respect to z. So, that has that has dimensions of inverse length square. So, dou square by dou rho square has dimensions of inverse length square similarly 1 by dou by dou rho has dimensions of inverse length. So, you need another dimension of length. So, therefore, you need another factor of rho.

Now, theta is a dimensionless quantity. So, angles are diamond they do not have any dimensions of length. So, you need 2 dimensions of length and therefore, you need one by rho square. So, it is always good to verify that your equation is dimensionally correct now similarly you can do the Jacobean for the truck for the transformation I will not bother with that.

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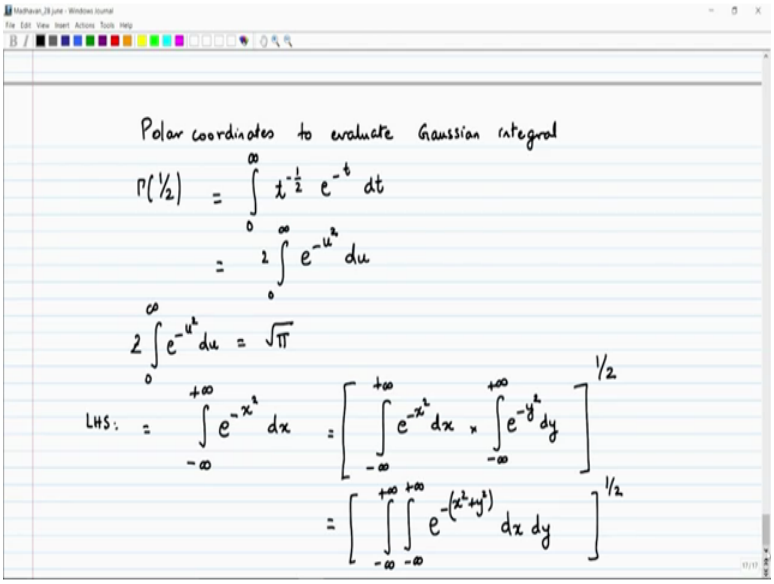

But now what I want to do next is to show is to show an application of polar coordinates to evaluate Gaussian integral.

So, if you remember when you are doing gamma function of half gamma function of half. So, what we said this was this was integral 0 to infinity t raised to minus half half half minus 1 is minus half e to the minus t d t we wrote this as we used a substitution by substituting by substituting t raised to half as u. We wrote this as twice integral 0 to infinity e to the minus u square d u, and we said that and we said that this integral e to the minus u squared d u is basically we what we said was that integral e 0 to infinity e to the minus u square d u twice integral 0 to infinity this is equal to root pi. And the now what we will do is we will actually show this we will actually show this expression we will actually show this using polar coordinates.

In order to do this let us write this right this left hand side as integral minus infinity to plus infinity because e to the minus u square is an even function e to the minus I will just call it x square d x I can use any variable for integration I just choose to use x. So, I can write now I can write this as integral minus infinity to plus infinity e to the minus x square d x times integral minus infinity to plus infinity e to the minus y square d y . So, so each of these is the same. So, whether you call it x or I call it y it is the same thing and so I will just raise this whole thing to the power half. So, this is nothing but this integral. So, I just end and I multiplied by same integral I just use a different variable y and the reason for using y will become clear. So, I wrote it in this form and now since x and y are independent variables I can write this as a double integral, integral from minus infinity to plus infinity, integral from minus infinity to plus infinity e to the minus, now I have e to the minus x square into e to the minus y square, so x square plus y square d x d y.

Now what I am going to do is I am going to use a trick I am going to convert now to spherical polar coordinates. So, what will do is will just convert to spherical polar coordinates. So, this integral we can you can write using spheric, you can write using plane polar coordinates.

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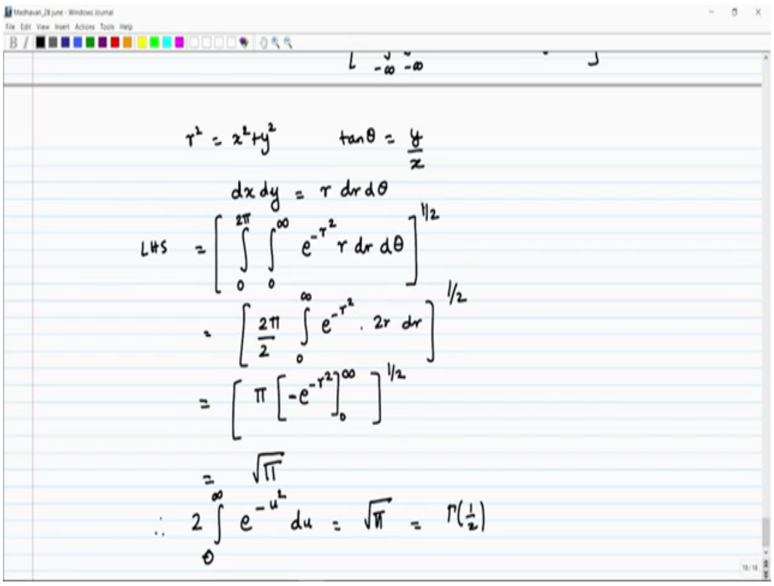

So, what you will write is you write r square equal to x square plus y square and you have tan theta equal to y by x. So, you are going to make the substitution and so and then and then d x d y this goes to r d r d theta and will put the range of integration. So, r goes from now we are we are letting x go from minus infinity to plus infinity. So, r will go from 0 to infinity theta will go from 0 to 2 pi. So, I can write my left hand side as equal to integral 0 to 2 pi integral 0 to infinity and what you have is we have e raised 2 minus r square r d r d theta and again the this whole thing is raised to the power half.

Now, you can clearly see that the integrand is independent of theta. So, I can just write this as 2 pi. So, the integral over theta will just give me a factor of 2 pi and then I have integral from 0 to infinity e to the minus r square, now I will just write it as 2 r d r and I will put a factor of 2 here and this whole thing is raised to half. And you can see why I did that because derivative of e raised to minus r square is e raised to minus r square into minus 2 r. So, I can just write this as pi times e to the minus r square with a minus sign from 0 to infinity this whole thing raised to power half. So, this will just give me now e to the minus r square when r equal to infinity this is 0, when r equal to 0 this is 1. So, I just gets square root of pi.

So, in this way what we have done is using this using this plane polar coordinates we managed to show that that integral e to the, we managed to show that integral from minus from 0 to infinity e to the minus u square d u equal to square root of pi and this is nothing, but gamma function of half, twice integral this equal to pi equal to gamma function of half. So, gamma function of half was e we have shown that that is equal to pi. This is just one example of doing integrals using different coordinates. Now often will find such will find such coordinates in various applications and you will often be working with the coordinate system that is most convenient, typically to describe the boundary conditions of the problem. So, to describe the geometry of the problem you will you use the appropriate coordinate system. So, suppose you have a system that is spherically symmetric then you know these sort of coordinates are more useful.

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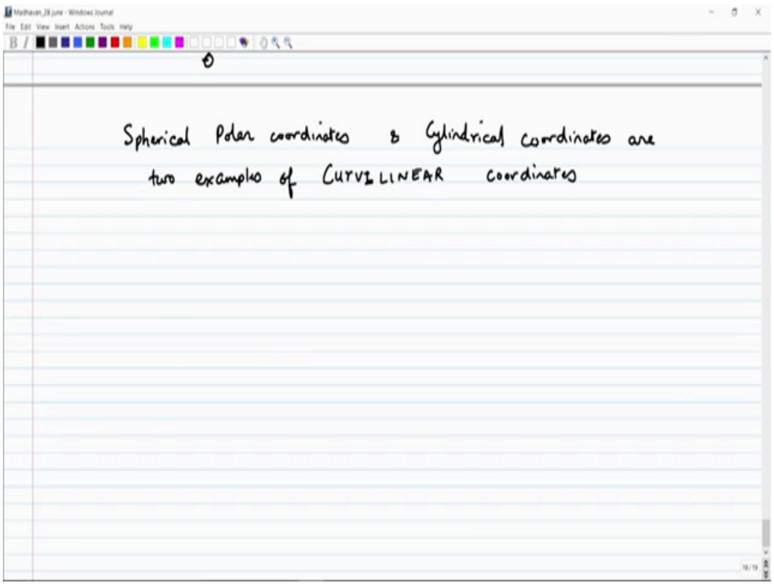

So, now, I just want to mention one thing that these this is spherical polar coordinates and cylindrical coordinates are 2 examples, examples of what are called as Curvi Linear Coordinates, Curvi Linear Coordinates and there are many more examples, there are many other examples such as electrical coordinates or prolate coordinates and so on which are used whenever you want to do and you know one of the most important applications of these coordinates is to actually do integrals. So, sometimes just as we saw in this case sometimes doing integrals are much easier in different coordinates especially when the geometry of the problem satisfies those coordinates.

So, I will stop this lecture. In the next lecture we will recap what we have done in this module and we will also look at certain practice problems.

Thank you.