Advanced Mathematical Methods for Chemistry
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Module - 03
Lecture - 03
Lecture 3 - Spherical Polar Coordinates

So in the last 2 lectures we looked at special functions, we looked at the step function the Dirac delta function and then we also looked at gamma function and the error function. Now these functions were defined in terms of integrals and these are very useful functions and we when you will see in your advanced physical chemistry courses that these functions appear very often. Today I am going to change the topic a little bit we are going to discuss about spherical polar coordinates; these are again things that you will see very often.

So, at least once you should work these things out completely. So, today I will talk briefly about spherical polar coordinates and the I will show one very interesting application of spherical coordinates in evaluating the value of a gamma function lets first work in 2 dimensions.

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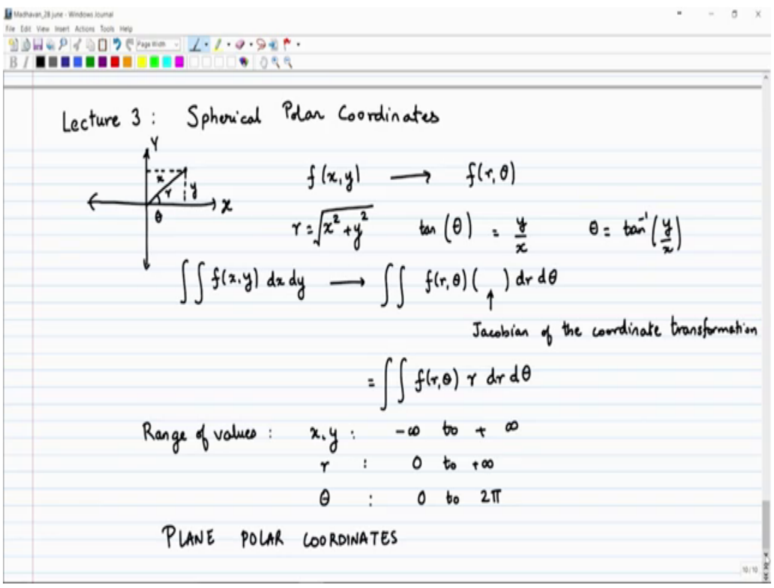

So, if you have x y space. So, typically your coordinate system is in terms of x and y and you write your functions as functions of x and y. So, any point in space has a certain x coordinate and the y coordinate ok.

Now instead of using x and y coordinates, very often we are interested in problems that have spherical symmetry or a circular symmetry. So, what you do is you define an r and a theta, theta is this angle with the x axis r is a distance of this point from the origin, and you say that r equal to x square plus y square under root theta. So, we see that tan theta equal to y by x or you can say theta equal to inverse tan inverse of y by x. So, now,. So, instead of f of x y we have we go to f of r theta. So, any function of x y is written as a function of r theta, and this is turns out to be extremely useful sometimes very often we do integrals.

So, when you are doing integrals integral f of x y, d x d y if you are doing a 2 dimensional integral now this goes this is actually equal to integral f of r theta, now instead of d x d y you would convert to d r d theta. So, will have d r d theta and you will have some object here which is called the Jacobean of the coordinate transformation. So, what is the Jacobean now I would not work out the details, but basically this Jacobean is this is just r, d r d theta and now what about let me explicitly write this as a double integral So, the first integral is over r and the second integral is over theta you have to put the appropriate limits ok.

Now what are the range of values. So, now, x and y they go from minus infinity to plus infinity r goes from 0 to infinity plus infinity. So, r is always positive. So, it is defined as the positive square root, theta now theta goes from 0 to 2 pi. So, when it goes to 360 degrees it the value of theta is 2 pi. So, these are the ranges range of values of x y r and theta. So, this is sometimes referred to as plane polar coordinates or sometimes it is also referred to as circular coordinates, now this is plane because you are in the x y plane.

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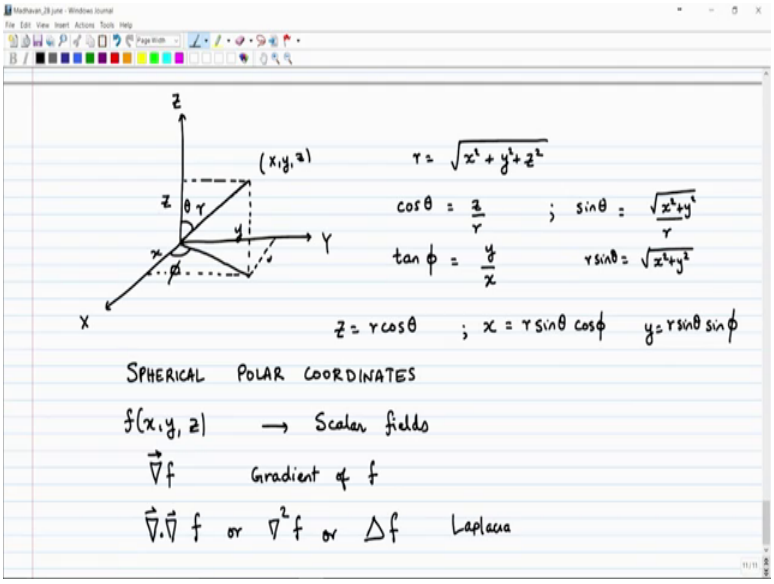

Now what happens in 3 dimensions? So, in 3 D you get what is called as spherical polar coordinates. So, here what happens is will you have x y and z, now you have some point whose coordinate is x y z then you have this it is line from the origin to that point. So, this distance from the origin third point is r, and now in this case your theta and phi have to be defined differently. So, what is done is the angle with the z axis is called theta and remember this point need not be in the x y it not it need not be at in this z y plane, it can be outside the plane. So, it can be in general it can be outside the plane.

So now the you need you need one more variable to describe it and that variable is chosen in the following way. So, you drop you project this vector on to the x y plane. So, you see where it where it falls on the x y plane and now you look at the angle that it makes with the x axis, this angle is called phi. So, what we did is we went from x y z to r theta phi what are the definition. So, clearly r is equal to square root of x square plus y square plus z square now if you just drop a perpendicular onto the z axis. So, this is the z coordinate now if you want to calculate the x coordinate. So, you can you can do it through these 2 steps first you drop a perpendicular on the x y plane then you then you project onto the x axis. So, this is the x coordinate, this is your y coordinate y coordinate. So, you can easily see that cosine of theta equal to z by r, and you can also see tan of phi. So, tan of phi is basically y by z; further you can you can you can see a few more things you can see that what is sin of theta. So, sin of theta is basically this projection and that is equal to square root of x square plus y square divided by r.

So now with this you can rewrite you can you can write z equal to r cos theta and what you can write is you can you can write x is equal to r sin theta. So, r sin theta is square root of x square plus y square. So, this implies that r sin theta is equal to square root of x square plus y square and so, I will (Refer Time: 08:55). So, this should be y by x. So, x will be r sin theta cos phi and y will be r sin theta sin phi. So, you can see that y by x is tan phi and it is satisfies this condition. So, this is a definition of the spherical polar coordinates. Now you can do you can do various things, now if you remember we where we went to functions of x y z we call them as scalar fields and you if you remember we define things like divergence of a scalar field or oh sorry the gradient of a scalar field, gradient of f and we also had a gradient you can also take a gradient dotted into gradient of f or del square f which is or which is also denoted by Laplace this triangle of f, which is called the laplacian of f.

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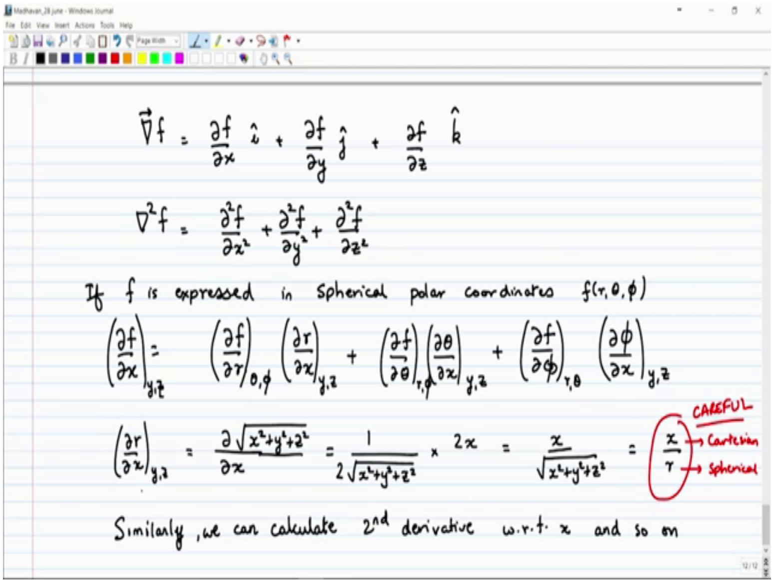

Now, if you remember the expression. So, we had gradient of f was dou f a dou x into I plus dou f by dou y into j, plus dou f by dou z into k. And the laplacian of f this was given by dou square f by dou x square, plus dou square f by dou y square, plus dou square f by dou z square ok.

Now what you can do is you can actually get expressions for each of these. So, if you had f in spherical polar coordinates. So, if f is expressed in spherical polar coordinates. So, if you had f of r theta phi then what you can do is you can write dou f by dou x as;

now remember when you keep will take dou f by dou x you are keeping y and z fixed. So, you can write it as dou f by dou r keeping theta and phi fixed times dou r by dou x keeping y and z fixed, plus dou f by dou theta keeping r and phi fixed times dou theta by dou x keeping y and z fixed, and you have dou f by dou phi keeping r and theta fixed times dou phi by dou x keeping y and z fixed. So, notice all I did was I wanted a derivative with respect to x of f. So, I take derivative of f with respect to r times derivative of r with respect to x, but f also depends on d theta. So, I take derivative of f with respect to theta times d theta by d x; similarly they also depends on phi. So, I also take that and this is the derivative with respect to x.

Now this if you know this function as a function of r theta phi you can write you can evaluate this. So, I want explicitly write these quantities that are constant, but you should remember that whenever you take derivative with respect to x, you are keeping y and z fixed when you take a partial derivative with respect to r or then you keep theta and phi fixed and so on. But I can write is this what is dou r by dou x keeping y and z fixed. So, then you have to write equal to you have to write r in terms of x y z dou by dou x of square root of x square plus y square plus z square. So, this is keeping y and z fixed. So, y and z are like constants. So, if I take a derivative of a square root. So, I get 1 over square root of x square, plus y square, plus z square.

Now I take d by d x of this quantity that is just 2 x y and z are constant. So, this is 1 1 1 over 2 I square root of x. So, this is just x divided by square root of x square plus y square plus z square, and you can write this as x by r, but you should be very careful. So, you can what a via mean you should be careful is because x by r is actually put this in this be careful when you write such expression, the reason is because they are in 2 different coordinate system. So, x is a in Cartesian whereas, r is in spherical polar spherical coordinates ok.

So, writing something like x by r is something that should be done with extreme care. Using this I can write the derivative with respect to x and once I have a first derivative with respect to x I can also calculate the second derivative with respect to x. So, similarly we can calculate second derivative x and so on. So, let me just mention a few things let me just write some of these partial derivatives that appear.

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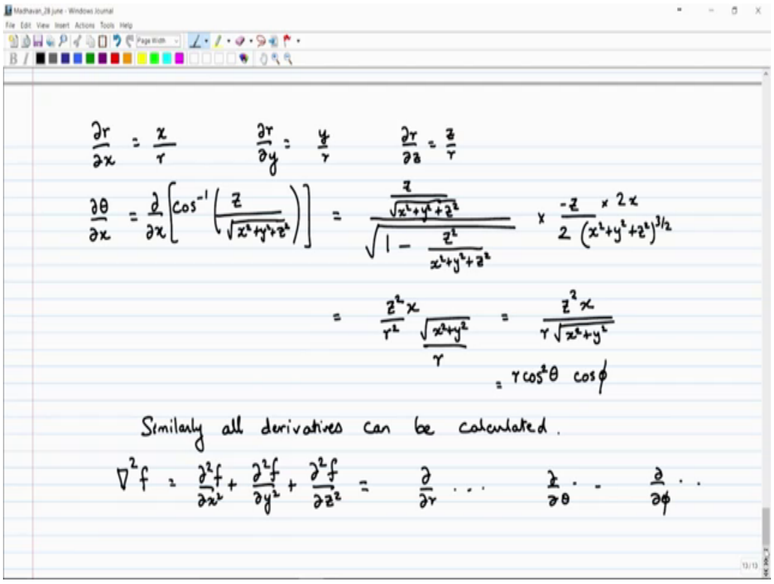

So, if you take dou r by dou x this I wrote it as x divided by r, dou r by dou y will be y by r, dou r by dou z will be z by r; now let us just look at some derivatives way of theta. So, what is dou theta by dou x? So, what is theta? So, we wrote theta as tan rather as cos inverse of z divided by r, now I cannot write r I have to write it as square root of x square plus y square plus z square and you are taking d by d x. See I wanted to take a derivative with respect to x keeping y and z fixed. So, therefore, I have to write it in this form now So, this is what you will get for d theta by d x now you have to write the derivative of cos inverse of some quantity.

So, this will give me a. So, derivative of cos inverse is just that quantity divided by square root of 1 minus now I will have z square divided by x square plus y square plus z square and now I have to take the derivative of this quantity with respect to x. So, what I will get is. So, it is you have something raised to minus half. So, it is. So, I will write z divided by 2 and what you have is x square plus y square plus z square raise to 3 by 2 and minus sin here, and then you have to take the derivative of x. So, you will get twice x again it looks very tedious, but you will find that lot of things will cancel ok.

So for example, the x. So, once we have done this I will just replace this by r. So, this is z by r this is minus z by r cube. So, I will have a z square by r square, and then I have an x that is (Refer Time: 18:58) around and then and then what do I have here now I have x square plus y square plus z square minus z square. So, that is x square root of x square plus y square and then divided by square root of x square plus y square plus z square that is just r square. So, I will have r divided by r. So, what do I get? So, I finally, get the expression is z square x divided by r square root of x square plus y square. So, and you can write this in a slightly different way. So, if you if you realize that z by r is. So, z square I can write as r square cosine theta. So, I will be left with r cos square theta and then x over x square plus y square is nothing, but cos phi. So, I will have r cos square theta cos phi ok.

So, similarly you can calculate all derivatives can be calculated and you can write a Laplacian and we can write an expression for del square f is equal to dou square f by dou x square, plus dou square f by dou y square plus dou square f by dou z square, I can write this in the entire thing in to in spherical polar coordinates. So, we can write this in terms of dou by dou r, dou by dou theta and dou by dou phi. So, we can write this expression; now if you work out this expression it is quite a long expression and I will just write it. So, you have to go step by step you have to calculate each derivative individually and you have to work it out. So, I will just write the final expression. So, this is something that you will use quite often in problems in quantum mechanics.

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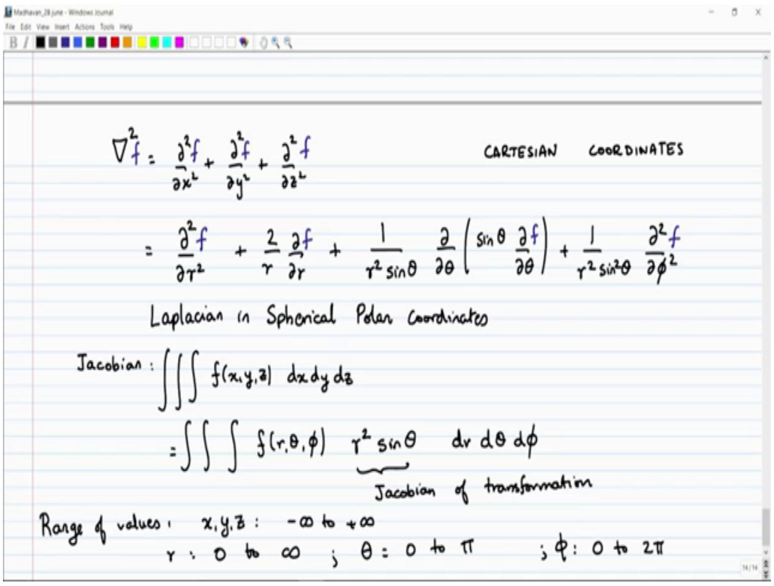

So, I will just write the expression for del square ok which is written as dou square by dou x square this is written in an operator notation dou z square. So, this is in Cartesian, when you write the expression for the Laplacian and Cartesian coordinates it just looks it looks very straight forward it looks like dou square by dou x square plus dou square by dou y square plus dou square by dou z square, now when you write it in spherical polar coordinates the expression is considerably more complicated, but you can works out. So, you have a dou square by dou r square term, then you have a term that looks like 2 by r dou by dou r, then you have a 1 over r square sin theta and you have dou by dou theta of sin theta dou by dou theta, and then you have a plus 1 over r square sin square theta dou square by dou phi square ok.

So this is the expression for laplacian in spherical polar coordinates and this I will written it like an operator. So, I have not shown the function that it is acting on I will not explicitly shown the function. So, I have just shown it like an operator and this is the operator that corresponds to the laplacian. So, if you had a laplacian of f then what you write is laplacian of f then you will have f in all these places. So, the derivative will be of f. So, here you will have 1 derivative and then you are take the derivative of this whole thing of sin theta d f by d theta, here will take a second derivative with respect to f. Now this is a very useful expression that you will see quite often another thing that will appear very often is what is called the Jacobean. So, this appears in suppose you have integral f of x y z, d x d y d z, it is a 3 dimensional integral. So, you are integrating over x y and z. So, then I can write this as I can I instead of x y z I can write this function of r theta phi and I have the 3 limits, now what I will have is instead of d x, d y, d z I will have d r, d theta, d phi times some quantity which is called a Jacobean ok.

So, this quantity what appears here is r square sin theta So, this is the Jacobean of transformation and now. So, this integral will be replace by this now the range of values. So, x y z go from minus infinity to plus infinity now r goes from 0 to infinity, theta goes from 0 to pi and phi goes from 0 to 2 pi. So, now initially it might seem a little confusing why theta goes from 0 to pi and phi goes from 0 to 2 pi, but we can see this by you can see this geometrically.

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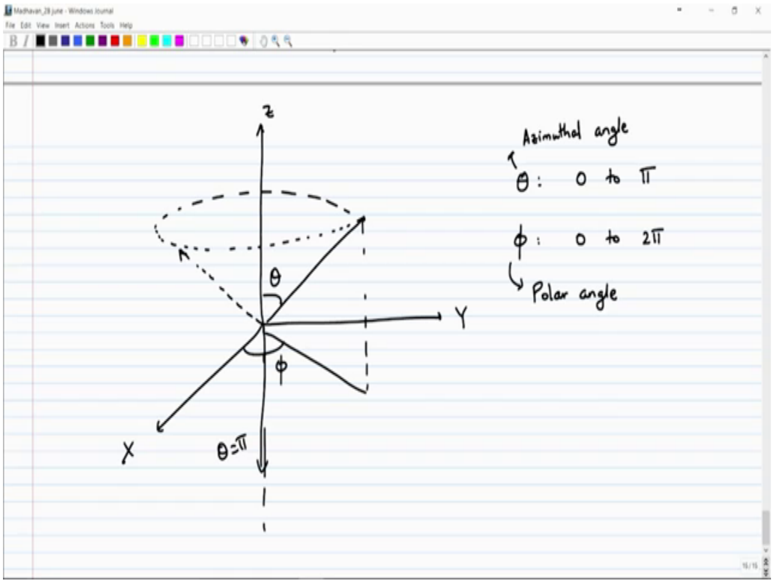

So, if you have if you have your coordinates x y and z, and we took some point and this point might be outside the y z plane and we said that this angle is theta. So, there is a this cone that goes like this and so, anywhere on this cone anywhere on this cone the angle with the z axis will be theta. So, whether you are here whether you are even if you are here at this along this line the angle will be theta. So, here also it will be theta.

So now theta can only go from 0 to pi because once you reach pi then all you are pointing along the negative z axis. So, when theta equal to pi you point along the negative z axis So, here theta equal to pi along this direction, and if you go more then as I said you know theta is only defined with respect to the z axis. So, you cannot go more than pi. Now what about phi? Phi is defined in the x y plane. So, this is my phi and clearly phi can go all the way from 0 to 2 pi, phi can go all the way are from 0 to 2 pi. So, therefore, we emphasize the theta goes from 0 to pi phi goes from 0 to 2 pi.

So, phi is called the Polar angle theta is called the Azimuthal angle So, I will conclude this lecture here. So, we have learnt about spherical polar coordinates and I have spent quite a bit of time discussing this what happens is you do spherical polar coordinates if you learn it very well then the learning other coordinate systems like the cylindrical polar coordinate system or elliptical coordinates becomes very straight forward. So, what I have tried to show you have tried to show you some of the things that you learn in spherical polar coordinates, and you know there are lot of formal derivations which I have skipped, but at least you will be familiar with spherical polar coordinates after this and you can you know where wherever you have to learn some new coordinate system it will be relatively straightforward.

Thank you.