Mathematics for Chemistry
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Module - 03
Lecture - 02
Surface and Volume Integrals

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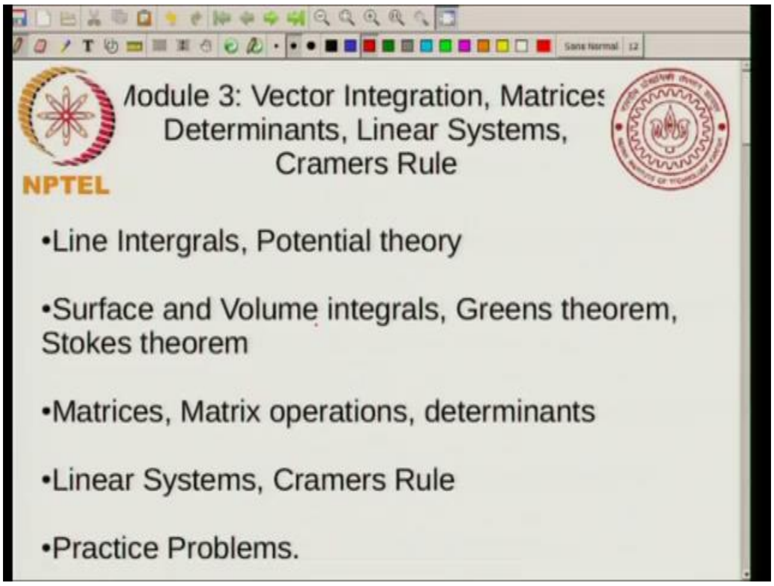

So in this lecture, I will be talking about surface and volume integrals and this is another way of doing a vector integration, which is slightly different from the line integrals that we saw earlier. And I will just be mentioning these and just mentioning a couple of theorems. I would not be spending too much time on these, but I just wanted to mention them for completeness.

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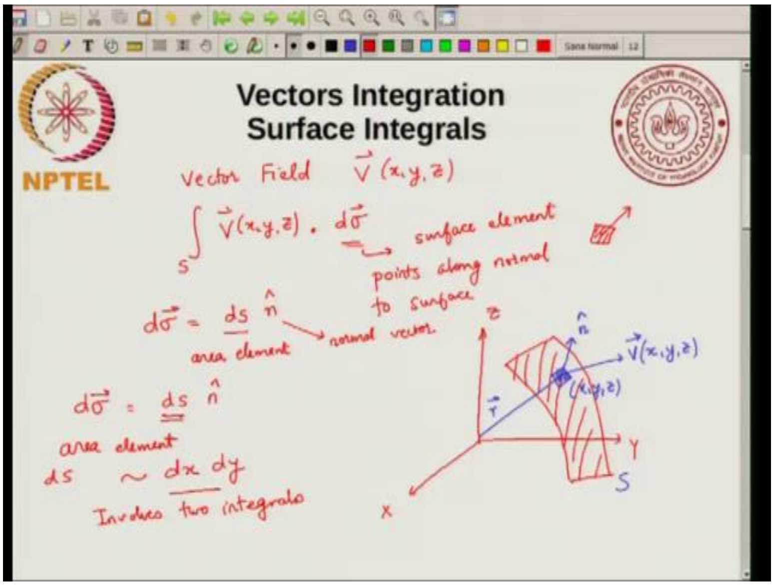

So, what is the surface integral? Surface integral is actually very similar to a line integral only thing is you are integrating instead of integrating over a line you are integrating over a surface. So, now, in this case a surface is a 2 dimensional object. So, it will be a 2 dimensional integral. So, instead of just having a d x or a d y you will have an integral over something like d x d y. So, what are the different surface integrals that you can have? So, you can define them in different ways, I will use the most common way in which we will be talking about surface integrals. Suppose you have a vector field V of x, y, z. So, it has 3 different components, then you can define your surface integral as integral V of x, y, z is sorry not x, y, z, I just want to take. Yeah, we can take x, y, z and you dotted into d sigma. So, d sigma and you integrate over some surface S.

So, this is the surface element, it is a vector. So, it is something like this. So, just this is a like will be a small region of the surface and it is a vector; it points. So, it points along normal to surface. So, in other words I can write d sigma as t d s; s is an area element times n hat; n hat is a normal vector. So, this is an area element, this is a normal vector. So, in the range of integration is the surface. So, you integrate over a surface S. So, just pictorially I will show you, what you mean is you are, you have. So, if you have X, Y, Z space now you have a vector field; vector field V is defined at each point. So, you have these vectors defined at each point in the space. Now suppose you want to do the integral over some surface.

So, if you want to integrate this vector field over the surface this is my surface denoted by S. So, suppose I want to integrate this vector field over the surface S then, what I imagine is, my imagine taking some small element of the surface and in this for the small element there will be a normal vector n hat; n hat that points normal to the surface. Now the vector field V at this small element, you will have a vector field that points in some direction V, eight points in some direction and it has some magnitude. So, if this point is r which is given by X, Y, Z then V of x, y, z is a vector at this point that points in some direction.

Now there is also this element of the surface also has a normal. Now we take a dot product of these 2 and you do this for each little element. So, you do this for each little element when you integrate over the entire surface, you add them up you will get the integral. So, this is the surface integral. Now notice that this d sigma equal to d s n hat and this d s is an area element and typically what will appear depending on the problem that you are doing, you will have an area element it includes something like d x into d y.

So, it will have something like d x into d y not exactly equal to, but it will have something that appears like a d x, d y. So, involves product 2 integrals. So, in general if you want to calculate a surface integral, you have to do 2 integrals; one over d x and one over the d y. Now in certain cases you might use spherical polar coordinates. So, instead of d x, d y you go to d r d theta and so on, but the basic idea of a surface integral is that since you are integrating or a surface, surface is a 2 dimensional object and so your integral will have, you will have to do 2 integrals. So, I would not talk too much about this in detail, but you will do some problems later on that involve these integrals.

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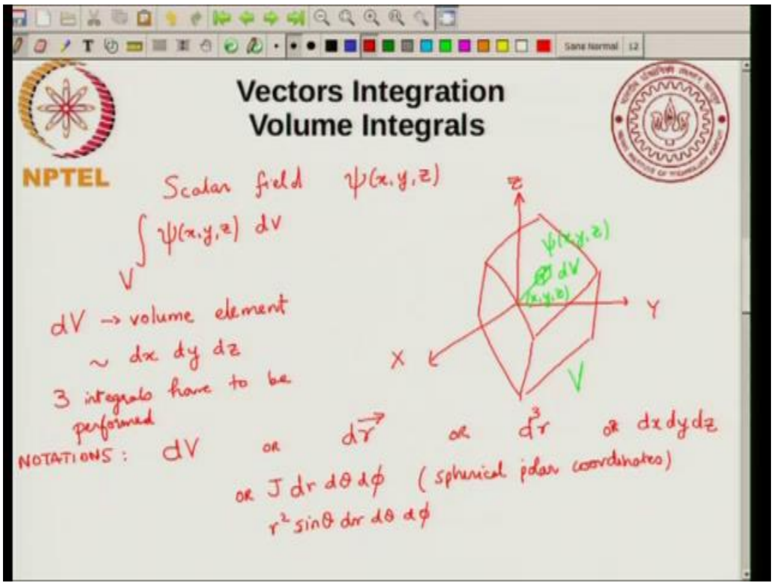

So, now we have talked about line integrals, we have talked about surface integrals. So, the naturally the next thing to do is to talk about volume integrals. So, that will be the next thing. Now here what you have is you can; now here what I will do is I look at scalar field. Now before I go to volume integral, let me just may emphasize one thing. Now notice that V here the way I have defined the surface integral, V is this, this is my surface integral. This is one definition of the surface integral and this is one popular definition. So, V is a vector, d sigma I have chosen it to be a vector. So, V dot d sigma is a scalar. So, whatever I will get will be a scalar and so my result will be a number.

So, now, for volume integrals, what we will do is we will start with a scalar field. Now my scalar field let me call it scalar field psi of x, y, z. So, if I take a scalar fields psi of x, y, z then, what I want to do is I want to do an integral over psi of x, y, z over a small volume element, over a volume element and I might integrate it over some volume V. So, what does this mean? So, again we go to our picture. So, this is our space X, Y, Z and you might have some volume that is shaped like this, I mean I am just showing some arbitrary shape just to emphasize that you know you do not need to have very symmetric shapes, you have some volume V. So, this is my volume V and you might have some; now imagine that within this volume V you take an infinitesimal volume element d V.

Now your scalar field, so if this point is let us say this point is x, y, z then the scalar field at this point is psi of x, y, z. So, what I do is I construct all these little little volume elements, I add all of them up. I calculate the psi at each of these little volume elements, I added up and I will get an integral over, I will get this volume integral. So, what is important about this? So, what is important is that d V is a volume element. It is a volume element; that means, you are integrating over an entire volume. Now a volume element typically has it is a 3 dimensional object. So, it has something like d x, d y, d z. So, you have to do 3 integrals. So, 3 integrals have to be done. So, in general you can write this in different ways.

So, sometimes instead of d V, you can use the symbols used vary; so d V, so notations. So, the commonly used notations are d V or d r vector, again d r vector is used to define to say volume integrals or you can use d cube r without the scalar sign. So, or you can just say d x, d y, d z; d x, d y, d z is if you are using Cartesian coordinates. So, in other coordinates, if you are using different coordinates you can always use, you can use I will put a J d r, d theta, d phi. So, if you are using spherical polar coordinates you can use d r, d theta, d phi. There is a factor that comes here, this is called the Jacobean of the transformation, but you know we will come to that a little later, but basically you need to do 3 integrals, in and you know this is in spherical polar coordinates. And in particular for spherical polar coordinates J is basically r square sin theta, d r, d theta, d phi.

So, I mean there are different ways to write this volume integral and often you will find that this, notations based on what kind of region you have. How you can specify your V? You choose the appropriate coordinate system. So, that is how much I want to say about volume integrals.

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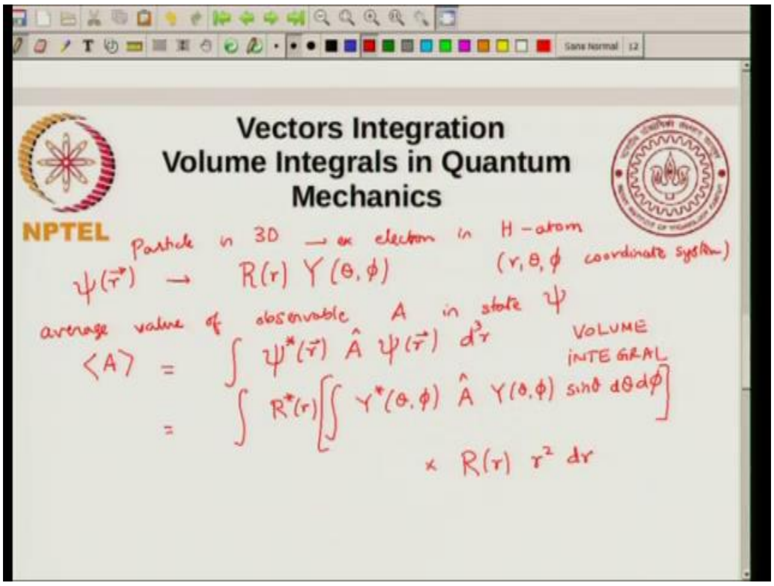

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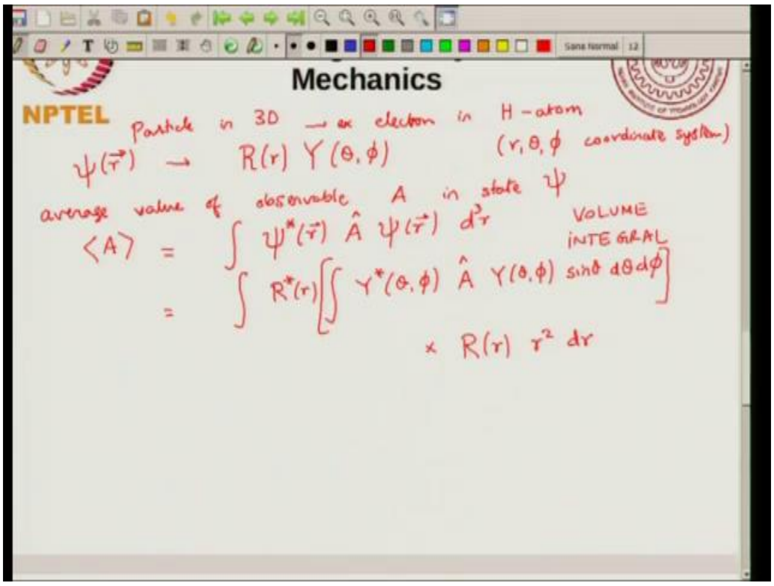

I just want to mention one thing that volume integrals you see them very often in quantum mechanics. Now suppose you have a particle in 3 dimensions like let us say, a hydrogen atom; particle in 3 D; so for example electron in hydrogen atom. So, now, this electron is defined by a wave function psi, which is a function of r, which most conveniently is written as a function of as a radial part that depends only on the r and angular part that depends on theta and phi. So, most can this angular part is denoted by Y and that is called the spherical harmonic and the radial part depends only on r. So, r theta phi is the coordinate system that you are using.

Now, any property you want to calculate involving psi of r involves integral. So, suppose you want to calculate, let us say the average value of observable A in state psi. So, when your electron is in state psi then, what is the average value of observable of some observable A? Then what you do is you denoted as average value of A, expectation value of A and to do this what you will do is you calculate an integral and that integral that you calculate is psi star of r and then you have A an operator, operating on psi of r. And then what you have is, d cube r or d r or d V. So, this is a volume integral and what is done typically in such cases is you separate this into 2 parts. You separate this into a radial part and you separate it into an angular part and what is done is depending on the observable. So, what is done is, you write this as 2 integrals, you write this as an integral over of psi star of, can we write it slightly differently.

So my psi is written as a product of this radial part and an angular part. So, you will have R star of r and you have Y star of theta phi and now you have this operator A and you have Y of theta phi and you have sin theta, d theta, d phi and you have and this multiplied by R of r, r square d r. So now just look back in the previous think, what I said is that your d x, d y, d z or d cube r is r square sin theta d r, d theta, d phi. That is a property of spherical polar coordinates. So, in spherical polar coordinates you have this r square, now r square will only look at the integral over R. It does not affect the integral over theta and phi. So, R this capital R and rs and the little r square they do not affect the integrals over theta and phi. So, so you can break up this integral in this way and this is something that you routinely do and you know whenever you calculate properties in quantum mechanics for 3 dimensional systems then you have these volume integrals. So, it is something that you get used to doing very routinely in quantum mechanics.

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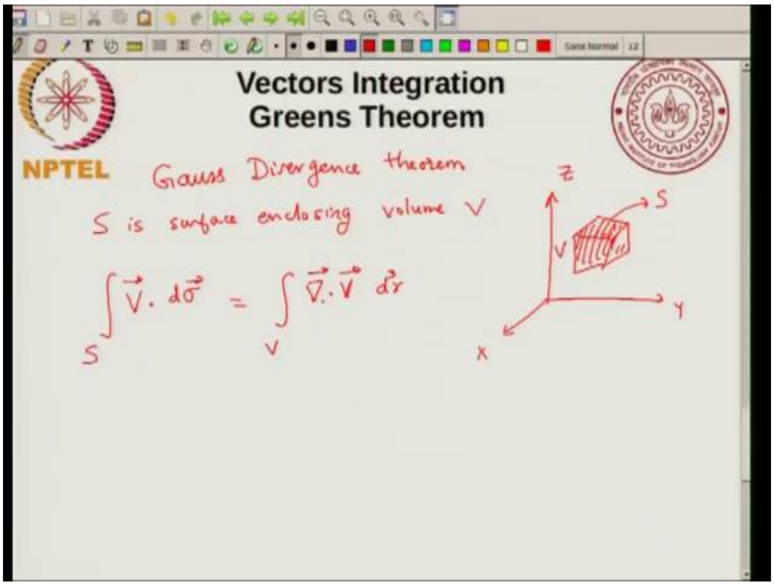

Now next we will just talk about Greens Theorem or this is also known as Gauss Divergence Theorem and this is very useful when you want to convert an integral between a surface integral and a volume integral and vice versa. So, what does this say? Suppose you have this X, Y, Z and let us say you have some volume V. So, you have some volume V and this volume, the surface enclosing this volume is S. So, S is the surface enclosing volume V then you have a nice theorem which basically says that if you have an integral over a surface of a vector field dotted into d sigma, which is the usual surface integral you can write this as an integral over a volume. So, here you are doing integral over 2 dimensions. So, now, you are making it a 3 D integral and what you have is instead of V, you have a divergence of V and d cube r. So, this allows you to go from volume integral to surface integral. This again is extremely useful I mean volume integral involves all these points in the interior, surface integrals involves only a points on the surface.

Now in some cases it is very easy to calculate the, it is much easier to calculate surface integrals and volume integrals. So, you will use it in the reverse way. So, if you have a complicated volume integral then you will calculate the, then you will convert it to a surface integral. In other cases the surface integral might be difficult to do and it might be easier to write the volume integral. So, based on your problem you can go from surface integral to volume integral and vice versa. This is known as gauss divergence theorem. Now obviously, you might ask is there a wave to go from surface integral to line integral? And the answer is yes, you can go from a surface integral to a line integral. So, that is what is called as Stokes Theorem helps you to go from a surface integral to a line integral.

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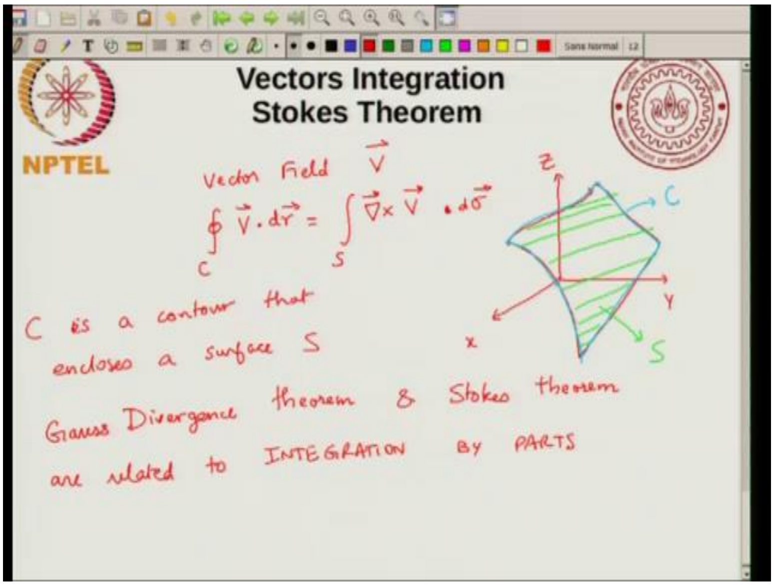

So, in this case you can write suppose you had a vector field V then you can write your integral over some curve, a line integral of V in the following way. I will just mention this again what is C? And what is V? So, you have X, Y, Z, you have some surface s this is S. S is the surface and I will just mark this contour or this curve that is enclosing surface C. So, C is a contour that encloses the surface S. So, C is a contour that encloses a surface S. So, and notice that it is a closed contour. So, it is a closed contour, I will just mark it with a closed loop here, yes; a c is a closed contour that encloses the surface S then, this line integral can be converted to a surface integral, can be converted into integral over S and what you have is something dot d sigma, d sigma is a usual surface integral element and what you have here is the curl of V. So, curl of V is a vector, this dotted into d sigma will give you a scalar. So, you have a scalar here and a scalar here.

So, in this way you can convert a surface integral to a line integral and vice versa. You can convert a integral over a closed contour to an integral over the surface that is enclosed by the contour. This is again and I mean there are lots of subtleties in this and you know this can be done and this is a very powerful theorem. This is called Stokes Theorem and these are extremely useful in especially in continuum descriptions, when you describe things as functions of variables of space. So, then these are very useful to do, I am just mentioning these for completeness. I will also mention one thing that both Gauss Divergence Theorem and Stokes Theorem. So, both these are in some ways related to are related to what is known as integration by parts. What I mean to say is that these are some sort of versions of integration by parts. So, they are some way related to integration by parts. In fact, if you look at standard books and see how they prove Greens Theorem and how they prove the Gauss Divergence and Stokes Theorem, they do use the method of what you have learnt about integration by parts. Notice that you know, in integration by parts I mean you have one term that has a derivative and one term that does not have a derivative and in the other case, the derivative is shifted to something else right. So, these are exactly manifestations of that for vector integrations. So, I will stop here with the discussion on vectors. In the next class we will start discussing about matrices.

Thank you.