Mathematics for Chemistry
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Lecture - 5

So far, we have looked at vectors we have seen, we have looked at products of vectors. We have looked at also how operators on vectors convert vectors to other vectors? We have also briefly looked at functions of vectors and we looked at this coordinate transformation, which is a very useful operation in keen various fields of theoretical chemistry. So, now next we are going to talk about differentiation with respect to vectors.

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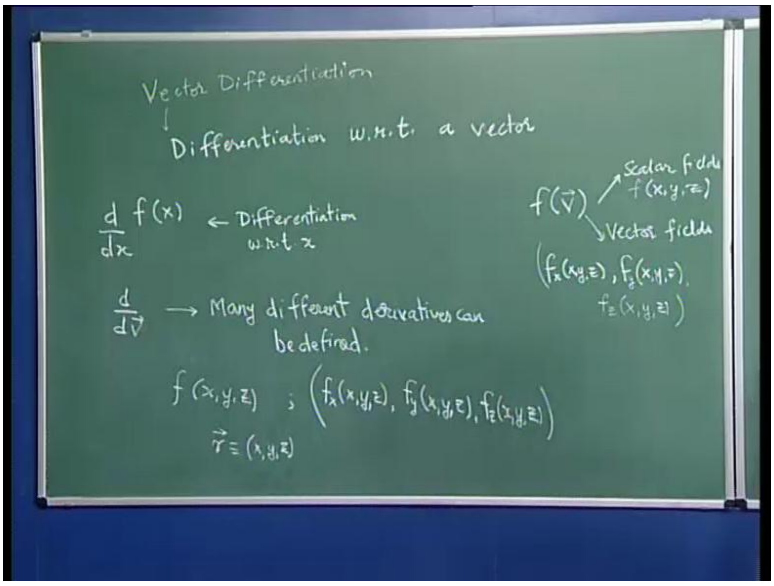

So, this is the topic of vector differentiation, and the idea here is the following that we have seen this is actually differentiation with respect to a vector. So, this is with respect to a vector; so the idea is that if you had a function f of a single variable, then we can define something like d by d x. So, this is differentiation with respect to x, where when x the simple scalar variable and d by d x is the usual derivative.

Now on the other hand, if you had function of vector so, we have already looked at functions of vectors and if you remember functions of vector are of two types. One is called the scalar fields. So, for example f of x, y, z and the other are the vector fields and these are of the type f x of x, y, z f y of x, y, z and f z of x. Thus the function itself has three components and each component is a function of x y and z. So, we have two kinds of functions scalar fields and vector fields.

Now we want to look at an operation, where instead of differentiating with respect to x, we differentiate with respect to a vector. So, we have something like d by d v of a vector. Now it turns out that, there are many ways of doing this. This is many ways, many different derivatives can be defined and what we will do is we will look at three very popular definitions of these derivatives. so and for the rest of this lecture I will be considering the coordinate base x, y, z. So, you have functions of x,y,z. So, you have scalar functions and you have vector functions. Vector functions will have three components. So, this is what I will be considering for the rest of this lecture.

So, when I say differentiation with respect to a vector, the vector will be that vector that has components x y z; so the vector r which has components x, y, z. So, we will try to differentiate with respect to r. So, wherever we have this d by d v the object with respect to which we are differentiating is r. So, now if you are just to think out of the box, how you would define a differentiation with respect to r. Now you can say r has components x, y and z. So, I could do various things. I could differentiate with respect to x, I could differentiate with respect to y, differentiate with respect to z and add them.

Ok or do various other combinations and each of these combinations and there are 3 such combinations, which are extremely useful and each of them has a name. And I will describe them briefly here. So, the first one is the gradient and one more thing I have to say is that, now you can take a derivative of either a function like this vector field with respect to x y z with respect to a vector or you can take a derivative of a scalar field with respect to this vector. And so there are lot of combination of things you can do and these correspond to various definition of these vectors of derivatives.

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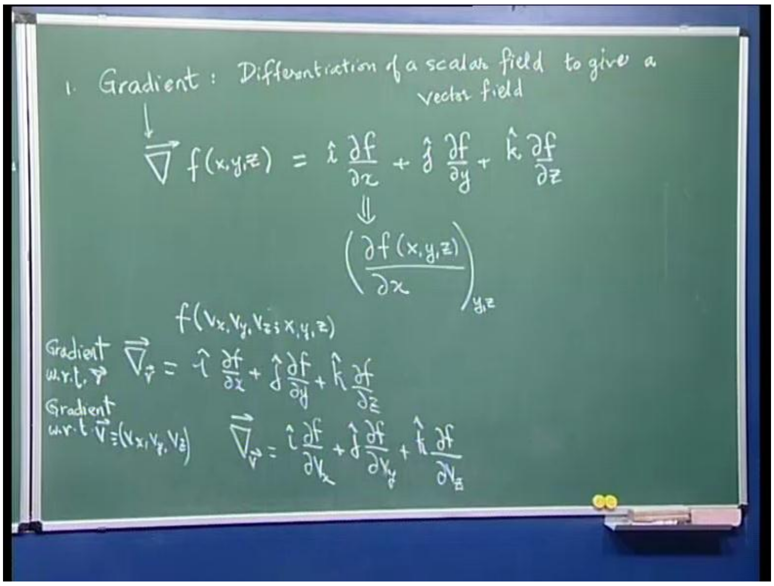

So, the first one we will consider is a gradient and a gradient corresponds to differentiation of a scalar field and it is always with respect to a vector and this gives a vector field. So, what this happens in the gradient is that you take a scalar field, you differentiate with respect to r and you get a vector field. And the definition of the gradient is as following so, the gradient is the symbol for the gradient is this and it is usually denoted as a vector, because when you differentiate, when this operates on a scalar field.

It gives a vector and therefore, this vector symbol is used on top of the gradient operator. So, when this acts on a scalar field it gives a vector and the definition of the gradient is following, this gives you i plus. So, you can differentiate this function. This is a function of many variables of x y z. So, you can take various partial derivatives and whenever you take partial derivative with respect to x you are keeping y and z fixed. So, you are taking a partial derivative of this function of x y z with respect to x keeping y and z fixed. So, I will write this explicitly, this is partial derivative of f with respect to x y and z keeping y and z fixed.

So, instead of writing this whole all these details, I will just use the short notation here. So, partial derivative of f with respect to x; this is partial derivative of f with respect to y. This is f with respect to z and notice that the gradient is a vector that points along this direction, along a direction and these are the three components of the gradient. So, you started with ((refer time: 08:29)). So, you took the derivative of a scalar field and what you got was a vector. Now I will just mention it briefly here, but I would not, we would not be dealing too much with that. Now here I took a gradient with respect to the r vector. So, this is gradient with respect to the r vector. You can now if your f can be written as a function of V x, V y, V z and let us make it slightly more complicated. So, it can be written both as a function of V x, V y, V z and as a function of x, y, z. So, the value of f at any point depends both on x, y, z and on V x, V y, V z.

Now, you can define a gradient with respect to just as you can define the gradient with respect to the r vector. So, this is gradient with respect to r vector and this will be defined in this form. So, it will be I, but you can also define a gradient with respect to the V vector. So, if I say V vector and V vector is just V x, V y, V z. So, how will this be defined?

So, in this case notice f is also a function of V x, V y, V z. So, the gradient with respect to V vector will be defined as i. Now instead of taking derivative with respect to x, you take derivative with respect to V x plus j to V z. So, you can define gradients with respect to any vector so long as your function is a function of those coordinates of that vector.

Now, for most of the course when I do not write this r, it is assumed when i just write a gradient without any without any vector symbol here, it is assumed that the gradient is with respect to the r vector or whatever which is the arguments of this function. So, let us take let us take a simple example of a gradient.

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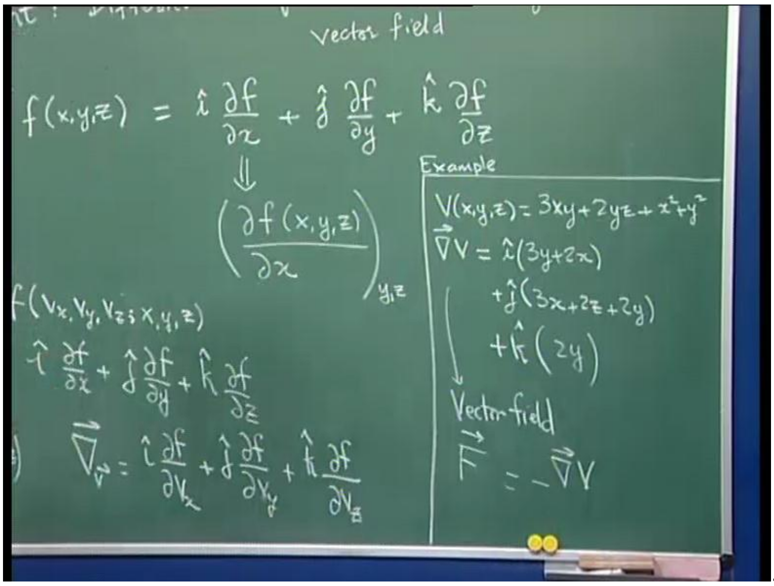

So, let us evaluate the gradient, I will give a function suppose I have. So, let me do it right here. If I have V of x is an example is equal to, I will take it as 3 x y plus 2 y z plus x square plus y square. So, this is a scalar field, it is a function of x y z. And if I take the gradient the, then this will have i and the i component is you take the derivative with respect to x. So, the first term will give you 3 y, second term will give you 0, third term will give you 2 x and the fourth term will give you 0. So you have 3y plus 2x and then plus j. Now in this case the first term will give you 3x, second term will give you 2z, third term will give you 0, fourth term will give you 2y.

And the k component, first term will give you 0, second term will give you 2y, third term will give you 0, fourth term will give you 0. So, the various components of the gradient are all functions of x y z and so your gradient is a vector field and that is what we said. We differentiate a scalar field and we get a vector field. So, this is the gradient operation. Now the gradient operation has a very important role in mechanics, often in mechanics the force is a vector and this is written as a negative gradient of the potential. So, if you have a type of force called a conservative force, then you can write it as a negative gradient of a potential and we will look at this example, in a little more detail. This is very useful when you are calculating the work done by a force and let us say displacing a particle or some such problem.

So, this is one very important application of gradients, but I mean gradients appear in various other fields also in thermo dynamics, in statistical mechanics, in quantum mechanics. So, you will see lot of application of this gradient operator.

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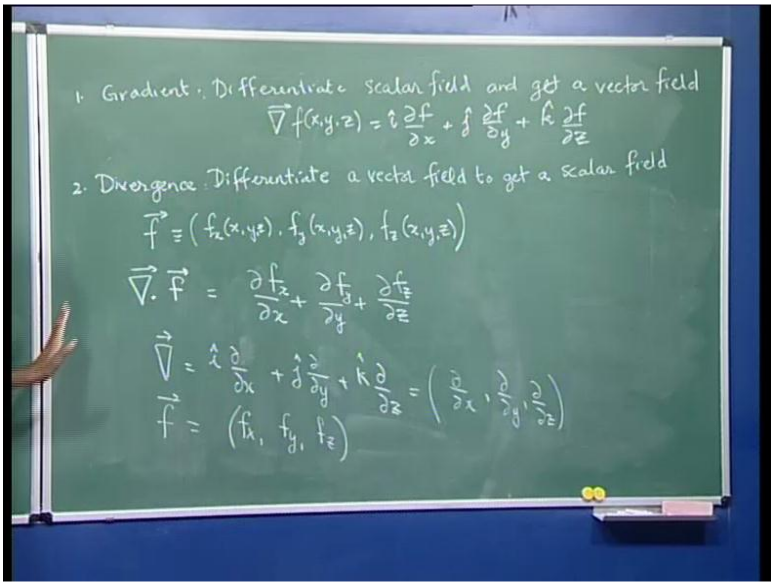

So, the first type of derivative we have was a gradient operator and what we said is that it is, you differentiate scalar field and get a vector field. So, in other words what you started off was a scalar and when you differentiated, you got a vector. So, we represented this by gradient operator and gradient of f of x, y, z as a y plus k. Now the next kind of vector derivative that we will see is something called the divergence. And in the divergence what is done is you differentiate a vector field to get a scalar field. So, here you have a vector, you have a vector field with various components.

So, if you had a vector field f with various components f z of x, y, z. Now the divergence of f is denoted as, it is written as del dot f and it will become very clear why it is denoted in this way. So it is written as del dot f and the value of this is partial derivative of f with respect to x plus partial f x with respect to x, f y with respect to y, with respect to z. So, you started with the vector and that has 3 components. Now you do the differentiation component wise. So, first component you differentiate with respect to x, second component with respect to y and third component with respect to z. You add them all up and you get a scalar and this scalar is the divergence. So, what you get here is a scalar, it does not have any components and so the divergence is the scalar. Now you might ask why is this notation used here? In order to see that, we go back to the gradient.

Now, when you took gradient of a function when you took grad f grad of f. You got I dou by dou x of f plus j dou by dou f of y plus k dou dou by dou z of f. So, in other words you can think of this gradient operator as an operator that looks like this. Sorry it is an operator. So in the operator form you write it as. In other words it is an operator that looks like a vector with three components. First component is the derivative with respect to x, second component is derivative with respect to y and third component is derivative with respect to z. And when this acts on an f, then you just put the f here. If it is acting on f you just put the f there. Now on the other hand if you dot it to some vector field like this what that means is you can imagine that you take this and you dot it into f which has 3 components f x, f y and f z and so you have two vectors.

So, just this has three components. So, you imagine as so you are dotting these 2 vectors. You are taking a dot product of del dot f in this particular direction. And what that looks like if you are doing a dot product, you would get exactly d f by d x and d by d y operated on y f y and d by d z operated on f z. Therefore, this notation is consistent with the idea of this dot product. However you should know that, this is not actually a dot product because dot product by definition should be commutative and which is not in this case. So, it is not a dot product. But, this symbol is used and it is used because it is fairly a very short notation and it is very convenient. So, this is the divergence, and what I will? And the third definition, so in the divergence you differentiate a vector field and you get a scalar field.

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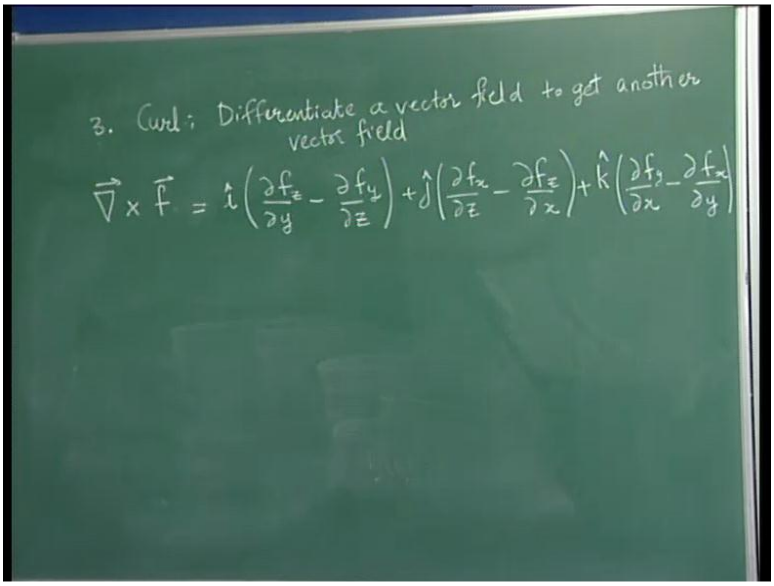

The next derivative that we will do is something called a curl. So, in a curl you differentiate a vector field to get another vector field. And I mean there are many ways to do this, but the definition of the curl, the symbol used is del cross f. So, you have a vector field f and the curl operator is you cross it with the del operator with the gradient operator and this has and the reason for this symbol will become obvious because the curl is defined as having components dou z.

So, in this case you took the derivative of the x component with respect to x, the y component with respect to y and the z component with respect to z. But, in this case what you are going to do is, you are going to take the derivative of the x component with respect to a z here and with respect to y. You do not take the derivative of the x component with respect to x and so if you if you think of these two vectors, then it looks as so you are taking the cross product, the usual cross product of these vectors. Therefore, it is this is the symbol that is used; so each of these derivatives plays a role in various areas.

The gradient is probably the derivative that you will see most often in both quantum chemistry and in classical mechanics because this is related to the potential theory, the force and potential theory. The divergence you have probably seen it in your courses on electricity and magnetism, but it also appears in something called the continuity equation in hydro dynamics. And the curl is an operator that is probably you do not see it as often.

But it does appear in electricity and magnetism and in general when you are talking about the effect of magnetic fields on molecular systems. So, we have seen these 3 kinds of definitions. And the next thing we want to do is to get some sort of way of understanding, what is the significance of each of these?

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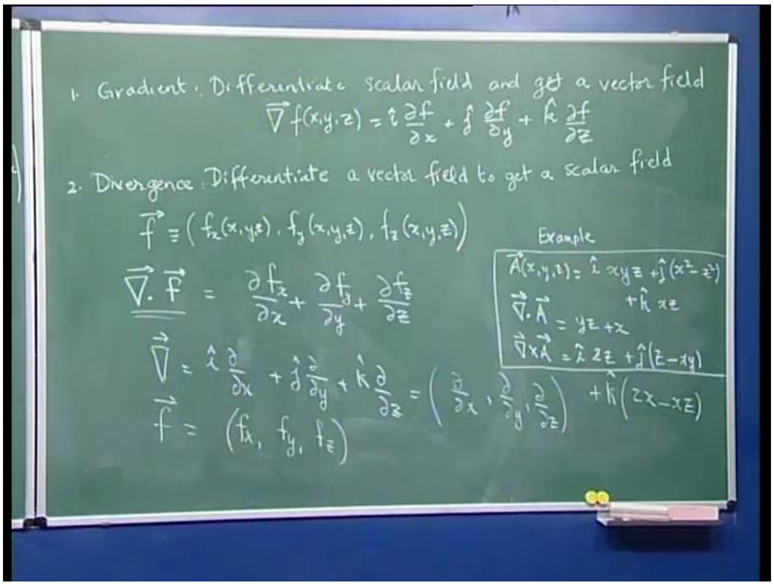

Before we do that, let me take some examples and I will take an example of the divergence. So, this is an example of divergence. Suppose you have A of x, y, z. This has 3 components. So, the first component is x y z, x into y into z, the second component is x square minus z square and the third component is x z. So, this is an example of a vector field where each of the components are functions of x y z and if you take the divergence of this. That means you take the derivative of this with respect to x, that will give you y z plus the derivative of this with respect to y that will give me 0 plus the derivative of this with z, that will give me x. So, this is the divergence.

So, the divergence is fairly straight forward to calculate. And the curl is also straight forward to calculate, only you have to take a few more derivatives here. So, the curl is a vector, the ith component involves differentiation of the z component with respect to y which gives me 0 and then differentiation of the y component with respect to z so that will give me minus 2z. So, this is 2 z y 2 z i as j. j component will involve derivative with respect to x of the z component that will give me z minus x y.

And the kth component will give me 0 kth component will give me 2 x here and it will give me minus x z. So, that is the curl of this vector. So, you can, you should be able to calculate the divergence and curl for any vector field just as you should be able to calculate the gradient for any scalar field. So, these are relatively easy to calculate and it is expected that, you should be able to do all these calculations.

So, let us look at the physical significance of each of these quantities. So, we have the gradient divergence and curl and let us look at the physical significance of each of these, starting with the gradient and here I want to give the full explanation. I will just briefly explain and you can look up one of the text books for references to find out to get a better understanding of this.