Mathematics for Chemistry
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Module - 02
Lecture – 03
Vector functions, scalar and vector fields, vector differentiation

In today's lecture, I will introduce vector functions or functions of vectors. In that I will talk about 2 types of functions what are called as scalar and vector fields.

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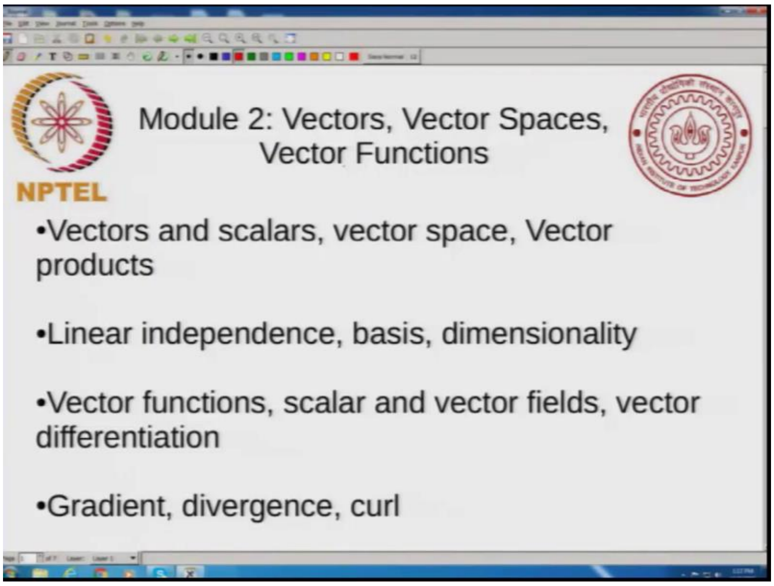

And then we will we will briefly mentioned vector differentiation, but the more details of vector differentiation I will talk in the next class, where we will talk about gradient divergence and curl.

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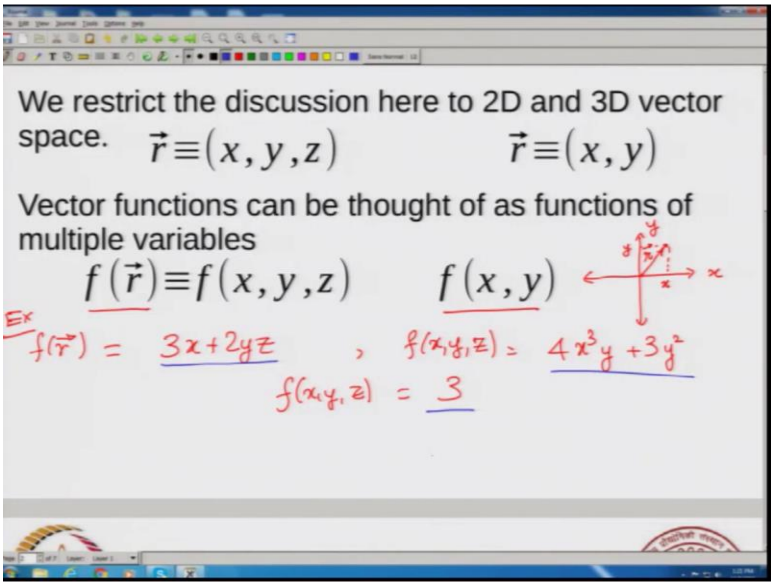

So, let us start with functions here we will restrict the discussion to 2 dimensional and 3 dimensional vector space. So, in if you have a 3 dimensional vector space, then this any vector can be written r as s in terms of three coordinates x, y, z. So, r is a vector in this vector space these are the components of r; x, y, z. So, this is just like a point in 3 D Cartesian coordinate system. If you have a 2 dimensional vector space then you have a 2 dimensional space and you can think of any you can think of an arbitrary vector r as having 2 components the x and y components. So, you can also think of it in in the x y plane in Cartesian coordinates and you can think of a vector at some arbitrary point in Cartesian coordinates. So, just to illustrate if you have 2 dimensional space you have x you know y and suppose you take an arbitrary point you can think of this as this vector r, this and these are the x and y coordinates x coordinate and this is the y coordinate.

So, you can think of a vector as a point in this 2 dimensional coordinate and therefore, I can represent it as r which is which has 2 components x and y and in 3 d space r has 3 components x, y, z. So, a function of a vector, you can think you can think of it as a function of multiple variables. So, a function of a vector means it is a function of r and r content x, y, z r is an x, y, z the information that x, y, z together give is exactly that information of r. So, I, so, instead of thinking of f of r, I can think of f of x, y, z or in 2 dimensions I can think of f f x y. So, a function of a vector can be just thought of as a function of multiple variables.

So, for example, if you can think of any function of multiple variables for example, f of r, this is example f of r equal to let us say 3 x plus 2 y is 2 y z. It can be any function you can multiply, you can take squares, you can do anything, you want or you can take or you can take f of x you, I can write it as a f of x, y, z is equal to 4 x cube y plus 3y square. Now, in this case an arbitrary function of x, y, z in this particular case it has no dependence on z, but even that is a general function of x, y, z. You can also have a function of x, y, z that has no y dependents or you can have a function that has no x, y, z dependence you can have. So, for example, even f of x, y, z if I equal to 3 this is also a function of x, y, z, so these 3 examples of functions of vectors.

So, you can you can do this in many different ways and the point as whenever you have a function of many variables, you can think of it as a function of a vector.

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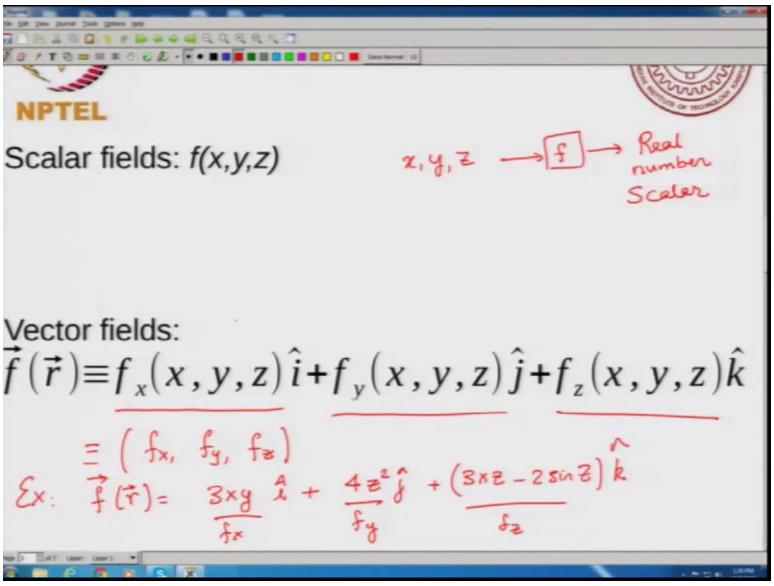

So, now there are 2 kinds of functions. So, so these functions of multiple variables, you can think of them as vectors they are also they are also referred to as fields and there are 2 kinds of fields 1 is called a scalar field and the other is called a vector field. So, in a scalar field your function that you have is basically a scalar; that means, that means you give x, y, z, you give it into the function and what you get is a real number. Real number, if it is a real function, if it is a complex, if it is a complex function you will get a complex number.

But essentially you get a scalar real number or a scalar. So, so this is called a scalar field and the examples that we talked about here are all examples of scalar fields. So, so scalar fields in scalar fields you have, you have the function which is just a scalar; that means, given x, y, z it returns a real number or a scalar. In vector fields, the function that you get for any x, y, z; you get a function which is which itself is a vector. So, f itself is a vector. So, f has 3 components. So, it has a x component which is again a function of x, y, z, it has the y component which is also a function of x, y, z and it has a z component it is also a function of x, y, z.

So, equivalently I can write this as fx, f y, f z and I keep in mind that each of the components themselves are functions of x, y, z. So, for example, I can have I can have an example where this vector field equal to 3 x y i plus 4 z square j plus 3x z minus 2 sin z times k. So, this is my fx this is my f y and this is the f z. So, so what we did here is we said that you know if this f x, f y, f z are all are all function are all scalar fields. So, actually f x itself is a scalar field fy itself is a scalar field f z itself is a scalar field. So, f x, f y, f z are scalar fields and these are components of the vector field f. So, these are 2 ways you can define functions of vectors and now we have these scalars and vectors fields and what are the examples where do you see this.

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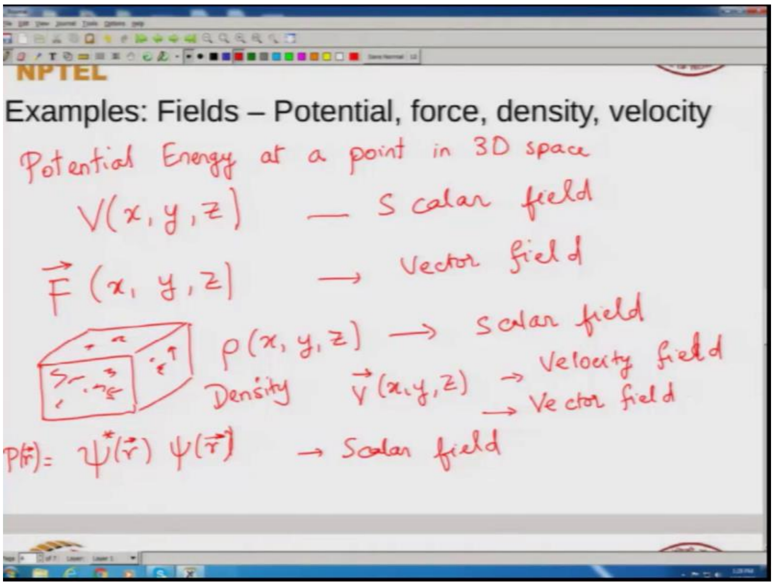

So, the most common examples of scalar in vector fields which will which will encounter is in potential theory. So, the potential energy, potential energy at a point in space, at a point in 3 D space, this is written as V of x, y, z. So, it is a function of x, y, z.

So, suppose you take any point in space, you ask, what is the potential energy? That is that is written as V of x, y, z. So, this is an example of a scalar field, because the potential energy is a scalar, now this potential energy actually, actually it might lead to something like a force at any point. So, so if you put a test charge at any point it a it might experience a force because of this potential energy so, you can ask what is the force at any point x, y, z, this is a vector field. So, this is one example of scalar and vector fields you can have many many such examples. Now one very common example that we that you learn in in statistical mechanics is you might consider you might consider a box, you might consider the system where you have lot of lot of particles let us say it might be a it might be a fluid system or it might be a system of gases. So, you have lot of particles and the density is not same everywhere. So, the density rho is a function of x, y, z. So, this is an example of a scalar field.

So, the density is an example of a scalar field. Now, now, if you have a fluid if you have a fluid then the particles at each point might move with different speeds. So, the velocity this is velocity, velocity field this is this is very commonly encountered in fluids and this is an example of vector field. So, so I just, I just wanted to show you some examples of scalar and vector fields that you that you may that you will encounter in various courses one is the scalar field and one is the potential energy which is the scalar field potential energy or just the electrical potential then you could have a force at any point. So, that should be a vector field.

Similarly, you could have a if you have a fluid then you can think of the density of the fluid at any point as a scalar field. You can think of the velocity at any point in the fluid as a vector field. So, these are some these are some examples of scalar and vector fields of course, there are many more examples, but I just wanted to say where you encounter these kind of objects. In fact, in fact as we said any function of multiple variables you can think of as a as a scalar field. So, so you might plot you might be calculating the density of particles like the like for example, you have a wave function psi of r and from this you calculate the probability at r as psi star, are psi of r.

Now, these are all this is a scalar field, because, you can calculate the probability of finding a particle at some point in space. So, that is another example of scalar field. So, I mean you encounter these objects all the time in various courses. So, so you should be aware of what scalar and vector fields are now. So, what we have done here is we have tried to define functions of vectors. So, we are tried to take vectors and we have tried to define functions of vectors and in defining these we came we came as there can be 2 types of functions. Functions which are scalars which are called scalar fields and functions which are vectors which are called vector field, scalar functions are called scalar fields; vector functions are called vector fields.

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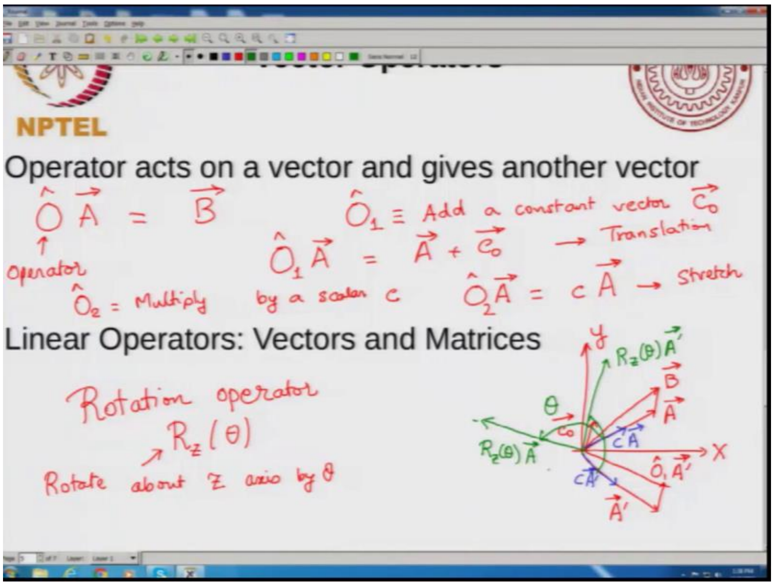

Now, there is another common terminology that is used when you are dealing with vectors and this is the idea of vector operators. So, an operator, operator is some object, so denoted by O hat, so operator is denoted by O hat. Now the operator has to operate on something. So, it acts on a vector. So, it might act on a vector A to give you another vector. So, it might give you some vector when I will just call it B. So, a typical operator acts on one vector, it gives you another vector, now A and B of course, belong to the same vector space. So, you can you can have an operator that acts on a vector space to give you; acts on a vector; in a vector space to give you another vector in the same vector space. So, now, these vector operators can do various things I mean they can it can; you can think of this as taking the vector and you know up and transforming it to another vector. Now, you can think of this as a vector field; you can you know you can think of

B as a function of A, but there are certain kinds of operators that we are that we will be really interested in and these are what are called as linear operators.

So, let us take an example, let us take some examples of operators. So, you could have an operator that takes and let us work in 3 D. So, in three dimensional spaces I can have an operator as this operator I defined as add a constant vector C 0. So, that is my operator. So, what does it do? So, suppose I take suppose I take operator acting on A, I have to what the operator does it adds the constant vector C 0. So, I get A plus C 0, now A plus C 0 is also a vector. So, A plus C 0 is also a vector in the same vector space. So, that is how this this operator works and will just for convenience I will call this O 1. You could have, you could have many different kinds of operators, you could have operator O 2. So, multiply A by a scalar, scalar c. So, then then for multiply I should not say multiply A multiply whatever the vector is by a scalar c.

So, for example, if you have O operator acting on A, you will get C times A. So, this is another operator (Refer Time: 16:01) let us be precise and call it O 2. So, so what you saw is you saw an operator that that adds a constant vector C 0, this is an operator that multiplies it by A constant A and just, just to inform you this is, a translation and this is a stretch. So, what do you mean by translation and stretch. So, I will. So, so what I want to say is that if you had A if you had a vector A and let us say let us say I will just take for convenience this as my C 0. So, then when I add when I add C 0 to A what I get is I will get a vector like this. So, this is my b b vector which is A plus C 0. So, so what it did is it took this vector and it and it moved this point up by it moved this point in the direction of C 0.

Suppose I had some other vector A, suppose I had some other vector here it would do the same thing. It would again move it up move it in this direction by this point. So, the new vector will be this. So, what the operator does. So, so if I take this as a prime then this is operator O 1, I have to appropriating on A prime. So, so that is why that is why this is a translation operator where it just where it just shifts or it just translates the vector by a certain amount.

Now, the other operation we said is called as stretch where what it does is it takes the vector and multiplies it by a scalar. So, you get a vector in the same direction and based on C it will be either be longer or it will be shorter. So, so the stretch operator, I will show this in blue. So, what it does is it takes A and it multiplies by C. So, this is my C times A if C is less than 1 then this length will be shorter, if C is greater than 1 it will be longer similarly it will take this and it will it will shrink it by the same factor. So, whatever the factor was here the same factor c times a prime. So, these are common operators.

Now, you can have other operators, you can as you see; I can take you can imagine an operator that does that does something called a rotation. So, it can take a vector rotate it by some angle. So, so you can have a just write it here, rotation operator I will come back to linear operators in a few minutes, but you can you can have an operator that does the rotation. So, what it does? So, I will just show this in green. So, it takes A and it rotates by some angle theta.

So, let us just call this r rotate by theta rotate let us say about some axis rotate let us say around z axis by theta. So, this is a rotate about z axis by theta. So, this is an example of a rotation operator and you can seem what it will do is: if this is this is my x and y plane it will take this vector A and it will give you this green vector which is r by this angle theta. So, r z of theta operated on A. So, so we will take any vector similarly we will take this vector A prime and it will give you it will rotate this by theta and it will give you something else it might give you something like this. So, so this is r z of theta into 8 prime.

So, essentially this is another example where it takes a vector and gives you another vector so. So, now, now we will come to a certain class of operators which are called linear operators.

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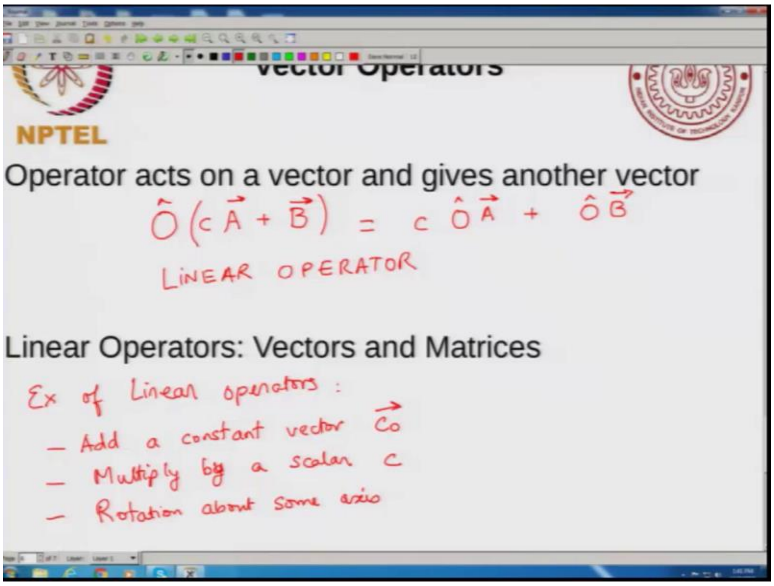

So, let us just come, come to the class of operators called linear operators. So, what is the linear operator? So, a linear operator you can you can think of it this way. So, suppose you have an operator O it acts on A on c times A plus B. So, operator should act on any vector it can act on any vector it should act on all the vectors in the vector space. So, so c times A plus B is another vector in the vector space.

So, if it operates on this if I can write this as c times operator on A plus operator on B. So, then this is called a linear operator. So, a linear operator is an operator which when its acts on a linear combination of vectors gives a linear combination of operator acting on each of the vectors so. So, now, linear operators are actually extremely common in very very important in quantum mechanics. In fact, the large part of the formulation of quantum mechanics is based on linear operators, but there is something else about linear operators what linear operators can do is they can only they can only there are only certain kinds of transformations on certain kinds of operators which are linear.

So, for example, you can have an operator. So, so this is example of linear operators. So, last time we said, we said you know add a constant vector c 0. So, that is an example of a linear operator and you can verify that it is trivially linear then multiply by a scalar c. So, that is also a linear operator then we talked about rotations, rotation about some axis.

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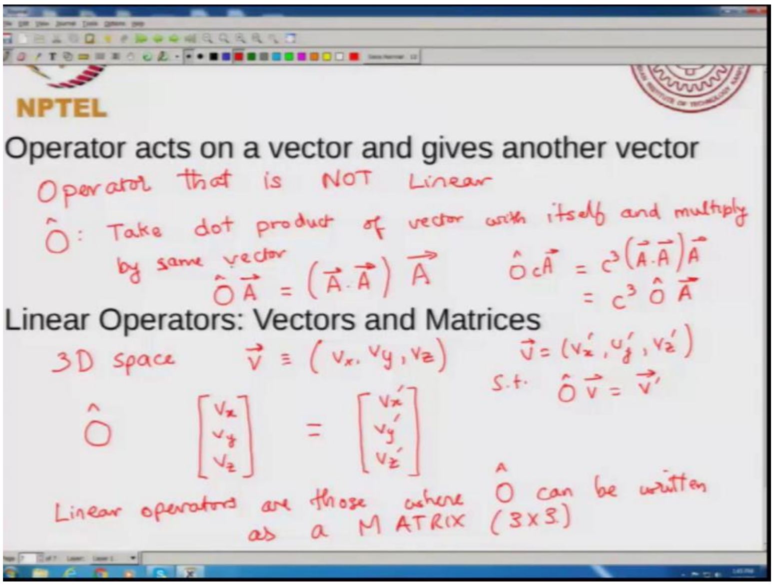

So, that is also that is also an example of a linear operator. What is an example of an operator that is not linear? So, an operator that is not linear. So, suppose I define my operator as something that that take dot product of vector with itself and multiply by vector by same vector.

So, what this does is it takes O and when acts on of certain vector A what it does is it takes A dot A. So, it takes the dot product and you. So, A dot A is a scalar. So, it takes this and multiplies it to A. So, now, you get a vector. Now, now, you can show that if you do this then you can show that this is not a linear operator because I mean, I mean it is fairly easy to show that it does not satisfy the it does not satisfy the condition for a linear operator and you can you can trivially show suppose I just take c A suppose I just take suppose I take O of c A. So, so this is clearly a constant times A. So, this is this is not equal to c times O of A, this is this actually c cube times O of A.

So, so it is c cubed times A dot A into A. So, this is c cubed times O of A. So, clearly it is not c time. So, of A it is not a linear operator, Now linear operators have something very they have a connection with matrices and you can see this in the following way see suppose I take suppose I take my vector. So, let us consider 3d space again. So, my vector v has components v y, v z. Now, I can think of my operator, I can; I will write this in as a column vector. So, v x, v y and v z and I have my operator here. So, here I have my operator and that gives me some other vector some new, new vector I will just call it we just call it v x prime v y prime v z prime.

So, this operator acts on v to give you v prime. So, we I will just define v prime equal to v x prime, v y prime, v z prime such that operator acting on v equal to v prime. So, once you write it in this form you can ask, what is the linear operator? So, you can have you can have I mean they there is no relation between v and v prime you can operate by any operator and you can get another vector now linear operators are those where are those where O can be written as a matrix a 3 by 3 matrix.

So, for linear operators you can generally write this operator O as a 3 by 3 matrix and so an arbitrary linear operator in 3D space can be written as a 3 by 3 matrix and you can you can easily show that if you, if you write it as a if you write this operator as a 3 by 3 matrix then this condition will hold the condition for a linear operator will hold. So, we will keep in mind that linear operator can be written as a matrix and or you can think vice versa matrix can be thought of as a linear operator on A on a vector you can think of it as a linear operation on a vector.

So, in the next class what I want to talk about is vector differentiation where since you can define a function of a vector you can also think of derivatives with respect to that function. So, so today we talked about scalar fields and vector fields we talks about functions of vectors now you can say you can ask what about derivatives with respect to these vectors derivative with respect to vectors and that may be the topic of the next class which will be vector differentiation where we will talk about gradient divergence and curl. So, I will stop for today now.

Thank you.