Advanced Mathematical Methods for Chemistry
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Module - 01
Lecture - 02
Vector Operations, Vector Products, Generalized Vector Spaces

Now, in the second lecture of this first week, we will talk more about vectors we will talk about vector operations, we will talk about vector products and then we will also talk about generalized vector spaces and just to recap.

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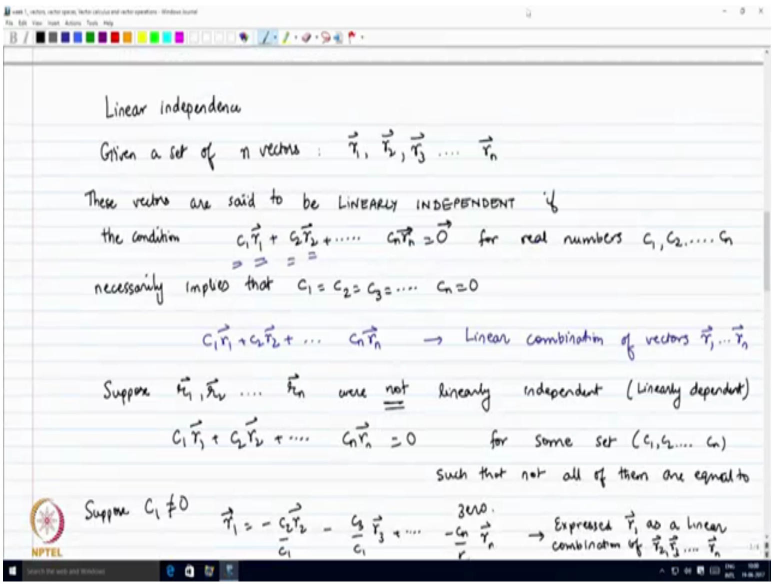

So, in the first lecture we talked the about the basics of vectors. So, we talked about what are vectors.

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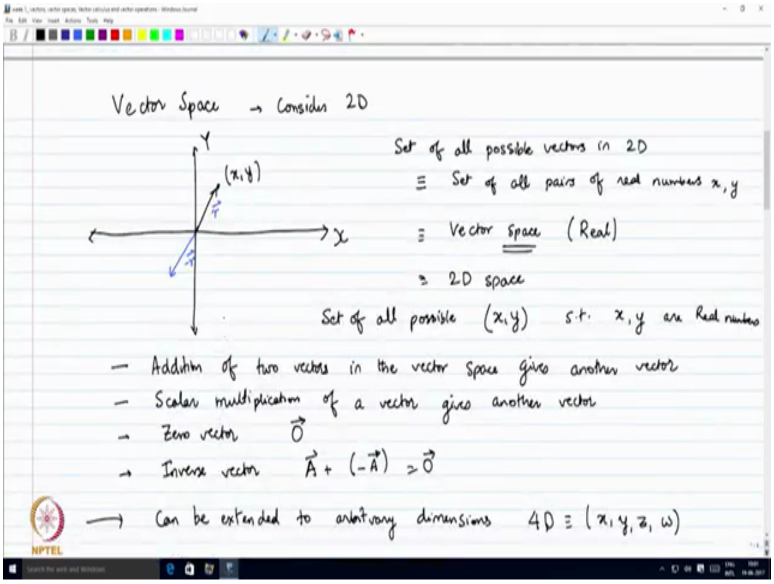

We talked about vector spaces and we talked about linear independence of vectors. So, we talked about to vector spaces linear independence, we talked about the concept of basis and dimensionality.

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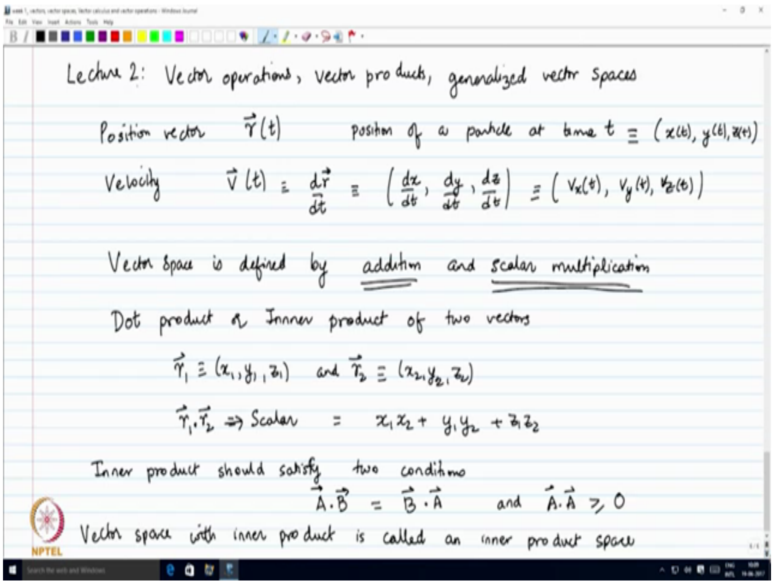

Now, now let us look at some other vector operations. Now before we do that let me let me mention a few vectors that you are familiar with from classical mechanics. So, for example, you are familiar with the with the position vector. So, the position of a particle r, so the position r this represents the position of a particle and it might be a function of time. So, r of t, so position of a particle at time t, this is a well known example of a vector that you might have encountered in classical mechanics. You have also seen vectors like the velocity vector. So, the velocity of a particle v at time t and what is interesting is that this is nothing, but d r by d t this is the time derivative of r, and the time derivative of r, is just given by d x by d t and d y by d t. So, it is a vector where each of the components are time derivatives of these vectors. And just to emphasize your vector r is in this case it is x of t y of t z of t in 3D space.

So if you are in 3D space then the position vector r is written as it has 3 components x y and t is z and each of them are time dependent. So, they are functions of time now the velocity is just a time derivative of the position. So, it has components which are just time derivatives and you can write this this is these components you might denote them as the x component of the velocity this is also a function of time y component of velocity and z component of velocity, we use it of t. So you have seen things like position vector velocity vector you can have acceleration which is a vector you can have force which is a vector and so on. So these are vectors are something that you have been seeing in in classical mechanics for a long time and they are also seen in different branches of physics and chemistry.

So, now when we talk about operations on vectors, the vector space is defined vector space is defined by 2 operations, namely addition and scalar multiplication. So, we know that if we if you add 2 vectors, you will get another vector and if you multiply a vector by a scalar you will get another vector.

So, addition and scalar multiplication are necessary to define the vector space. So, you have to know how to add vectors you have to know how to multiply them by a scalar now there are other operations you can define and these are additional things that you defined on the vector space. For example, there is one operation called dot product dot product or inner product. So, what you do is your, you define the dot product or inner product of 2 vectors. Now suppose you have 2 vectors r 1 which is denoted by x 1 y 1 z 1 and r 2 which is denoted by x 2, y 2, z 2, then the dot product r 1 dot r 2 this is a scalar. So, this is a scalar, this is a scalar and which is equal to x 1 times x 2 plus y 1 times y 2 plus z 1 times z 2.

So, this is the usual this is the definition of the dot product. It is also referred to as inner product. So, dot product or inner product and this is how you usually define it in 2D or 3D space. And this is I should emphasize that this is not the only definition of the dot product there can be other definitions of the dot product, which I would not go into I would not go into that they there is a formal meaning of what can constitute an inner product. So, a dot product or an inner product inner product should satisfy 2 conditions.

I am writing the 2 main conditions there are other conditions which I am not writing here. So, the 2 important conditions that they should satisfy is that A dot B. So, if you take 2 vectors A and B when you take the inner product the dot or the dot product. So, this should be equal to B dot A and A dot A is always if you take an inner product of a vector with itself then it should always be greater than or equal to 0. In fact, it is equal to 0 only if a equal to 0 it is greater than or equal to 0 and it is equal to 0 only if a equal to 0.

So if these 2 conditions are satisfied then you can you can define an inner product in any way that these 2 are satisfied. So, this this usual way of taking the inner products just by just by multiplying it component wise and adding up is just one way of taking an inner product, but there can be other ways of taking the inner product. So, long as they satisfied this rule then it is a valid inner product. So I would not talk I would not speak more about the dot product, I will come back to this this dot product or inner product when we are talking about generalized vector space, but I will just emphasize that vector space with inner product is called an inner product space.

So, this inner product space is a kind of vector space, that where the inner product is defined. You could have vector spaces where no inner product is defined that is perfectly fine, you could have vector space where dot product is not defined vector space is defined only by addition and scalar multiplication, but if you have a vector space where an inner product is also defined which satisfies these conditions then it is called an inner product space.

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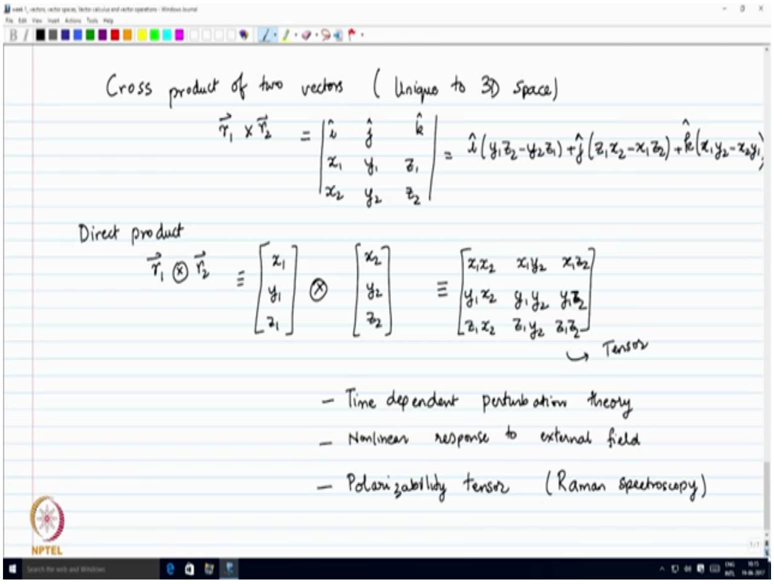

So now I there can be other kinds of vector products that are already that are also defined, and you could you could also define things like cross products cross product of 2 vectors. So, if you had 2 vectors let us say r 1 cross r 2 this is actually the cross product is unique to 3D you cannot define a cross product in 2D 2 dimensional space. So, if you had 2 vectors r 1 and r 2 in 3D then you can define a cross product and you know how to define the usual cross product.

So if r 1 has components x 1 y 1 z 1 and r 2 has components x 2 y 2 z 2 then you write this as a determinant I j k and you write the components x 1 y 1 z 1 x 2 y 2 z 2. So, you write this in this form and this is a vector. So this gives a vector. So I can write it as I into y 1 z 2 minus y 2 z 1 plus j into z 1 x 2 minus x 1 z 2 plus k into x 1 y 2 minus x 2 y 1. So, this this is the cross product and clearly it is a vector. So, the cross product of 2 vectors gives you another vector.

So we saw that the dot product of 2 vectors gives you scalar the cross product of 2 vectors gives you another vector. And you can also have other kinds of products these are not the only kind of products, you can also define many different products of vectors. So, for example, suppose you had you can define something called the direct product. So, the direct product and I will just use a notation. So, suppose you had suppose you have the same 2 vectors r 1 and r 2 then r 1 you take a direct product with r 2. Now this I will denote it by a matrix. So I will just show it as a matrix, I will show it in the matrix notation.

So, what I do is, I take x 1 and I take. So let us write this in in matrix form. So, suppose you had x 1 y 1 z 1 and you take a direct product with x 2, y 2, z 2. So notice I have used I have denoted x, I have denoted r 1 and r 2 as column vectors then the result of this direct product is something is an object called a tensor which is which is actually which can be represented in a matrix form. So, x 1, x 2, x 1, y 2, x 1, z 2, y 1, x 2, y 1, y 2, y 1, z 2, z ,1, x 2, z 1, y 2, z 1, z 2.

So I can represent this by a matrix. So notice what I have done is I have taken x 1 and I multiplied it by x 2, I have multiplied it by y 2 I have multiplied by z 2 and I have taken all these products unlike in the cross product, where I took suitable combinations of these products here I kept all the 9 products. So what I get is a 9 dimensional object and this is a tensor this is actually a tensor. I mean tensors are again quite important in for example, these play a role in time dependent perturbation theory, perturbation theory, so for example, or you can see in non-linear response to external fields.

So, for example, you can have something called the polarizability tensor. So, for example, if you take a molecule and you put it in a strong electric field. Then if the molecule the molecule may not have it is own dipole moment, but it might get polarized due to the electric field and due to this polarization of the molecule it might induce a dipole moment. So, this pole this the tendency of a molecule to get polarized is represented by a tensor called the polarizability tensor. So this is one place where you will see tensors appearing.

So for example, this plays a role in Raman spectroscopy. So I mean you will see tensors in advanced quantum mechanics and spectroscopy courses, but what I wanted to emphasize through this is that, you know you it is not you know vector products can be defined in many different ways. There are no there is no unique way of multiplying vectors, but you can define several different ways to multiply vectors.

Now next I want to generalize the idea of vector spaces. So, we have seen 2D and 3D vector spaces. Now we can easily construct as he said vector spaces can be generalized can be generalized to many dimensions.

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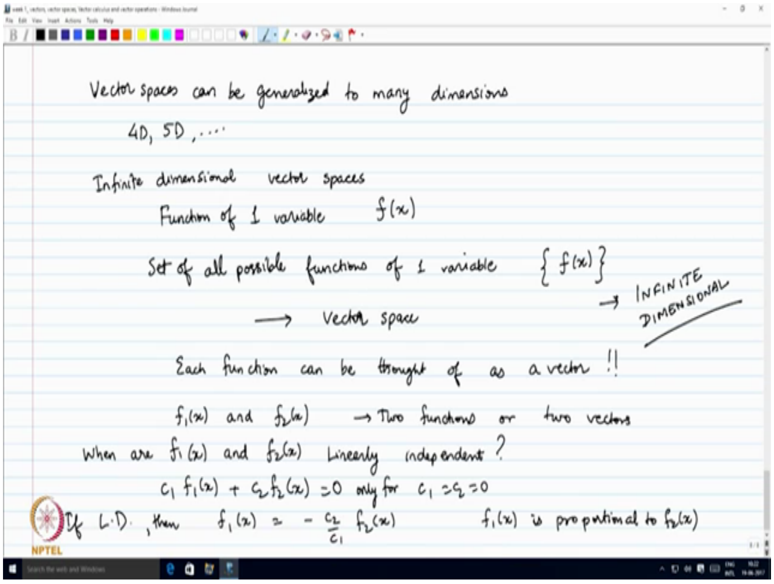

You do not need to look only at 2D or 3D vector spaces. You can look at you can look at many different dimensions. So we already saw 4D for example, you can go 4D 5D and so on. Now you can also go to a different type of vector space which is called the infinite dimensional vector space vector spaces.

For example, I will just give one example of an infinite dimensional vector space. So if we take function of one variable. So, for example, I say f of x. Now, f of x is a function of one variable. Now you consider the set of all possible functions, of one variable. So, we are taking the set and let me denote by curly braces. So, this set f of x of all possible functions of a single variable x. And let us say for convenience that x is a real number it does not matter. So, if you take the set of all possible functions of one variable; that means, this you can easily show that this is a vector space and why is it a vector space because you add any 2 functions, you will get a third function which is also a which is also a function of one variable.

If you multiply a function of one variable by a scalar you will get another function of one variable and the clearly is 0 is also a function of one variable, is a constant function you can have 0 which is a constant function of one variable, you can have a negative of a function which is the additive inverse of the function. So, clearly the set of all possible functions of one variable is a vector space. It satisfies all the necessary conditions to form a vector space.

So, you can think of functions as vectors. So, each function can be thought of as a vector. This is a very important idea and it is actually central to all of quantum mechanics. Now each function can be thought of as a vector, now what you can do something else you can ask suppose you had f 1 of x and f 2 of x. Suppose you had 2 functions you as I said you can think of them as 2 vectors or 2 vectors.

Now you can ask a question are these 2 vectors linearly independent. So, when are f 1 of x and f 2 of x linearly independent, and in this case the answer is that if you take c 1 f 1 of x plus c 2 f 2 of x equal to 0. And you say that c 1 and c 2 are both are not equal to 0 or not both 0 and for some if they are linearly independent if c 1 f 1 of x plus c 2 f 2 of x equal to 0 only for c 1 equal to c 2 equal to 0. So, if this condition is only satisfied when c 1 equal to c 2 equal to 0, then you say the vectors are linearly independent. If this is satisfied for some c 1 and c 2, which are both not 0 then I can write f 1 of x equal to minus c 2 by c 1 f 2 of x or I can write f 1 of x as a scalar, minus c 2 by. So, c 1 is a scalar. So, I can write it as a scalar multiple of f 2; that means f 1 of x.

So, if linearly dependent, then we can write this form and then f 1 of x is proportional to f 2 of x. So, 2 functions are linearly dependent only if one is proportional to the other. So, any 2 functions that are not proportional to each other will be linearly independent. And this; obviously, implies that the number of basis functions number of linearly independent functions is infinite; you can have infinitely many functions that are not proportional to each other. In fact, I can take any 2 functions and multiply them and I will get a function that is not proportional to either of them.

So, basically what I want to emphasize is that this set of all possible functions is an infinite dimensional space. So, this is an infinite dimensional vector space. And so we can see this space of functions as an infinite dimensional space, you need not you can you can construct several other different infinite dimensional vector spaces which I would not get into, but let me just conclude this lecture by mentioning that you can also define inner products on space of functions.

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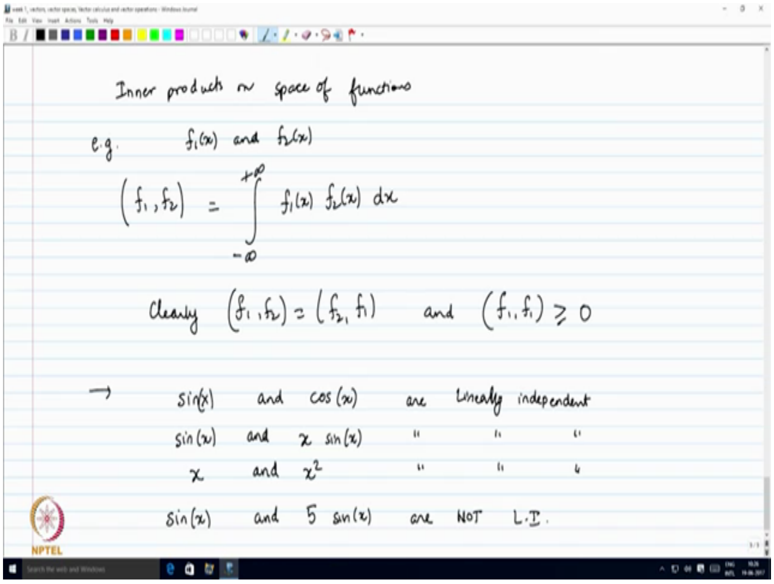

So, one example this is an example. So, suppose you had f 1 of x and f 2 of x these are functions their inner products I will just write it as f 1 comma f 2. So, these are these are vectors you be think of them as vectors. So, you may define them in this form integral f 1 of x, f 2 of x d x, over whatever the range of x is. So, if x goes from minus infinity to plus infinity it goes over that range. So, over the entire range of x this would be a valid definition of inner product, because clearly f 1 comma f 2 equal to f 2 comma f 1 and f 1 comma f 1 is greater than equal to 0. Because f 1 comma f 1 will give you f 1 square then f 1 a square of any number has to be greater than or equal to 0. And so the integral of a square of a number of a function has to be greater than or equal to 0.

So, you can also define inner product on these on these infinite dimensional spaces and again such inner products or things that you will see very regularly in quantum mechanics. And what I have tried to show you in the first 2 lectures through this idea of linear independence and basis is that you can generalize the concept of vectors to greater than 2 or 3 dimensions you can in fact, go to infinite dimensions you can look at spaces of functions and you can you can look at all kinds of spaces.

So just to conclude let me mention that suppose you take a function sin x, sin of x and cosine of x. These are linearly independent. Similarly, if you take sin of x and x sin of x, the x sin of x is some other function these are also linearly independent. You can take x and x square these are also linearly independent, but you can take something like sin x and let us say 5 times sin x, these are not linearly independent because. So, the only functions that are linearly independent are those which are related to each other by a constant. So, if you take the ratio of them you should get a constant this independent of x only those functions are linearly independent and this clearly shows that the space of functions is infinite dimensional you can have infinitely many functions that are linearly independent.

So, your basis set has infinitely many vectors. So in the next class I want we will go to other things, you can do with vectors we will go to vector differentiation and functions of vectors and so on.