Mathematics for Chemistry
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Lecture - 2

So far, we have studied what we mean by vector spaces and what we mean by vectors to recapitulate. Vector space is a collection of objects called vectors, and this collection satisfies some basic properties and the important properties for in a vector space are that it is close to addition and scalar multiplication. So when you add two vectors you get another vector and when you multiply a vector by a scalar you get another vector. So, the axioms of a vector space are related only to addition and scalar multiplication.

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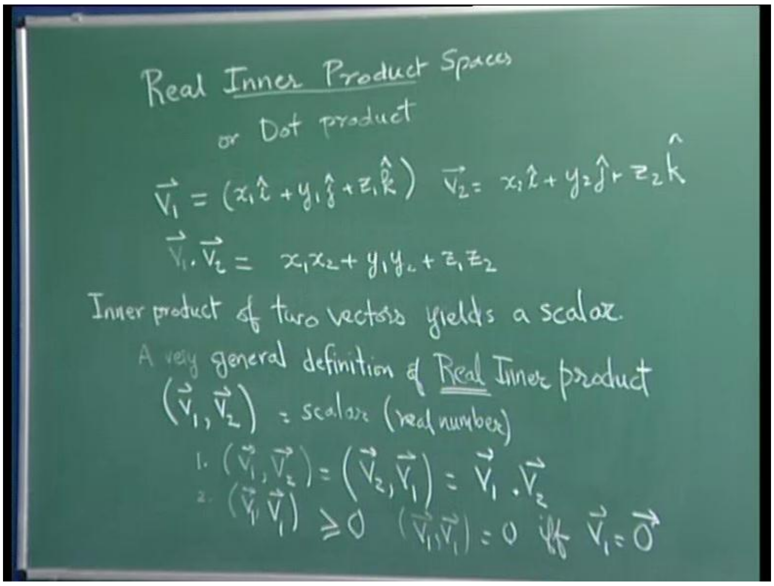

So, the axioms of a vector space do not talk about the product of two vectors or multiplying two vectors and this is the next topic that we will talk about. So, vector multiplication it is not necessary for real vector space that you need to define multiplication of vector space of vectors, however there are spaces called real inner product space, and these are spaces where an inner product of two vectors is defined. So, these are special kinds of vector space in addition to this we will look at three kinds of products of vectors the first is called the dot product or the inner product, the second is called the cross product, and the third is called the direct product, or the tensor product.

So, let us look at real inner products spaces and this is the first kind of product which is called the inner product or the dot product you all probably know how to take the dot product of two vectors in say 3 dimensional Cartesian coordinates. So, in 3 dimension Cartesian coordinates, if you have a vector V 1 denoted by x 1 i plus y 1 j plus z 1 k, and you had a vector V 2 denoted by x 2 i plus y 2 j plus z 2 k. Then you will then the inner product of these two vectors is denoted by V 1 dot V 2, and the inner product of these two vectors gives you a scalar and the value of the scalar is x 1 and x 2 plus y 1 y 2 plus z 1 z 2. So, thus we say that inner product of two vectors yields a scalar, and for this reason this is also, sometimes called the scalar product, it is called the scalar product inner product or dot product, and this is this is the procedure for taking the inner product of two vectors in 3 dimensional space.

However, this procedure is restricted to vectors in Cartesian coordinate system of 3 or more dimensions. Or even two dimensions however we want more general definition of an inner product. So, in more general a very general definition of inner product, general definition of real inner products and I used the term real because we are dealing with real vector spaces and in this in a real in a real inner product space the inner product will be a real number. So, the inner product is denoted by inner product of two vectors V 1 and V 2 is generally denoted by this bracket. So, this is the this is the notation for inner product of two vectors V 1 and V 2, and this is a scalar or a real number. Now, this is defined for any two vectors and you can have depending on the vector space you are considering you can have the appropriate definition of the inner product.

And in fact there is no unique definition of inner product and you can define many inner products and any that satisfies two conditions is a valid inner product. The first condition is the inner product is commutative so, V 1. So, the inner product of V 1 and V 2, this is specific to a real inner product. So, inner product of any two vectors is equal to inner product same of the two vectors in the taken in the opposite direction. So, for example, in this case you can clearly see that if i take V 2 dot V 1 then i will get x 2 x 1 plus y 2 y 1 plus z 2 z 1, which is the same as x 1 x 2 plus y 1 y 2 plus z 1 z 2. Then the second condition is that the inner product of any vector with itself. So, if i take a vector V 1 with V 1 should be greater than equal to equal to zero, and V 1 dot V 1 is equal to 0 if and only if, V 1 is the 0 vector. So, they the only case when the inner product of a vector with itself can be 0 is if the vector is the 0 vector, and the 0 vector we had we had mentioned that, this is a vector in the vector space such that you add any vector to it you get the same vector. So, we can define the inner product of two vectors, and any product defines. So, that it satisfies these two conditions is a valid inner product. I will be using i will be using two symbols for the inner product, i will be i will be using either this symbol or i will be using this symbol V 1 dot V 2, this is not restricted to 3 dimensions we will see that. We will see how we can extend this concept of inner product to other kinds of vector spaces.

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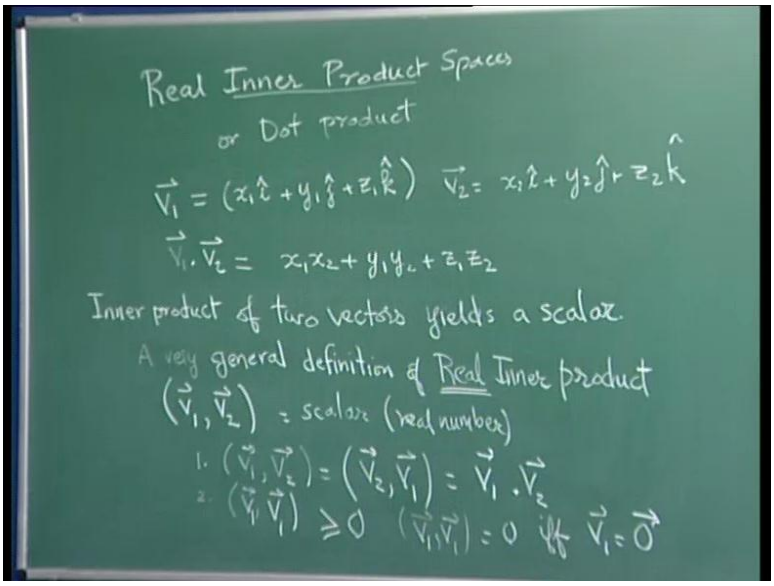

In addition to this I have not stated in the in the formal definition of the inner product has some other conditions regarding associativity and distributivity. But I have not stated them here and I will assume that they are satisfied by the inner product that you are considering. So, let us look at some examples of inner products the first example, is the usual dot product. So, before we go to some examples of inner products I want to mention what we mean by a real inner product space a really inner product space is nothing but, a vector space for which you have defined an inner product.

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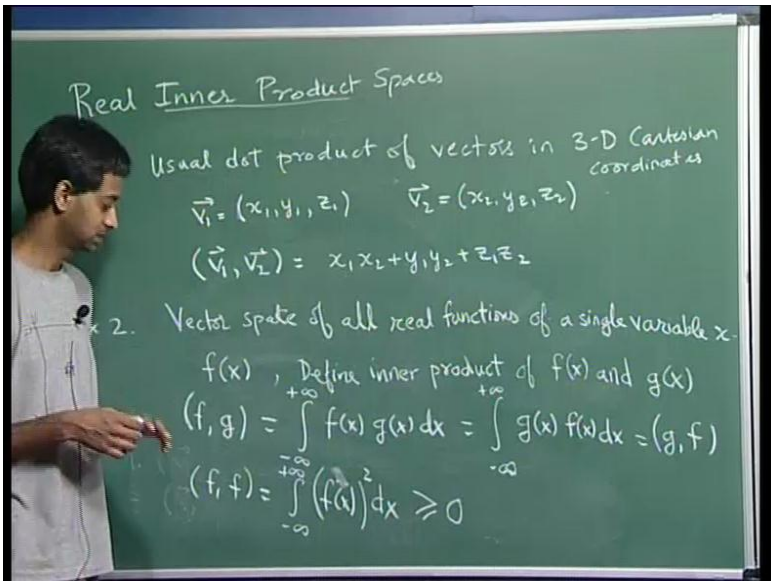

So, a vector space for which the inner product is defined is called a real vectors real inner product space. Now, let us look at some examples of inner products example one is the usual dot product of vectors in 3-D Cartesian coordinates. So for example, you can say V 1 is equal to x 1 y 1 z 1 V 2 is equal to x 2 y 2 z 2, then the inner product is equal to x 1 x 2 plus y 1 y 2 plus z 1 z 2. And we are seen that this satisfies the axioms for a real inner products inner for a real inner product.

So, this is an inner product in the 3-D Cartesian coordinates in 3 dimensional vector space and. So, the 3 dimensional vector space with this definition of the inner product forms a real inner product space. The second example is suppose you had vector space of all real functions of a single variable. So, in that last class we saw that the space of all real functions of a single variable F of x, where f of x can be any function of a single variable, it can it can be polynomial, it can be trigonometric, it can be exponential, it can be an exponential of a logarithm, it can be it can be almost it can be any function, and this forms of vector space. And if you look at this vector space then, we can define an inner product define inner product inner product of f and g of x. So, f of x and g of x are two functions of x. So, both these are members of this vector space.

Now, we define the inner product of f of x and g of x in this form f comma g is equal to integral f of x g of x d x over the range of ox. So, if this is define from minus infinity to plus infinity if x goes from minus infinity to plus infinity then this would be the range of integration of this. Now, the question is this valid inner product. So, in order to verify that this is the valid inner product you will see if it satisfies the axioms of an inner product, and the first axiom is f comma g should be equal to g comma x g comma f and you can clearly see that I can always write this integral in this form. I can always switch the order of f and g and. So, I can write the integral in this form and if you look at this and look at the definition of f comma g you will see that this is the definition of g comma f.

So, clearly f comma g is equal to g comma f inner product of a f f and g is indeed commutative. The second property that we have to ensure is that f comma f is greater than or equal to 0. And if you look at from minus, this is integral minus infinity to plus infinity f of x square f of x i will write it write it this way d x f of x square d x and now, what you have is that the integrand is positive at each value of x. So, clearly this is greater than or equal to zero, and it is only equal to 0 when f of x is equal to zero. So, the point is that where f of x can have both positive and negative values but, the square of f of x is always non negative. So, it is always greater than or equal to 0 and. So, this integral will be greater than or equal to 0.

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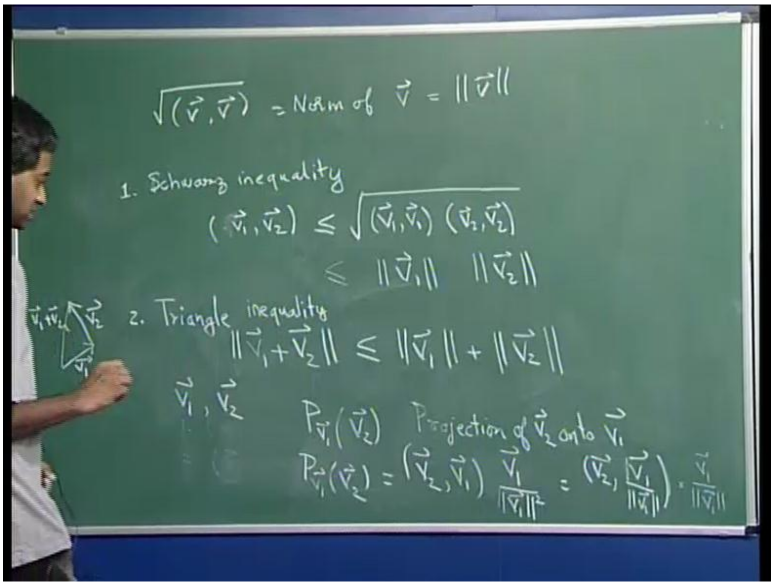

So, we can see that we can see that this definition of inner product is a valid definition and now we can construct an inner product space of functions of a single variable x, and this inner product spaces is closely related to the hill birds space that you will see in your quantum chemistry courses and. Therefore, it is good to be exposed to this sort of thinking. Now, this definition of inner product; so we have defined the inner product in terms of two basic axioms one is one is that it should be commutative and the other is that it is norm or the inner product of vector with itself should be greater than or equal to zero. Now, the inner product of any vector with itself this is the square root of this quantity is called a norm of the vector norm of V and it is denoted by.

So, one of the conditions of the definition of inner product is that the norm should be greater than or equal to 0. Now, this definition of inner product immediately implies two properties of inner product and the first property is that inner product satisfies the Schwarz inequality. So, any inner product any inner product will satisfy the Schwarz inequality any real inner product which satisfies the two axioms of real inner products space will also satisfy the Schwarz inequality. So, the Schwarz inequality says that inner product of two vectors V 1 and V 2 is always less than or equal to square root of inner product of V 1 with V 1 times the inner product of V 2 with V 2.

In other words it is less than or equal to the norm of v one times a norm of V 2 times of norm of V 2 and this is called the Schwarz inequality. This is true for any inner product space. So, we looked at two very different looking examples of inner product and I will leave it has an exercise to you to try to show that indeed both this way both these vector spaces satisfy the Schwarz inequality. The second axiom the second property that they satisfy and actually it is not just one property there are whole series of properties that follow from this one is called the triangle inequality. And this states that the norm of V 1 plus V 2 is always less than or equal to norm of V 1 plus norm of V 2.

So, the way to think of this is i mean if you imagine called angle inequality. If you imagine V 1 and V 2 to be vectors in the in the usual 3 dimensional space, then V 1 might point in this direction. So, if this is V 1 this is V 2 then V 1 plus V 2 will be this V 1 plus V 2. So, this is called the triangle inequality, because the norm of this vector and the norm is directly related to the length through the length of this vector is less the sum of lengths of these two vectors of. So, in other words the length one side of a triangle is always less than the sum of the length of the other two sides. So, this is the generalization of this of this to other vector spaces gives you something called the triangle inequality.

Now, based on the triangle inequality there are other geometric inequality which are related to the triangle inequality called the parallelogram inequality. But, we would not mention it here. Now, I leave it as a exercise to you to also look up the proofs of these inequalities. So, you really understand what is meant by these inequalities. Now, the inner product is extremely useful in all of coordinate geometry. But, in addition the inner product is the quantity that is very widely used in quantum chemistry. The inner product allows us to define something called a projection. So, projection if I had vector V 1 and a vector V 2 then, I can define something called the projection of V 2 on V 1. So, projection onto V 1 of the vector V 2; so this is called projection of V 2 of V 2 V 2. So, I am using this symbol for the projection of vector of. So, you are projecting vector V 2 on to vector V 1 and this can be defined in terms of the inner product. So, I can define this as V 2 comma V 1, V 1 norm of square.

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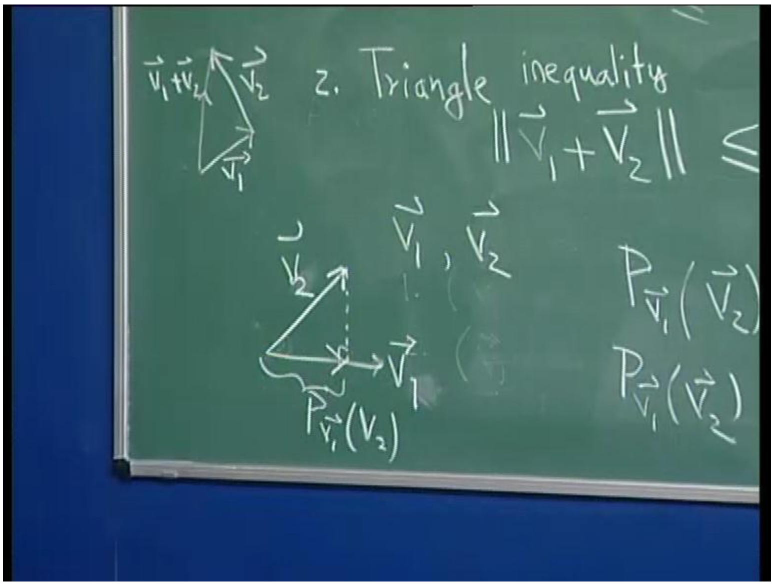

So, essentially the way to think of this you can you can think of this as two parts the first part is you can think of this as V 2 projected on to the unit vector in the direction of V 1 that is V 1 divided by norm of V 1. So, this is a first part. So, it is an inner product of V 2 with a unit vector in the direction of V 1. But, this gives a scalar and the projection turns out to be a vector. So, in you want a vector in the direction of V 1. So, you multiply by a unit vector in the direction of V 1. So, the projection of one on to other is if you had a vector V 1 and you had another vector V 2 and the projection is nothing.

But, this is the projection. Sorry, I will do it the other way, I will call this we have V 2 and V 1. So, you want the projection of projection of V 2 on to V 1. So, projection of V 2 on to V 1 is this vector. So, notice that it is a vector it is in the same direction or as V 1 and it tells something about the inner product of V 2 and V 1. So, if you think of the inner product of these two vectors, if these are two vectors in the usual Cartesian coordinate then the inner product of the dot product it is just V 1. The absolute value of v 1 times absolute value V 2 into cosine of this angle and V 2 cosine of this angle is nothing but this length. So, the projection is nothing but this length multiplied by a vector in that direction. So, once again I want two emphasize that the projection that we defined I try to explain it in terms of the usual vectors in 3 dimension.

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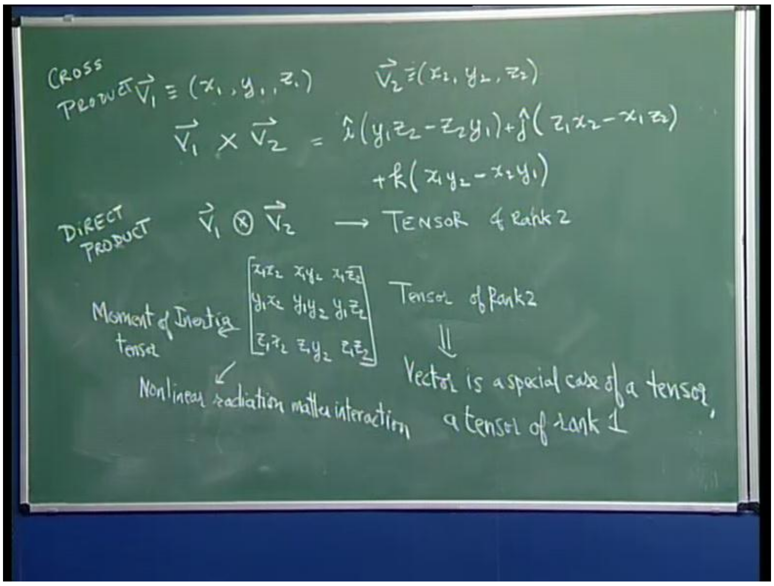

But, it is possible to define these projections for any inner product space. So, all you need once you have the definition of inner product and the definition of a norm you can always define a projection of a vector on to another vector now. So, this is as much as I want to say about the dot product or the inner product. Now, the next kind of product and this is something that you have seen is called the cross product. Now, it turns out that the cross product is unique to 3 dimensional space.

So, in that sense it is not as general as a dot product or an inner product but, it is unique to 3 dimensional space in 3 dimensional space if you have two vectors V 1 by x 1 y 1 z 1 and you had vector V 2 given by x 2 y 2 z 2. Then, the cross product of these two vectors gives you a vector and that vector has 3 components and the 3 components of the vector are given by. So, the i component is related to y 1 z 2 minus z 2 to y 1 the j component. So, the j component is related to z 1 x 2 minus x 1 z 2 and the k component is simply x 1 y 2 minus x 2 y 1. So, the cross product notice that in the dot product you just had x 1 multiplying y 1 x or sorry x 1 multiplying x 2 y 1 multiplying y 2 and z 1 multiplying z 2.

In the cross product you have x 1 multiplying either z 2 or x 1 multiplying y 2. So, x 1 that does not multiply x 2 but, instead multiplies these 2. So, the cross product is different from dot product. In that sense and it is unique to 3 dimension because the cross product two you need you need to have this anti symmetrisation possible and that is possible in 3 dimensions. So, I would not mention a lot more about the cross product since I assume that all of you know how to take cross products I will briefly the third kind of product. And the next thing is the direct product and I am not going to talk too much about this because this is not as useful in the standard at in usual m c s level chemistry but, in more advanced course you will see this product appearing again. So, the direct product of two vectors. So, if you had vector V 1 and you had vector V 2 then this yields an object called a tensor i. So, it yields an object called a tensor and this is the tensor of rank two.

So, what is the idea of the direct product? So, here in the in the dot product we multiplied x 1 by x two in the y 1 by y 2 z 1 by z 2. So, you multiplied the terms corresponding to the same component together in the cross product you multiplied x 1 by either y 2 or z 2. Similarly, you will always multiply y 1 by either x 2 or z 2. So, you always you multiplied terms with of one component with another component you never have any term where the same component is repeated in this cross product tensor the direct product is something that combines both these and it says that you can multiply you look at all possible combination of products. So, if you look at all possible products that you can generate then there are nine possible products, and it is typically represented in this matrix of form.

So, the nine possible products are x 1 x 2 x 1 y 2 x 1 z 2 then you can have y 1 x 2 y 1 y 2 y 1 z 2 and you could have z 1 z 1 x 2 x 1 y 2 z 1 z 2. So, notice that along the diagonals of this direct product, you have the terms that appear in the dot product. So, dot product is the sum of these diagonal element, and the cross product is related to the element that you see in the cross product appear here. But, you go from two vectors with the components to an object with nine components and this object called a tensor of rank 2 and it is called rank 2, because you have a row and a column and essentially it is a direct product of two vectors. Now, we would not talk much about tensors but, all the one useful way to think about tensors is that these are objects that are generalization of the concept of vectors.

So, in this theme a vector is a special case is of a tensor and it is a tensor of rank 2 of rank 1. So, vector is a tensor of rank 1 and you can go ahead and you can say that even a scalar tensor of rank 0. So, tensor is a generalization of the concept of vector. So, we started with scalar then we went to vectors and you can go to tensors and tensor is a generalization it can have arbitrary ranks and we usually in chemistry applications. We usually restrict to tensors of rank 2 3, or even sometimes 4.

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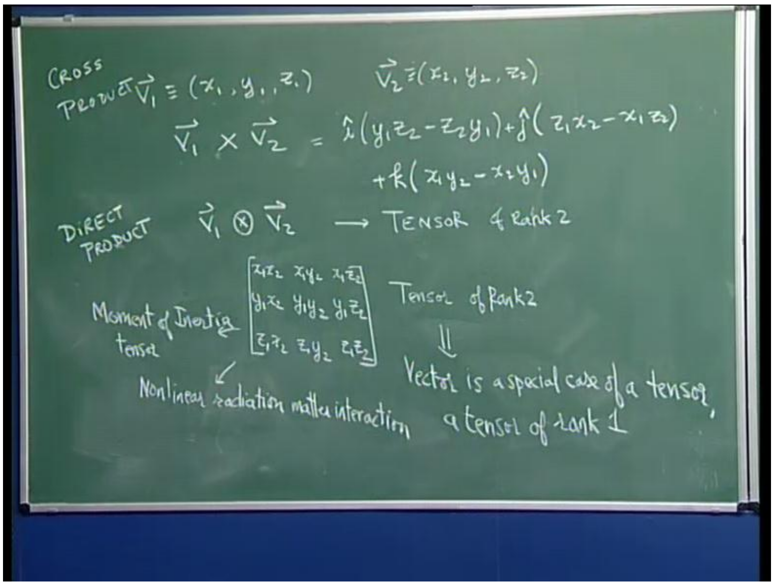

These appear in a two there are two prominent places where you will see the tensors one is the moment of inertia of tensor which appears when you are analysing rotations of a molecule. The other place where you see tensor is when you are trying to analyse non-linear optical phenomenon. So, the two places where it appears I will repeat again one is the Moment of Inertia tensor, and this appears when you are studying rotations your rotation of molecules. The other is the non-linear radiation matter interaction and in this in non-linear radiation matter interaction which is essential to the development of laser and other liner optical phenomena in that you have tensors corresponding to the polarise ability, and the hyper polarise ability of the medium.

So, we have seen that the vector the product of two vectors can be defined in many ways and we have seen at least three useful definitions of products, I want talk about all the scalar triple product and vector triple products. These are simple extensions of the dot product and the cross product involving more than two vectors. The next concept that I want to discuss here is what is called as linear independence. And linear independence and two related concepts are basis and dimensionality.

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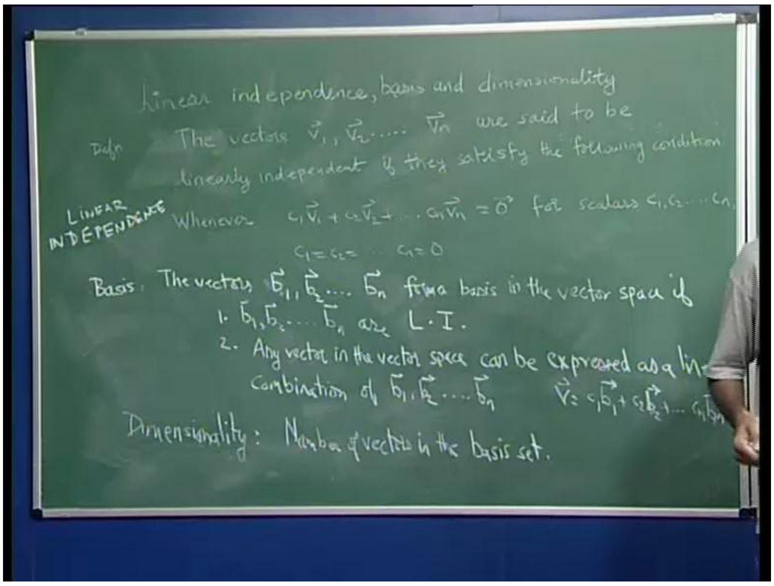

So, what is meant by linear independence and first I will give the definition of linear independence and then, I will try to explain it with examples, this concept will become a lot more clear when we start discussing matrixes and there you will use this concept of linear independence very it is used it is used very often, and the in study of matrices or in solving a system of linear equations. So, let us look at linear independence what is definition of linear independence. So, the definition a set of vectors, V 1 V 2 up to n up to V n is said to be linearly in a set of vectors are said to be actually probably I should say vectors V 1 V 2 up to V n are said to be linearly independent if they satisfy the following condition.

So, what is the condition they should satisfy whenever c 1 V 1 plus c 2 V 2 c n V n equal to 0 for scalars c 1 c 2 up to c n then c 1 equal to c 2 equal to c n equal to 0. So, i will just go through this once again a set of vectors is said to be linearly independent, if they satisfy this following condition. The condition is that whenever you have a linear combination i imply each vector is multiplied by scalar and then this vector is added to next vector, and whenever this linear combination of vectors gives you the 0 vector, for some scalar c 1 c 2 up to c n. Then, the only what that is way that the possible is this each of these is equal to 0.

So, what we are saying is that you have a set of equations and you solve for all the c 1's and c 2's up to c n and if you are only solution that you get for this is the trivial solution where all of these are 0. Then, these vectors are said to be linearly independent. So, in other words this expression gives you the set of equations from which you solve for each of this c 1 c 2 up to c n now it is clear that c 1 equal c 2 equal to up to c n equal to 0 is valid is a solution which satisfies this equation. Now, if there is no other solution then these vectors are said to be linearly independence. So, this is the definition of liner independence, and this is definition. So, if these vectors V 1 v 2 up to V n satisfy this property then these vectors V 1 up to V n are said to be linearly independent.

So, this is the definition of linear independence, if there exist some combination of where of c 1 c 2 up to c n such that not all of them are 0, that means you are saying that these set of solutions have a non trivial solution. Then, these vectors are said to be linearly dependent. So, if there exist no other solution other than this then they are said to be linearly independent, and if they are not linearly independent they are said to linearly dependent. So, we will give some examples of this but, before we go the examples, I want to define these two other terms the next is a basis. So, a set of vectors.

So, the vectors V 1, I will deliberately used the term vectors b 1 b 2 up to b n from basis in the vector space, if they satisfy two conditions the first condition is that b 1 b 2 up to b n are linearly independent. So, I will use the term l, I for linearly independent. So, all these vectors are linearly independent the second condition is that any vector in the vector space can be expressed as linear combination of b 1 b 2 up to b n And by linear combination, what I mean is exactly something like this where you have some scalar multiplying V 1 plus some scalar multiplying V 2 and so on. So, any vector suppose if you have an arbitrary vector V then you can express that as some scalar I will say c 1 b 1 plus c 2 b 2 up to where all these c 1 c 2 etcetera are scalars.

So, any vector in the vector space there should be no expectation every vector in the vector space that means every vector each and every vector in the vector space should be or should be expressible in this form so and then, and then these vectors if it is. So, if these set of vectors satisfy both these conditions first they should be linearly independent, and secondly any vector in the vector space should be expressible as a linear combination of these vectors if they satisfy these two conditions. Then, these vectors are said to form of basis in the vector space. Now, if you have a combination of vector such that any vector can be written as a linear combination of these vectors then this combination these vectors are said to span the vector space v. So, when you say when you say you have certain vector that span the vector space V what you mean is that any other vector in the vector space V can be expressed as linear combination of these vectors. Again I emphasize that we will come back.

And we will look at examples of these but, first let me define one more quantity and you have seen all these before in different forms. So, but it is good to see the formal definition so that you will be able to use this concepts even where even for other cases. So, the dimensionality is nothing but, the number of vectors in the basis. So, if the basis set contains 3 vectors then you say it is 3 dimensional vector space if the basis set contains four vector you say it is four dimensional vector space and so, on. So, the number of vectors in the basis is called the dimensionality of the vector space.

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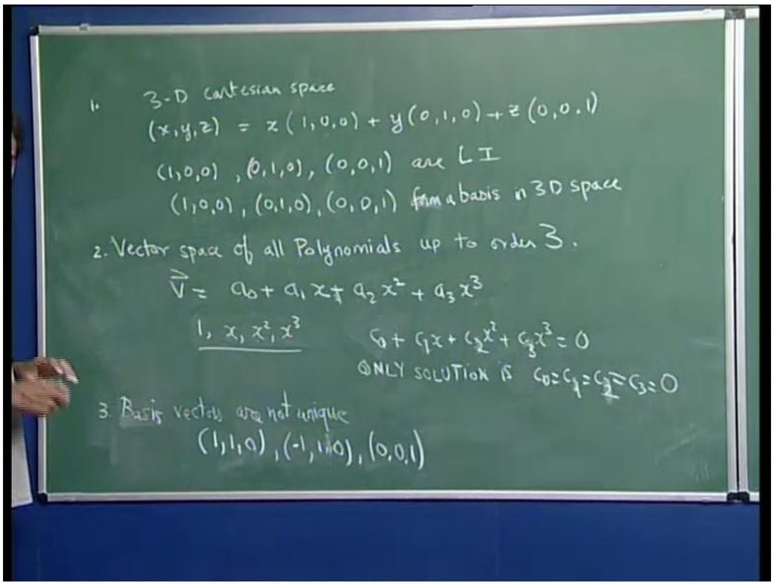

Now, with this definition of the basis you can also show that the maximum number of vectors that can be linearly independent is the dimension of the space you cannot have in a 3 dimensional vector space, you cannot have four vectors be linearly independent. So, the maximum number of vectors that can be linearly independent is equal to the dimensionality of the space and i leave this as an exercise for you to work out. So, let us now look at some examples of basis vectors. So, in the usual 3-D Cartesian space, we have a vector that is x y z and any vector can be written as a linear combination. So, it can be written as a scalar x multiplied by 1 0 0 plus a scalar y multiplied by 0 1 0 plus a scalar z multiplied by 0 0 1. So, these vectors 1 0 0 0 1 0 and 0 0 1 they span the entire vector space.

Now, the next question is are these 3 vectors linearly independent and it is easy to show that 1 0 0 0 1 0 and 0 0 1 are linearly independent and again I will leave this as an exercise for you to try you take a linear combination of these and you show that if the linear combination is 0 then each of the scalars multiplying this have to be 0. So, I will it again I will leave that as an exercise for you to show. So, this is the first example. So, these are linearly independent and span the vector space. So, 1 0 0 0 1 0 and 0 0 1 they are basis or they or they form a basis in 3 D space. So, 1 0 0 0 1 0 and 0 0 1 form a basis in 3 D space. Next let us look at another example this is the vector space of all polynomials up to order 3 and. So, this is in this vector space any vector any vector V is written as a 0 plus a 1 x plus a 2 x square plus a 3 x cube where, x is the variable of which we are taking the polynomial.

So, the set of all these all possible vectors. So, all if you take all possible vectors you will get all possible polynomials up to order 3 and this forms a vector space and now the question is what would be a suitable basis for this vector space and you can easily show that the vectors 1 x square and x cube. So, this vector these four vector they form a they form of a basis for this vector space you can easily see that 1 is a vector because one can be written as 1 plus 0 x plus 0 x square plus 0 x cube. So, 1 implies a 0 equal to 1 and all other 3 are 0 and. So, that is also that is also polynomial of not order 3 but, it is less than or equal to order 3. So, it is order 0 x is also polynomial of whose order is less than or equal to 3.

Similarly, for x square and similarly, for x cube and you can show that any vector can be written as a linear combination of these vectors. So, this forms a basis and you can also show that these are linearly independent. So, you cannot if I take any combination of these if I take c 1 plus c 2 x plus c 3 x square plus c 4 x cube equal to 0 the only way this can be satisfied is if each of these coefficients is 0. So, the only solution is this c 1 equal to c 2 equal to c 3 is equal to sorry if the c 0 c 1 c 2 c 3.

So, c 0 equal to c 1 equal to c 2 equal to c 3 equal to 0. So, all of them have to 0 and that is the only solution because this is a polynomial in x can take any arbitrary value and the only way this is satisfied is if each of these terms are 0 and that means each of the coefficient have to be 0. The other thing I want you to notice are that are that basis vectors are not unique. So, there are many types of basis vector that you can have for example, in 3 D Cartesian space you can have you can have these set of basis vectors but, you can also show that the vectors 1 1 0 minus 1 1 0 and 0 0 1 this also form a basis.

So, in order to prove this you have to show two things first is that these 3 vectors are linearly independent and the second part is that any vector can be written as a linear combination of these 3 vectors and again I leave this as an exercise for you to work out. So, you show how you can you can take first you show that these 3 vectors are linearly independent which is relatively easy to show. Then, the second part you have to show that you can write any vector as a linear combination of these 3 vectors. So, then what the important point is that the basis vectors are not unique.

So, you can have many different set of vectors which form a basis now notice that since we were dealing 3 D Cartesian space you can have only 3 vectors in the basis since the dimensionality of the space is 3 since you have 3 vectors in the basis in this case the dimensionality was four because you have four vectors in the basis. So, the dimensionality of the vector space is equal to the to the number of vectors in the basis and that does not change even if you change the basis. So, you can whether you use 1 0 0 0 1 0 and 0 0 1 or 1 1 0 minus 1 1 0o and 0 0 1 the dimensionality of the vector space remains the same.

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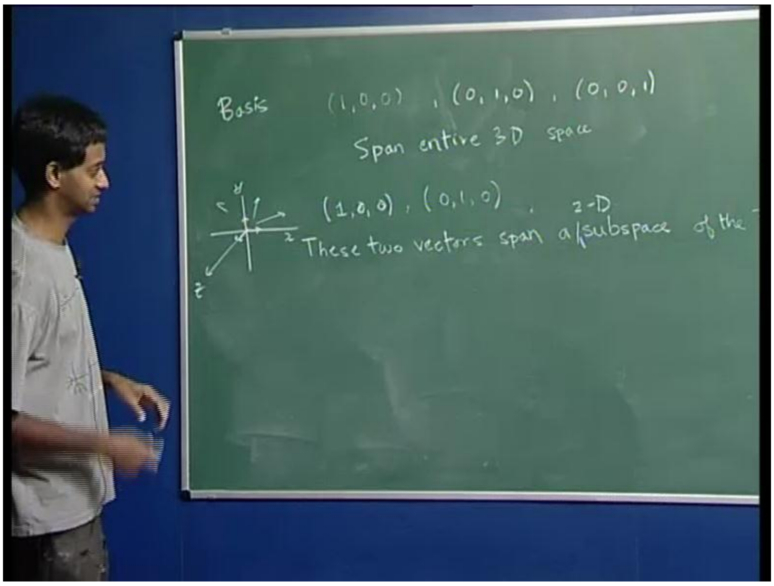

So, we saw that the vectors, 1 0 0 0 1 0 0 0 1 these form a basis. So, these are the basis vectors and these 3 vectors span the entire vector space. So, we say that they span entire 3 D space. So, that means any vector in 3 dimensions can be written as linear combination of these 3 vectors, and if we take all possible linear combinations of these 3 vectors you will get all the vectors in the 3 D space now suppose you take the linear combination of just two of these vectors. So, you take a linear combination of instead of the 3 vectors in the basis you take a linear combination of these two vectors.

So, then if you take all possible linear combinations of these two vectors then, you will span a sub space the sub space of the 3 D space and in this case this sub space is the two dimensional sub space. So, this is a two dimensional sub space. So, if you take a partial list of the vectors in the basis and you take all possible linear combinations of these two vectors you will get a vector space but, that is a sub space of the 3 dimension of vector space. So, since you took only two basis this is a two dimensional space and you can easily see that that these two span the entire x y plane. So, they if you have x y and z now these 3 span the entire space entire three-dimensional space the x y z coordinates; whereas if you just take linear combinations of these two vectors then of or if you just take liner combinations of these two vectors you will get all the vectors in the two-dimensional space. So, you will just span this plane and that is a sub space of this full three-dimensional space.