Chemistry Atomic Structure and Chemical Bonding
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Lecture – 14
Linear Vector Spaces and Operators: Dirac's Bracket Notation

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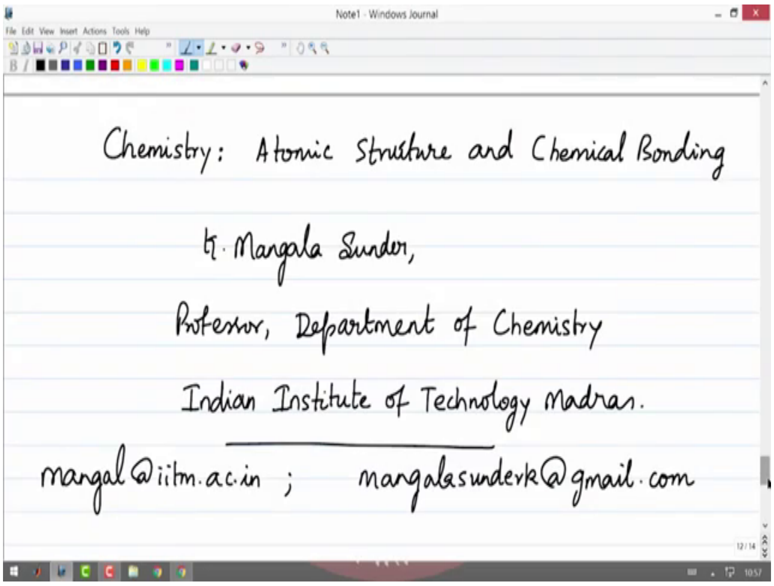

Welcome back to the lecture in Chemistry on the topic of Atomic Structure and Chemical Bonding. My name is Mangala Sunder. I am a professor of chemistry in the Department of Chemistry, Indian Institute of Technology, Madras, India and my email coordinates are given here as mangal at iitm dot ac dot in and mangalasunder k at gmail dot com.

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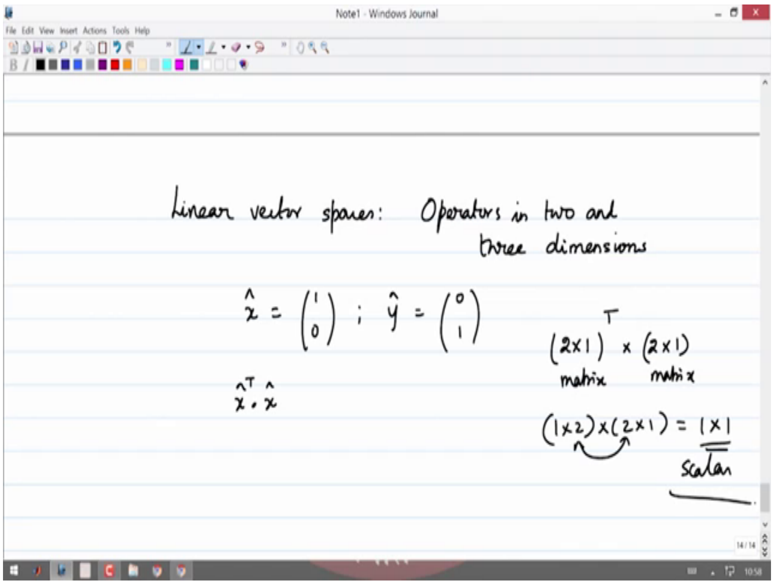

We shall continue this lecture from the previous one with the linear vector spaces where we discussed vectors in two and three dimensions and now the same thing we will continue with a defining operators in two and three dimensions. For that let us recall the definition of the vectors using matrices column vectors namely x in two dimension as 1 0 and y in two dimension as 0 1.

Now, what we did so far was to take x dot x the transpose was on the left side and therefore, you could see that it was a 2 by 1 matrix transpose multiplying a 2 by 1 matrix. And so, you had 1 by 2 multiplying the transpose of that is 1 by 2 multiplying 2 by 1 and in the matrix of course, this gives you the product 1 by 1 which is a scalar. Now we shall get what are known as tensors, basic tensors.

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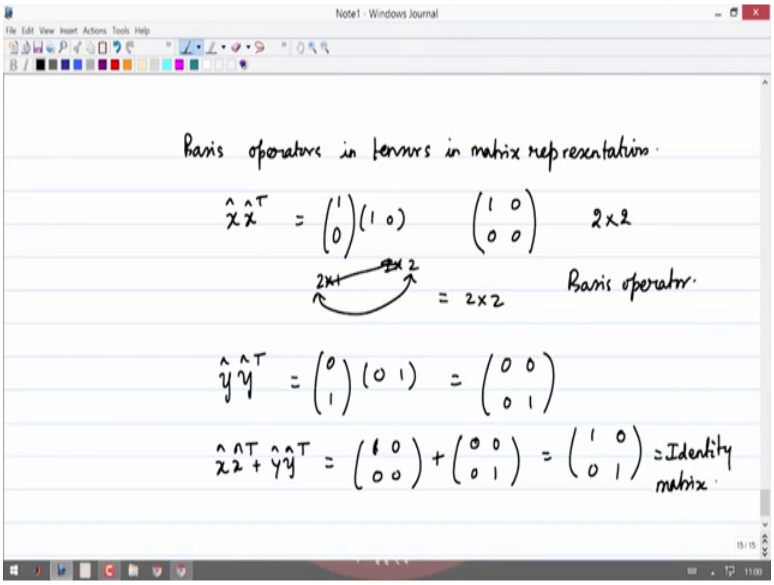

Basis operators or tensors in geometry represented using linear algebraic quantities. So, let us form x x T direct product. Now xx T is the row multiply sorry, is the column multiplied by the row. Now please remember this is a 2 by 1 matrix and this is a 1 by 2 matrix. The product is a 2 by 2 matrix and if you do the simple matrix multiplication, you can see that this gives you the 2 by 2 matrix 1 0 0 0; 2 by 2 matrix this gets cancelled off. So, you get 1 by 2 sorry 1 by 2 gives you 2 by 2. So, this 1 gets cancelled off.

So, you get a 2 by 2 matrix 2 by 2. This is known as a basis operator. Likewise if you form y y T unit vectors y y T you will see that this is 0 1 multiplying 0 1 which will give you 0 0 0 1. And interesting that if you add x x T to y y T, you get the unit matrix namely 1 0 0 0 plus 0 0 0 1 which is 1 0 0 1. This is the identity matrix.

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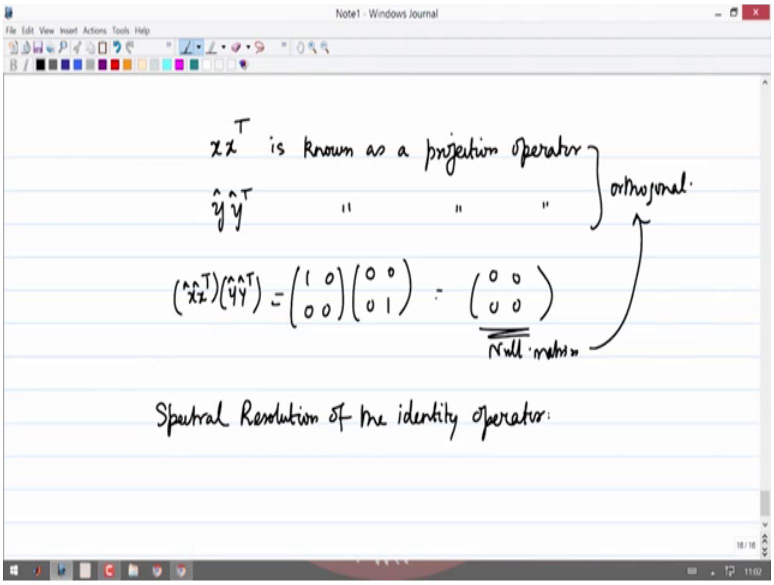

And it is important to recognize that xx T is known as a projection operator and likewise yy T is known as the production operator such that and they are both orthogonal. Because x x T multiplied b y y T you will see that 1 0 if you do 0 0 0 1 which is x x T y y T only is unit vectors. If you do that you see you get, 0 0 0 0 null matrix.

Therefore they are orthogonal projectors and they are such that the sum of the 2 projectors gives you identity. This is in mathematics, in linear vector spaces this is generally known as an example of the resolution of the identity operator; spectral resolution of the identity operator. And in what way is it important to us in quantum mechanics, why we need to study these things; we shall see it in a few minutes.

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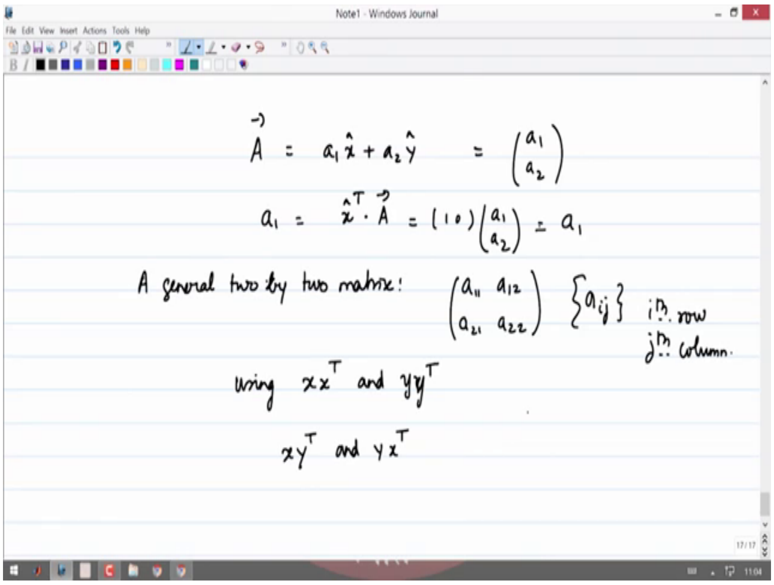

Now, I have a vector A which is in 2 dimension a 1 x plus a 2 y. I said a 1 is the projection of x T on A. You know this is in matrix notation, this is a 1 a 2 and the projection this is 1 0 on a 1 a 2 and that will give you a 1. So, this is the projection operator, this is the projection of the vector to give you the component of the vector.

Now, if I represent a general 2 by 2 matrix a 1 1 a 1 2 a 2 1 a 2 2 to indicate the row column elements. So, a ij is the element of the ith row and jth column element. If we do that, then to represent this using the operators that we have written down namely x x T and y y T, I will find out that these 2 are not enough, but i also need to know what is x y of T and y x of T.

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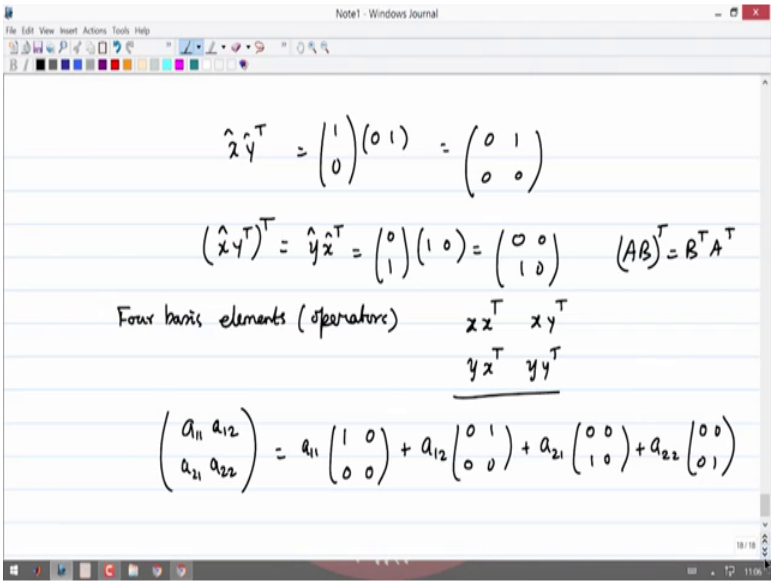

Now, what is x y of T? X y of T is the column 1 0 and the row 0 1 and this you can write immediately as 0 1 0 0. What about x y of T transpose which is y x of T, you remember in matrices if you write A B transpose, you should know that it is B transpose A transpose. So, if you do that if you write this, then you see that this is the column 0 1 for the y and the row 1 0 for the x of T and you know what this will give you is this will give you 0 0 1 0. Therefore, now we have four basis elements or operators x x of T x y of T y x of T y y of T is easy to remember that because you know this is nothing, but the four quantities that are formed from x x T y y T x and y.

Now, these four elements are such that if you write a 1 1 a 1 2 a 2 1 a 2 2, you know in matrices using the elementary matrices. This is nothing other than a 1 1, 1 0 0 0 plus a 1 2 0 1 0 0 plus a 2 1 0 0 1 0 plus a 2 2 0 0 0 1. Now, you see immediately the representation of the operators coming into picture for us.

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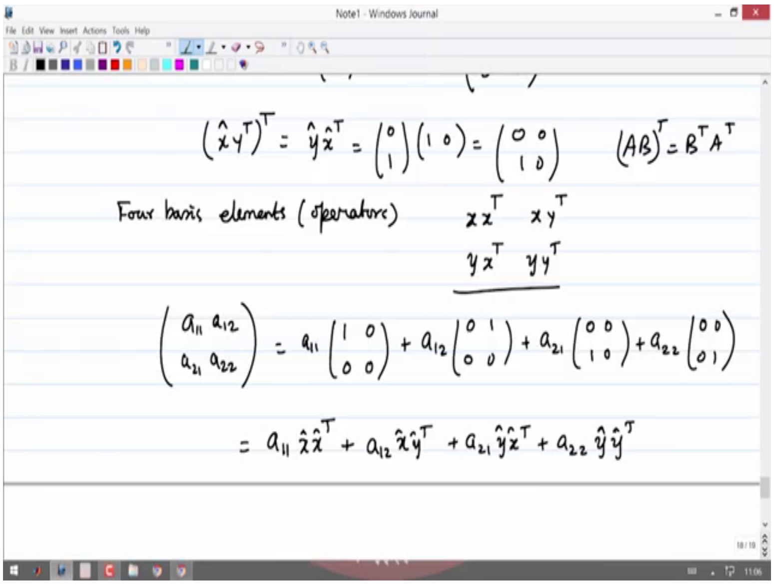

So, now you can see that this is nothing other than a 1 1 x x of T plus a 1 2 x y of T plus a 2 1 y x of T plus a 2 2 y y of T. So, this is also known as the resolution of an operator in terms of basis operators, exactly the same way that you had a vector written in terms of the basis vectors and the components of the basis vectors. You have now any 2 by 2 matrix which is which will represent an operator in the basis of x and y any 2 by 2 matrix is now resolved into the four component operators that you have the x x of T y y of T and x y of T and y x of T. This is a mathematical way of writing an operator in terms of the four basis operators quite; obviously, when you do this in three dimensions.

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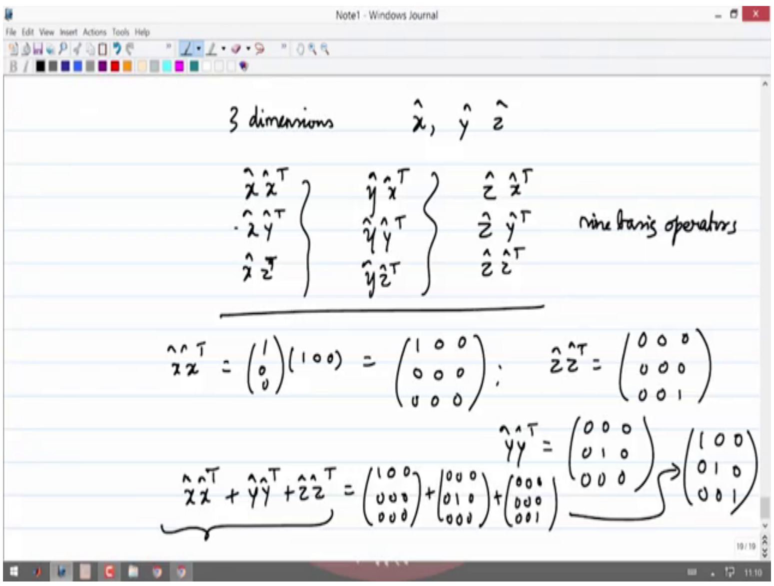

You know the vector is represented in three dimension by a column with 3 elements, 3 rows. Therefore, you can see not if you have x y and z in three dimensions y and z; when you can form 9 quantities namely x x of T x y of T and x z of T and likewise with y x of T y y of T and y z of T and the z x of T z y of T and z z of T.

So, you have nine basis operators each of which is three dimensional, in the sense it is a 3 by 3 matrix nine basis operators the same way that you had three basis vectors xy and z for writing any arbitrary vector A in terms of the components. Now you have any arbitrary operator in terms of the corresponding square dimension. If it is three dimension, it is nine operator elements; If it is three two dimension, four operator elements that is what you have to remember. So, this is easy to write that down, I will write a couple of them x x of T you know is a 1 0 0 multiplying 1 0 0 and that will be the 3 by 3 matrix even here. And now you can see that all the other things are similarly 3 by 3 matrices with one in only one place out of the 9 and the rest of it being 0.

So, zz of T for example, is 0 0 0 0 0 0 0 0 1 and y y of T is 0 0 0 0 1 0 0 0 0. Now you see again the beautiful identity with respect to these things namely x x of T plus y y of T plus z z of T. Yes, you can see that it is 1 0 0 adding all these three matrices 0 0 0 0 1 0 plus the third one 0 0 0 0 0 0 it is 0 1 and so, that gives you the identity matrix 1 0 0 0 1 0 0 0 1.

So, this is the spectral resolution of the identity operator in three dimension and this extends to any n dimensions and of course, it is also extends to complex spaces where the numbers that we have are not real numbers, but complex numbers. And therefore, we have a complex linear vector space, which is the fundamental entity and fundamental description for defining or what is called the basis for defining the operators and the matrix elements and then calculating them for measurements and experiments. Therefore, this is the formal basis to that.

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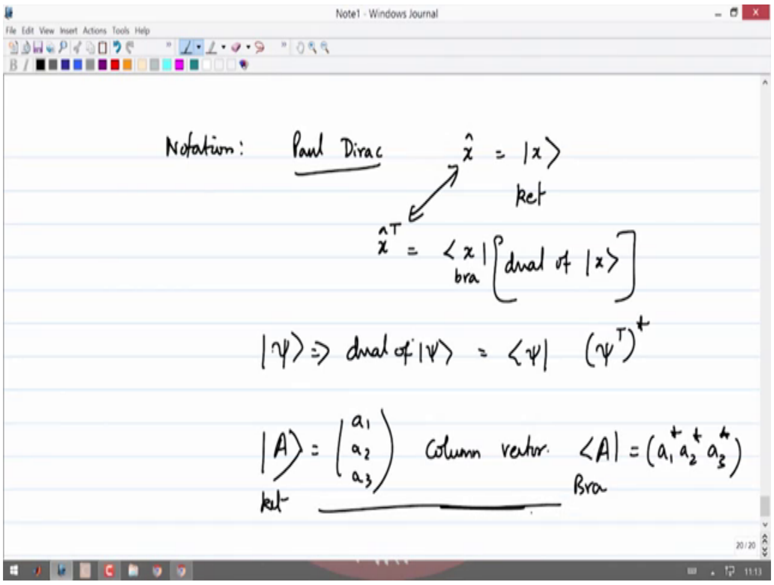

Now, let us write the notation that was first introduced by professor Paul Dirac. Paul Adrian Morrison Dirac is a founder, one of the founding fathers of Quantum Mechanics and his book on the Principles of Quantum Mechanics is still almost like a bible for the whole field. Paul Dirac introduced the notation that the abstract vectors that we wrote he wrote this as a ket. And then of course, he also introduced the x of T as the bra vector x. Since these are real the relation between the ket and bra is a transpose of the quantity. If the basis vectors are complex in nature, then the relation between the ket and bra will not be just to the transpose, but it will be transpose complex conjugate.

Suppose we have a psi which is a complex vector if it is given, it is dual. This is called, the bra is called the dual of the ket vector. The dual of psi will be psi and this will be basically psi T star, in terms of geometric representation if you have to do that or in terms of say linear vector algebraic representation. It is a transpose of psi also with the complex conjugate what is the example for example, if you have a as a 1 a 2 a 3.

This is a ket vector which is written as a column vector the dual the bra vector this is the ket vector. The bra vector is a 1 star a 2 star a 3 star. So, you see that it is not only the transpose of this column vector into a row vector, but it is also the complex conjugate of the elements in. This is the formal definition of the bra ket and the scalar product of 2 vectors or vector with itself is written as A A with the connector C.

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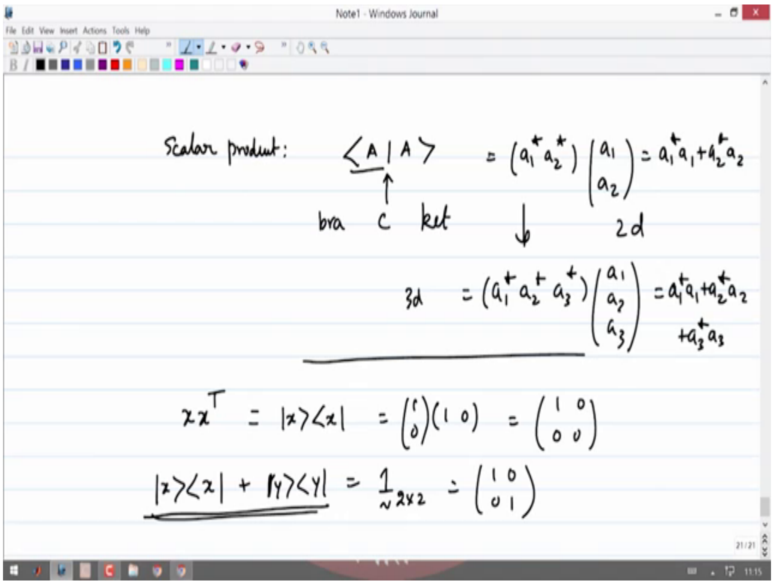

So, this is called the bra and ket. So, basically bracket was defined into a left component and a right component and a connector which is basically the relationship between them, but the bracket means something more should be there like an operator should be there and so on.

So, in this case of course, you can write the bra vector is a 1 star a 2 star in 2 dimensions multiplied by a 1 a 2 in 2 dimensions gives you a 1 star a 1 plus a 2 star a 2. And in three dimensions, this will be this is 2 d and in 3d this will be a 1 star a 2 star and a 3 star multiplied by a 1 a 2 a 3 giving you a 1 star a 1 plus a 2 star a 2 plus a 3 star a 3. Anyway this is for introducing A to be a complex number. We will not concern ourselves with the complex numbers for some time. Therefore, if you write to these things are usually transpose of each other we can neglect the star because the real number its complex conjugate it is itself imaginary part is 0.

Therefore a 1 star is the same as a 1 tells you that a 1 is a real number. So, if you deal with real numbers we do not need to worry about these stars. Now using this let us see, x x T is now formally defined as x ket multiplied by the x bra because the x ket is of course, 1 0 and the x bra is the transpose of this which gives you 1 0 0 0. Therefore, you have the relation x x plus y y in two dimension is the identity operator in two dimension which is usually written as a matrix in 2 by 2 and that is 1 0 0 1. This is the formal way of writing what we wrote a few minutes ago in terms of the adding the operators to give the identity operators.

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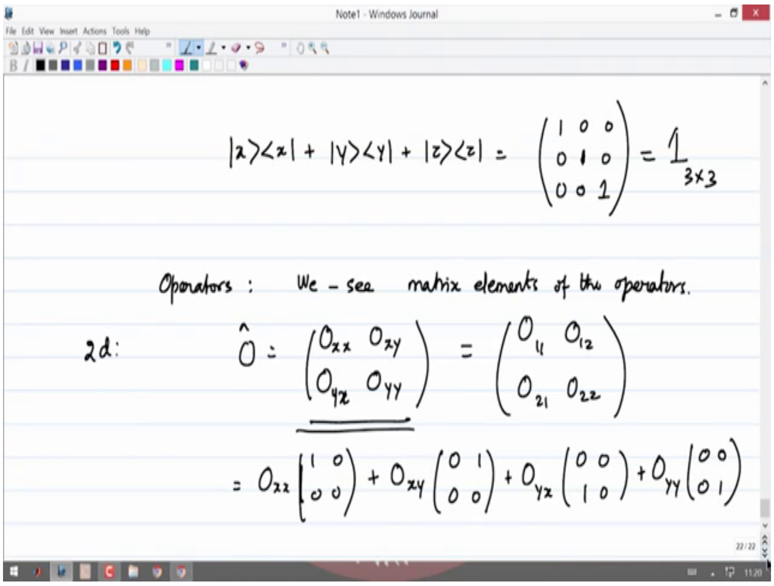

And likewise in three dimensions, the formal relation is x of x plus y times y plus z times z and so, you have giving you identity 1 0 0 0 1 0 0 0 1 and so, this is the identity in three dimensions. And the same thing extends to n dimensions, if you have really n dimensional space and so on.

Operators using the bracket rotation and we will see what are known as the matrix elements of the operators. We start with two dimensions. So, a general operator has a two dimensional matrix representation given by x x x y x z sorry this is y x O yy. I think you remember that we wrote this also as O 1 1 O 1 2 O 2 1 O 2 2 to represent to the row and column indices, but let us use.

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This notation x x y y xyz so, if you look at this carefully, this is O x x times 1 0 0 0 plus O xy times 0 1 0 0 plus O yx times 0 0 1 0 plus O y y times 0 0 0 1. Now, you have already represented these things in terms of ket bra states.

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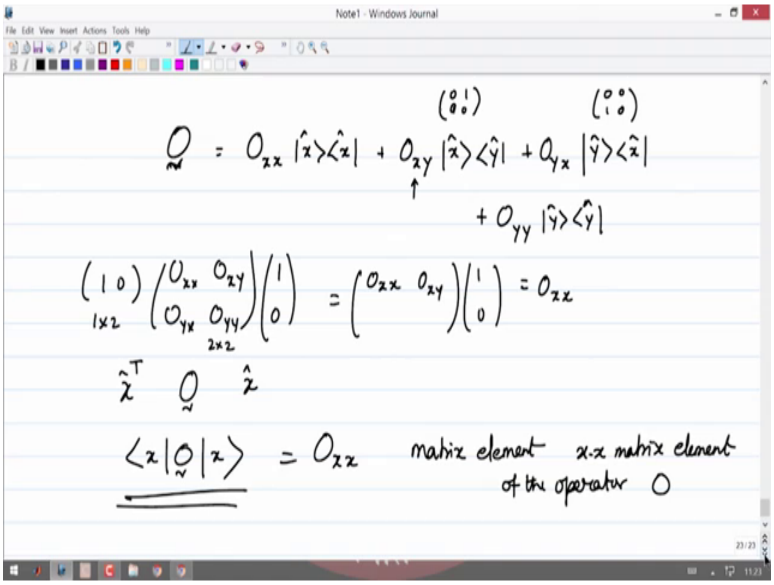

Therefore if I write the operator O with the with something making underscore so, what we do is its O x x times x x plus O xy remember the left is given by that. And O y x is given by y x plus O yy given by y times y right this is the matrix 0 1 1 0 and this is the matrix 0 1 0 0. This is the matrix 0 0 1 0.

Now, if I project this is O is a matrix of this type xy O yx O yy. If I multiply this matrix on the left with say, x and on the right with say again x T, so, what I have is x T O x I mean there are of course, these things are all written to give you some unit vector in the vector space. So, if you do this, this is also written as x the operator y and x; if you do this the matrix multiplication immediately gives you this answer. You can do the first 1 1 0 O x x, what will you get? You will get 1 0 multiplying O x x will give you O x x and then 1 0 multiplying the second.

So, this is 2 1 by 2, this is 2 by 2. So, you will get 1 by 2 which is the next 1 0 multiplying the second row will give you oh x y and this multiplied by 1 0 gives you on the right gives you O x x. So, this quantity is O x x is known as the matrix element. In this case it is known as the x x matrix element of the operator ohm. So, you can see that.

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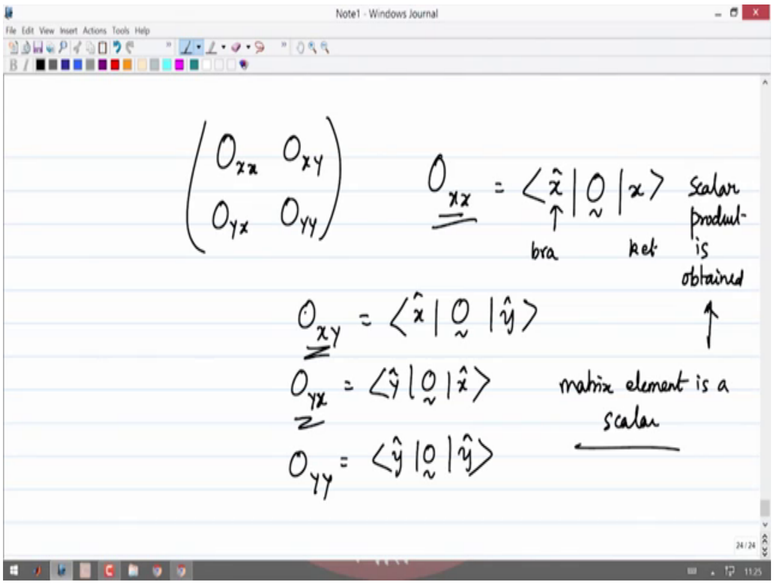

Oxx xy O y x O y y if you write this matrix the first element O x x is the matrix element x the operator O and x column. So, this is the bra ket likewise you can write immediately O xy it is easy for you to verify that this is x the operator O times the vector y and O y x a scalar. Please remember these are all numbers or scalars.

But these are all also numbers of scalar the entities inside here or vectors or operators such that a scalar product is obtained. Therefore, the matrix element is a scalar. So, O yx if you have to continue, it will be y O x and likewise O y y as a scalar. If you continue it is y the operator O and the vector y.

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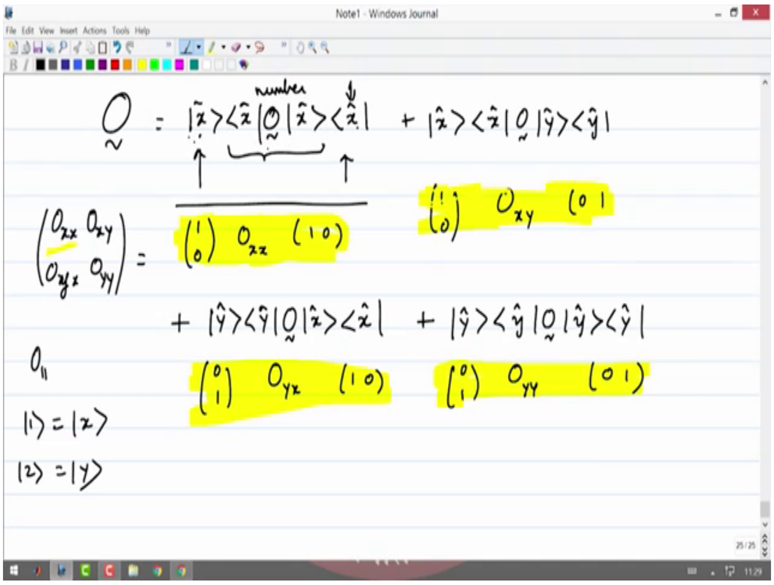

So, now, there is a very nice way of writing these things namely O. The operator is go back the element x x is given by that. Therefore, the way you would write it as x x O x x.

So, what you have done is to introduce the element inside in between the 2 please remember this is a number. So, what you have done is to write the ket vector the number O xx and the bra vector 1 0 that is less this 1. Likewise this is for the first element O x x and in the same way you can write to this as x O x y is x O y y could always keep these hats on to say that they are also vectors unit vectors and so on.

So, this is nothing, but 1 0 O x y and this is 0 1 and the third one is O y x which will be y y O x and you have x. So, this is 0 1; this is the matrix element O y x, this is y and this will be 1 0 and the last of course, when you write this as y y O operator y y which gives you the quantity 0 1 O y y and 0 1. So, what is important is the four terms that know lets highlight that. The operator O is now written; the operator O xx O xy O yx O yy is now written as a sum of four terms this one; a sum of the four terms that you have here, second one is here and the third one is this and the fourth one is this.

Therefore if you have to do this for arbitrary number of dimensions, a b c d e f I mean these are all basis vectors. You will see that an operator is therefore, represented if in that dimension; if it is n. There are n basis vectors the operator has an m by n matrix representation and each element of the operator is connected with the basis element indexed as 1 or 2 or 3 or 4 etcetera. The same way that you have indexed to this 1 O x x with let us do that O x x if you do that it is indexed with O 1 1.

So, what is your vector 1? Your vector 1 is x, your vector 2 is y. Therefore, these are the matrix elements representation that is an operator is now represented in terms of the basis operators and the corresponding matrix elements.

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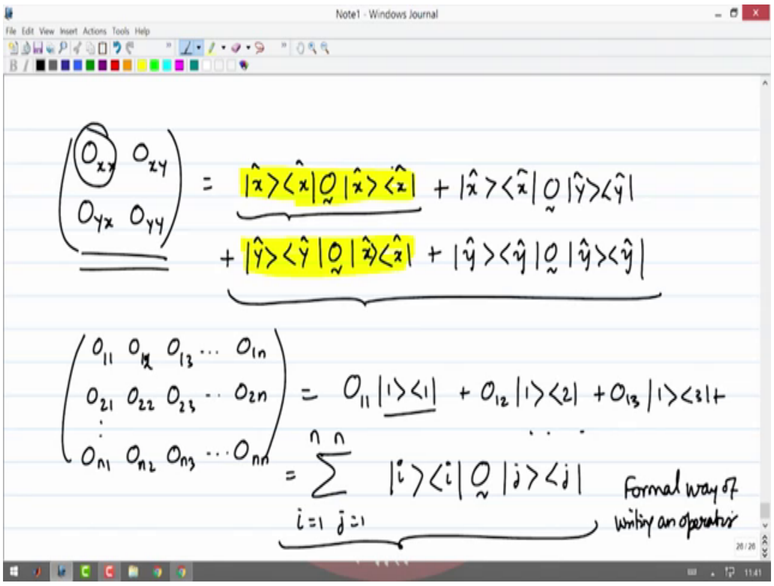

This is nothing other than O 1 1 1 1 that is the basis vector 1 for this n dimensional problem and likewise O 1 2 is the basis vector, basis operator O 1 2 O 1 3 is the basis operator 1 3 and so on. So, it is easier to write this as sum over i is equal to 1 to n, j is equal to 1 to. This will be i i O j j this is the general representation for the operator in quantum mechanics using linear vector spaces namely using the matrix representation and this is formal way of writing an operator.

So, all of this gives you some handle on how to represent vectors and matrices using vectors and operators using matrices main namely column vectors and row vectors and then column matrices and column row matrices. And you have a general field. Now let us do the formal mathematical statements of some of these linear vector spaces. Let us write down a few statements.

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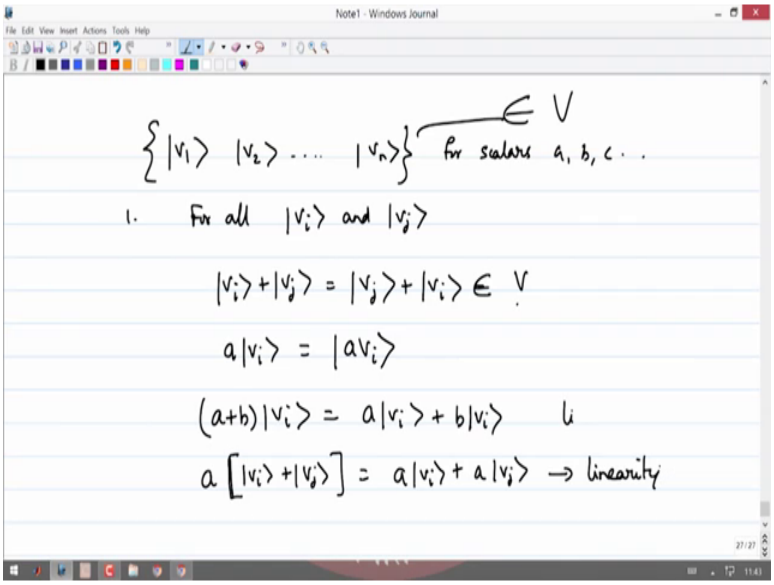

If we have a linear vector space defined by a collection of vectors v 1 v 2 v m and for scalars arbitrary scalars a b c etcetera. First one, for all v i and v j, the sum vector v i plus v j is equal to the commuted sum v j v i and is an element of the vector space V. All of these are elements of the vector space V.

Secondly, any number scalar multiplying the vector v i is also written as the new vector scaled vector a b i. The sum of 2 numbers v i can also be distributed as a v i plus b v i linear. The a on 2 vectors v i plus v j is also a on v i plus a on v j. This is the linearity.

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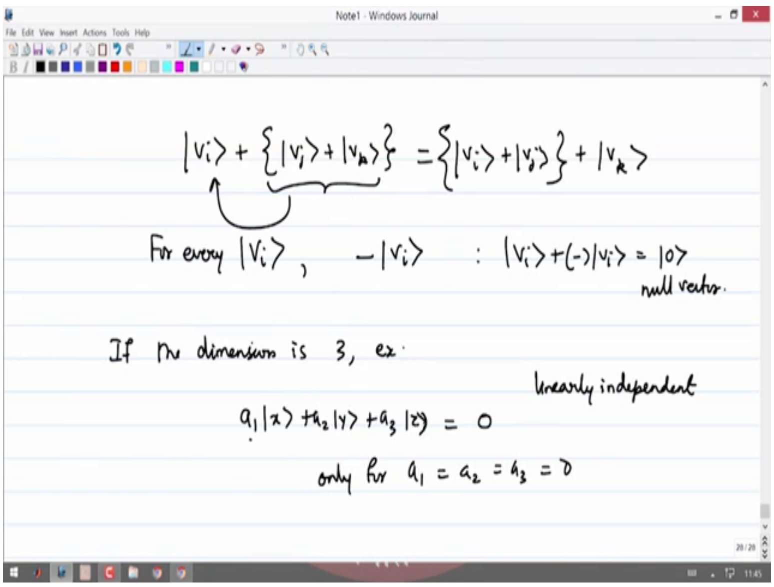

Likewise associativity if you have it v i plus if you add to other vectors v j v k and then you add the sum of this to this vector. This is equivalent to doing this summation v i plus v j first and then adding it to the vector v k. And for every v i you shall also have a minus v i minus 1 times v i such that v i plus minus 1 times v i is the null vector 0.

If the dimension is 3; for example, if I write a 1 times x plus a 2 times y plus a 3 times z; if i require this to be 0 and x and y and z are orthogonal and linearly independent vectors, linearly independent vectors. The definition of linear independence is that this sum is 0 only for a 1 is equal to a 2 is equal to z 3 is equal to 0. That is it is not possible for me to form a linear combination of all the basis vectors using any scalar such that the sum of that is equal to 0. That is not possible unless the scalars themselves are 0. The sum of this will always be some vector.

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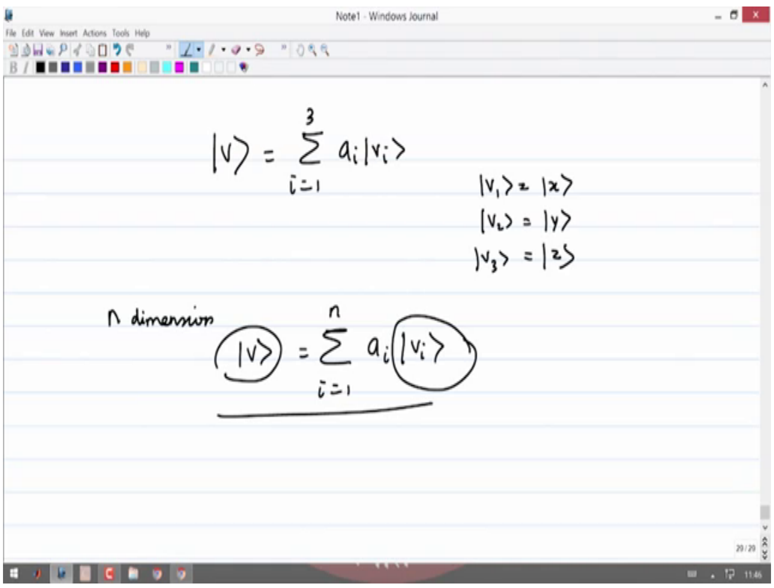

Therefore this tells you that any vector v for example, can be represented in 3 dimensions by 1 2 3 a i times v i. And we used for v i the v 1 as x and v 2 as y and v 3 as z earlier. But if it is in the n dimension, then the same thing holds good for the vector v in n dimension except that the sum is no over. All the n dimensional linearly independent vectors with coefficients a i v i. This is the representation of any arbitrary vector in y n dimension in terms of the basis vectors in n dimension and these basis vectors are independent.

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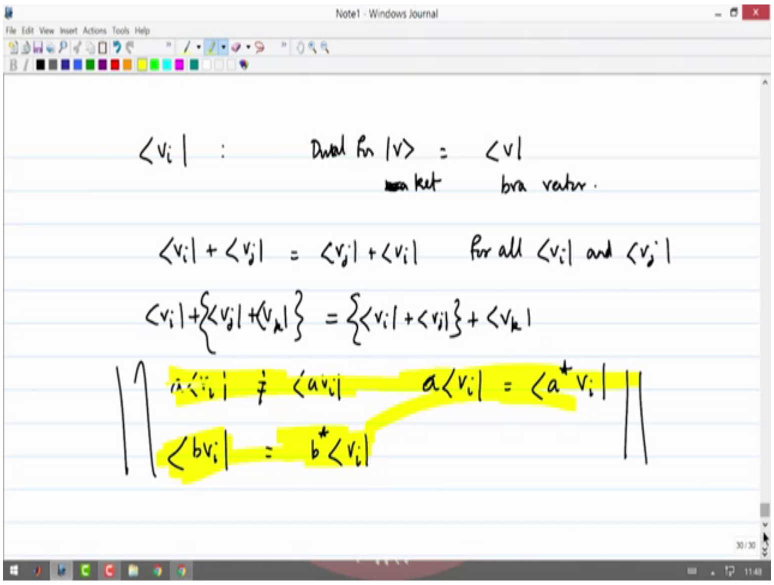

Now what about the complex conjugate or the ket vector v i? The dual it is called, the dual for v is written as v. This is bra this is sorry this is ket and this is the prostate bra vector. The relationships are still the same for summation v i plus v j is the same as v j plus v i for all v i v j elements of this space, for all v i and v j. And likewise the distribution that v i the associativity that you have v i plus v j plus v k, you have the association of these 2 and then you form the sum this is equivalent to the sum v i plus v j first and then summing this to the v k, the third one.

The most important differences a times v i is not a v i, but a times v i is a star, the complex conjugate of v i that will go in and likewise if you have a b vi inside if the vector is let and if you want to take the scalar out; the scalar has to be the complex conjugate v on v i. So, this is important, I will highlight that this is important with respect to the properties of the scalars with respect to the bra vector and the ket vector.

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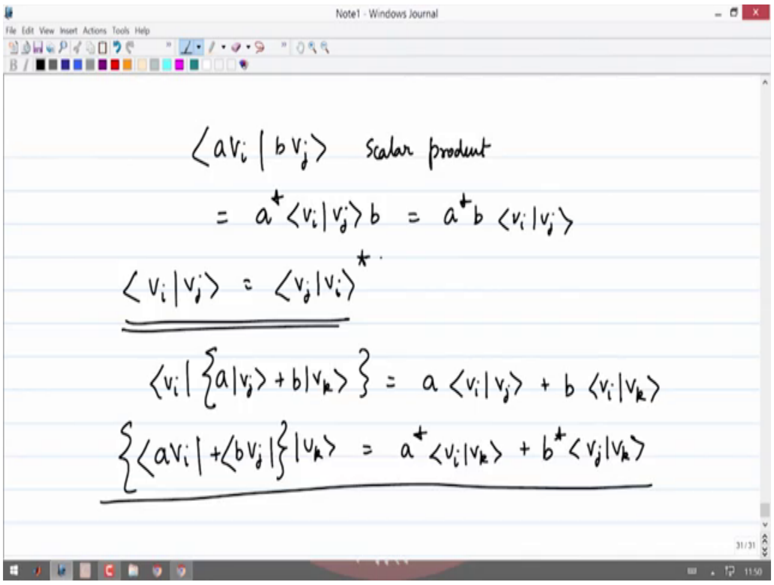

So, therefore, you can see that if you write a quantity such as a v i, if you write a quantity such as a v i and you write another b v j and this is the scalar product or the inner product, then you know this is equal to a star v i v j times b which is a star times b v i v j. Therefore, if you have a vector psi no, we if you have a vector v i v j, you know that this is v j v i star. This is the relation between the scalar products with the vectors in the order i j ket the bra ket with respect to ket bra this one.

If you interchange the order the scalar product is the complex conjugate. And the last step that I would like to write is that if you have a vector v i forming a scalar product with a v j plus b v k, then the scalar product is a times v i v j plus b times v i v k and lastly if you have a v i plus b v j. If this forms the scalar products with v k, then this is given as a star v i v k plus b star v j v k. These things are important that there is a star associated with the bracket the bra vector. Any scalar associated with the bra vector if it has to be taken out of the bra vector, then its a complex conjugate that you have to worry about. So, these are important we will use some of these things as we go along when we study the matrix representation until then.

Thank you very much.