Chemistry Atomic Structure and Chemical Bonding
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Lecture - 06
Elementary Mathematics: Introduction to Matrix Algebra
Part II

So, let us assume the matrix multiplication here, I have given an example on the screen, which are fundamentally important for this course also.

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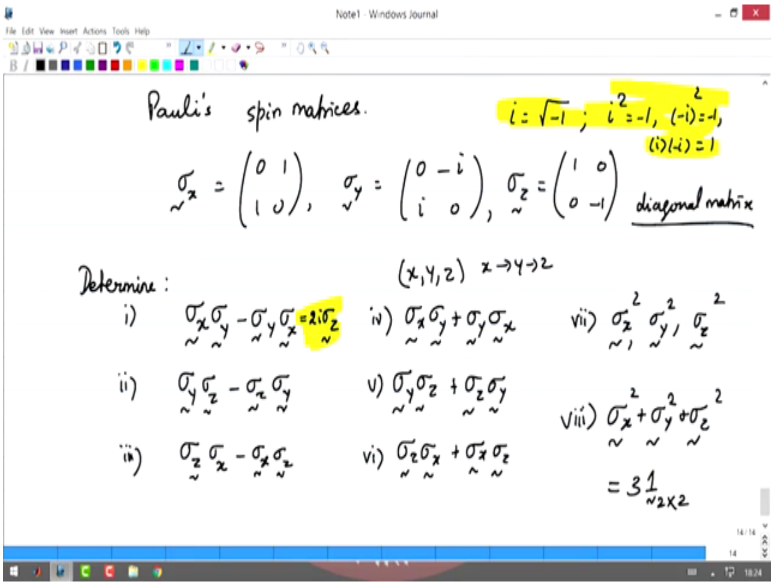

Therefore, I have chosen these special matrices called they are called the Pauli spin matrices in honor of professor Wolfgang Pauli, who first introduced them in understanding. In our understanding of the spin quantum number and as a property of the, systems nuclei and electrons and other particles ok.

So, you have the x component, this is called the x component of the Pauli spin operator. It is a 2 by 2 matrix, the y component of the Pauli spin operator, which is the 2 by 2 matrix, but it has an imaginary quantity, i and minus i and i and the imaginary numbers of course, you, you know the algebra of all the imaginary, complex numbers. You know i is defined as the square root of minus 1 and likewise, i square is minus 1 therefore, and likewise minus i whole square is also minus 1 i into minus i is 1 ok. Keep that property in by i mean keep this in mind and then you have sigma z, which is the z component of the Pauli spin operator with the 1 0 0 minus 1, this is a diagonal matrix.

It is diagonal matrix, because it has all the off diagonal elements to be 0. It has non-zero elements, only along the diagonal. Now, these matrices obey very special properties called anti commutation rules, in the sense that if you take the product of the matrix sigma x sigma y and then take the commuted product sigma y and sigma x and add them, find out what answer you get and there are three such commuted properties, which involved x y y x y z z y z x x z. So, it is sort of cyclically x y z. So, it is like x to y to z and if you take the differences between those matrices, you will also find that, these matrices do not commute with each other sigma x does not commute with sigma y. Therefore, the difference is non zero. The answer is actually 2 i sigma z ok.

In this case and likewise you can find out the other answers also determine sigma x squared, sigma y square and sigma z squared, you will find out that these are nothing, but identity matrices 3 times, the identity matrix 2 by 2 ok. So, these properties are important therefore, even though it is matrix multiplication and elementary things, please keep some of these special matrices will keep coming again and again ok.

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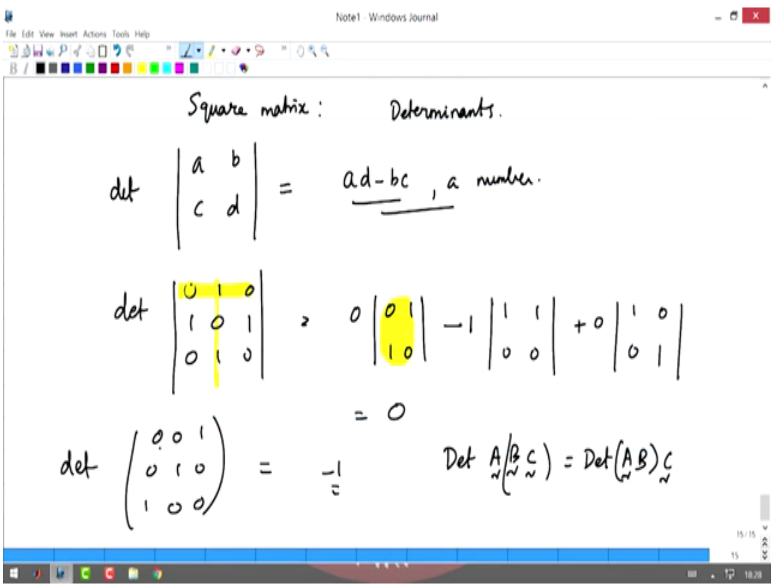

Now, let us move to the next property of the matrices. Particularly the property of the square matrix ok, a square matrix is one in which the rows and columns of the matrices have the same number. There are 2 by 2 3 by 3 4 by 4. It is not square matrices can have what are called the determinants and the determinant is something you are already familiar with for any array. If you have a b c d as a matrix, the determinant is written by the symbol and that is a d minus b c which is n number.

So, let us calculate the determinant of a 3 by 3 matrix 0 1 0 1 0 1 0 1 0, you can see in calculating the determinant, please recall your high school or the previous mathematical mathematics that you studied, that you can expand the determinant along any given row or along any given column. So, let us expand this, along the first row. If we do that it is 0 times the, if you do 0 then it is the cofactor of 0 is 0 1, which is, which is called a minor 0 1 1 0. And since, you go to the second element, the sum of the indices row plus column index is odd. This will be a minus sign and you will see that it is 1 times 1 0 1 0 and the last 1 is 0 times 1 0 0 1.

So, if you take any element 0 for example, then all you would do is, in doing the matrix multiplication, you will delete that row and you will delete that column and. So, the rest of it is 0 1 1 0, which is what is here and in the same way the minor of 1 will be deleting, deleting this column and this row. So, what is left over is, sorry not this one in determining the minor of 1, you will delete this column and this row. So, what is left over is 1 0 1 0, which is what is here of course, the answer for this is 0, if you do a matrix such as this 0 0 1 0 1 0 1 0 0, if you want to calculate the determinant of this matrix, then it is clear that the first two are 0.

So, you do not need them and the last one is plus 1 times whatever is the minor and the minor is minus 1. So, the determinant of this matrix is minus 1. And you can also verify that the determinant of A B C is the determinant of A B times C, because you know that matrices obey the associativity determinant of is also, it also follows the same properties. Now, there are matrices for which the determinant is 0.

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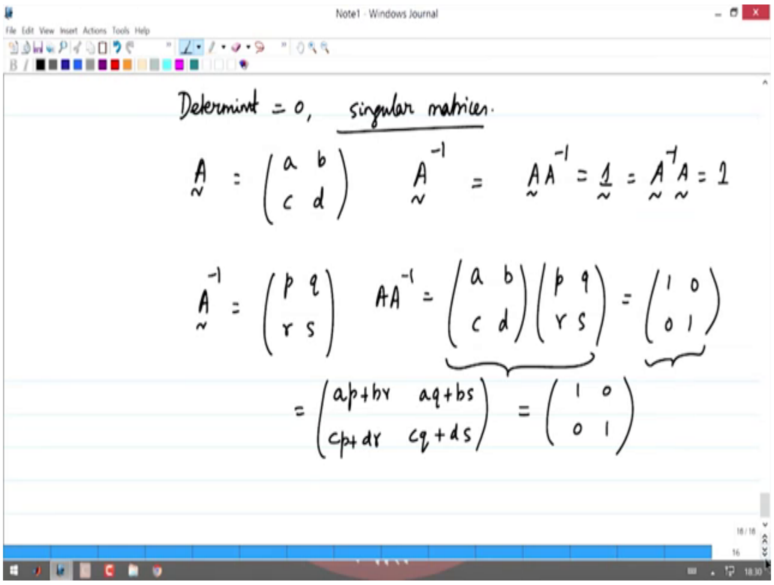

And these are called singular matrices, the singular matrices are such that if you want to define an inverse for the matrix A suppose, you have a matrix a b c d and an inverse is to be defined, A inverse the property of the inverse is that A times A inverse is the identity matrix and it is the same thing as a inverse and a. So, in that sense they commute ok. This is the property of the inverse.

Therefore, if A is of a b c d and you want to calculate A inverse and let us write this as p q or s then A, A inverse would be a b c d multiplied by p q r s and that should give me the identity matrix namely 1 0 0 1. And since this is a matrix the elements of this matrix should be the same as the elements of this matrix. So, let us calculate them, it is a p plus b r that is the first row first column then the first row, second column is a q plus b s likewise c p plus d r and c q plus d s this should be 1 0 0 1.

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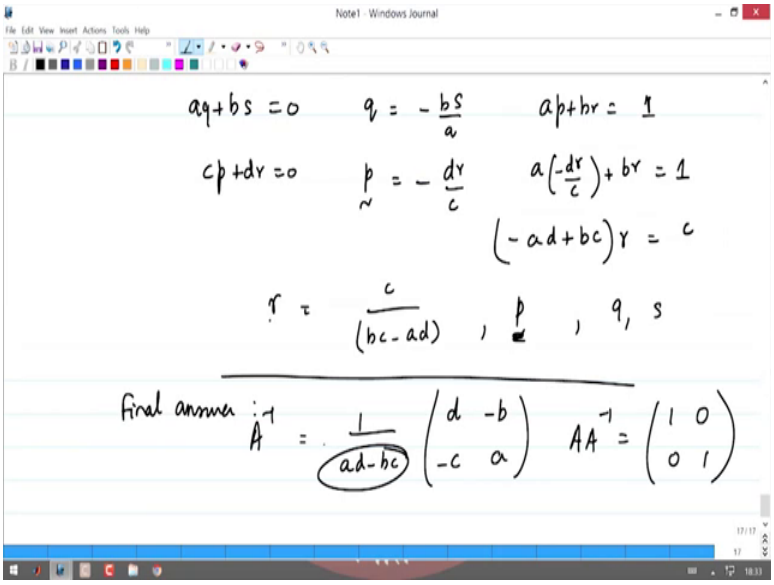

Given this, you can immediately see that the element a q plus b s is 0 and since we are interested in finding out p q r s in terms of a b c d which we know. So, we can write q is equal to minus b s by a and likewise, this element c p plus d r is equal to 0 and. So, I will write p is equal to minus d r by c we also have the property that a p plus b r is equal to 1 and since we know that p is minus d r you have a times minus d r by c plus b r is equal to 1. So, this gives you immediately minus a d plus b c times r is equal to c. So, what is r; r is c by b c minus a d and once you know r, you can immediately find here. Since r is connected to p, you can immediately find p.

Therefore, you determine p you determine similarly, q and you determine s. What is the final answer, the final answer will turn out to be 1 by a d minus b c times. The final answer is 1 by a d minus b c times the matrix d minus b minus c a. It is easy to verify that if this is A inverse then A into A inverse actually gives you, the matrix 1 0 0 1 ok. Now, what is important is this factor a d minus b c please note that a d minus b c for this matrix is nothing, but the determinant of a therefore, it should not be 0.

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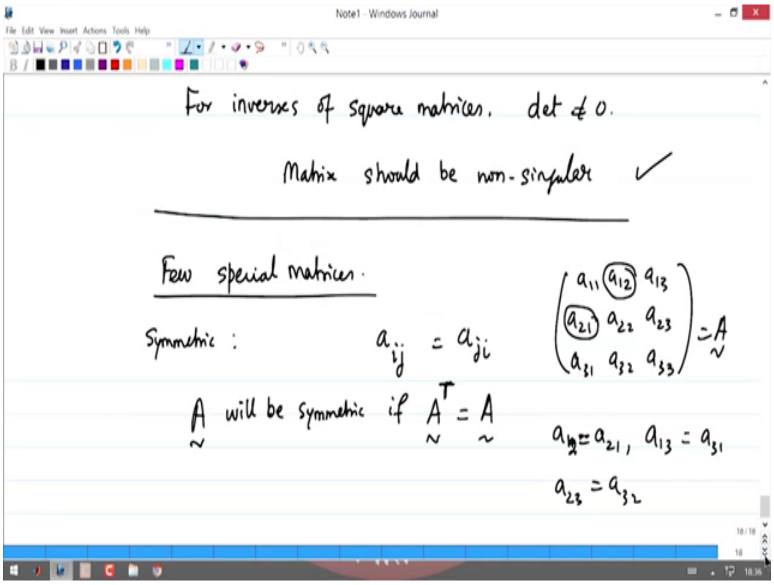

Therefore, for inverse to exist the matrix should be non singular. For inverses of a square, of square matrices determinant should not be 0, matrix should be non-singular in my lecture, notes. Of course, I will give you a very clear formula for inverses of a general matrix in terms of what are known as the determinant as well as the cofactors of each elements, but here we have seen that. So, likewise it is easy to, calculate inverses and inverses are very important, wherever they exist the, it is important to find the inverse and associate the properties of the inverse with certain types of matrices.

In the next and the final, the part of this particular lecture; I shall introduce you a few special matrices, in which inverse will have a critical role ok. Now, a matrix is a symmetric matrix, if the element a i j is the same as the element to a j i that is the matrix a 1 1 a 1 2 a 1 3 a 2 1 a 2 2 a 2 3 a 3 1 a 3 2 a 3 3, if you write this as a matrix, this a will be symmetric; If the transpose of the matrix, which is obtained by transposing the rows and columns of any given matrix is equal to the matrix itself.

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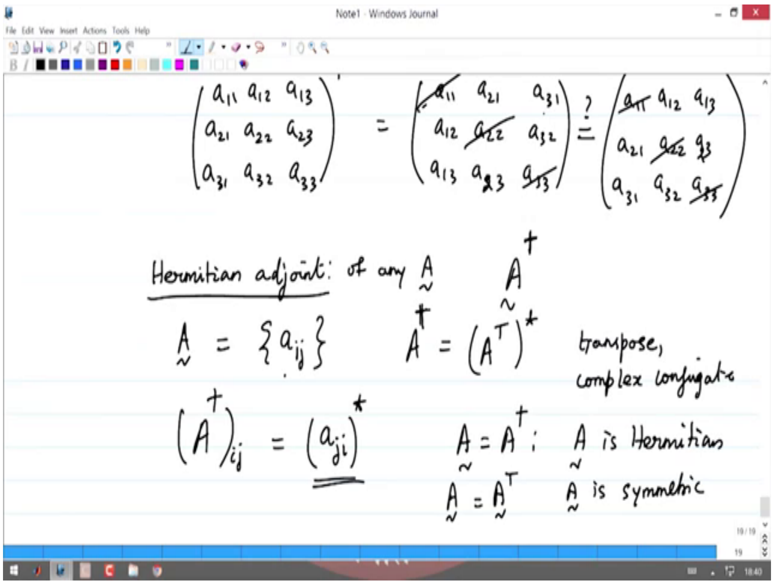

Therefore, a symmetric, if you have a 1 2 and a 2 1 or the same, a 2 1 likewise, a 1 3 and a 3 1 are the same and a 2 3 and a 3 2 are the same. That is also easy to see, because the transpose of this matrix a 1 1 a 1 2 a 1 3 a 2 1 a 2 2 a 2 3 a 3 1 a 3 2 a 3 3. You take the transpose of this matrix, you are basically transposing this, column into a row or this row into a column. So, let us take this row, then it becomes for the first row becomes the first column a 1 3, the second row becomes the second column a 2 3 and the third row a 3 1 a 3 2 a 3 3 ok.

If this where to be equal to the original matrix a 1 1 a 1 2 a 1 3 2 1 a 2 2 a 2 3 a 3 1 a 3 2 a 3 3, then you see that there is no problem with the diagonal elements, because they do not, transpose themselves. They are all equal, but a 2 1 should be a 1 2 and a 3 1 should be a 1 3 and a 2 3 should be a 3 2, which is what I have written here. So, this is required if A t is equal to A. Now, this is for symmetric matrices. Now, if the elements are complex, you would see that, we can define in a similar way, what is called the Hermitian adjoint.

The Hermitian adjoint of any matrix a is denoted by of any a is denoted by the symbol, A dagger and if the matrix of A is denoted by the elements a i j then A dagger is the elements of the matrix A transpose star, transpose complex conjugate. Therefore, if you write A dagger i j is a j i star ok. There matrix is transposed and it is complex conjugate, this is the element, this is defined as A Hermitian adjoint of A. It does not tell you anything about, whether A is the same as Hermitian adjoint of A dagger that is A is equal to A dagger. It does not tell you anything that for every matrix A, we can define a Hermitian adjoint.

If the element is real then the Hermitian adjoint is given by the transpose of the matrix, the elements of the transpose of the matrix, a matrix is Hermitian only if A is equal to A dagger then we say A is Hermitian, in the same way we say, when A is equal to A of t, we say A is symmetric.

So, the Hermitian includes complex numbers and therefore, the complex conjugation is important in the definition Hermitian adjoint and Hermitian matrices that is in matrices for which the matrix and it is Hermitian adjoint are equal. They are fundamentally important. In fact, all observable quantities in quantum mechanics in the matrix formulation are represented by a Hermitian matrices actually in mathematical parlance, it is, they are represented by what are known as the self adjoint matrices.

But for our course, if we keep the, terminology simple and Hermitian matrices are very-very important in quantum mechanics all eigenvalues are eigenvalues of Hermitian matrices that we will eventually, find then the other important property of a matrix other important type of a matrix is known as orthogonal type.

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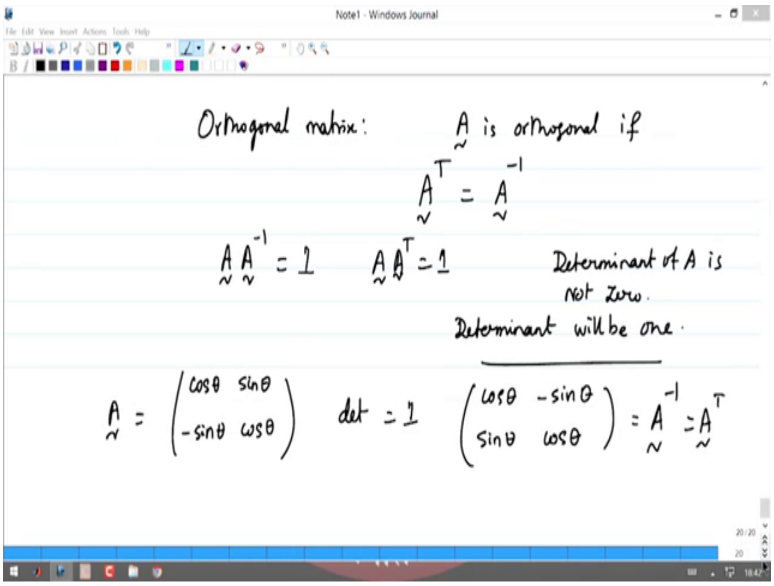

Your matrix is orthogonal, if A is orthogonal. If A T, the transpose of A is equal to the inverse of A that is A A inverse, if it is 1 then it is the same thing as saying A A T is equal to 1. Since, clearly inverses involved the determinant of A should not be 0, A is not 0.

In fact, it will turn out to be 1 ok so, because 1 in also determinant of A A T, involves determinant of A in the denominator. Therefore, you would say that orthogonal matrices or matrices for which the transpose of the matrix is equal to the inverse of the matrix or you compute the inverse by simply transposing the matrix.

So, if I have a matrix like cos theta sin theta minus sin theta cos theta then I know that the determinant of this matrix is 1, it is cos square theta plus sin square theta minus of minus sin square theta and the, this matrix is orthogonal. Its inverse is the transpose namely cos theta minus sin theta. The first column becomes the first row and the second column is the second row sin theta, cos theta is A inverse.

If this is A and this is nothing, but the transpose of the matrix. So, here is a very simple example for what is known as a transpose and the inverse. These are for real elements, if you have complex elements, then 1 does not define an inverse in this way or the, orthogonal in this manner, but 1 defines what is known as the unitary matrix.

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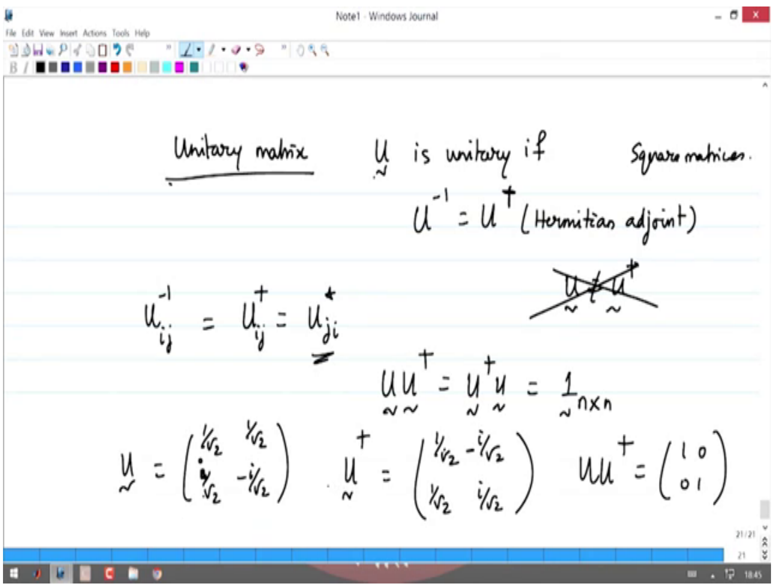

A unitary matrix u is unitary, if u inverse is equal to u dagger the Hermitian adjoint, u is not Hermitian that is u is not equal to u dagger in general ok. No, therefore, the inverse of the matrix is the same as u dagger. So, u dagger is of course, you know is u j i star ok.

u i u dagger i j is u j i star the rows and columns are inversed in, I mean transpose and complex conjugate.

Therefore, this is the same as the u inverse i j. So, the property is u U dagger, which is the same as u dagger u and that is equal to 1 ok; obviously, all are square matrices. We are not talking about any other at this point ok. So, this is the identity matrix therefore, if u is n by n, this will be and an identity matrix of n by n. What is the example of a unitary matrix? Very simple 1 by root 2 1 by root 2.

Let me do i by root 2 and then I write 1 by root 2 minus i by root 2, I take this matrix then it is inverse, if this is u it is inverse is u dagger and u dagger is the transpose of the matrix 1 by root 2 i by root 2, but also complex conjugate. Therefore, i becomes minus i for the first column, becomes the first row and the second is 1 by root 2 i minus i by root 2, which becomes plus i by root 2 ok.

If you multiply these two matrices, you will see u U dagger is 1 by root 2 times 1 by root 2 plus this. You will see 1 by 2, that is 1 and the second, column is minus i by root 2. This i by that is also 0 and likewise this is 0. So, this is u U dagger is 1 0 0 1. So, this is an example, a very simple example of a unitary matrix in two dimensions is even now, what I have not said in conclusion, I should state that.

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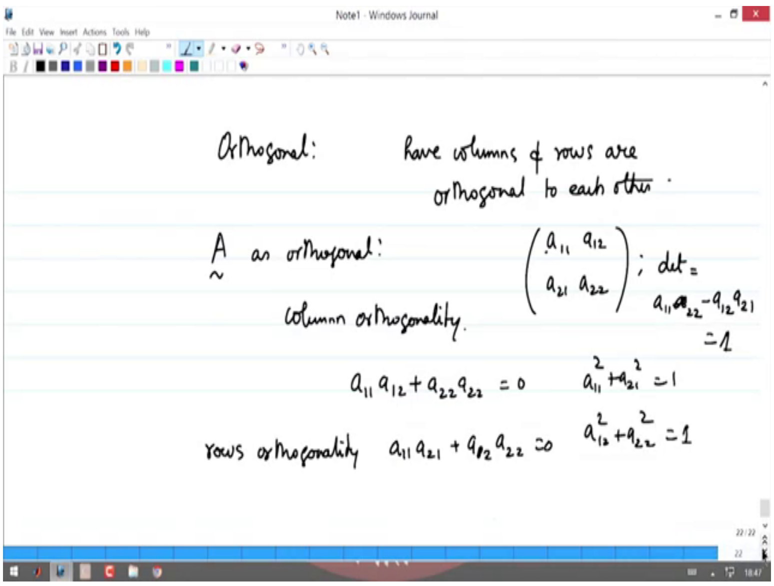

Orthogonal also means the following orthogonal matrices have columns and rows which are orthogonal to each other or orthogonal to each other and or normalized. So, if I take A matrix a as orthogonal then the property of this column orthogonality, it is the following a 1 1 a 1 2 a 2 1 a 2 2. Please remember the determinant is 1 which is a 1 1 a 2 2 minus a 1 2 a 2 1. This is 1 and the column orthogonal to essentially means column 1, multiply the element by element within column 2 will give you the answer 0 a 1 1 a 1 2 plus a 2 1 a 2 2 is 0 and likewise the rows will also be orthogonal row.

Orthogonality will be a 1 1 a 2 1 plus a 1 2 a 2 2 that is 0. What about rows by themselves; a 1 1 square plus a 2 1 square that will be 1 and likewise, a 1 2 squared plus a 2 2 square will be 1. So, the rows and columns are normalized and the rows and columns are orthogonal to each other, this is for an orthogonal matrix for a unitary matrix. One of the rows that we take in the product of two rows has to be the complex conjugate of the row itself and therefore, when you say you.

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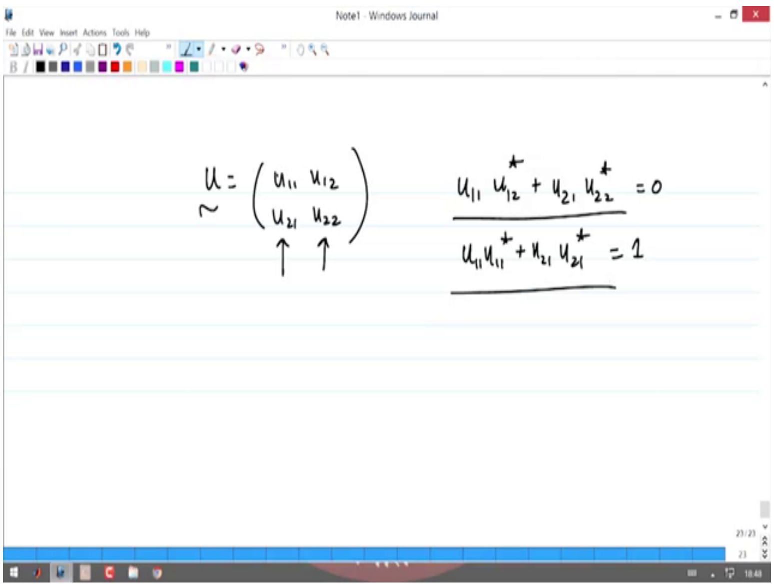

Suppose, you write to the matrix u as u 1 1 u 1 2 u 2 1 u 2 2 that is a simple example then the column orthogonality essentially means column 1 is orthogonal to column 2. So, you either take column 1 real, but then you multiply with the complex conjugate of column 2 plus u 2 1 u 2 2 star that is 0.

So, this column multiplied by the complex conjugate of this column is 0. It does not matter which one is taken as a complex conjugate, because if a number is 0, it's complex conjugate is also 0. So, if you take this row, this column and you take the complex conjugate of it, it is still 0. The other thing is the ortho, the normalization essentially means u 1 1 u 1 1 star plus u 2 1 u 2 1 star that is equal to 1.

Therefore, unitary matrices are such that the rows and columns are normalized and the rows and columns are orthogonal, but remember you have to take the, real products for the row normalization. The real products for the column normalization, but you have to take the one column or one row to be complex conjugate of the other column, these are properties of the unitary matrices.

We will have a lot of occasions to see these things in the next lecture and then many others, but keep these properties in mind. This lecture is pretty long, but this is a fairly quick revision of some of the matrix properties. I am sure you have seen and let us continue with the, the linear algebraic representation of some of these matrices in the next lecture.

And also look at the eigenvalues and eigenvectors for some of these matrices and the connection between them and quantum mechanics in the a few lecture. So, I would believe that this module will have a few of these, lectures together and it is important preliminary for understanding quantum mechanical calculations in a large scale. We will continue with the matrix algebra in the next lecture until then.

Thank you very much.