Advanced Mathematical Methods for Chemistry

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Module – 02
Lecture – 02
Special Matrices – Symmetric, Orthogonal, Complex Matrices

In this lecture I will talk about what are called as special matrices, and you know I have used the word special, but basically we will be looking at matrices that are symmetric orthogonal.

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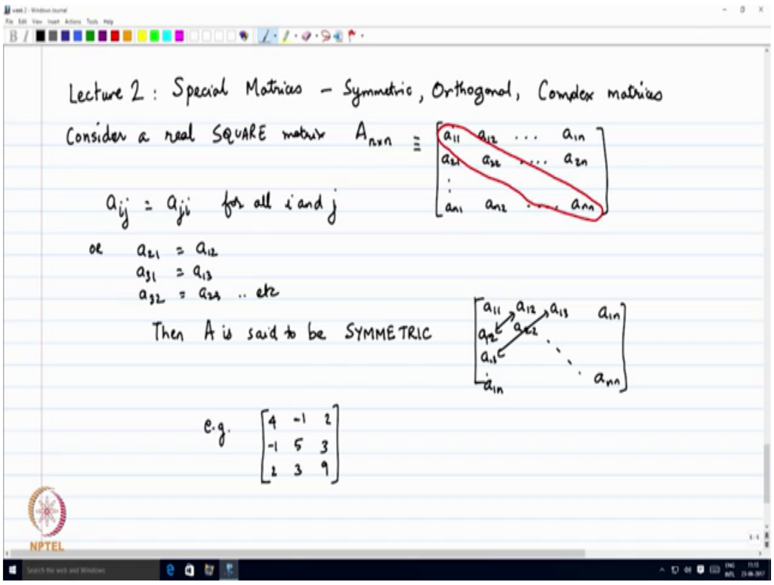

And we will be looking at complex matrices and the corresponding and the complex matrix corresponding to symmetric and orthogonal real matrices.

So, first let us consider real I will use a word square matrix A and I will say n cross n. So, it has n rows and n columns, it is a square matrix, the number of rows and columns is the same. Now if you consider a real square matrix and again will uses notation that we that we are familiar with a 11, a 12 upto a 1n, a 21, a 22 upto a 2n, a n1, a n2 upto a nn. Now in this matrix this set of elements this is called the diagonal elements of the matrix. So, these are called the diagonal elements of the matrix. So, the elements along the diagonals are referred to as the diagonal elements. So, the matrix and these are called the off diagonal elements. So, all the others are called the off diagonal elements.

Now, suppose you had a real square matrix and n cross n square matrix; such that the a i j equal to a j i for all i and j; that means, or I can say a 21 equal to a 12, a 31 equal to a 13, and all the way and then and then similarly a 32 equal to a 23 and so on. So, if you have this case then A is said to be symmetric So, A is said to be a symmetric matrix and it is very obvious what it will look like. So, what will it look like is that you will have a 11, a 22 upto a nn along the diagonals, then whatever you have here a 12 the same a 12 you will have here a 13, a 13 and so on a 1n, a 1n. So, these 2 elements will be same these 2 elements will be same and so on and the end you can do for all the other elements too. So, an example of a symmetric matrix I will just take a 3 by 3 matrix and show you what a. So, suppose you have let us say 4, 5, 9 minus 1 minus 1, 2, 2, 3, 3. So, this is clearly a symmetric matrix. So, a symmetric matrix is one kind of special matrix.

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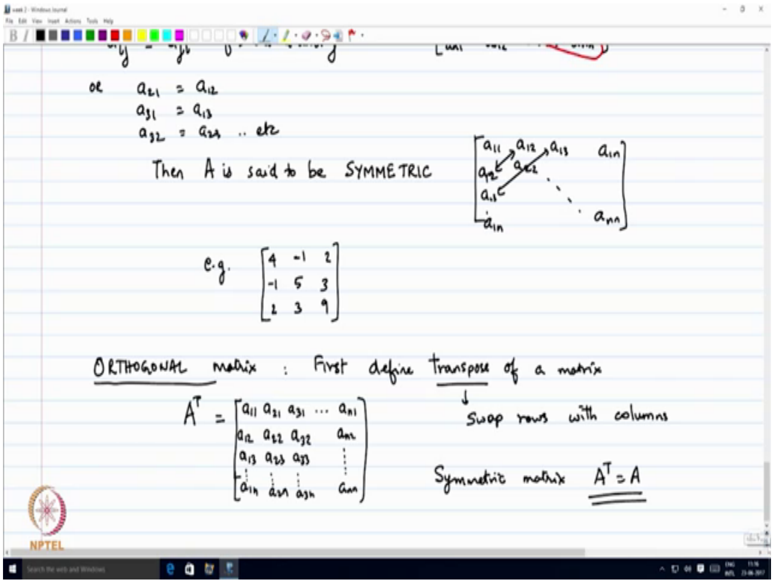

Now, the next matrix that I want to talk about is what is called an orthogonal matrix. In order to describe an orthogonal matrix let me define. So, first define transpose of a matrix. So, A transpose is equal to. So, A transpose is also a matrix. So, it is denoted by this way and what you do is you basically swap the rows and columns, if A is given by this form. So, if A is given by this by this expression. So, A transpose is also an n by n matrix and what is done is a 11 and then you put a 21, a 31 upto a n1, a 12, a 22 and a 13 all the way upto a 1n here and in this case a 21, a 22 now what you will have is a 23 all the way upto a 2n, a 32, a 33 all the way upto a 3n, a n2.

So, this is a transpose of A and you can clearly see what happened is you just change you just swapped the off diagonal elements, you kept the diagonal elements the same and you swap the off diagonal elements. So, basically you transpose means switch rows and columns, swap rows with columns. So, the transpose of a diagonal matrix is defined in this way and what you can. So, we can clearly see that for a symmetric matrix A transpose equal to A. For a symmetric matrix A transpose is equal to A; now let us go to the next thing which is a diagonal matrix and here or an orthogonal matrix.

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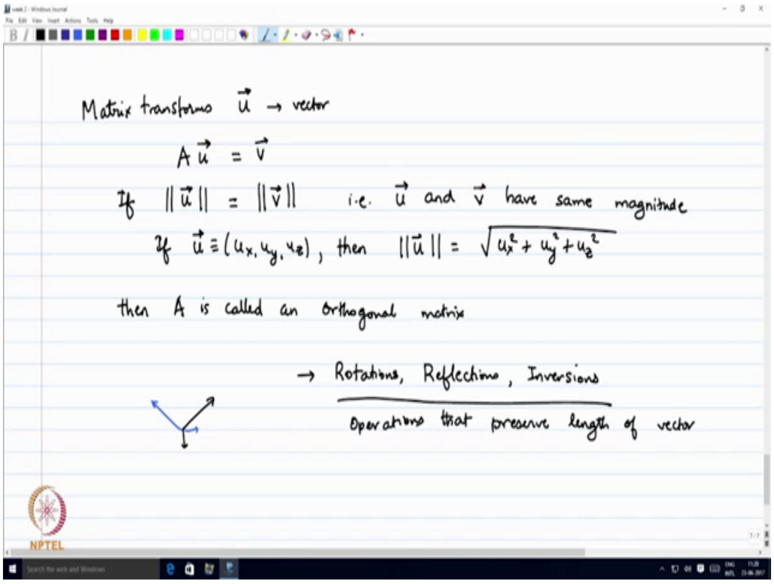

So, now let us get back to a matrix as a transformation of a vector u which is a vector. So, A u equal to v. So, it takes u it transforms it is a linear transformation, it gives a vector v. So, if the norm of u equal to norm of v that is i e u and v have same magnitude, and we are talking about the usual norm. So, if u is equal to u is given by u x, u y, u z then norm of u is equal to square root of u x square, plus u y square plus u z square. So, that is a usual way you take the length of a vector.

So, if a matrix a transforms a vector such that it preserves it is norm and this is true for any vector. So, matrix a is such that whichever vector it takes it transforms it in such a way that it transforms it to a different vector which has a same norm as the original vector, then A is called an orthogonal matrix, if it transforms a vector such that it gives it just another vector with the same magnitude then a said to be an orthogonal matrix.

Now, in order to see, what does it do? So, suppose you had a vector and you transformed it to another vector that had the same magnitude, you could have a different vector you could have another vector let us say that looks like this and this might be transformed to some vector that has the same magnitude something else. So, such a transformation is referred to as an you know. So, the matrix corresponding to such a transformation is referred to as an orthogonal matrix.

Now, orthogonal matrices you can immediately see that what is an operation that would take a vector and transform it to another vector that has the same magnitude, you could have things like rotations, reflections that means, if it just takes each vector and rotates it by a certain angle then you will get another vector with the same magnitude you could have reflections. So, you could you could you could reflect each vector, you could have inversions. So, you could take a vector and point it in the opposite directions that would be an inversion of the vector, you could reflect it about a plane. So, you could take each vector and reflect it about a plane and so on. So, these are examples of operations that preserve the length. So, these are the kind of transformations that we will see.

Now, there is another property of this orthogonal matrix which we will see, and in order to in order to see that property we will define something called a inverse of a matrix.

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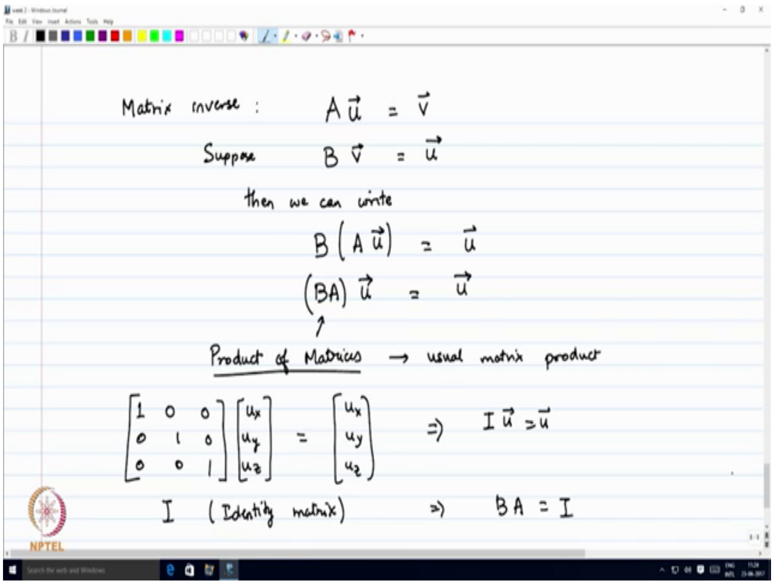

So, we can now in order to do this you we said that a matrix is an operation. So, matrix, if you had a matrix a operating on A vector, you get some other vector v. Now suppose B operating on v gives you back u, suppose you find some other it should it should not have the arrow on this suppose you find some other matrix B which operates on v to give you back u.

So, then we can we can write as B operator on v and instead of v I will write A u equal to u and so now, A and B are matrices and you can show that that this is just this I can write as BA operating on u is equal to u. So, BA is a product of 2 matrices, this is the usual matrix product and I expect you to know the usual matrix product if you are not familiar with it is no problem you can learn it very quickly, but if you take this product of 2 matrices and you operate on u you get exactly u.

Now, what is a matrix that that operates on a vector to give you back the vector. So, what can be a matrix? So, suppose I take I will just take a 3 dimensional vector let me take u x, u y, u z to give you the same may the same vector u x, u y, u z. So, now, what I should have here is you can easily show that if i take 1 0 0, 0 1 0, 0 0 1, if I take this matrix operate on this vector I will get back this vector so clearly. So, this implies that I times u equal to u where this matrix is called I matrix identity matrix and now when you take the product of B and a. So, this also implies that B times A equal to I identity matrix. So, thus what you can say is that if B times A is identity matrix.

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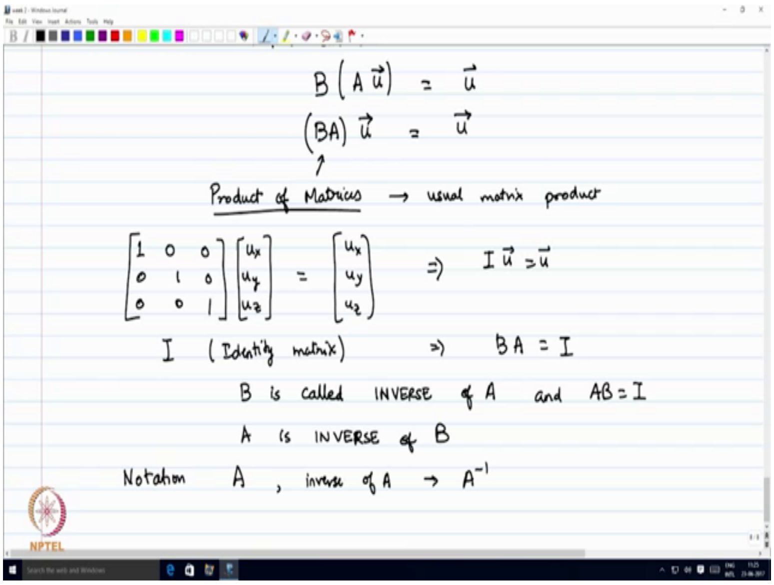

So, then B is called inverse of A and you can do this the other way also B is called the inverse of A, and A times B is also equal to identity.

So, A is inverse of B. So, in other words A if B is inverse of A, then A is inverse of B. So, this is the idea of inverse. So, in general notation is A inverse of A is denoted as A inverse. So, if you have a matrix A then inverse of A is denoted as A inverse.

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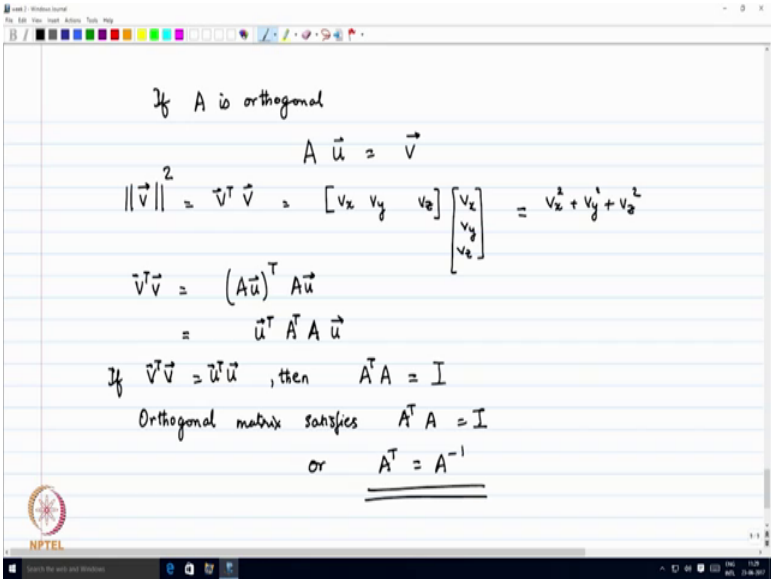

So, now we can go ahead and we can look at these orthogonal matrix, say the orthogonal matrix has a very special property for the inverse. So, if A is orthogonal then what we said is that A operator on u gives me v such that u and v have the same magnitude. So, now, suppose. So, the norm of v I can write as in this form. So, I can write it as v transpose v. So, v transpose is given by this. So, v x, v y, v z, this is a transpose of a matrix that is not square. So, and v is v x, v y, v z.

So, I can define the transpose even for a matrix that is not square. So, I had a 3 cross 1 vector it is transpose will be a 1 cross 3 row vector. So, and if you take the usual matrix product this is just v x square plus v y square plus vz square. So, norm of v square, this is norm of v square. So, now, suppose I take v transpose v now. So, that is A u the whole thing transpose A u, now A u transpose I can write as u transpose A transpose. So, whenever you take a transpose of a product it is product of the transpose, but in the in the opposite direction. So, you have to switch the order and then you have A times u.

So, if v transpose v is equal to u transpose u, and just put vector signs everywhere. So, this v transpose v is equal to u transpose v u that is norm of v is equal to norm of u then we must have A transpose A should be equal to the identity matrix, because if A transpose A was identity then this will be identity times u which is just u and u transpose u. So, thus orthogonal matrix satisfies A transpose A equal to identity or A transpose equal to A inverse. So, this is what gives you what is called an orthogonal matrix. So, an orthogonal matrix you can just do the transpose of the matrix you can calculate the inverse and you can check whether the matrix is orthogonal or not. So, this is when A is real.

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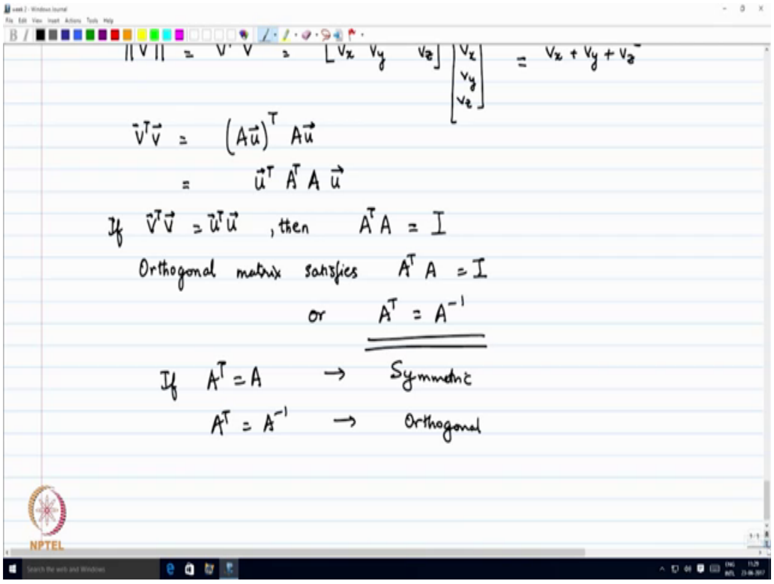

So, we have seen that if A transpose equal to A then it is symmetric, if A transpose equal to A inverse then it is orthogonal ok.

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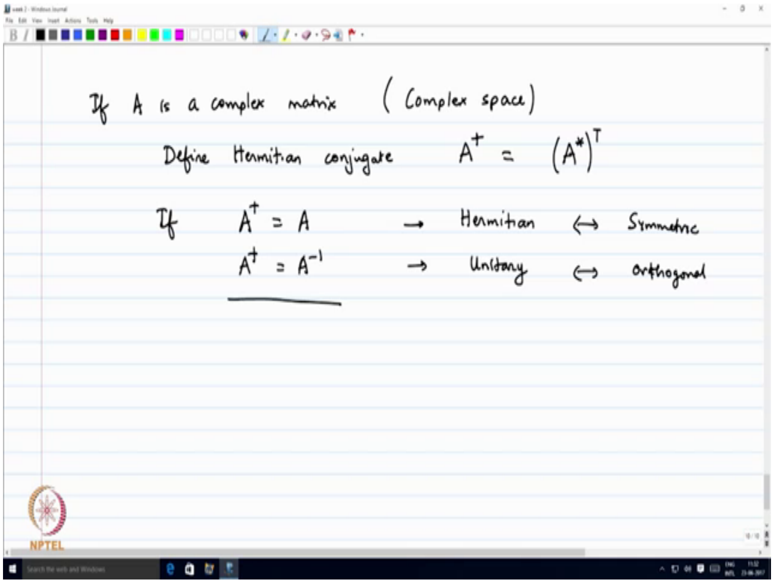

Now, suppose A is a complex matrix. So, if A is a complex matrix. So, this is actually a complex space which is which you often find in quantum mechanics is called a Hilbert space. So, you can also defined matrices on this complex space then define what is called a hermitian conjugate. So, which is given by A dagger. So, this is equal to you take A, you take a complex conjugate of A and then you take a transpose. So, you take each element of A and you take and you replace it by their complex conjugate and then you take the transpose this is called the hermitian conjugate.

So, if A dagger equal to A then matrix is called hermitian, and if A dagger equal to A inverse then it is called unitary. So all you did is instead of having A. So, for a symmetric matrix we had A transpose equal to A, for a hermitian matrix you have A hermitian conjugate is equal to A, similarly for a orthogonal matrix you had A transpose equal to A inverse for a unitary matrix you have A hermitian conjugate equal to A inverse. So, the hermitian and unitary are the equivalent of symmetric and orthogonal matrices for real matrices. So, it is a generalization of symmetric and orthogonal to complex matrices and you know this of unitary transformations or orthogonal transformations is again extremely useful in several areas of chemistry.

So, I will stop this discussion on special matrices we look more closely at rotation matrices in the next lecture.