Mathematics for Chemistry
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Module – 04
Lecture – 18
Special Matrices – symmetric, orthogonal, hemitian, unitary

We have seen how to calculate the rank of a matrix, how to calculate the inverse of a matrix, then we have seen how to calculate eigenvalues and eigenvectors of the matrix. So, today we will be talking about certain what I call special matrices.

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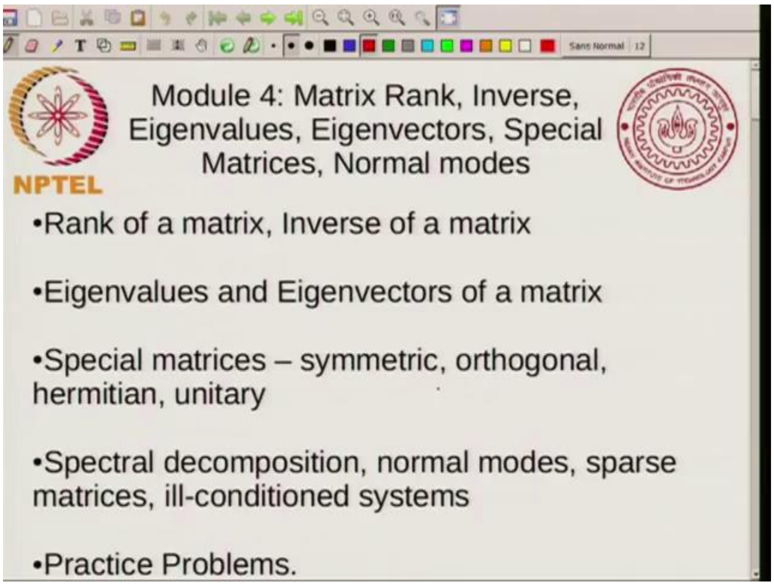

And the kinds of matrices that will be talking about are symmetric, orthogonal, hermitian and unitary matrices.

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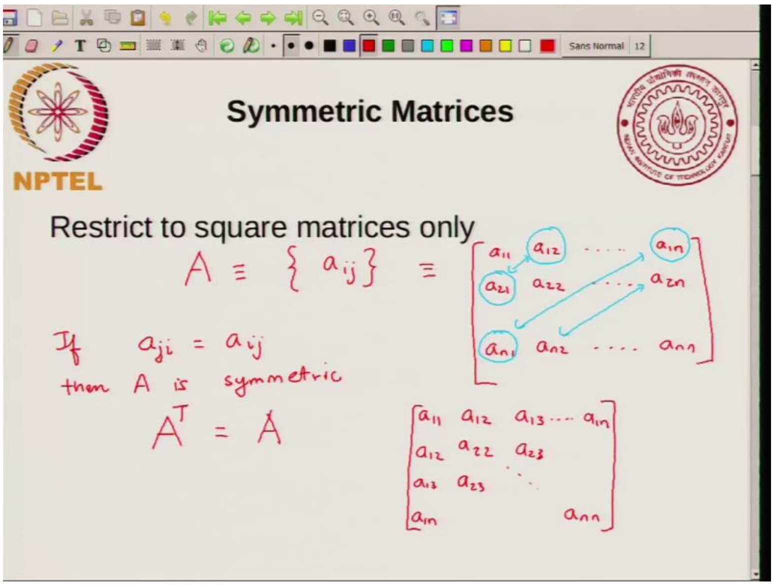

So, let us start with symmetric matrices. And again as we have been doing earlier we will restrict to square matrices only. So, if you have a square matrix; let us say A which is composed of the usual coefficients which we denote as a ij. This is our usual matrix which we have been using. So, you have a 11 a 12 up to a 1n; a 21 a 22 up to a 2n; a n1 a n2 up to a nn. So, this is our n by n matrices.

Now, this matrix is set to be symmetric if the off diagonal elements, if any two off diagonal elements are identical. So, if a 21 is the same as a 12 and so on for all the off diagonal elements. So that means, a n1 will be the same as a 1n and so on. So, if all the sets of off diagonal elements are basically the same then we say that the matrix is symmetric. So, mathematically we can write this in two ways. So, if a ji equal to A ij then A is symmetric. So, if the ij and the ji-th elements others are identical then the matrices set to be symmetric.

Now there is another way to write this you can also write this as A transpose is equal to A. Remember A transpose is the same as A with the off diagonal elements swap. So, A transpose has a 12 here instead of a 21 and so on. So, these are basically the same thing. So, a matrix is set to be symmetric if either you can say A transpose equal to A or if you want to look at the individual coefficients you can say a ji equal to a ij. So, what will a symmetric matrix look like? So, it looks like a something like all the diagonal elements will be as you always had.

Now, the off diagonal elements; so if this is a 12 this will also be a 12, if this is a 13 this will also be a 13, and if this is a 1n this will also be a 1n. So, all the off diagonal elements will be identical to each other. And the matrix will have the appearance of symmetry. So, it looks very similar across all these. Similarly I should also mention here. So, if you have a 23 this will also be a 23. So, both these will be a 23 and so on. So, symmetric matrix is one kind of special matrix.

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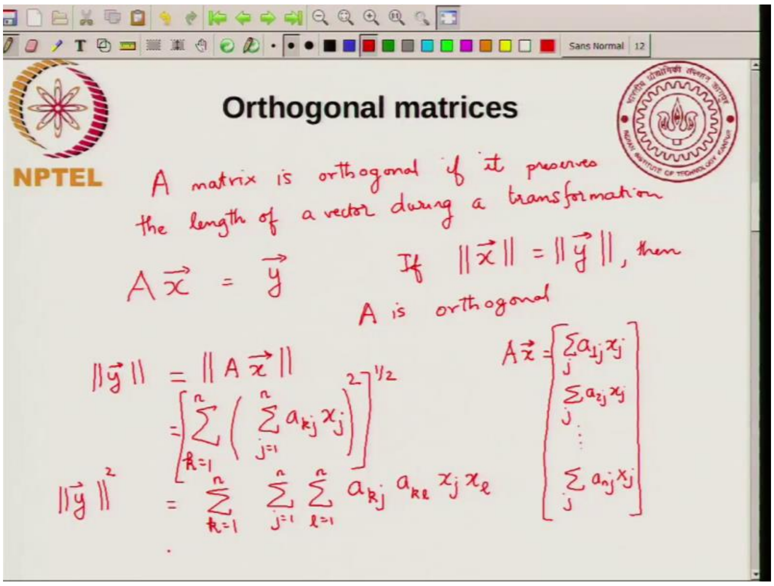

The next kind of special matrix is what is called as orthogonal matrix, and let us just remind ourselves. For a symmetric matrix we had A transpose equal to A. Now an orthogonal matrix is; we can write this in two different ways and orthogonal matrix usually we think of an orthogonal matrix if you can; I will I will say that: A matrix is orthogonal if it preserves the length of a vector during a transformation.

So, it is very important. Suppose you had A matrix and it operates on a vector x to give you y. Then a set to be orthogonal if the norm of x is equal to the norm of y. So, then the length of these vectors is preserved after the transformation. Then we say that A is orthogonal. It should be for all vectors. So, for any vector when a matrix acts on any vector it preserves the length of that vector, then such a matrix is set to be orthogonal. Now what are the conditions for orthogonality, can we find some conditions in the coefficients. And yes, we can do that.

So, if I just take norm of y, so this will be norm of A x and the norm of A x; A x I can write as A times x as various elements, so the elements will be a 1j x j sum over j and then you will have sum over j, a 2j and so on all the way up to sum over j, a nj x j. So, this will look like a vector. So, A x will look like a vector way, these are the components by usual matrix multiplication. So, if you use matrix multiplication these are the components of A x. So, the norm can be calculated as the sum of squares of each of these components. So, I can write the norm as in the following way.

So, I can write the norm as sum over I will just use an index k equal to 1 to n. And what I will do is this is the k-th row, so I will write this as sum over j equal to 1 to n a kj x j and this whole thing has to be squared. This entire thing has to be under the square root So, this is the norm of the vector. And now what you are doing is. So, you are squaring a sum means you are multiplying the sum by itself and it is not hard to see that this will turn out to look something like this it is. So, I will just write norm of y square. So, this will look like sum over k equal to 1 to n.

Now you have one some and you are squaring it, so when you square or sum of terms then it is like making a double sum. So, what I will write this is some over instead of j I will right j equal to 1 to n sum over l equal to 1 to n; and what I have is, I have a kj a kl x j x l. So, this is exactly the square which I wrote in this form.

Now what this implies is that; now this should be exactly equal to sum over x j square. So, if this has to be an orthogonal matrix this whole thing should be exactly equal to sum over x j square. So, what that implies is that this sum over k; if I change the order of the sums what I will get is sum over j equal to 1 to n sum over l equal to 1 to n. And what I have is I will have an x j x l and then I have a sum over k equal to 1 to n a kj a kl.

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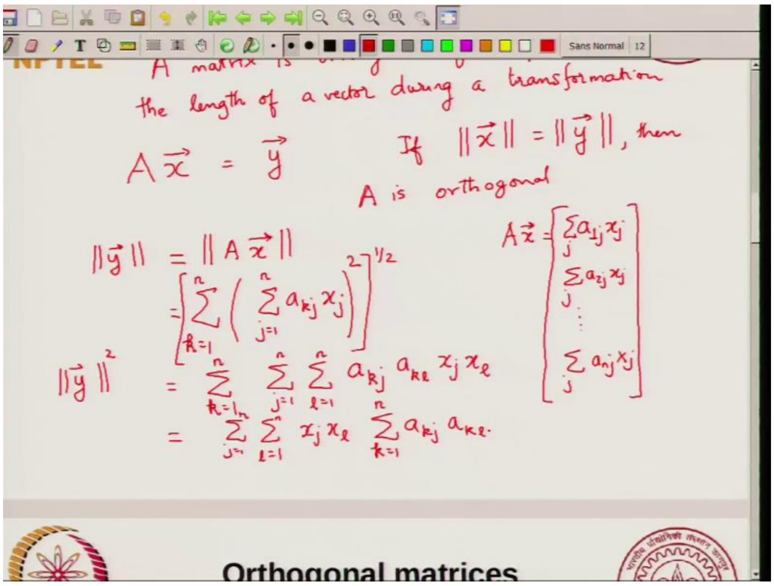

Now if this matrix A has to be orthogonal then the norm of y square has to be is the same as norm of x square.

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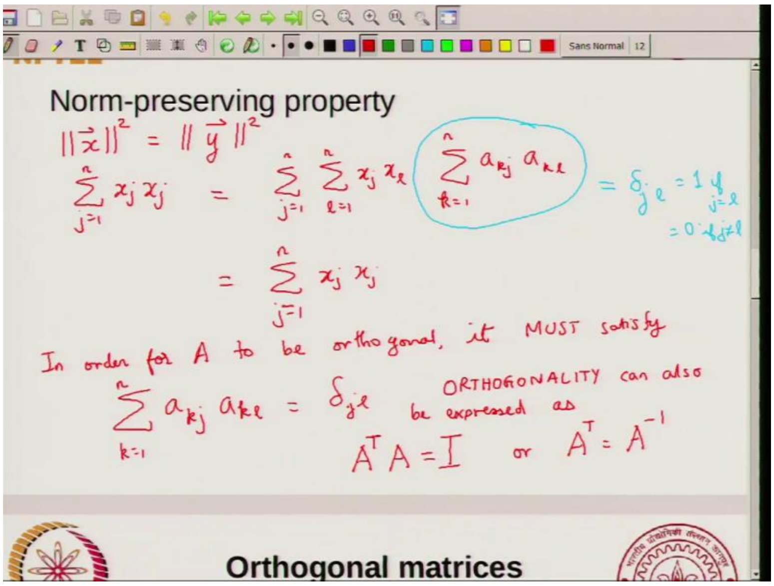

So, if a is orthogonal, then you can immediately write that you should have the condition norm of x square should be equal to norm of y square. And now if you use this expression for norm of y square you know that norm of x square is nothing but sum over; I will use the index j equal to 1 to n x j x j, I will just write instead of writing x j square I am just writing it as x j x j. So, this is what you mean by that the squared norm of x. And this should be identical to; what we have here is you have a sum over j equal to 1 to n and additionally you have a sum over l equal to 1 to n x j and you do not have x j into x j you have x j into x l. And not only that you have this additional term which looks like sum over k equal to 1 to n a kj a kl.

Now you can just take a look at this, you immediately realize that in order for this to be true what should happen is that this whole thing here; this whole thing should be such that it should be 1 if j equal to l and it should be 0 otherwise. In other words this whole thing should be what is called that this should be equal to delta j l. So, this is equal to 1 if j equal to l equal to 0 if j is not equal to l. So, if this is satisfied then you can immediately see that I can replace this whole thing by delta j l. And now when I sum over l equal to 1 to n only the term where l equal to j will contribute. So, what I will get is nothing but sum of j equal to 1 to n x j x j, so that is the only term that will contribute.

In other words, the condition for A to be orthogonal is exactly this. So, in order for A to be orthogonal it must satisfy sum over k equal to 1 to n a kj a kl equal to delta jl. Now, what is this sum over k equal to 1 to n a kj a kl. That means, what you doing is you are taking the j-th an l-th column and the elements of the k-th row and you are multiplying them together. It should get 1 if j equal to l and you should get 0 otherwise. In other words, what this says is that different rows or different columns of the matrix if you think of one row of a matrix as a vector and another row of the matrix has another vector then these two vectors should be orthogonal to each other; that is what you are saying.

If you are orthogonal to each other then you take a dot product of two different rows you will get 0. And additionally if you take the length of any row or any column you get 1. So that is the meaning of this orthogonality of this matrix A. Now additionally we can write this in a slightly more compact notation. So instead of writing it in this way I can express orthogonality in a slightly different way. So, I can write orthogonality implies; orthogonality can also be expressed as; so I can write this as A transpose A. So, A transpose is a matrix when you multiply it by a you get another matrix and this product should be equal to the identity matrix or you can write A transpose equal to A inverse.

So, this is the same thing as what we said here; either you can say A transpose A equal to identity or you can say A transpose equal to A inverse or you can write this in terms of coefficients a kj; a kl sum over k should be equal to delta j l. So, these are what it takes for a matrix to be orthogonal. And in each of these three conditions are identical to each other.

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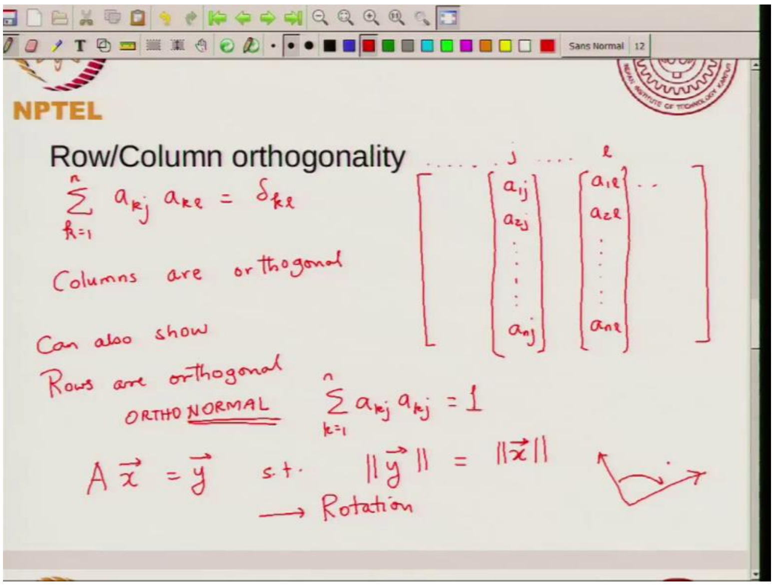

So, what I mentioned here is that the rows and columns should be orthogonal. In other words if you; we said that you know sum over k equal to 1 to n a kj a kl equal to delta k l. So what that means is that; so if I take the j-th column then the elements of the j-th column, so if you go to the j-th column then the elements of the j-th column are given as a 1j a 2j up to a nj. And then I take the l-th column then I will have a 1l a 2l up to a nl. Now what you can see is that in this sum what is appearing is a kj and k goes from 1 to n. So, it comes a 1j a 2j a 3j all the way, and then a kl that is a 1l a 2l up to this. So, what you are effectively doing is you are taking this vector and taking a dot product with this vector. So, essentially you are taking the dot product of these two vectors. And that dot product should be 0 if you take two different columns; if you take the same column that dot product should be 1.

So, this is what you mean that any two columns are actually orthogonal to each other. So, columns are orthogonal. And similarly I leave it as an exercise for you can also show rows are orthogonal. And more precisely we should use the term ortho normal. So, ortho normal means it is not only a to two rows orthogonal, but if you take a dot product of any column or any row with itself you get 1.That means, you can say a kj a kj sum over k equal to 1 to n, so now I have take an l equal to j this is equal to 1. You take the dot product of any row with itself, you take the norm of any row vector or column vector you get 1.

So, this is the property of orthogonal matrices. And what we have already seen is that orthogonal matrices player a very important role because, any orthogonal matrix when it acts on a vector it gives a vector such that norm of y equal to norm of x. So these orthogonal vectors have this non preserving quality. And therefore, now if we just think in terms of physical picture, so this will look like a rotation.

So, you say that you take a vector and you rotate it and you get another vector, then the length is not changing. You are just rotating it, so the length is not changing. Such so a matrix that does this orthogonal an orthogonal matrix is like a matrix of rotations. So, like a matrix that rotates a vector. And this is one of the most important applications of matrices. And we will see this in a subsequent class.

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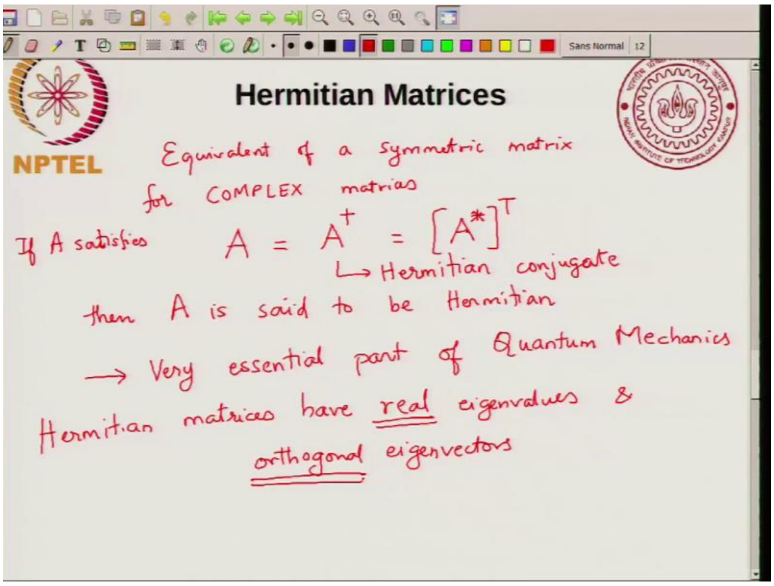

Now, I will define a few more special matrices which you will encounter in various courses. One is what is called Hermitian matrices. So, a hermitian matrices is very much like a symmetric matrix; think of this as the equivalent of a symmetric matrix for complex matrices.

So, here we are not talking about matrices with elements which are real numbers, but we are talking about matrix whose elements are complex numbers, then hermitian matrices.

So, if this matrix has A equal to A I will put a dagger sign. So, this dagger is what is called the hermitian conjugate. And what does it do; what does this dagger does. So, A dagger is nothing but you take your matrix, you take each elements you take it is complex conjugate, so this is a complex conjugate and then you transpose it. So, you do A transpose And you do a complex conjugate. So, you do both these operations then you will get what is called a dagger which is called the hermitian conjugate. So, if a matrix is equal to its hermitian conjugate then you say the matrix is hermitian. So, if A satisfies this relation then A is said to be hermitian.

You can clearly see that this is like a symmetric matrix. So, it is like A transpose, but you do not just stop A transpose you also take a complex conjugate. So, it is like the equivalent of a symmetric matrix for a complex matrix. And this is a hermitian matrices are again these are very essential part of quantum mechanics. The hermitian property of various operators is a very essential part of quantum mechanics. There are some nice properties of hermitian matrices.

So, hermitian matrices have real eigenvalues and orthogonal eigenvectors. So, if you take any two eigenvectors for two different eigenvalues they will be orthogonal to each other. And eigenvalues of a hermitian matrix are strictly real they cannot be complex; in fact, this as part of the foundations of quantum mechanics, where you invoke hermitian property for all operators that correspond to real observables.

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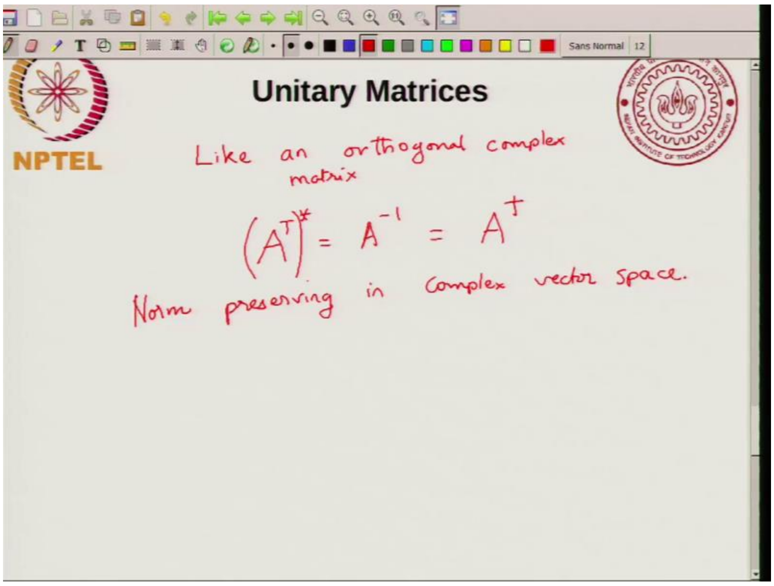

Just for completeness I will tell what is an unitary matrix. So, a unitary matrix is like an orthogonal matrix for a complex matrix. So, it is like an orthogonal complex matrix. Remember in orthogonal matrix you had A transpose equal to A inverse. Now what you do for a unitary matrix is you will take a transport and you will take a complex conjugate. So, A inverse equal to A dagger. So, this is what is meant by a unitary matrix. So, if A satisfies this condition then it is said to be unitary matrix. And, so you can think of a unitary matrix as a equivalent of an orthogonal matrix for a complex space. And unitary transformation is something that when you operate a unitary matrix on a vector or another matrix you will get something that preserves the norm of the vector. So this is norm preserving in complex vector space.

So, if you having a complex vector space then the norm incidentally also involve the complex conjugate. It is not just a simple dot product, but you also have to take a complex conjugate. And the unitary matrix is a matrix that preserves the norm of this vector during a transformation. So, this is what I want to say about the unitary matrix.

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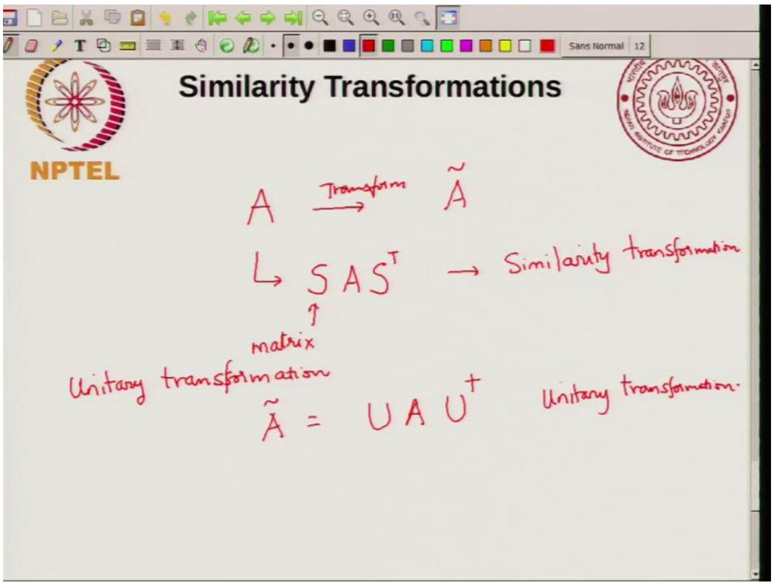

Now, I will just mention briefly that there is something called a similarity transformation. Suppose you have a matrix A. Now you can take this matrix A and you can transform it to A tilde. And there are several ways to do this transformation. One way to do this transformation is you essentially you take A and I will just write this. So, suppose you take S A S transpose. So, I am just taking some matrix A and I am doing S A S transpose, this is called as similarity transformation.

So, one very common transformation that is used in quantum mechanics is called a unitary transformation. So, what you do is you take A tilde equal to U A U dagger; where U is a unitary matrix. So, this is called a unitary transformation. So, you will do this transformation using a matrix U. So, such transformations of matrices are often used to change from one coordinate system to another.

So, I will stop the lecture here. In the next class, we will talk more about matrix diagonalization, spectral decomposition. And then in the last class of this module we will do some practice problems.