Mathematics for Chemistry
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Module – 04
Lecture – 17
Eigenvalues and Eigenvectors for a Matrix

So, we have seen the meaning of a rank of a matrix and the inverse of the matrix in the last lecture. Today I will be talking about eigenvalues, eigenvectors of a matrix.

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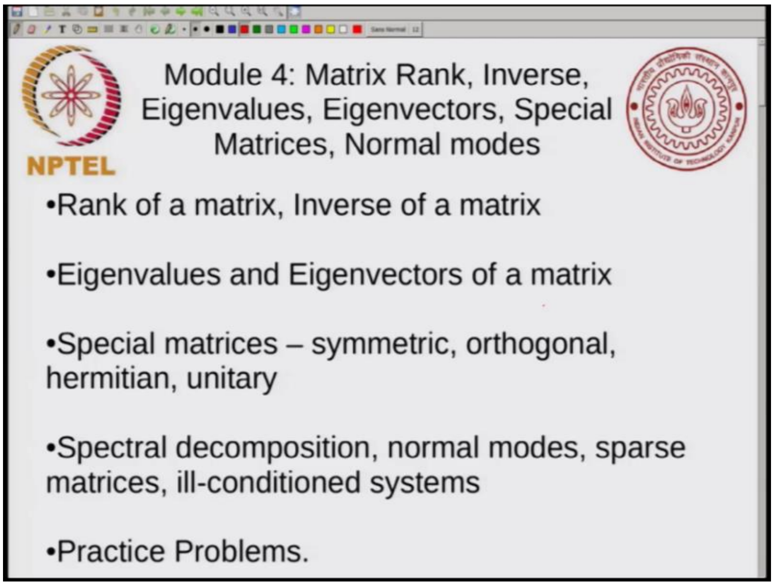

And I want to emphasize that this is probably one of the most important areas of linear algebra to find eigenvalues and eigenvectors of matrices and it is used in all branches of science and engineering. So, let us get to the discussion of eigenvalues and eigenvectors.

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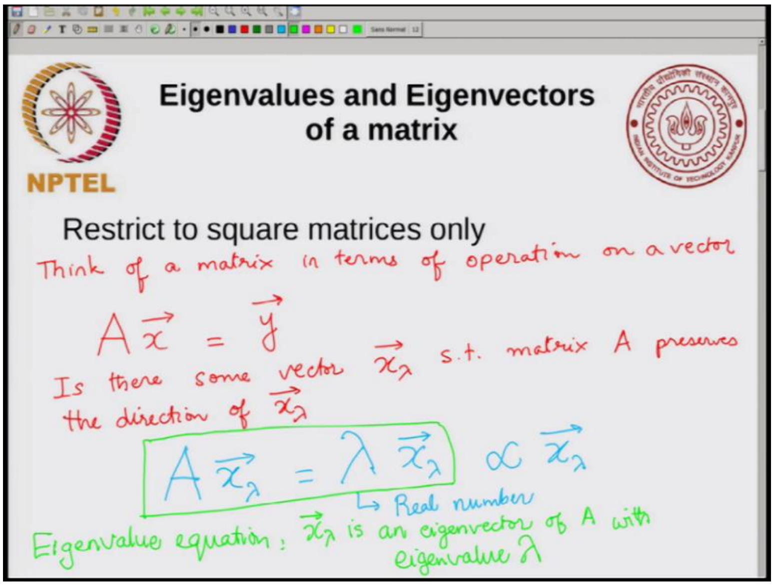

In order to do this we will restrict our discussion to square matrices only and that is where eigenvalues and eigenvectors are defined. And in order to do this we will just mention that it helps to think of matrix in terms of operation on a vector. So, for example, you could have a matrix A and that operates on a vector x, and when this matrix operates on a vector it will give you another vector. So, I will just call that vector y. So, matrix operates on a vector to give you another vector. And now we say what is the relation between x and y; is there any relation between x and y. In general x and y they can be completely different vectors.

Now for a matrix; now we ask the question is there some vector I will call it x lambda such that matrix A preserves the direction of x lambda. So, the question we are asking, is there some vector x lambda such that the matrix A preserves the direction of x lambda; that means what you mean to ask is there a matrix and I will use a different color for this because this is an important equation. So, for the same matrix A when it acts on this particular vector x lambda it gives you something that is proportional to x lambda; it gives you a vector that is actually proportional. And this constant of proportionality I will call it as lambda.

So, lambda is the constant of proportionality, this is a scalar or a real number; real number if you are dealing with real matrices. Now the question is we are saying that for any given matrix A that can be certain vectors x lambda such that when A operates on x lambda it gives a vector that is proportional to x lambda. In other words this is proportional to x lambda. So, if this is the case then this equation is called an eigenvalue equation, this is refers to as an eigenvalue equation. And what we say is that; x lambda is an eigenvector of matrix A with eigenvalue lambda.

It is very important to get the sense of the statement. What we mean is that x lambda is an eigenvector of the matrix A corresponding to the eigenvalue lambda. So, it is not that you cannot generally define eigenvectors and eigenvalues you have to talk in reference to a particular matrix. And always for a given matrix there can be many eigenvectors and many corresponding eigenvalues. So, it need not be unique.

So, now how do we solve for eigenvalues? What we said is that, we just mentioned that this equation is called the eigenvalue equation. And in general for a matrix they can be more than one eigenvalue then there can be more than one eigenvector. And we will just go ahead and try to see what you need to do to calculate the eigenvalues and eigenvectors.

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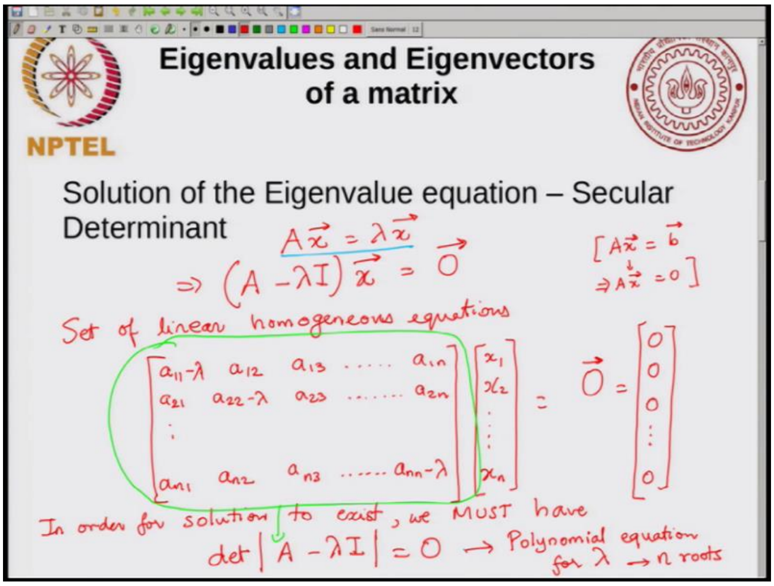

So, what will do is will start with this equation; will write A x equal to lambda x, and what will say that that implies A minus lambda times identity times x equal to 0 vector. So, what I did is I just took the lambda to the left I multiplied it by identity so that I get a matrix. And this is A minus lambda x equal to 0. So, it is the same as the above equation, I just rewrote it in a slightly different form. But the advantage of writing in this form is that now looks like a set of linear homogeneous equations.

If you remember this looks exactly like your set of linear equations where you had something like A x equal to b; we had this was the general linear system that we had. Now in this case what you have is something like A x equal to 0. So, this kind of equation is called a homogeneous equation. So, you have some matrix A instead of A I have A minus lambda I in this case, but when it operates on x you get the 0 vector. That means, my system of equations looks like this. So, if my A has usual if you use the explicit notation for a then you have a 11 and then you have minus lambda times I. So, identity matrix just has one along the diagonals. So, lambda times identity will just have lambda along the diagonals and you are subtracting that from a, so what you will get is you will get a subtraction of lambda from the diagonals. And the off diagonal element will have no change. So, it will be a 12, a 13 and so on up to a 1 n if it is an n by n matrix and so on.

So, you have a 21, now we will have a 22 minus lambda a 23 a 2n and a n1, a n2, a n3, a nn minus lambda. So, this is a matrix and what you have is this multiplied by x; x is a vector I will just give it some coefficient x 1, x 2 up to x n it is equal to 0. I should explain what this 0 is. So, this is your 0 vector which is basically a vector with all elements 0. So, this is a column vector, n dimensional column vector all elements are 0; this is an n dimensional column vector that is your x. And this is the matrix where you have along the diagonals you have a 11 minus lambda, what you are doing is you want to solve the set of equations.

Now the nice thing about this is a set of homogeneous equations. Now in order for them to be consistent and solution to exist; so in order for solution to exist we must have determinant of this matrix that is determinant of A minus lambda I that is actually this whole matrix. So, the determinant of this matrix should be equal to 0. Only if the determinant of this matrix equal to 0 can we have solutions of this problem.

So, notice now we just come back to the eigenvalue equation for a minute; this equation, this eigenvalue equation. Now what we are going to do is we are going to take this equation and solve for both the x and lambda. And we solve for x and lambda with the same equation you are going to solve for both x and lambda. Now when you set the determinant of A minus lambda I equal to 0 then you will get a polynomial equation for lambda. So, this is a polynomial equation A for lambda. And we will see an example of this in a minute. And you can see just by looking at the product along the diagonals you can see that you will have lambda raise to n power coming in this determinant. So, this determinant will contain a term that that has lambda raise to n. So, it is an n-th order polynomial equation. And in general you will have n roots. That means, the number of eigenvalues is equal to the dimension of the matrix. So, you have n eigenvalues for this equation.

Now, next is you want to take those eigenvalues and solve for the eigenvectors. So, as we said earlier our goal is to determine both the eigenvalues and the eigenvectors. So, corresponding to an eigenvalue lambda; I should mention that here I have not put x lambda explicitly because I am using all these subscripts on x, but if you want you can put an x lambda it is just a notation. Now when you solve for the eigenvalue coefficients; how will you solve for these eigenvalue coefficients?

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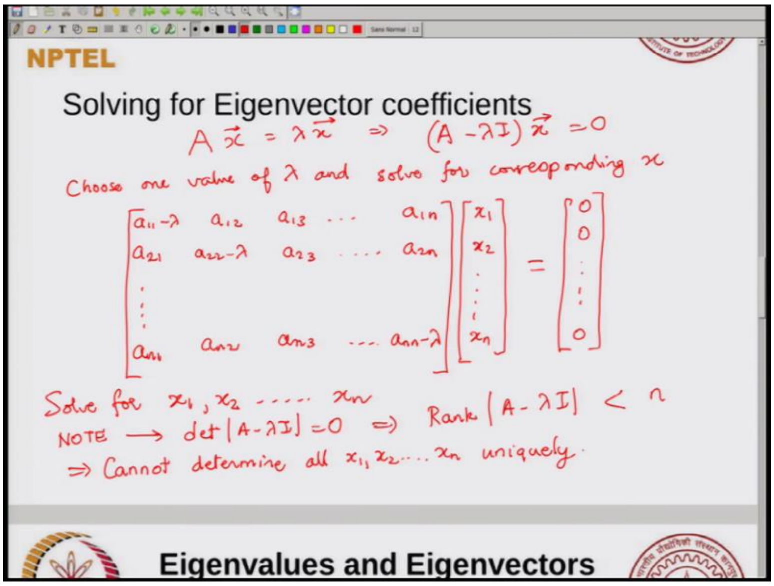

So, again you go back to our equation: you say you had A times x equal to lambda x. And this implies A minus lambda I x equal to 0. Now we choose n value of lambda and solve for corresponding x. What I mean is if you choose a value of lambda then this determinant is this matrix A minus lambda I is well defined. So, you have a 11 minus lambda a 13 and so on up to a 1n; and a 21, a 22 minus lambda a 23, a 2n, a n1, n2, n3, a nn minus lambda. This is your A minus lambda I and then you have the coefficients of x which I will have x 1 x 2 up to x n. These are the coefficients of the x vector and this should be equal to 0.

So, you do it to solve for x 1 x 2 up to x n. Note that the determinant of this matrix equal to 0 implies; these equations are actually dependent equations. That means, a rank of A minus lambda I is less than n. That means, the rank of this matrix is less than n and that basically implies that you know cannot; so this implies that you cannot determine all x 1 x 2 etcetera up to x n uniquely. So, there is no unique choice of these x 1 x 2 up to x n. In fact, typically what we do is we take one of them to some number and you express all of them in terms of that single coefficient. So, we will see an example of how to do this, but the point is you should keep in mind that whenever you have eigenvectors you cannot determine the eigenvector uniquely. And there is another reason for this, and I will just mention this right here. It is fairly easy to see.

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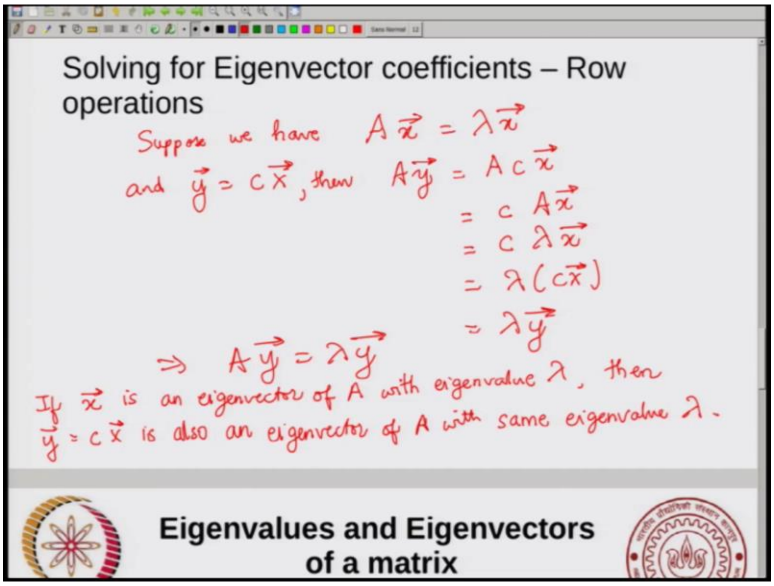

I will also mention that you can solve for these eigenvector coefficients using row operations, and we will see an example of that. But before that I just want to mention that suppose we have A x equal to lambda x and y equal to c times x; y is a constant times x, then A y is equal to you can see easily this is A times c x now c is just a scalar so you can take it to the left of the matrix and so on and. So, I can write this as c times A x and

A x is nothing but lambda x. So, I can write this as c times lambda x or I can write this as lambda times c x or I can write this as lambda times y.

So, what I have is that this implies that A y equal to lambda y. So, what this implies is that if x is an eigenvector of A with eigenvalue lambda then y equal to some constant times x is also an eigenvector of A. And it is not just it is an eigenvector of A with same eigenvalue lambda. That means, if you have an eigenvector then you can just multiply it by a constant you will get another eigenvector with the same eigenvalue. And that is why we say that eigenvectors cannot be determent uniquely by this procedure. So, eigenvectors are not unique, you can take any eigenvector multiplied by a scalar you will get another eigenvector with the same eigenvalue.

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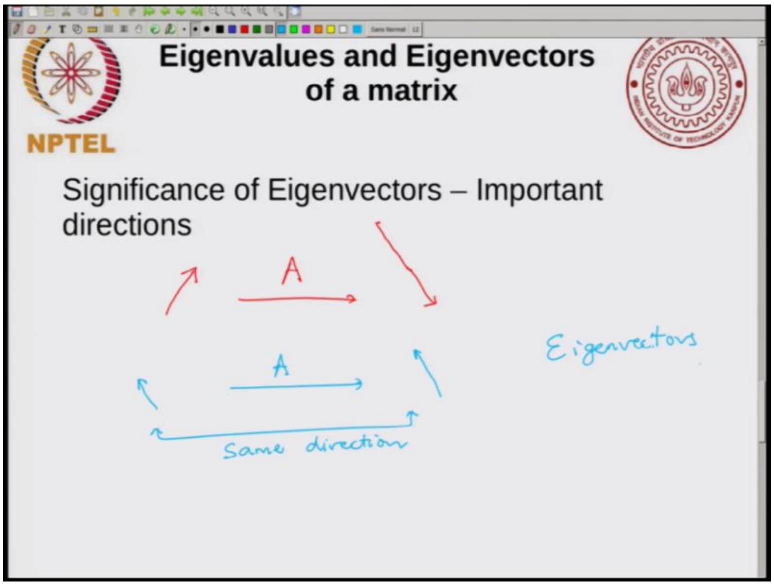

Now, I will just mentioned one thing before we take an example. So, what is the significance of eigenvectors? So, you can think of eigenvectors as important directions. And, so what I can think of is suppose I have a vector like this. So, this is my vector I am just showing it as an arrow. Now when I operate it by this matrix A then I might get some other vector like this; that will in general point somewhere in some other direction it might have a different length also I will just show it expanded it might look like this. So, I by operate this vector by with this matrix A and I get something else.

Now there you can do this for various vectors. And what you will find is that is that there are certain vectors, I will show this in the light blue color. So, there are certain I would say directions certain specific direction, any vector pointing in this direction will have the property that when I operate it on it by a I will get another vector in the same direction and maybe it is slightly longer or may be slightly shorter. But whatever it is the point in the same direction. So, these 2 are in the same direction. So, this is for eigenvectors.

So, eigenvectors have this property that when they are operated. So, eigenvectors really represent some very specific directions such that when the matrix operates on vectors in those pointing in those directions it will give you another vector pointing in the same direction. And these are you can think of these as important directions of your system.

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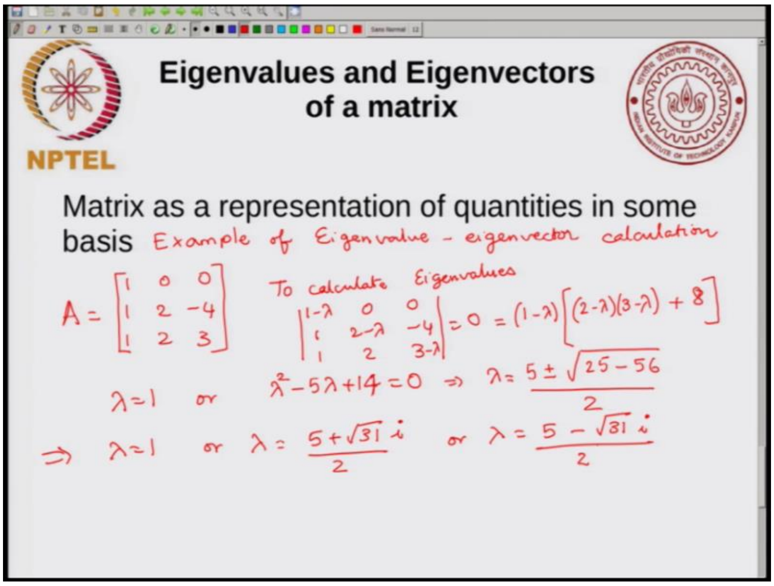

So, now let us take; I will just mention this briefly that your eigenvalues and eigenvectors there is another way to think you can think of your matrix as a representation of some physical quantity in some basis. And this will be an important theme that we will discuss when we are seeing applications of matrices and quantum mechanics. But first let us do an example of an eigenvalue, eigenvector calculation.

And I will take a very simple example just to illustrate what you need to do in order to calculate eigenvalues and eigenvectors. So, let me take a matrix A that looks like 1 0 0, 1 2 minus 4, 1 2 3. And I ask you to calculate the eigenvalues and eigenvectors of this. So, calculate eigenvalues and eigenvectors of this matrix. So, to calculate eigenvalues; so we use the secular equation which says that this determinant 1 minus lambda 0 0, 1 2 minus lambda minus 4, 1 2 3, this determinant has to be equal to 0; so 3 minus lambda. Now what you can do is you can multiply this out.

In this case you have the first row has just one non 0 element. So, when I multiply this out I will get 1 minus lambda times I will get 2 terms I will get 2 minus lambda into 3 minus lambda plus 2 into 4 is 8. And this has to be equal to 0. So, immediately you can see that lambda equal to 1 will satisfy this. So, 1 root of this cubic equation is lambda equal to 1. So, lambda equal to 1 or now if I just expand this out I will get lambda square minus 5 lambda plus 14 equal to 0.

And this implies lambda is equal to 5 plus minus, so will be 5 plus minus. So, what do you have? You have 5 square is square root of 5 square is 25 minus; so you have 14 into 4 is 56 divided by 2. So, this implies. Therefore, what you say is lambda equal to 1 or lambda equal to 5 plus root 31 times i, i is the unit imaginary number divided by 2 or lambda equal to 5 minus root 31 i divided by 2. So, these are the three roots of this secular equation and these are the three eigenvalues. So, we have calculated the three eigenvalues. Now what we need to do next is to calculate the eigenvectors.

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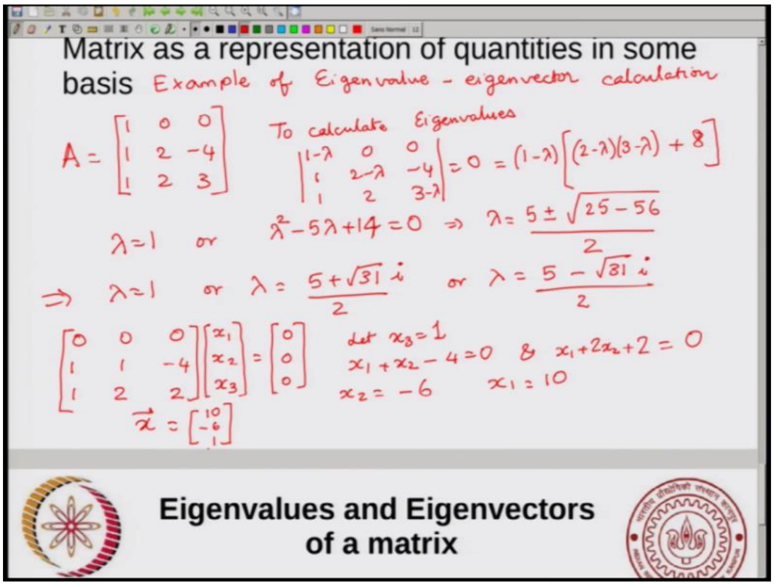

So, I will take one example let us take lambda equal to 1. If you take lambda equal to 1, so I will calculate the eigenvector corresponding to lambda equal to 1. What I do is I take lambda equal to 1 and I put it in my equation. So, what I will get is my equation which is shown in over here. So, what I am going to do is I am going to put lambda equal to 1 and this in the in an equation of this form. And what I will get is the following equation. So, I will get 1 minus lambda now lambda is 1, so I get my equation 1 minus 1 is 0 0 0, 1 2 minus 1 is 1 minus 4, 1 2 2; this times your eigenvector I will just give it some coefficients x 1, x 2, x 3. And this has to be equal to 0 0 0.

And what you can do is you can take let us say for convenience we will take; since I said now you have only 2 equations and you have three unknowns. So, you can choose one of the unknowns arbitrarily. So, let x 3 equal to 1, then what you have is you have 2 equations x 1 plus x 2 minus 4 equal to 0 and x 1 plus 2 x 2 plus 2 equal to 0. And you can go ahead and you can just subtract this equation. So, what you will get is x 2 equal to minus 6 and x 1 equal to 10. So, my eigenvector corresponding to this is basically given by 10, minus 6, 1. So, this is my eigenvector. So, notice what I have to do is I have to choose one of them arbitrarily; in this case I just choose chose x 3 equal to 1, I could have also chosen x 1 equal to 1 or x 2 equal to 1 then I would have got appropriately I would have got all these other quantity (Refer Time: 25:18). So, basically my eigenvectors are proportional to this 10, 6, 10, minus 6, 1.

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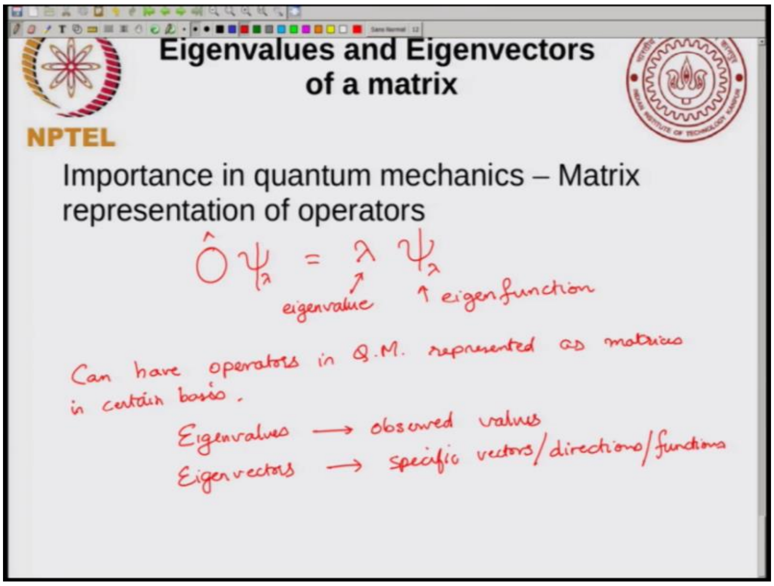

Now before we conclude this lecture I just want to say why eigenvalues and eigenvectors are very important in quantum mechanics. In quantum mechanics the eigenvalue equation is has the following form. Suppose, you have an operator O and it operates on some states psi, you get lambda times psi. Then you say that in, I will put just put a subscript lambda; then you say that this is called an eigenfunction of the operator O and this is called the eigenvalue. So, this is the typical eigenvalue equation that you write in quantum mechanics.

And now if you are using a certain basis to represent your functions, then you are state functions they look like vectors, and your operators look like matrices. So you can have a operators in quantum mechanics represented as matrices in certain basis. This is the very important way to think about quantum mechanics. In fact, some of the earliest developments of quantum mechanics were done using the matrix algebra. And once you do that then the significance of eigenvalues represents observed values, and eigenvectors. Again these are specific vectors or directions; or in this case you can also think of the mass functions.

So, there is a very natural use of eigenvalues and eigenvectors in quantum mechanics.