Symmetry and Group Theory
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Lecture No. 18
Back to Transformation Matrices

So we familiarised ourselves with how to classify molecules according to symmetry we talked about symmetry operations and theorem answer for and so forth. And then we went on to talk about symmetry operations in the language of matrices and we wrote something called matrix representation. I think lecture 3 title was matrix representation. And after that we talked a lot about matrices basically because if you want to write a matrix presentation you better know what matrices are all about.

Today we come back to matrix representation once again we revisit the same issue but with a little more background on matrices. Before we do that it is always better to behave like a bowler, go back a few steps and then coming to deliver. So let us go back a few steps and make sure that we have not forgotten the A B C's required here, right. This is what we have been doing last few days; we are talking about transpose, we talked about adjoint.

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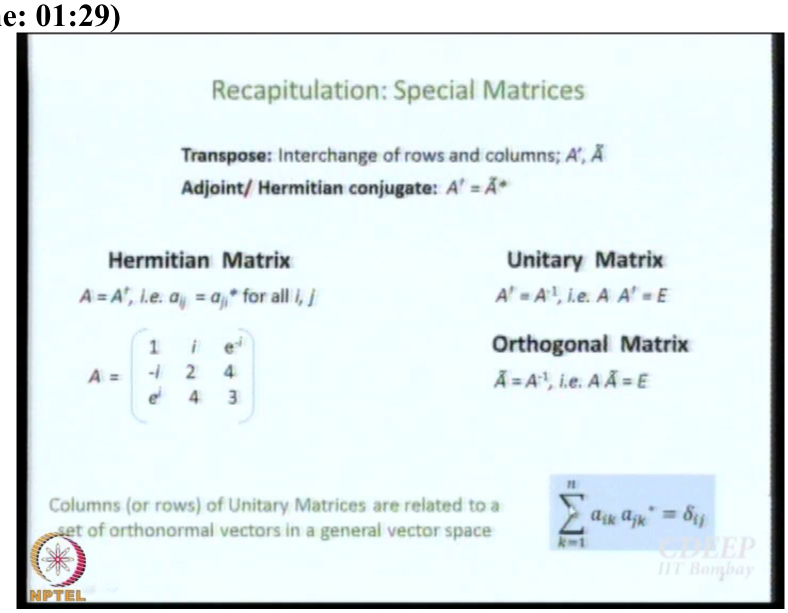

What is sometimes called hermitian conjugate, and we talked about hermitian matrices and unitary matrices. Since you all know this, in fact, we tested this in last class also; tell me, what is the hermitian matrix? Yeah, red black t-shirt, what is your name? First tell me your name Sumith. So, there is two Sumith in class. So Sumith tell me what is hermitian matrix? A = A transpose.

Somebody wants to say something about that hermitian matrix? A, A dagger A adjoint not transpose, right.

A transpose will be a special case if it is a real matrix right. Hermitian matrix is A = A dagger, A transpose would be correct provided all the elements are real there is no imaginary element. And what is the unitary matrix? The other Sumith, so the hermitian matrix is A = A dagger, what did you say? A into ok right A= A dagger is hermitian matrix and A inverse = A dagger is unitary. It is very easy to remember hermitian is A= A dagger and unitary is A inverse = A dagger or A, A dagger = E, Sumith, no confusion with unitary anymore? Good.

And what is an orthogonal matrix? Orthogonal matrix is a special case of unitary matrix where all the elements are real. When you work with real matrix then A transpose = A inverse makes it orthogonal. And today we are going to see some examples of orthogonal matrices. You have already seen some examples earlier; today you are going to see more. And today they are going to be more relevant to symmetry, right. This is another thing we have derived; right that columns or rows of unitary matrices are related to set of orthonormal vectors in a general vector space right where I demonstrated this right?

And how do you write it in summation form? Sum over k = 1 to n, aik aij star = del ij. What is the meaning of sum over, what is the meaning of this let us expand, aik, what is aik? aik then ai1 ai2 ai3 so and so forth. Are you going down the column or are you going from left to right in a row like this or like this? Like this right. Thus the first one i, the first subscripts denotes the row number. Second subscript denotes the column number, right. So when ai1 then ai2 ai3 and so on and so forth right.

We are going from left to right in a row so that the row number is constant and the column changes. Is that alright? And then what you have? You have ajk star that = Del ij. So when j = i then it is1 and when j = anything other than i it is = 0. And that is how we define orthonormal vectors right. This is something that we have demonstrated.

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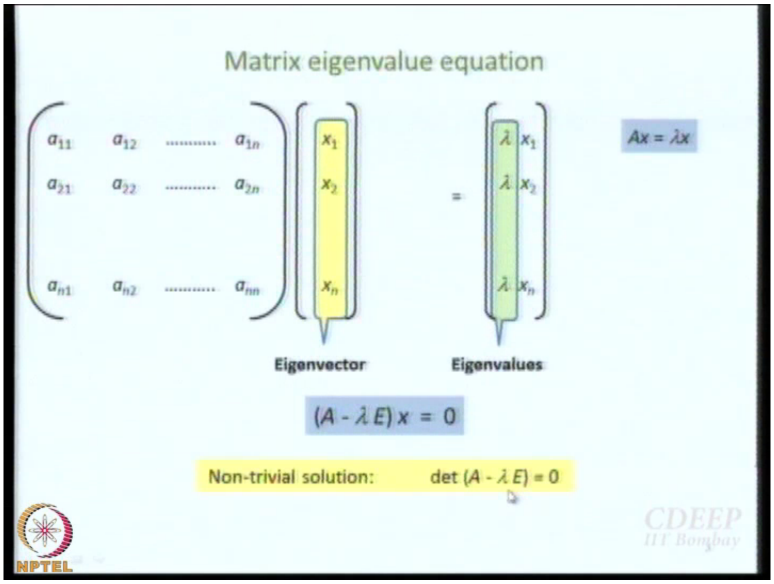

And we have talked at length about the eigenvalue equation. And we said that and what happens is you can have the situation where a square matrix multiplies with and eigenvector X1 X2 X3 X4 so on and so forth Xn to give you same column and same vector multiplied by eigenvalue Lambda. And that happens when you write it in a matrix eigenvalue form AX=Lambda X. A is the square matrix; x is a column matrix consisting of X1 X2 X3 etcetera. Lambda is the eigenvalue constant scalar and then you have X. So, the small x is also matrix do not forget that, right.

Eigen vector, Eigen value and then we have demonstrated in last class that we can rewrite this equation in more convenient form and that is A= A - Lambda E multiplied by X = 0, right. now if you get a equation like that non trivial solution will also come when you have det A - Lambda E = 0.

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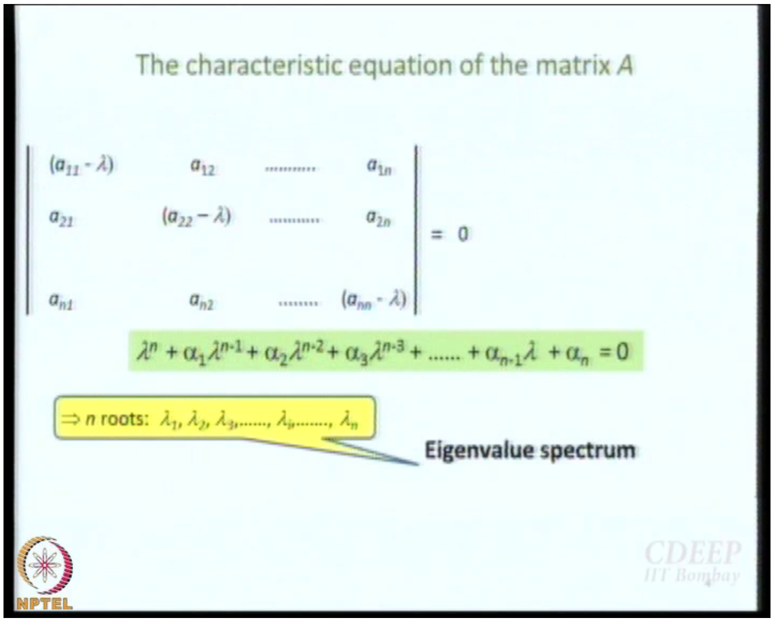

Write out this determinant this is a secular equation that is to get. As you said, the secular equation occurs in many, many places where you solve such a system of equations, ok. Now, when you expand this matrix have you all clear that we are going to get on the left hand side a polynomial in Lambda of the order n right. You know how to expand matrices right. Now when you equal equate that to 0 quadratic equations gives you how many roots. Quadratic equation gives 4 roots.

Just because you got a square two roots quadratic means to the power 2. Why it is called quadratic quite interesting thing. Let us see how many have forgotten since it is to the power 2 right, a squared + bx + c square = 0, why it is called quadratic then? What is the Quadra? Quadra is 4, the answer is very easy A square, bx, c, 0 there are four terms that is why. You perhaps give the right answer it is such that you touch your nose like that anyway. So this n roots that you get, they form what is called the eigenvalue spectrum, alright

So for each of these n roots you can write A matrix Eigenvalue equation, ok. So now, it is better to add subscript to matrix eigenvalue equation and write it as Axi = Lambda i i ok, i denotes which root you are working with. And then, what we said is that this xi, is all column vectors so instead of writing n number of equations, it is better to write one equation and combine all the column matrices into one square matrix it is n by n. When you do that you can write it like this A capital X = Capital X Lambda.

What is Lambda? Lambda is a diagonal matrix right, and in its diagonal it has Lambda 1, Lambda 2, Lambda 3 all the roots, ok. Finally we realise that if you perform a symmetry transformation, a similarity transformation of A, using x then you get Lambda. This is one way of diagonalizing a matrix. Perform a similarity transformation using the matrix of the eigenvectors. That should give you a diagonal matrix which will tell you all the eigenvalues. And I think in the last day we have worked out a sample where we worked out the lambdas and found out what is x. Of course you can do that for any Matrix that you have.

Another important point that we made was X transpose X dagger X= E or X is a unitary matrix. No Surprise because we already said that columns or the row of the unitary matrix are associated with orthonormal vectors and we are working with vectors right, the eigenvectors fine. That is a unitary matrix.

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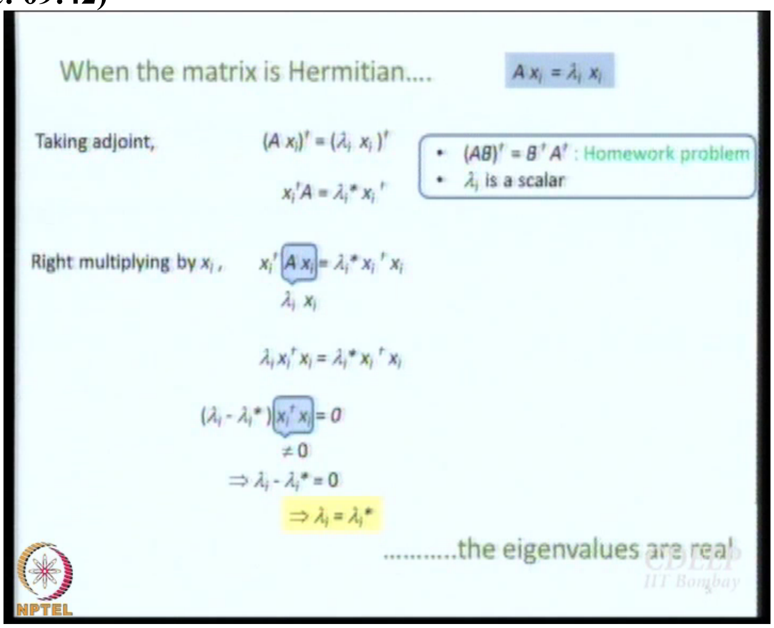

And then we went on to prove something more when the matrix is hermitian first of all we see that the eigenvalues have to be real which is in-line with what we study in quantum mechanics, Quantum chemistry.

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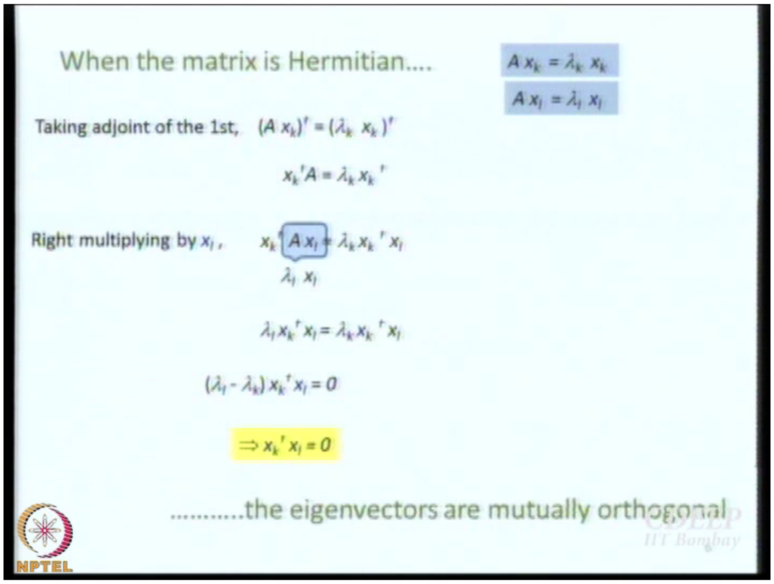

Secondly we also understood that when the matrix is hermitian then the eigenvectors are mutually orthogonal. That is why everybody likes the matrix operators and I mean hermitian operators and hermitian matrices because you get mutually orthogonal eigenvectors and you get real eigenvalues very easy to handle from any system, right. And there is lot of practical utility as well. And then finally we talk a little bit about similarity transformations.

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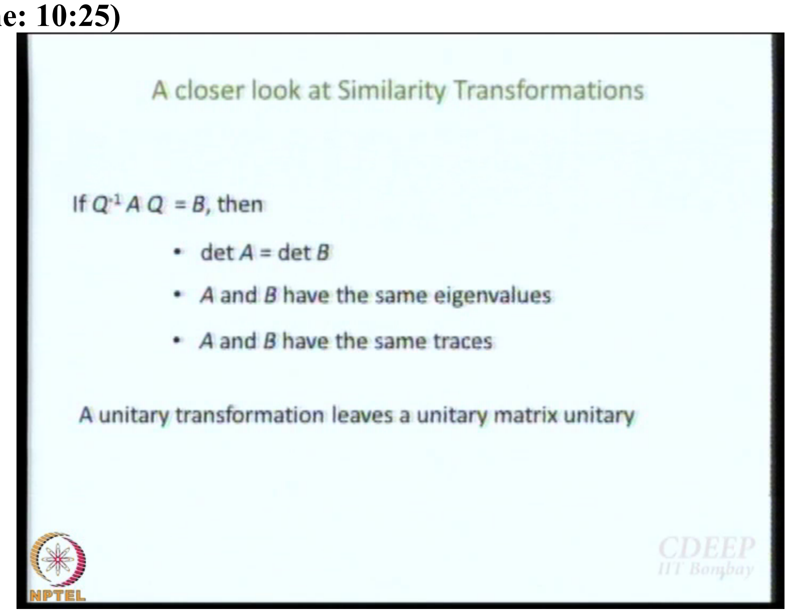

If A and B are conjugate to each other then we learn that det A=det B, we learn that A and B has to have the same eigenvalues, they have the same traces. And lastly we said that a unitary transformation leaves a unitary matrix unitary. Some questions about the way we derive it I suggest you just to go through Bishop's, there it is worked out, so it should not be a problem. The question is why are we suddenly doing this maths in a chemistry course.

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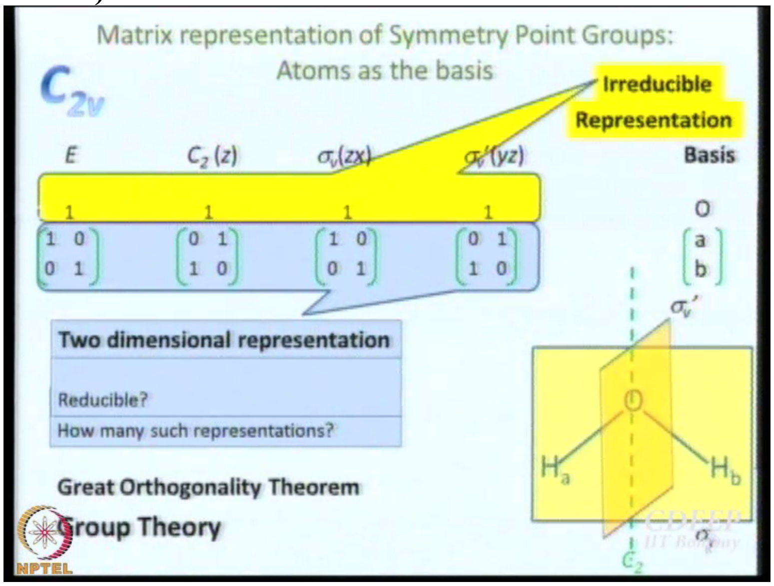

Doing all this maths because do not forget where we have taken off from the discussion of symmetry that was our closing slide, right. We are talking about C2v, water ok, very simple molecule, we keep on saying as simple as water, even though that is not chemically correct. You should not say as simple as water at the most you can say as simple as hot water. Water is an extremely complicated liquid, so many hydrogen bonds making and breaking all the time.

If you heat it some hydrogen atoms are not there then it will become a simpler liquid. Water should not be in the liquid in the first place you know that right. Why should we say that water should not be a liquid? Yeah. Once again I mean little bit of what we learnt in our childhood H2S, H2S is a gas in periodic table sulphur is below low oxygen. So, H2S is a gas and then why H2O be a liquid. It is a liquid because of hydrogen bond right. That is why it is a strange liquid; it is an unusual liquid that is what it makes life unusual as well because life is all about water.

So, blame it on hydrogen bonds, anyway. So, water belongs to C2v here water in the representation for C2v right using the atoms, oxygen HA and HB as the basis, ok. And we have obtained two representations one is the one dimensional representation which has to be reducible and the other is the two-dimensional representation we left the topic with the question is this two dimensional is reducible or not reducible or irreducible? If it is reducible how do I reduce it? How do I know whether it is reducible or irreducible? And how many irreducible representations are there.

So you said that answer to this will come from great orthogonality theorem which comes from group theoretical treatment of the problem of symmetry. And in order to be able to do this group symmetry theorem treatment we need to know all that he studied about matrices ok. So, now that we are little more informed about the matrices, now that our memories are refreshed, let us see what we can say about these matrices.

1001 is very boring unit matrix but 0110 is a hermitian matrix? It is a unitary matrix? It is an orthogonal matrix. Just work it out. What is the transpose? If it is unitary then it will be orthogonal of course, right it is a real matrix. So first let us work out the transpose. 0110 what is the transpose, is the same so A = A dagger or A transpose what would you call it? Hermitian, yes it is hermitian, it is unitary? How do you know? You have to find the inverse and what is the inverse of 0 1 and 1 0.

Since they are just asking that it is unitary or not we can take a shortcut and multiply 0110 by itself see what you get multiply 0110 by itself. Do not be a spoilsport then let other workout as well. Multiply 01and10 by itself. Hold on with the answer. I am getting 2-3 5 and 8 0 1 1 0 multiplied by 0 1 1 0 what is the name I forgot again Kamal right Kamal. What you are getting? 1001. What about you Anchal? 1001, unit matrix, so everybody has got 1001. So what do I get A = A transpose.

What I can also say sorry A transpose = A inverse, A = A transpose and A transpose = A inverse so it is unitary and of course this orthogonal also it is a real matrix. It is everything, right. Everything and of course the same holds for 1001. What is the inverse of 1001? 1001 what is the transpose of 1001, same thing, ok, right.

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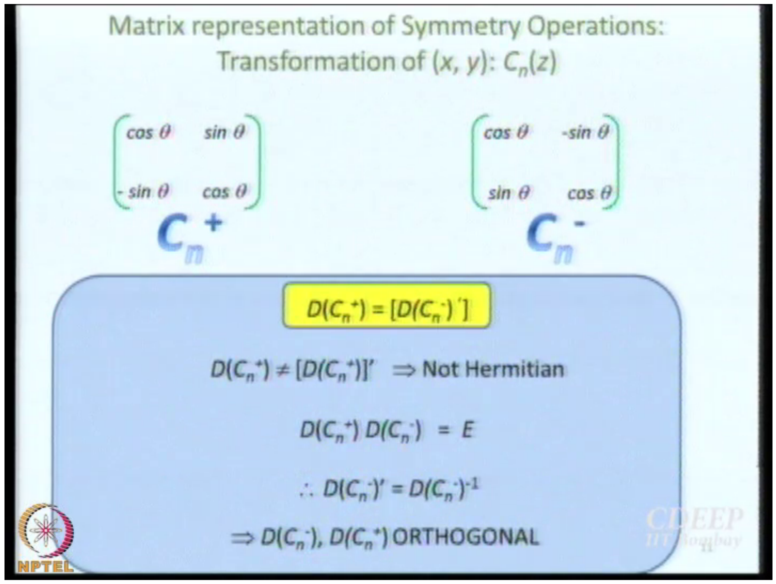

Now let us turn our attention little more complicated matrix that we have encountered earlier. Remember this matrix, we have used that the coordinates of the point xyz as the basis and we have worked out these matrices for the Cn rotation. For Cn plus we got cos theta sin theta 0 minus sin theta cos theta 0 001 and for Cn minus we have got cos theta minus sin theta 0 sin theta cos theta 0 001 right. Remember, either remember or believe me, right. These are the Cn plus and Cn minus matrices for Cn plus and Cn minus operations that we got in the general representation.

This matrix can also be block factorised in this manner. What is meaning of block factorise? Leave all the zeros outside the two lines ok. Then you have a 2 by 2 blocked here and you have a 1 by 1 block here ok. 1 by 1 block is again 11. So let us not worry about it. Let us only work with 2 by 2 blocks. Now what does the two by two blocks deal with? Which part of the basis? What is the basis here? xyz the coordinates, right.

Out of this z is unique, it forms the basis by itself, irreducible representation, it forms a representation by itself ok, x and y are here. Why do I call it a two dimensional representation? Because the half diagonal elements are not zeros ok so I call it a 2-dimensional representation. Another way of thinking is what is the basis here? X and y, right, how many elements are there, 2, 1 is x and other is y so the dimensionality of the basis is defines the dimensionality of the representation. The reason is why we have half diagonal, why is it we have half diagonal elements as non zero. What does it mean?

In a transformation what do diagonal elements stands for? What do half diagonal elements stands for? What do we are revising it is very easy to forgotten what we discussed earlier but if we do not remind ourselves all this, we do not understand what is going on afterwards. So, basically we are revising. What is the meaning of diagonal elements in this transformational matrix? Which one diagonal or half diagonal what you say I am sorry, diagonal elements, denotes the contribution of the particular vector into its own transformed form right.

And half diagonal elements, contribution of a vector in a transformed form of another vector right, see this sin theta for example. There is a contribution of y in x dash right, x dash y dash = cos theta sin theta - sin theta cos theta multiplied by xy. So x dash = cos theta x + sin theta y is that right. So the sin theta is coefficient of y in x. Similarly -sin theta is the coefficient of x in transformed y is it not? What is y dash? Y dash = -sin theta x + cos theta y right, half diagonal elements are contributions of particular element of the basis in a different transformed element.

And this subscripts tell you where the contribution is coming from and the where the contribution is made, ok. So now, now that you have a two dimensional representation let us what work with that. Let us forget about z, let us talk only about transformation of x and y. Because x and y jointly forms the basis here so far as we can see and the whole point here is that x and y get mixed. When you turn you cannot represent transformed x as pure x. It is a mixture of x and y, fine.

So now what do we what can now we say about these matrices? With the background of last 3 or 4 classes, what do you say about these matrices? The first point to note at the north transpose of each other and henceforth what I am going to do is I am going to call these matrices as D that is the notation followed in Bishop's book. So the transformation matrix going to be denoted as D and when I write d i j that means the matrix elements in matrix D, so are you ok with this? DCn + = transpose of DCn -.

You see this cos theta if you want to transpose you need to take the -sin theta here -sin theta and this -sin theta has to come here minus sin theta this cos theta remains where it is ok because these are transpose of each other, Shiva questions? Answered ok, we will get more answer as we go along. Second point to note is this. What is the condition for the matrix to be hermitian we said? A must be = A dagger or everything is real and A must be = A transpose.

Are any of these matrices are equal to its transpose? No, right since you have not equal it to transpose they are not hermitian. Earlier in the earlier example we have encountered matrices which are hermitian as well as unitary as well as orthogonal right. Here these matrix two matrices are definitely not hermitian right. Next what is DCn + and DCn -? Multiply it together and see, first row first column what is it cos theta into cos theta + sin theta into sin theta cos squared theta + sin squared theta. What is cos square theta + since square theta, it is 1.

So first row first column is 1, first row second column is cos theta - cos theta sin theta into - sin theta - cos theta sin theta + sin theta cos theta that is 0. Second row first column, -sin theta cos theta + cos theta sin theta is 0 and second row second column -sin square theta + cos square theta, that is a problem minus, minus plus and so not minus, no problem sin squared theta + cos squared theta. I also I also need to see that everybody is awake, so this is unit matrix right. What does it mean? That means the DCn plus is inverse of DCn minus yeah exactly.

But even before we go there now see we have reached something interesting. You could have said that DCn Plus is inverse of DCn minus instead of doing all this, right. Think of rotation by one 120 degrees. This is plus this is minus or they are not inverse to each other right. It is just that we are worked it out for a more general case little more vigorous. So DCn plus is the inverse of DCn minus that means what we now get to see is that geometry is actually reflected in the agenda is just that you need to able to read it.

Geometrical changes are actually being reflected in the relationship between the transformation matrices, right. Now I hope you are not forgotten this DCn + = DCn - transpose, right. I can write into instead of DCn plus I can write DCn minus transpose. DCn minus transpose = DCn minus inverse. Rahul's said is that right if Rahul has said that correctly. These are orthogonal matrices ok if the transformation matrix is real and then orthogonal. This is a demonstration for that you can take from other bases workout other matrices and check whether they are orthogonal or not, ok.

Hermitian is not a necessity but orthogonality will be there. That is why we can invoke the great orthogonality theorem. If it is not orthogonal, how will orthogonal orthogonality play a role that is why we are getting very slowly? Fine so much for your Cn+ Cn-. What was the basic remember the coordinates right basically we are talking about transformation of a point right. Now let us do it in a little different way.

But before that if I write cos theta sin theta if there is a possibility that I myself will goof up. So instead of cos theta sin theta I would like to work with some value.