Symmetry and Group Theory

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Lecture No. 19
Matrix Representation Revisited

The value I like is the 120 degrees. Let us talk about the C3 rotation, what is DC3? What is cos theta? When theta = 120 degrees.

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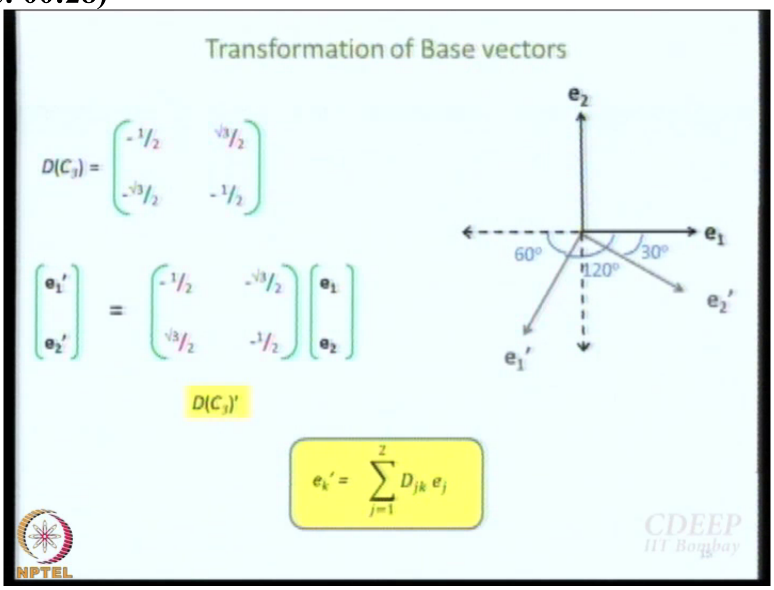

And what is sin theta? Root 3 by 2 right minus half or plus half 120 degrees, minus sure, why minus? All sine then yeah, so this is the matrix right very good Sahu is right cos theta sin theta minus sin theta cos theta becomes minus of root 3 by 2, minus root 3 by 2, minus half that right. What are you transforming points coordinates of the points. Now let me do it in a little bit different way instead of transforming the point, let me transform the axes. This is what I want to do I want to transform the base vectors now instead of transforming the point.

And I want to see what kind of matrix we get once again as we will see the result we get is something that is very much in line with common sense right. Let us proceed let us draw something otherwise it will be a little problematic what are base vectors? Base actors are vectors their react with acid vectors even vectors as some other meaning in biology. So what are base vectors please tell me? XYZ and something more, XYZ are directions then I had the right answer, time. Time is fourth dimensions no do not make things more complicated then they have to be. But I heard the right answer, be brave and give the right answer. X Y and Z direction is right and what is other than the reaction ijk yes.

What is i j k? Unit vectors write ijk is correct unit vector is along X Y and Z and just to be in the same page as Bishop we call it e1 e2 and e3. So do not get scared right e1 e2 e3 is nothing but ijk right. Let me draw and here I do not do not even need e3 because we are working only with X and Y. So let us say these are the base vectors X and Y e1 and e2, e1 along X and e2 along Y. What will I do? Now I will take in clockwise direction by 120 degrees right. Let me do that 120 degree, this is what it will be right.

e1 dash transformed e1, length is a same do not forget even though does not look the same for some reason. But that to my poor artistic skills all lines here are the same ok. 120 degrees angle between e2 and e2 dash is also 120 degrees I do not think my poor artistic skills it is the screen is messed up perspective is ok everything is in the plane there is no perspective. The screen ratio has changed in order to be compatible with that. Actually is looking ok with that my screen is looking strange anyway fine.

Angle between e2 and e2 Dash is also 120 degrees right, you just write e1 dash and e2 dash in terms of e1 and e2 very simple ok. In order to do that just because we are going slow let us also draws the arrows for -e1 and -e2 right -e1 and -e2. This is -e1 this is -e2 right, right or wrong. There is right transpose, transpose of right this is -e1 this is -e2 not very difficult to understand ok. Now since while you are at it, let us also write down what is the angles are, what is the angle will be 60 as really.

How was 60? 180-120 let me ask sometimes questions easy also and what is this angle? This angles this you are taking it as insult your intelligence so you are not responding to it or not. This is 25 degrees then how 30? 120-90 very good write are you clear about these angles. Now it is very easy to fill in this matrix. I want to write it as e1 dash = A into e1 + B into e2 ok how will I do it? Simple vector addition components do the trick. What I have to work out is what is the e1 component of e1dash? What is the e2 component of e2 dash? Right, all the components will be written here is it not. So, noww tell me what is this if I draw a perpendicular line e1 dash today e1tricks e1 axis.

What will it be? Yeah lauder, -half and if I draw perpendicular on e2, what it will be, -root 3 by 2 are you looking for that this length, this is one so if I draw a perpendicular here, what we learnt in school is that it will start with the equilateral triangle and draw a perpendicular bisector. So, if this side is 1 this side will be half and since it is of along -1 -e1 it will be minus half. And similarly this will be by Pythagoras theorem root 3 by 2.

So e1 dash = -half e1- root 3 by 2 e2 - half e1 - root 3 by 2 e2 correct. What is e2 Dash? E2 Dash = root 3 by 2 e1 and then minus half e2, is that right. This is the matrix that we get -half -root 3 by 2 root 3 by 2 -half right. Now you see 2 transformation matrices 1 is DC3 associated with transformation of the coordinates that is -half root 3 by 2 root 3 by 2 -half. And other one we get is the transformation of the unit vector of the base vectors that is -half - root 3 by 2 root 3 by 2 minus half.

Do they have anything to do with each other or not they are transposed right. This matrix that I get by using the unit vectors of base vectors of the basis is the transpose off the transformation matrix that I get when I use the coordinates as the bases is that right is that wrong? It is right. Now ok let us write most difficult think first and then we will come back to the nicer and easier thing after that. Come on this is what we are talking about let us see whether we understand this or not.

I am saying ek dash = sum over j, I do not know I have written j = 2 do not get carried away by this example where j = 1 to n, j = 1 to n Djk ej right what I am doing here is that generally it should be row multiplied by column. But here when I am working with unit matrix I can use that same transformation matrix that I get from transformation of coordinates but multiply by row not by column that is what gives me some over j Djk ej. What is the meaning of this Dkj ej? K is constant right. What is the first substitute and what is second substitute.
First substitute is row and second substitute is column, now that substitute is so second substitute is column. So what we are saying is that we are keeping the column constant we are going down the column row number is changing right.

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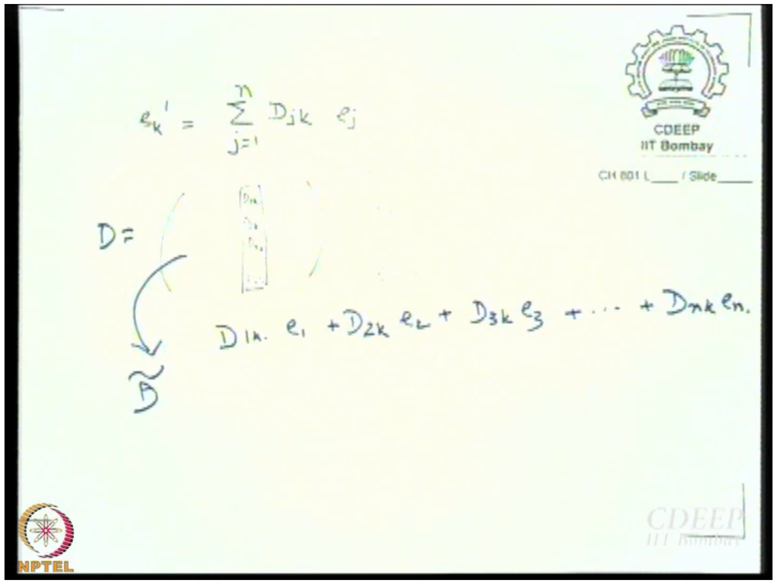

What does this mean? This is my matrix ok k is constant I am summing over j, that means I should go down the column. What is this? D1k this is D2k then D3k so and so forth lost you have Dnk right. What I am multiplying with it ej so e1 e2 en. So this would mean, I do not think that I would have written so much. D1k e1 + D2k e2 + D3k e3 + so and so forth + Dnk en ok, why am I doing that in this because the matrix that I am actually multiplying with is this transpose?

This is D, I am actually working with D transpose right, actually multiplying by the row but what I want to do is I still want to keep the matrix that I got from transformation of coordinates and not axes. That is why I am multiplying with column that is the only reason. First look this might look little bit strange it is not. Do not forget what happened here I hope you cannot see it. Do not forget what has happened here. I am working with DC3 prime not with DC3. I am talking about transformation of coordinates.

DC3 is the transformation of matrix that you get for operation of C3 on the coordinates. When I say coordinates what do I mean? Position vector can I say that is the position vector that is moving xyz is changing, that means position vector is going from here to here right like this ok. Now we will come back to this but before that let me write this DC3 Prime is nothing but DC3 minus or DC3 inverse rather, we learnt that. DC3 inverse now she does it make sense. What I am saying is that the transformation matrix which I get by using the position vector as the basis.

Is the inverse of transformation matrix I get when I transform the base vectors? What does that mean, and here of course plus minus clockwise and anticlockwise rotation right.

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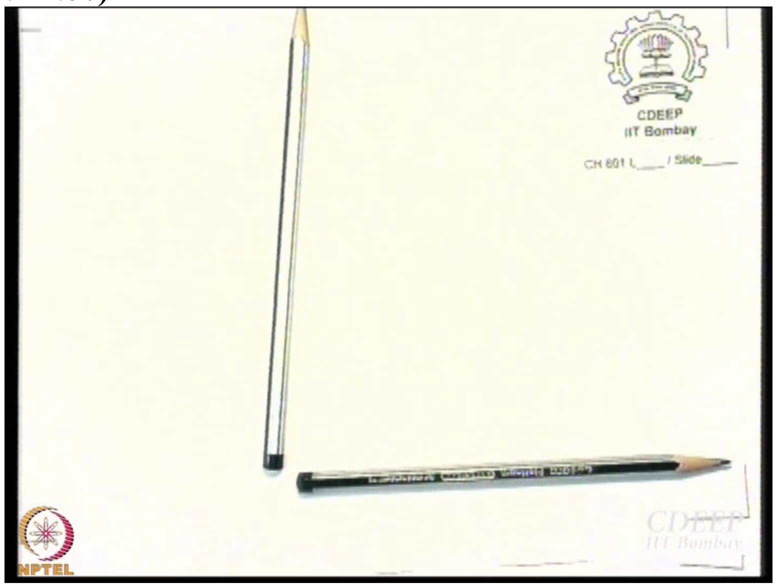

Now see these are my base vector ok, this is my position vector do you see that clockwise rotation of position vector is same as the anticlockwise rotation axis is it not, that is what it means. Clockwise rotation of the position vector what it does is it decreases the angle between X and the position vector. Instead if I rotate the axis base vectors then also the same thing happens right. So, the matrix that I get for clockwise rotation of the position vector should be the same as matrix that I get for anticlockwise rotation of the base vector and vice versa.

Now does it make sense right, this is what it is, that is what we need to do if there is any question please ask me for you to go ahead. Two kinds of people they do not ask questions. Those who have understood everything and those who have understood nothing, I assume that everybody has understood everything. Is this notation clear now ek dash = some over j 1 to n, I tempted to change it, ek dash = some over j = i to n D jk = ej, ok and the most important take home message is that the transformation matrix of position vector and therefore the axis.

They are just in words of each other, here they are happens to be opposite of each other this is something which we are going to use again. Please do not get confused when I write it in this fashion because what it implies really multiply column by column, do not forget why we are writing it. Do not forget what DA is, D denotes the transformation matrix of the point the coordinates not the axis alright let us move on.

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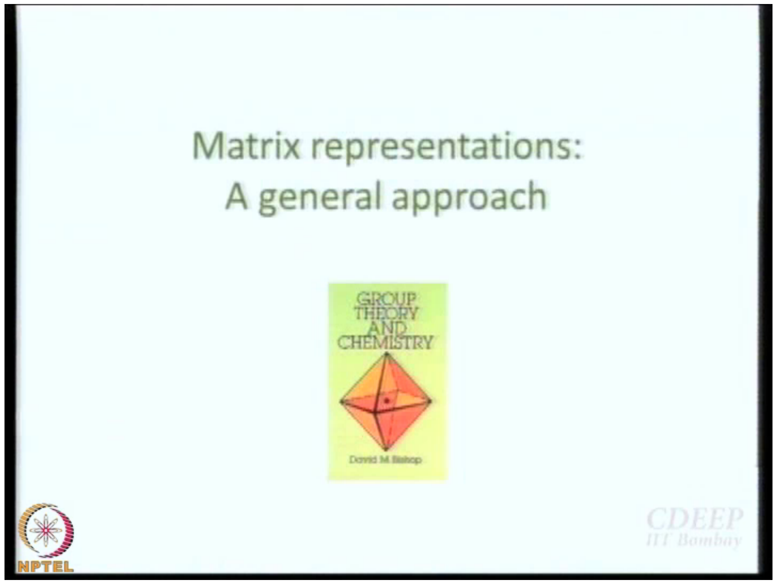

Now the point is this we have all those matrices and we know that it is possible by similarity transformation to get the diagonalized matrices. So it should also be possible by similarity transformation to get at least block diagonalized matrices. So what you could try to do it you take any molecule and use any bases that you want workout the matrices and find suitable matrices that well similarity transform this matrices into block diagonalized form and then you stay blocks as irreducible representation ok that sounds possible.

What are the problems with this? Why do we not want to do this? You want to do this you could have done this, if you read Harrison Bertolucci book example they have worked out how you can block diagonalized the matrix C5 group, C5 group it is worked out. What would be the problem that would be; what would be the problem of approach like that? Would there be any problem or that will be fine.

Bigger the matrix more the complicated, moreover you cannot just use the matrix to do the similarity transformation there right. We already know which matrix will work at least one kind of matrix we know already. There is a n by n matrix then I think we have convinced ourselves that this eigenvalue vectors matrix that we have X that can be used to similarity transform and get diagonalized matrix completely diagonalized forget about block.

But that is obviously not the way to go because that would mean is that that would mean is that there is no you irreducible representation that is more than one dimensional. Similarity transformation using the X matrix gives you a completely diagonalized matrix right. So if that was the way to go that would be then no; that means irreducible representation have to be; has to be dimensionality 1, that sounds little bit strange. Besides when you do a similarity transformation you should do the same similarity transformation on every matrix.

And every matrix is not going to have the same eigenvalue eigenvector right, so, just eigenvector matrix does not work. Maybe there some other matrix maybe what is work out in Harrison Bertolucci's book but what is the problem how you find the matrix it is back breaking, it is a group force method right. Just look at those matrices that I have given in Harrison Bertolucci book they are ugly. They actually give a block diagonalized form but they are ugly. Secondly point is what do I, use as bases and which molecule we have used.

As I discussed earlier water is C2v, Ch2 Cl2 is also C2v write is just that the matrices in Ch2 Cl2 maybe double the size of the matrices that will get for water at least two more elements will be there if we only use the atoms. Using molecule is not very smart way of doing things. That point is that question we ask how many reducible representation are there that is not the answer. So as we see the representation depends on the basis right what basis you use dictates which representation shows up.

It is very possible that the representation for which is not very easy for us to imagine what the basis is going to be and remember this question we are going to show you example of such bases. We are going to show you examples of such representation for which it is not very easy to think of a base. So that group force approach is not such a great way of going. So what should we develop what is that we should develop is general theory, something that works for everything ok.

And finally you should have a machine the black box into which we will feed any molecules we want any point group we want. And this box is going to give us whatever answer it can about that molecule at least the question that we are asking at this stage. It should be able to tell us how many reducible representations are there. What are the dimensionalities of those reducible representations? What are those reducible representations ok? If these 3 answers come then that is good enough we do not need anything more rest we will see ok.

So, what I am trying to tell you for the last 10 minutes is that just by trying out different combinations and similarity transformation is not a good way to go. We must develop something which is more general right. So, let us go ahead and do that.