Symmetry and Group Theory
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Lecture No.6
Transformation matrices and Matrix representation:

Let us do something very simple once again what will do if is work out this easy ones here. I will give you little bit of difficult ones to do at home and next Friday we start with this ok. What to say you remember whatever is that we have discussed so far in the language of geometry. But then if you really want to work out your methodology by which you can do things very easily or let me the computer do it the only way in that in which it is going to happen is if you translate all this into the language of algebra. And we perform this translation geometry to algebra by using all our familiar friend matrices ok what about matrices, matrices are very additive numbers is it not. So, let us see how that happens.

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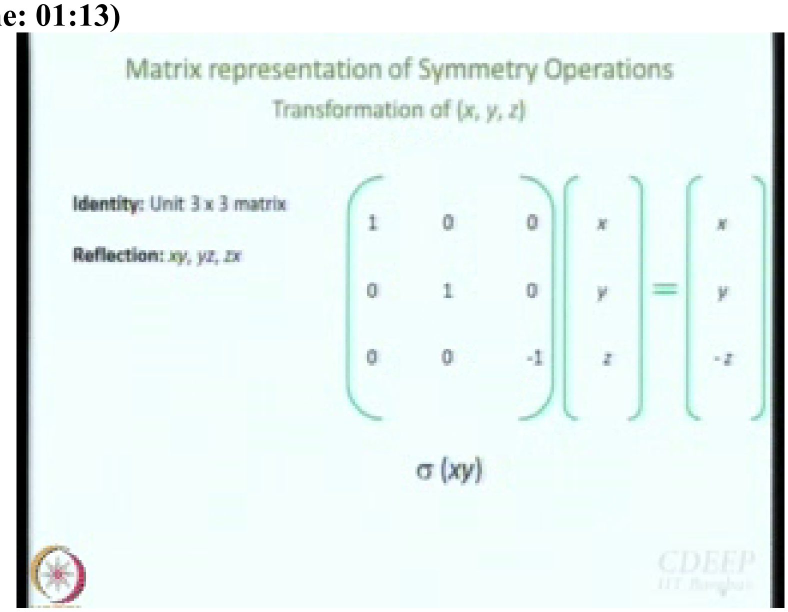

So, let us say I am talking about the transformation of your point of coordinates xyz ok, xyz. Identity matrix is very easy to workout this is actually the identity matrix unit 3 by 3 matrix because if you perform C1 or E then what happens to xyz is x remains x, y remains y and z remains z no change, so the transformation matrix is going to be 100 010 001 ok. Now let us think of reflection and keep things simple let us talk about xy yz and zx ok. What happens when you perform reflection with respect to say xy plane what happens to x what happens to y what happens to z, x remains same y remains same and whatever z, z becomes manageable I think all will understand that ok.

So, x remains x, y remains y, z remains z that z becomes Sigma -z sorry what will the matrix that is child's play for you 100 then right, 100 010 00-1 this is the matrix. So, what one what have you got you have got the matrix representation of reflection with respect to xy plane ok very simple no difficulty so far. Now tell me what will be the matrix be for yz it is variant y and z will remains same so the x will change sign x becomes -x right -100 010 00-1 001 sorry and zx, yes. Now before going any further let me state something that is perhaps obvious.

I like to draw your attention for these elements here that is something that comes handy later on. The diagonal elements the octagonal elements what is the meaning of diagonal elements and what is the meaning of octagonal elements? That is what I want to ask you. See on the right hand side what do you have? You have the transform co-ordinate is it not right and what is this? This column where, these is the additional coordinates, each element on the matrix basically gives us the contribution of one of the original coordinates in each of the transformed coordinates.

Let me put that in a complicated manner ok look at this first one the 11 element. This multiplied x will come here is it not what is this x, the x basically 1 multiplied by x + 0 multiplied y + 0 multiplied by z ok. So, this 11 element the transformation matrix tells us about the contribution of the original first element in the transformed first element, make sense Bala make sense very scary, very good. What about the second one the problem here it is 0 but still latest thing when it was non 0 what will retirement, contribution of the original y in transformed x right.

What is this 12 up to 1 what do you call it what is the element number 12 right row number column number, row number first column number second. So, the 12 element stands for contribution of second original coordinates in the first transformed co-ordinate ok what about this 0 here 13 it stands for contribution of z in transformed x, contribution of the original third element in the transformed first element ok. So, what will be workout to 21 22 23 31 32 33 so now if you focus on 11 element 22 element and 33 element the diagonal elements would not you agree with me when I say that this stands for contribution of a particular element in its transformed of that is that so.

What is 11 it is a contribution of x in x contribution of original x in transformed x. What is this 22 element contribution of original y in transformed y. What is it 33 element contribution of original z in transformed z do you agree with this. It is quietly obvious to many of us but interest is not there but I want to stress this point, it is important to what matrices mean. It is not just any of you remembered ok. The diagonal element stands for your contribution of an element in itself after transformation.

Orthogonal elements stand for contribution of a co-ordinate in another transformer co-ordinate is it not. So, see here what us happened is that here x y and z are not mixed they either remain what they were or at most they have change sign x and y remain the same is it as change sign and there is no xy mixing ok that is why you have a diagonalized matrix here. The transformation matrix is such only the diagonal elements of the non zero. The orthogonal elements all 0 when you have matrix like this that is mean physically that there is no mixing of coordinates.

X remains x or becomes –x, y remains y or become –y, z remains z or becomes -z but there is no mixing x with y and y with z and z with x makes sense you see identity there is no question of mixing either deflection with this plane taken they do not cause mixing of coordinates fine what about rotation.

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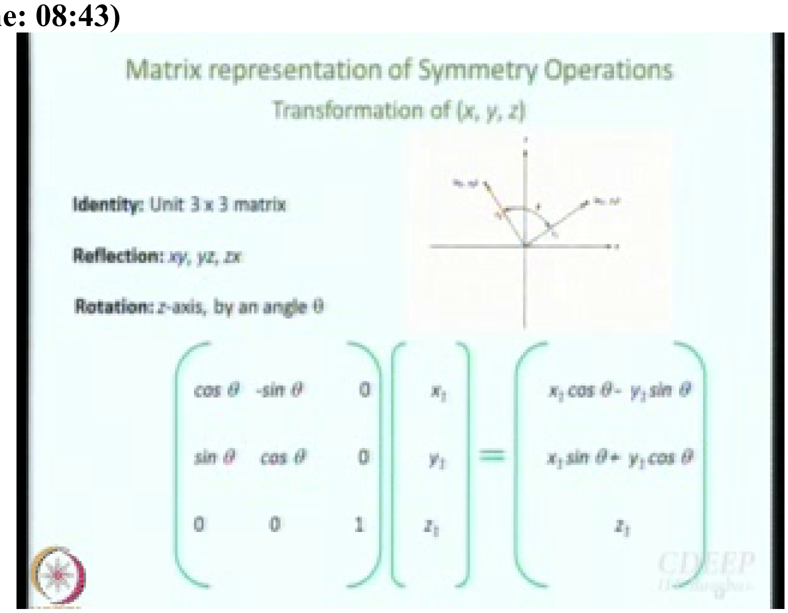

It is customary to take the z axis as rotational axis, z is always unique ok. So, if you turn with respect to z then what will happen you start with what you have written x1 y1 z1 the original coordinates x2 y2 z2 the transformed coordinates. Since zx is there rotational axis I think it is not very difficult to understand z2 is just equal to z1right. So, z does not mix with x or y right so you can write part of the matrix right z remains by z itself it is unique.

Because you are performing a rotation with respect to z so I can actually fill in these elements here 33 element is going to be 1 and this orthogonal elements involved z what is this contribution of what in what z1 in transformed x, x2 right. What is this contribution of z1 in transformed y yeah what is this x and z and this one is contribution of y and z ok. Since z does not, z is at top so does not mix with x and y in this case right it likes to be x itself.

So, actually I can fill in all this, what we left is this block here the 2 by 2 block is that I have to fill ok and here you see I cannot have something that is very simple because what is happened if you have turned, now think of the projection of the position vector on xy plane ok, x1y1 has becomes x2 y2 no way in which you can your present x2 just in time of x, y just in terms of y there is a mixing because this point has x and y component, this point also have x and y component the mixing is there ok.

Can you workout this expression what is x2 equal to in terms of x1 and y1 what is y2 in terms of x1 and y1, it is perhaps better to write you can work it out looking at the board it will be great it is not possible it is obvious that it is understand then it is this something to do with cos theta and sin theta is it not that is very obvious. I will give you the answer please work it out, if you can you cannot then we will work it out in class next day. This is a answer x1 cos theta -y1 sin theta and y2 is x1 sin theta + y1 cos theta then tell me what will be the matrix now cos theta - sin theta and sin theta cos theta this is the real transformation matrix.

And this is the beginning of something important because you see actually you can divide this matrix into two blocks you can draw a line like this and you can draw a line like this because the story that these matrix tells us as the result of, you know the rotation with respect to z what we are able to do is that we have been able to create two different classes of coordinates x and y mix with each other right. So, they give rise to this 2 by 2 block and z remains what it was so that gives rise to the 1 by 1 block all these 0's are useless.

So, the minus sign will be used, I can draw a line like this and I can draw another line like this, so essentially I done is that I have divided the matrix into two parts or as a call 2 blocks, 2 by 2 block and a 1 by 1 block which is of the number alright this is the beginning of something that is going to be very useful for us later on ok. Please work this out by yourself this is worked out in very nicely Carton book is also here but then Harrison Bertholysis book is there it is where it is work out all that details ok.

So, we close this today and next day what will do is start from here, we talked about the transformation matrix and then we take little bit of mathematical interview because what we need to do we need to rewind ourselves about the properties of matrixes and then we will see that and we will use something called group theory we are going to show you that all the symmetry operations formed what is called a group. Are you familiar with the term group not political group or anything mathematical group? Are you the term group.

What are the properties of the elements of the group have to satisfied not mentioned obvious first property is identity, identity do not neglect the obvious ok. So, we just remind ourselves what is the properties of the group and then we are going to demonstrate that this symmetry operations actually formed groups ok and then little bit of properties of matrices from there we will see how one can use group theory where ever something called great orthogonality theorem.

And then comes to the application part using this great orthogonality theorem we learn how to construct character tables and using character tables we will construct symmetry adapted linear combination we will see what they mean and that is what will allow us to go into description of molecular orbital theory from the point of view of symmetry.