Symmetry and Group Theory

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Lecture - 18
Matrix Representation of Symmetry Operations

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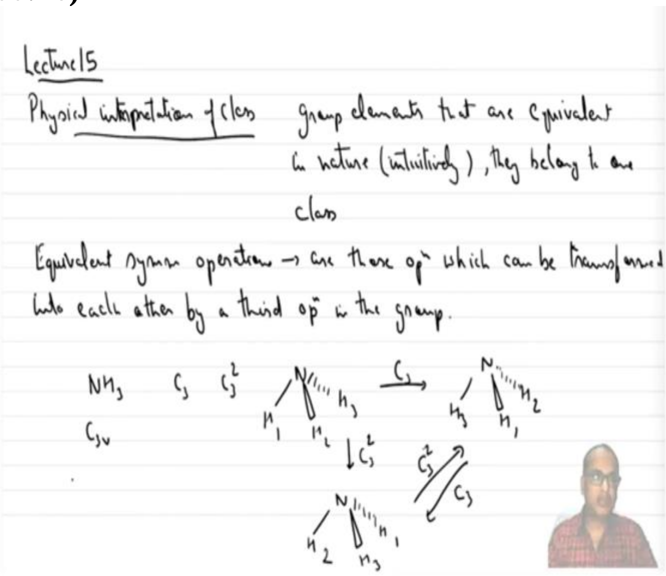

So, in the last class we were discussing classes. So, let us continue the discussion and let us see the physical meaning of what do you mean by class, physical interpretation. So, by now, if you have worked out classes for NH3 molecule, and C4v molecule, which we were discussing in the previous class. So, if you have worked out the classes for these 2 molecules, you must have realized that classes are the group elements that are equivalent in nature intuitively, I must say at this point.

They belong to one class. So, for example, C3 and C3 square they seem equivalent and then they belong to same class 3 sigmaVs of NH3 they belong to one class. So, what do you mean by equivalent symmetry operations? So, let us see, because if we can identify equivalent symmetry operations, we can simply group these equivalent symmetry operations in one class and we do not have to actually calculate all the similarity transformations for individual group elements, that will be easier.

So equivalent symmetry operations are those operations which can be transformed, I will give you two definitions for this, into each other by a third operation in the group. So, what do I mean by saying that? Let us say if we are considering NH3 molecule, the point group is C3v.

So, C3 and C3 square are equivalent symmetry operations that is effect of C3 or effect of C3 square can be inter converted between each other by a third symmetry element.

So, let us without wasting time let us see what do I mean by that? Let me write down NH3, 1, 2, 3. So let us operate C3 on this and we will also operate C3 square. So here C3 square, C3 anticlockwise will give you, the 3 goes to 1 so, 3, 1, 2 and C3 square will give you 3 comes here, 3, 2, 1. Now these two operations must be related by a third symmetry element. So, let us say if I want to go from here to here what symmetry operation I can use, so that I can call this equivalent. Can you find out one?

So, if I do so, I can say that this is C3 in this case actually this is the same but these 2 are basically the effect of the two are still interrelated by an element in the group and similarly here also I can go by this will be by C3 square and this will be by C3. So, idea is basically that the two symmetry operations are equivalent if the result of the two things, two operations can be interconverted into each other. It can be by a third element or by one of the, basically one of the elements of the group. In other words, we can also say that, let me write down the exact definition.

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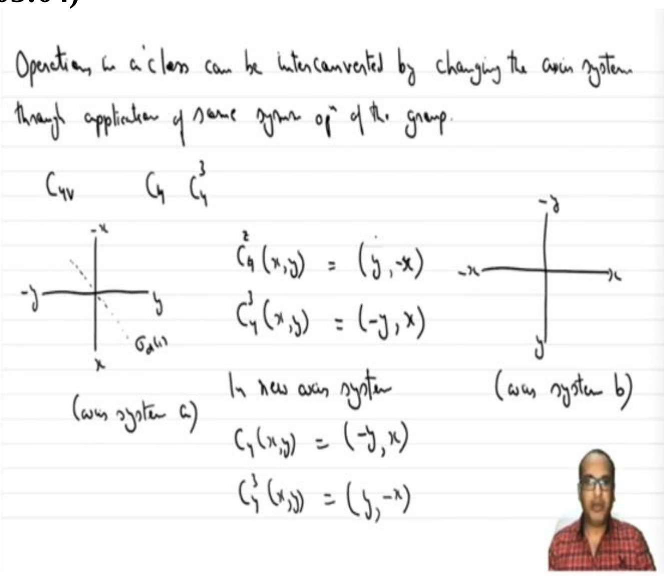

Operations in a class can be interconverted by changing the axis system, we will see an example of this, through application of some symmetry operation of the group. So, let us consider C4v point group. So, what I am saying is operation in a class can be interconverted by changing the axis system through application of some symmetry operation of the group.

So, the meaning is, so let us consider C4 and C4 cube, which belong to same class we should have all worked out by now. So, the effect of let us say, let us take the coordinate system.

So, x, y, –x, –y this is the axis system, axis system I would call as A. Now if I do a C4 operation on to x, y, C4z my axis around z. So, what happens to x? x goes to anticlockwise, so x moves to y, and y moves to –x. This is the effect of this particular operation. Now similarly, let us say what is the effect of C4 cube on x, y. C4 cube will be 270 degree rotation. So, x goes to –y and y goes to x. Now let us say that if we change the axis system, so that by one of the elements which is sigma-D1, this is the plane sigma-D1.

Sigma-D1 is part of this C4v group. So, if we change the axis system we go to y, x, –y, –x. Now in this, let me name it as axis system B. Now in this new axis system which is obtained by application of one of the group elements let us apply this C4 operation on x, y again. So now, if I do on to x, y what do I get? So again, I am doing x anticlockwise rotation, so x moves to –y and my y goes to x, now if I do C4 cube on x, y, what do I have? So, x moves here that is y and y move to –x.

Now you see that the effect of C4 was earlier y - x, now effect of C4 is - y x. So, the effect of C4 and C4 cube are interconverted by changing the axis system and the axis system is changed by one of the symmetry elements of the group. So, what I am saying over here is operations in a class can be inter converted, so operations in a class can be inter converted. So, operations in the class can be inter converted by changing the axis system from A to B through application of some other symmetry element which is sigma-D1 here.

So, this should be very clear this is the physical significance because basically what we are trying to say is that, when I am fixing certain elements in a class that means their effect is interconverted, so it is like changing the axis system and doing the same operation again. So that means, so if C4 is doing certain operation in one axis system, and C4 is doing certain other operation in another axis system then C4 cube should also give me the same result as the previous axis system or the one of the axis systems.

So, the idea is that, if we change the axis system the 2 symmetry operations change their result and then they are called as equivalent symmetry operations and thus they are classified into same class. Now we have understood the physical significance we know how to classify and now, we will see later that why this is so important, why finding elements which belong to one particular class is so important that we will see in matrix representation but that will come maybe 1 or 2 lectures later. So, this finishes the discussion for subgroup and class.

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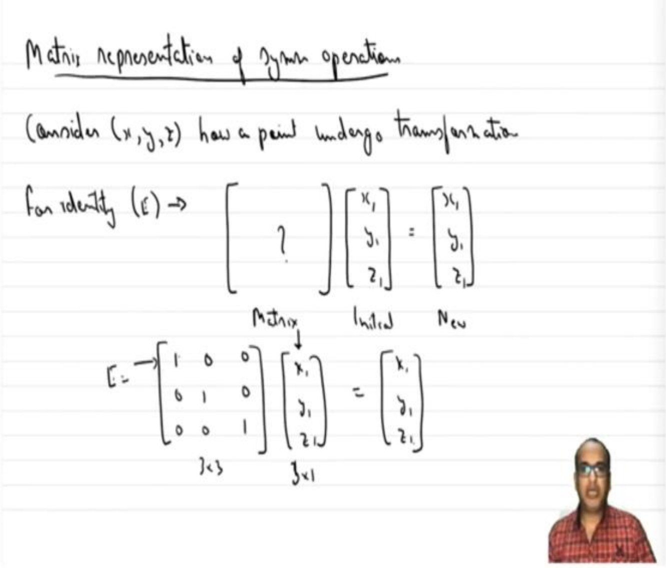

The next important topic is Matrix representation of symmetry operations, these are operators, so all operators by definition can be written as a matrix representation if we know the proper basic sets. Let us work it out let us see, let us consider a coordinate system x, y, z and let us say how a point x, y, z undergo transformation due to this symmetry operations. So, let us first consider for identity E. So, let us say we are trying to find a matrix representation for E. So, this is the matrix which we do not know, this is the matrix.

Now initial coordinates of the system are x1 or of a point are x1, y1, z1, this is the initial location of the point and this is the final location, new location you can say. Now new location in case of identity will not be different it will be same as x1, y1, z1 because identity operation does not change anything in the molecule or to the point. So that means E should be a unit matrix of order 3. 3 cross 3.

So that is very easy to see. Now if you do this multiplication, this is a 3 cross 3 matrix and if we multiply x1, y1, z1 which is 3 cross 1, so what we will get is a 3 cross 1 matrix. And we all know how to multiply here, matrix. So, x1 multiplies with 1 + y1 into 0 + z1 into 0 which will give you first element here, x1. Similarly, x1 into 0 + y1 into 1 + z1 into 0 will give you y1, x1 into 0 + y1 into 0 + z1 into 1 which gives you z 1. So that is how you will determine matrix representation for E. So now, let us look at other symmetry operation.

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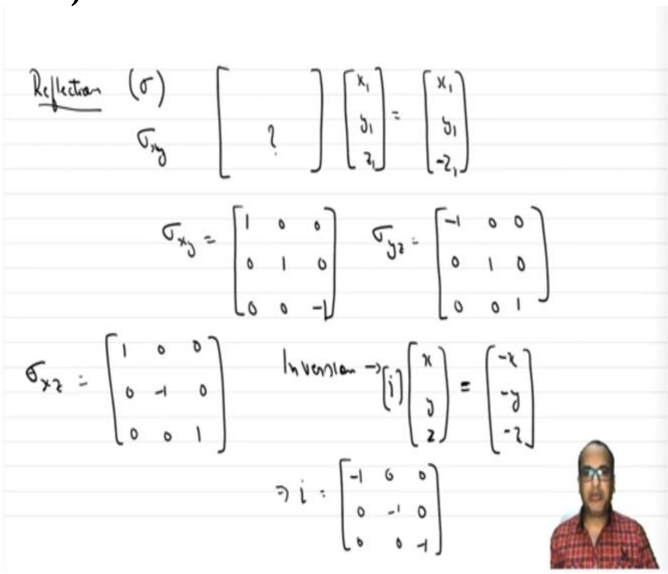

Next in the line is let us start with the easier ones first and then we will move to the complex ones. So, for reflection, let us say sigma. So again, let us write down the unknown one as question mark. The initial, let us consider this as sigma-xy may be. We have to consider one plane, so you can consider any plane. So, if we have x1, y1, z1 the initial point will move to, because x1 and y1 would be lying on sigma-xy, so they will not change their locations. So they will be same.

Then z1 will move to –z1, z1 will go to -z1. So that means what do I have? This matrix for sigma x y, because x1 and y1 are not changing anything they will be 1 and 1 at the diagonal and since z is going into minus sign you can write z as negative. Similarly, you can write for sigma-yz, this will be - 1 0 0, 0 1 0, 0 0 1 and for sigma-xz it will be 1 0 0, 0 - 1 0, 0 0 1. So this is easy to see, reflection is easy.

Now also look at inversion, so in an inversion operation what happens to x y z, i matrix, x goes to -x, y goes to -y, z goes to -z. So, this implies i matrix is nothing but negative unitary. This should also be very clear, there is no confusion in this. So now, let us look at where we need to do some calculations for rotation.

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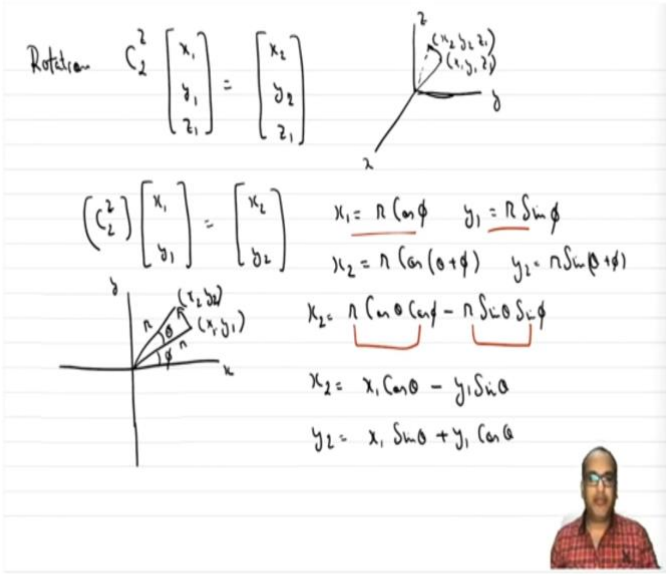

So, let us consider C2z rotation where z is collinear because it will be easier to see. So, C2z rotation on x1, y1, z1 gives rise to, so now, x1 will move to x2, y1 will move to y2, z1 will remain at z1. So, what do I mean? I mean if this is x, y, z and we have a point in plane which is x1, y1, z1 which can be represented like this then I am moving to a certain point in space which is by application of C2z which is now defined with the coordinate as x2, y2, z1, my height does not change.

So, if I am fixing my z1, I can also reduce this to a 2d problem where I can say that x1 by application of C2z matrix my x1 y1 is actually changing to x2 y2. So, this is only for solving it a little easy so that we are converting into a 2D problem. So, let us see what it means. We have x, y, x1, y1, moves to x2, y2. Let us call this angle is phi and this angle is theta and let us call the length of this point or distance of this point from origin as r which remains unchanged, because we are only moving in this direction.

So, this is my rotation. So, if we want to write now x2, y2 in terms of x1 y1, how do I write? so let us see, x1 can be written as r cos phi and y1 can be written as r sin phi. It is the basic trigonometry. Now let us say if we are trying to write x2 in those terms, x2 will be equal to r cos theta + phi because that is the total angle theta + phi. So, x2 can be written as r cos theta + phi. And y2 can be written as r sin theta + phi.

So now let us try to expand this x2 is nothing but r cos theta cos phi - r sin theta sin phi that is my expansion for cos theta + phi. So now I know that r cos phi is x1 and r sin phi is y1. So, I can write x2 as x1 cos theta - y1 sin theta. So, similarly, if you expand y2 sin theta + phi what you will get is, x1 sin theta + y1 cos theta. So now, if I write this in matrix form what do I get?

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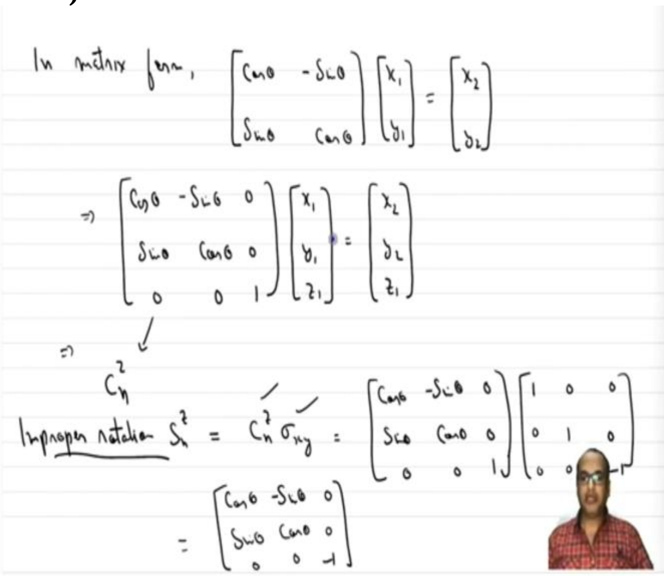

In matrix form, the above equation can be written as cos theta - sin theta and we have sin theta, cos theta into x1 y1 which gives me x2 y2. So now again introducing the z axis in the system which is not changing, so we can say this implies cos theta, - sin theta, 0, sin theta, cos theta, 0, 0 0 1, I am only extending the whole thing into third dimension, which is z, which does not change. So, notice that I am writing z1 as z1 y1 goes to y2, x1 goes to x2 whereas z1 remains as z1.

So that means, this implies that this particular matrix is my representation for C2z. Now I can take any angle or Cnz this is not; we have not explicitly set any angle here. So, this is for Cnz let me also correct it the previous one here, so let us say this is C n z. So now, if I want for C2z what I will have to do is, my theta will be 180 degree. So accordingly, the values of cos theta and sin theta will be placed here and that will be the matrix for C2z.

Similarly, if I want C3z my angle will be now 2 pi / 3 and then if it is C4z it will be 2 pi / 4 and so on so forth. So, you can easily calculate a rotation matrix or matrix representation for any kind of rotation. Now next is for improper rotation which is Snz. So, we all know that improper rotation, Snz can be written in terms of Cnz into sigma-xy, so sigma-xy because that sigma is perpendicular to Cnz, so that has to be very clear.

If we are taking our rotation axis along z axis, then the sigma has to be the perpendicular plane. Now if we can obtain this matrix easily because we know that the matrix representation for this as well as this. So, let us just multiply the 2 matrices. We have cos theta - sin theta 0, sin theta cos theta 0, we have x and y unchanged and z goes to - z. So, the only difference we will have is that we will have this, I am just writing everything same and instead of +1 over here, we will have, the only difference is instead of +1 over here we will have -1.

Which defines that now z1 actually goes to -z1 for improper rotation and the x1 y1 will still go to x2 y2 whereas z1 will go to -z1 that is the meaning of improper rotation. So that should be very clear. So, if that is clear, we will move to how to write matrix representation. In next class we will see how to write matrix representation for various point groups. So that is all for today. So, thank you.