Symmetry and Group Theory

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Lecture – 20
Symmetry and Group Theory - Tutorial 4

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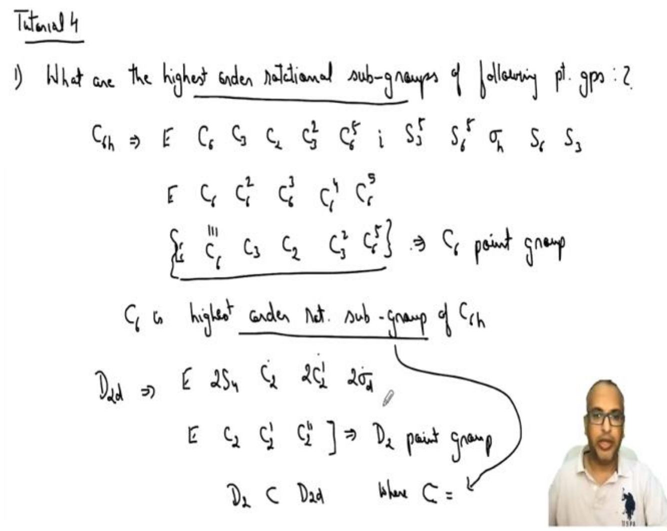

Welcome back so in this week tutorial we will be discussing some of the practical applications of point group. So far what we have learnt. So, let us see some of the kind of questions which try to change the words, so that the question appears very difficult but then what is the approach to solve such kind of questions? So, let us and will try to work out at least 4 questions of different types.

So, let us see the first one is what are the highest order rotational sub-groups of following point groups? So, question is asking that what are the highest order rotational sub-groups? So sub-group as you know is the set of group elements which follow all four properties of that particular of the group out of that particular point group. So, let us say if we have C6h. So now we should know how to find out what are the symmetry elements or symmetry operations present.

So, let me just list down for C6h. I have written it here with me. So, you have E, C6, C3, C2 these are all the group elements or symmetry operations C3 square, C6^5 each of this is a different class, then we have S3^5, S6^5, sigma-h, S6, S3, so these are the set of elements now it is saying that what is the highest-order rotational sub-group so for rotational sub-group you have to consider the rotational elements on these which is your rotational axis that is C6.

So, C6 is the highest order axis. So, let us see if we generate all the operations from C6, do we get a sub-group out of this? So that will be E, C6, C6 square, C6 cube, C6^4, C6^5 and C6^6 will be E. So now this is equivalent to C6 then this will be C3. So, we have C3 here. Now this will be C2, we have C2 here, this will be C3 square, we have C3 square, and this will be C6^5. So, these are the elements which contain only rotation pure rotation.

So, we wanted to see if the pure rotation sub-group is present. So yes, our subset is present we do not know whether it is sub-group or not. So, let us see so if we look at just these 6 elements this actually forms a point group for the cyclic group C6. So, if we look at C6 point group, then that is composed of only these elements. So E, C6, C3, C2, C3 square and C6^5. So, we can directly say that yes this is a C6 is a highest-order rotational sub-group of C6h.

So that was easy so you can do the idea is you have to find out only the elements which composed of rotational operations and then see whether it is forming. So, in this case we already know that it is forming a C6 point group. But ideally you should be testing it for all four group properties that all four group properties like closure associativity, inverse and identity all four are conforming to this set of elements.

So, then we can say that C6 is the highest order or rotational sub-group. So similarly let us look at another one. So, we have D2d here so now what are the elements present or the group of this thing present the D2d will be symmetry operations will be E, 2 S4 and we have C2 and 2 C2 prime and 2 sigma-Ds. So now we are only interested in the rotational things. So, this is not rotational this is reflection this is rotation and reflection.

We only want the rotation, so the rotational sub-group will be E, C2, C2 prime and we can call it a C2 double prime or we can call it 2 C2s here. So basically 3 C2s which are perpendicular to each other that is our subset. Now this subset does it belong to a particular point group or not we have to identify. So, if we look at yes it does belong to, so the point group is D2 here, let me just also look at the literature yes.

So, if we say that this belongs to D2 point group, and thus you can see this is the highest-order rotational sub-group of D2d. So, D2 is the highest-order rotational sub-group of the D2d. I am just saying D2 is a subset of D2d. So, we have a subset is meaning highest-order rotational sub-group. So, I hope this is clear this is the kind of questions which is sometimes asked in different types of exams.

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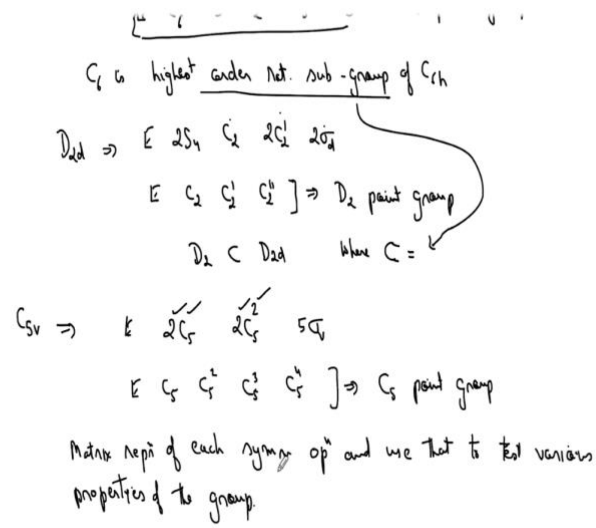

So, I thought it will be interesting to cover this C5v. So now C5v what are the group elements under C5v? We have E, 2C5. So, 2 operations given by C5, two operations given by C5 square and 5 sigma-Vs. Now what is the highest-order rotational sub-group so we cannot consider this one. So, we have E if you consider the operations generated by C5 now, so this will be C5, C5 square, C5 cube, C5^4 these are the operations that will be generated.

So, all these following any point group, yes so this will be a C5, point group. But do we have all the elements which are present here in this. So now that again we can test by looking at if all of these elements all of these do, they conform to the associativity, closure and all the properties. So individually we have to work it out pick up any example and start working on it or else what you can also do is when you are testing these properties you can take the matrix representation of each symmetry operation and use that to test various properties of the group.

So, once you do the matrix representation, you do not have to imagine a molecule and do all the operations to find out the property. So, take x, y, z as the basis create a matrix representation for all of this and find out whether if all these are following the properties of the group are not. So, this is one type of questions.

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$E \quad C_5 \quad C_5^2 \quad C_5^3 \quad C_5^4 \;] \Rightarrow C_5$ point group

Matrix repn of each symm opn and use that to test various properties of the group.

2) What is the point group obtained by adding/deleting a given operation?

C_3 point group + i operation $\longrightarrow$ New point group?

$E \quad C_3 \quad C_3^2 \quad i \quad \ldots ? \ldots$

Group follows closure property. $C_3 i$ or iC_3 = ?

Find out the matrix repn of each of the elements, and keep finding the products or squares.

So, let us look at another type which is actually a little difficult not difficult but you need little imagination. So now say what is the point group obtained by adding/deleting a given operation. So, let us say you are given a point group let us say you are given a C3 point group. And now to that C3 point group let me write down C3 point group, to this C3 point group, you are adding a inversion operation.

So, what is the new point group? How do you find out this? So, there can be enormous number of combinations I have just taken one example here but you can have different type of examples. So how do you approach what is the approach if you know the approach you can solve any given problem. So, but you should know the approach for these kinds of problems. So, for C3 point group what you have is a list on the elements group elements.

You have E, C3, C3 square and on top of that you are now adding i, now adding i is not just adding i so if you add i to this what additional elements are also added that one has to identify. So how do you identify that so the very easy thing is that group always follows closure property group follows closure property. So that means what you have to do is you have to create the products of different elements.

And see what is the resultant which you are getting now that resultant may belong to the already existing element or may give you some additional element. So, for example if we do a C3 into i or i into C3 what do we get? Let us see if we get a new operation. So now that new operation can come here. So how to do that, let us see. So again the easy way is to write down the matrix representation for the two because you do not know how the molecule will change let us say if we have C3 and some molecule which is of C3 point group.

Now if we are adding i operation how do we change the molecule. What is the symmetry of the new molecule? That is impossible to predict. So, best ways to find out the matrix representation of each of the elements and keep finding the products or squares of different elements because that is bound to give you a new element unless all the elements are completed all the elements of the new group are completed. So let us see how does it work out.

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$$C_3 = \begin{bmatrix} -1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & -1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad i = \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} \quad C_3 i = \begin{bmatrix} 1/2 & -\sqrt{3}/2 & 0 \\ \sqrt{3}/2 & 1/2 & 0 \\ 0 & 0 & -1 \end{bmatrix} \Rightarrow S_6$$

$$\cos\theta = 1/2 \quad \theta = 60^\circ \quad n = \frac{360}{60} = 6$$

$$S_6 = \{E, C_3, C_3^2, i, S_6, S_6^5\}$$

↳ test the set of group elements for

✓ closure property

✓ associativity

✓ inverse

✓ identity

So, for C 3 and i, for C3 we have learned that the matrix representation can be written as minus half, minus root 3 / 2, 0, root 3 / 2, minus half, 0, 0, 0, 1. And for i, matrix representation can be written as -1, 0, 0, 0, -1, 0, 0, 0, -1. Now if I do C3 into i, what do i get? It is a unit matrix with negative signs so multiplication is easy. So, all you have to do is just change the signs over here. So that means I will get half, minus root 3 / 2, 0, root 3 / 2, half, 0, 0, 0, -1.

Now what kind of a cemetery operation is this? So, if you want to define this matrix representation as a single symmetry operation what kind of operation is this? Now first of all it is not a pure rotational operation why it is not a pure rotational operation? Because a pure rotational operation would never give you -1 in the z, -1 corresponding to the z basis. So that means if z is getting converted to -z that means there is a reflection involved.

So, it has to be a rotation and reflection. So now rotation and reflection mean that this is some sort of a rotation x y, now what is the angle that angle we can identify by looking at the value so if we have cos theta is equal to half, we have theta is equal to you can say 60 degree. So that means this is if my n will be 360 / 60, so this will be 6 so that means this will be a C6 kind of rotation this was C3 rotation this is C6 rotation now.

Now if this is C6 rotation and this is sigma h corresponding to it so this would become S6. So now what do you have obtained this you have gone to a little higher number of elements. So, you have obtained S6 now S6 if you calculate the square of it so that will be S6 square. What else do we have? S6 square, so that will be C3, S6^4 will be a C3 square. So, what you will have is S6^5 which will be the independent operation.

Now S6^5 will also come as a product of one of these maybe it will be from i to C3 square or so and so forth. Now this follows all the group properties of course you have to test it I am not testing it here I am just telling you once you have identified S6 you know that S6 alone would give you S6 as well as S6^5. So, I have included this operation here but what you have to do is you have to test the set of group elements for closure first of all closure property.

And then associativity, so once the closure property is fulfilled, then only you can go for a test for associativity, inverse, and identity. So, these 4 properties have to be fulfilled and then you can say that now the new group is nothing but S6 point group. So, from C3 by just adding one symmetry element you have gone to S6 point group. So that otherwise it is difficult to imagine that what will be the point group by deletion or addition of a symmetry element.

So same thing can be done by addition or for deletion of element also. So again, this is an important question I have seen this coming in different exams. So that is why I thought I will bring it up here.

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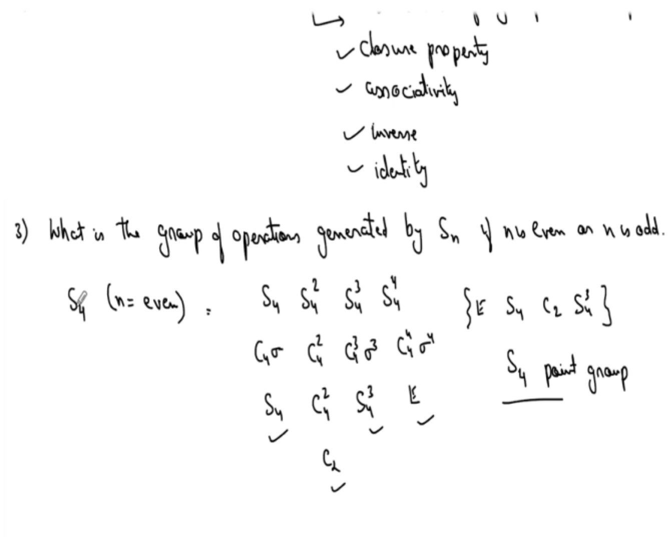

So now let us ask a third question is, what is the group of operations which are generated by Sn if n is even or n is odd. So let us take each of this case with example, so let us say if n is even. So, let us consider S4, so n is even. So now what are the operations that will be generated? So, S4 will generate S4, S4 square, S4 cube, S4^4 now each of this is called as C4 sigma, so this is an independent operation.

So, we will keep it as S 4 now this will be C4 square sigma square is E, so this is nothing but C4 square and this can be then written as C2. S4 cube can be written as C4 cube and sigma cube. So, you can simplify it as C4 cube into sigma. So, nothing can be so you cannot simplify it further.

So, S4 cube will be there S4 to the power 4 will be C4 to the power 4 and sigma to power 4 both our E so you have E.

So, generating operations from S4 you get 4 different elements which is E, S4, C2, S4 cube. Now these are the set of elements which will form S2n or S4, point group. So that is easy to identify, so for n = even if we are generating operations of S4 you will get S4 point group back.

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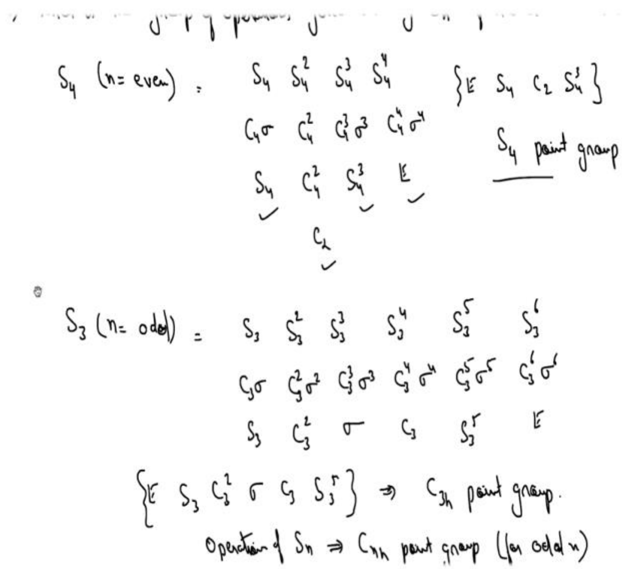

Now let us say for n = odd what is the case so let us consider the simple case of 3 because 5 will be too long. So, n = odd, so let us say what are the operations which are generating S3, S3 to the power 2, S3 to the power 3, S3 so we have to keep going till we hit E. So, let us say if we have already hit E at S3 to the power 3 or not. So, S3 will be equal to C3 sigma so which is nothing but S3 again this will be C3 square sigma square.

So sigma square you see so you can write it as C3 square, S3 cube will be C3 cube and sigma cube, so you will have this is C3 cube is E, and sigma square is E, so you are left with one sigma, so you have one sigma over here and what else we have so you are still not got E, so we have to keep going S3 to the power 4, will be C3 to the power 4 and sigma to the power 4, sigma to the power 4 is E and this is C3 to the power cube is E. So, you are left with one C3 operation.

So again, we are not getting E so move further. So, this is C3 to the power 5 and sigma to the power 5, nothing will go to E. So, we are left with C3 square and sigma square. So that would mean you have S3^5 back, S3 to the power 6 you have C3 to the power 6 sigma to the power 6 which is E. So, after that you do not need to generate more operations because that will give you an S3 again.

Now so what we have got is E, S3, C3 square, sigma, C3, S3^5 these are the set of operations which we have got. Now this set of operations what is the point group for this? This will give you a C3h point group. So that means if we are generating operations using S3 axis or Sn axis where n = odd then we will generate Cnh point group. So, in general we can say Sn will give you Cnh point group.

So, operations of Sn where n is odd for odd n we will use Cnh although it appears that it is a S3 axis only then, but still it pops out sigma out of nowhere, pure rotational elements out of nowhere, by just doing operations of S3 you are getting a Cnh point group. So, these are also kind of questions which are asked in different type of exam. So, it is important to cover this. Let us look at one last question and then we can stop for today so let us see.

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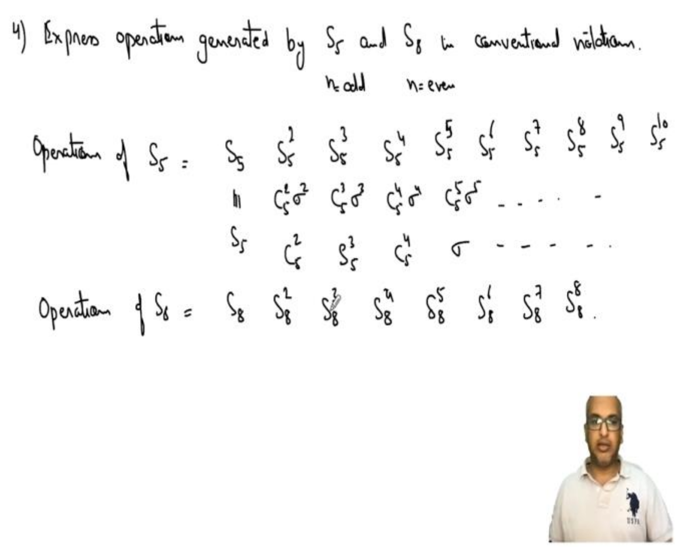

So, the fourth question is express operations generated by S5 and S8 in conventional notations. So now this is easy now that you have learned how to generate different operations of S5. So basically, here they have taken 2 examples where n is odd and n is even. So, for even n, you have to keep going up to, so, S8 to the power of 8 and for S5 we have to go up to the power of 10. So why I am saying that let us just look at it again. So, operations of S5.

So, what all operations S5 will generate and you have to put it in conventional notation, what is the conventional notation? So, S5, S5 square, S5 cube, S5^4, S5^5, S5^6, S5^7, S5^8, S5^9, S5^10 we have earlier seen that only when we hit S5 up to our Sn raised to the power 2n we will hit E otherwise we will not hit E. So, we have to keep going at least up to the 2n one part. So, S5 is nothing but S5, so there is no change in conventional notation what is S5 square? So, we have C5 square into sigma square, now sigma square is E. So, we can write it as C5 square.

So, although it is C5 square but it is an operation generated by S5. So, this is what it means by conventional notation. Now again C5 cube sigma cube. So, this does not conform to anything, so we will keep it as S5 cube only. Again, this will be C5 to the power 4, sigma to the power 4, this is cancelled. So, we will be left with C5 to the power 4, C5 to the power 5, sigma to the power 5. So, we are left with only sigma and so on so forth. So now you can actually calculate.

So, these are the conventional notations for the operations generated by S5. Similarly, we can work out operations of S 8 in the same manner. So here we have to go to S8 to the power 2, S8 to the power 3, S8 to the power 4, S8 to the power 5, S8 to the power 6, S8 to the power 7, S8 to the power 8. So, this will give you and then you can figure out whether it will be S8 or C8 or sigma and so on so forth, or E. So that is how you can generate different operations by rotation-reflection axis and find out the corresponding conventional notations.

So, we have learned today how to work with different type of problems related to point groups which is which can be sub-group or related to multiplication tables when we are trying to find the closure property and so on and so forth right. So that is all for today. So next let us see what is there for next class. And we will come back with next week’s tutorial.