Symmetry and Group Theory

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Lecture - 17
Sub - Group and Classes

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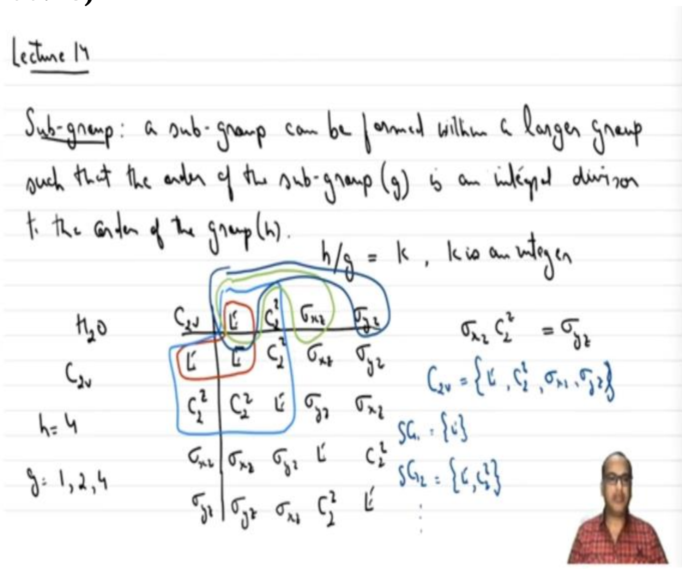

So, welcome back everyone. We have seen in the last lecture, how to write group multiplication tables. And we have also seen the detailed properties of groups using some solved examples. Let us now see how a group can be divided into smaller subgroups. So, what is the definition for a subgroup? Subgroups can be formed a subgroup, so subgroup can be formed within a larger group such that the order of the subgroup, let us call that order as g, is an integral divisor to the order of the group which is h.

So, in other words, if you take h / g, this should be equal to k, where k is an integer. So that should be very clear. So, now, let us take an example, let us take, let us quickly write a GMT group multiplication table for water. The water is C2v point group, this is E, C2z, sigma-xz, sigma-yz. So, we will see that how within this group, we can find a subgroup using GMT. So, subgroup by definition, the subgroup should follow all the 4 properties of group, like the closure, associatively, identity, and inverse.

So that is understood, because from the name it is subgroups C2z, sigma-xz, sigma-yz. So let me write easy ones first E into E will be E, and C2z into C2z will be E, sigma-xz into sigma-xz will be E again, sigma-yz to sigma-yz will be E, that is easy. And then the first row E into anything will be C2z will be same, it is like multiplication with 1. Similarly, here this will also be same. Now the rearrangement theorem says that no 2 elements in a group in a row or column can be repeated.

So, in this row we have seen that C2 and E are already there and in this column sigma-xz is already there. So, the only option to write here is sigma-yz and you can also test that if I apply, so the meaning of writing sigma yz is that if I apply C2z first and sigma-xz, I should have sigma-yz which can be easily tested and I leave it for you to test it on this molecule. And now the fourth element here, the only option is sigma-xz. It is like solving sudoku puzzles.

So, again, so we have E, C2z, sigma-xy, so the only option we have a sigma-yz and now sigma-xz. Here we have E, sigma-xz, sigma-yz, so we are left with C2z and we are left with C2z here. So that is a quick way to write a group multiplication table. Now let us see that the order of this group is h = 4. So, the subgroups can only be of order, so g can take values of 1, 2 or 4.

Because these are the only options where k is an integer, if let us say if you consider g = 3 then 4 / 3, this 4 / 3 would not be an integral divisor and thus a subgroup of order 3 cannot be formed in this particular case. So, subgroup of order 1 can be formed and subgroup of order 2 can be formed but not necessarily. So, it may or may not be present but these are the only subgroups which may be present. So, let us see the first thing is the subgroup of order 1.

E will always follow all the properties of subgroup, so E will be a subgroup always. So, let us now see, do we have any other subgroup of order 2, so E, C2z, C2z, E, so if you notice that this will be another subgroup, similarly if you think that E, sigma-xz, sigma-xz, E that will be another subgroup, so let me paint it with a different color. So, you can see that, so this is a different sub group and then we have another subgroup which is with E and sigma-yz.

So, it will have different subgroups of order 2, similarly now, subgroup of order 4 is basically the full group, so that also does not count. So, basically there are 2 subgroups of order 1 will be, let us say if we call it as C2v has the elements E, C2z, sigma-xz, sigma-yz, I can always say that subgroup 1 will be E, subgroup 2 will be E, C2z and so on. So, we can write subgroup 3, G3 will be this is not the order, so group 1, group 2 or we can say subgroup 1, subgroup 2, subgroup 3 will be E, sigma z, sigma xz and subgroup 4 will be E sigma yz.

So, I hope this is very clear. So, subgroups basically can be found within larger groups and the order of the subgroups have to be integral divisor. So that should be very clear. Now let us look at the other classification of group elements into smaller units which are called as classes.

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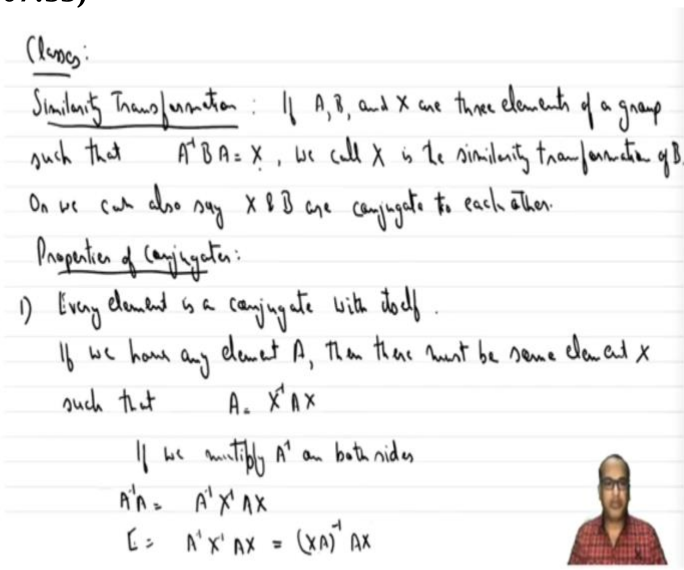

So, before we actually try to understand what is a class, let us first try to understand, we will come back to this classes but we first need to understand an operation called as similarity transformation. Some of you already know this from other courses, but let us try to work it out here, similarity transformation. For example, if you are taking an NMR course, the similarity transformation is also discussed there.

So, the idea is if A, B, and X are 3 elements of a group such that A inverse B A = X, we call X is the similarity transformation of B, or we can also say X and B are conjugate to each other. What does it mean? We will come to that. What is the physical meaning of that? So, the definition is clear so similarity transformation, if A, B, and X are 3 elements such that A inverse B A = X then we call X is the similarity transformation of B or we say that X is the conjugate of B and we will show that B will also be conjugate of X.

So, let us try to look at few properties of conjugates under similarity transformations. So, properties, first property is every element is a conjugate with itself. So, this means that if we have any element A then there must be some element and we will show how to prove it, some element X or at least 1 element X such that A = X inverse A X, this is the definition from similarity transformation.

Now we are seeing that there has to be 1 element X in a group, if we have an element A there must also be an element X in the group such that this relation holds. So that A is a self conjugate. So, now, how do we prove this? So, let us see if we multiply A inverse on both sides what do we get, A inverse A. So, we have A inverse X inverse A and X, this implies that we have E = A inverse X inverse A X which is equal to, if you remember that the inverse of the product is equal to product of inverses in opposite order. So that means, we can write A inverse X inverse as X A whole inverse into A X.

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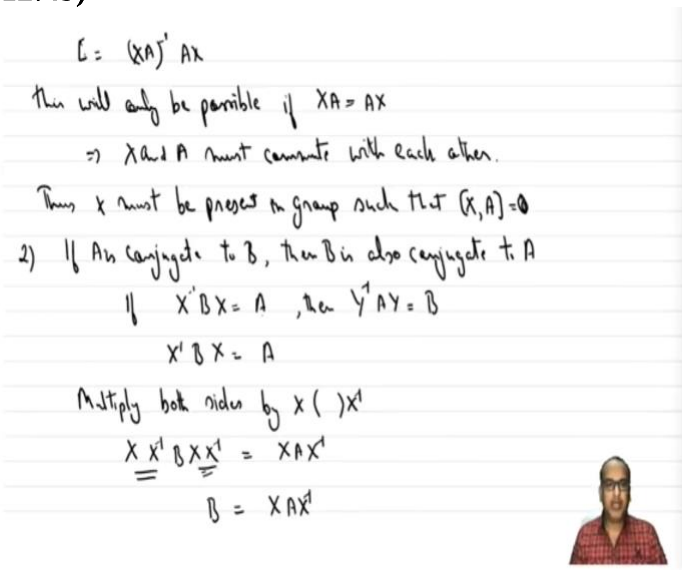

And this will only be possible if, let us go to so E = X A inverse AX this will only be possible if X A = A X, then only we can write that, this will be A X whole inverse and then the A X inverse into A X will be E. So that implies that X and A must commute with each other that means, you must have an element X which should commute with the element A to prove that A is a self-conjugate. Thus, X must be present in group such that, so we know that there is always an element E which commutes with all the elements. So, there is definitely an element E present, which commutes with all the elements and thus we can say that A is conjugate to itself.

So, now let us look at the second property. If A is conjugate to B, then B is also conjugate to A that means both are related to each other by similarity transformation. So, now let us see what does it mean mathematically? That means, basically what we are trying to say is, if we have X inverse B X = A then, we must have an element Y such that Y inverse A Y = B.

So, we are saying that if A is conjugate to B, then B must be conjugated to A where A, B, X and Y all are elements of a group. So, now let us start with this X inverse B X = A and we can multiply both sides by X, X inverse. So, what do we get? X X inverse B X X inverse = X A X inverse, we can do that, matrix multiplication. So, now what do we have here, so this goes to E, this goes to E, so basically what we have got this B = X A X inverse but we wanted Y inverse A Y = B.

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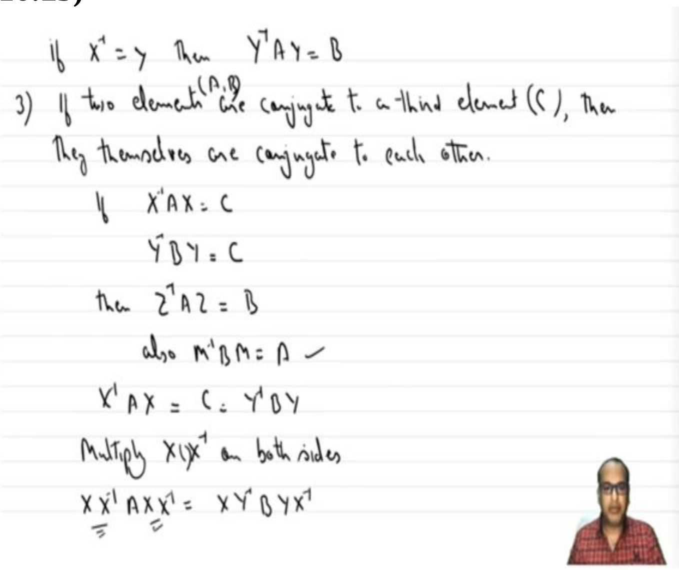

So, now, this is possible only if say if X inverse = Y, then we can write the above relation as Y inverse A Y = B. Now we know that in a group, each element must have an inverse so that means, Y must be present as a X inverse and thus, since Y is present, so we can say that the B is also a conjugate of A. So, if A is conjugate of B using A, so then B is also conjugate of B using Y for a similarity transformation. I hope this is clear. Let me know if it is not.

So, the third thing is like if two elements are conjugate to a third element, when I say element I mean group element not simply elements, to a third element, C let us say, if two elements let us call them A and B, if 2 elements A and B are conjugate to a third element then they themselves are conjugate to each other. What does it mean? So that means, what I am trying to say is if X inverse A X gives you C, Y inverse B Y gives you C, then there must be an element Z in the group such that Z inverse Z = B.

Then and then there must be another element of M let us say, also you can show M inverse B M should be equal to A because we have already shown this, so I am not going to show this part. So, this we have already shown if A is conjugate of, B is conjugate of A then A is conjugate of B and all. But the point here is that if C is conjugate of A, C is conjugate of B then A and B are conjugate to themselves.

So, now, how do we prove this? So, again, let us start with X inverse A X = C = Y inverse B Y and now multiply X X inverse on both sides, then what do we have here? X X inverse A X X inverse = X Y inverse B Y X inverse. Now this side, this becomes E, this becomes E, so we are left with A.

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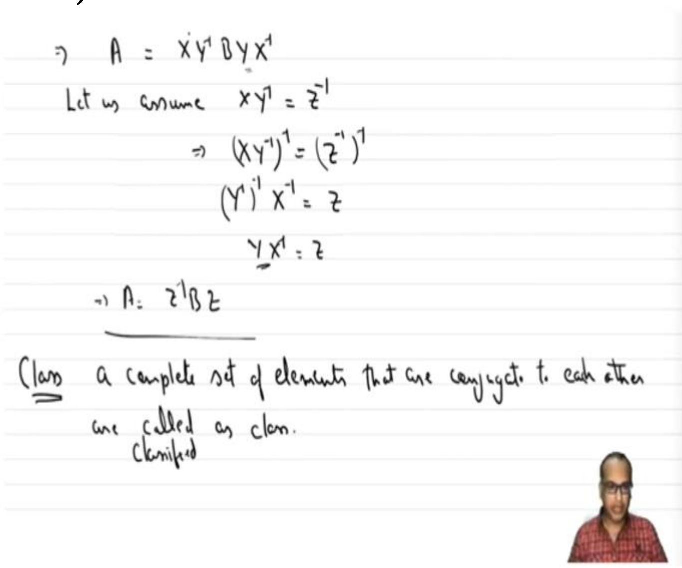

And we have, here we have X Y inverse B and we have Y X inverse. So, now let us assume X Y inverse = Z inverse this comes from properties of group. So, if we have Z inverse over here and now if we take inverse of the whole thing X Y inverse of the whole thing then we get Z, now this thing we can write it as Y inverse, inverse and X inverse which is now equal to Z. So, this becomes Y X inverse. So, this term becomes now equal to this. So, this implies that A = Z inverse B Z.

So that means, if X and Y are elements of the group, Z is also an element of the group because it is related by a product relation or combination relation, thus A and B are proved to be conjugate of each other. So that should be very clear. So, now, coming back to definition of class, now that we have understood what is a conjugate, so let us look at the definition of class. So, a complete set of all elements, group elements or symmetry operations that are conjugate to each other are called as class or classified as class. So, let us see what it means? So, let us quickly look at some group which will have some classes.

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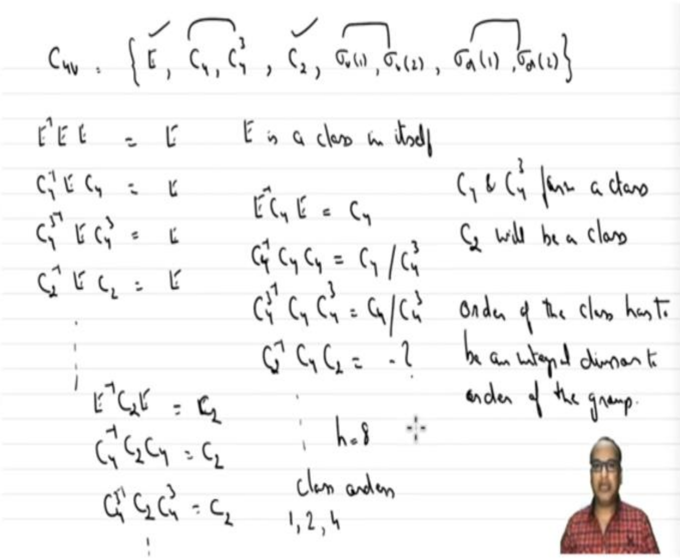

So, let us look at C4v the operations are E, C4, C4 cube then you have C2 then you have sigma-v1, sigma-v2, sigma-d1, sigma-d2. Now to identify the class elements in this C4v example, you can take anything like square parameter. So, to identify what are the elements which are forming a class you have to take similarity transformation of each element using by each element. So, what do I mean?

So, let us take, if I am taking similarity transformation of E by E inverse E, C4 inverse E C4, C4 cube inverse E C4 cube, C2 inverse E C2 and so on. So, what do I get here? In all these cases you will see that I will get E nothing else. So, then we can say that E is a class in itself. So, E always forms a subgroup and similarly, E forms a class also. So, E is a class in itself. Now let us also look at other operations. Let us see, let us look at C4.

So, if you have a group multiplication table, finding these products is much easier, so that is where the importance of group multiplication table but let us look at this. So, E C4 inverse E, What do I get? C4, let us say if I do C4 inverse C4 C4. So, what do I get if I do this multiplication? So, C4 into C4 will give me C4 square and then C4 inverse will be equal to, so let us, shall we do that or we should either get C4 or C4 cube. I am leaving it as a home exercise for you to do it, because there is not much time now.

So, let us try to make a point. So, let us C4 cube inverse C4 C4 cube, this should also get C4 slash C4 cube either of this will come out as an answer but what you have to do is you have to, if you write this group multiplication table, it is easier because then we know what is the product of it. Otherwise, what you can do is you can actually take a molecule do this operation and see what you are getting. Similarly, do it for C2 inverse C4 C2 and see what we are getting.

So, now, when I do these operations on C4, I get either C4 or C4 cube. Similarly, when I do these operations these similarity transformations on to C4 cube, I get either C4 and C4 cube. So that means, this tells me that C4 and C4 cube form a class. C2 will be a class so, again try to identify whether C2 will be a class in itself, just like we did for E or C4, again do it for C2. So, what I mean is then you have to do all the operations to identify what are the conjugates of C2, C4 cube inverse C2 C4 cube and so on.

So, calculate and every time you will get C2 as an answer. There is no other element which you will get. Similarly, if you do similarity transformations of sigma-v1, you will get either sigma-v1 or sigma-v2. So that means this sigma-v1 and sigma-v2 will be forming a class. Similarly, here if you do a similarity transformation of sigma-d1 you will get either sigma-d1 or d2 and if you do a estimate on sigma-d2 then you will get either sigma-d1or d2.

So, these 2 will form a class, these 2 will form a class, these 2 will form a class this will be a class in itself, this will be a class in itself. So, now try to work out yourself taking an example, let us take an example if you want an easier example maybe take NH3 for C3v and see what are the elements which are forming a class. For class also there is a condition that order of the class just like subgroup, order of the class has to be an integral divisor to order of the group.

So, thus the order of the group here is 1, 2, 3, 4, 5, 6, 7, 8. If h = 8 the class orders which are possible are 1 integral divisor 2, 4. But it is not necessary that all such integral divisor orders would form a class. Because now you will see that there is a class of order 1, there is a class of order 1 and there is a class of order 2, 2, 2.

But there is no class present for order 4 in this particular case. So, this is the condition but it is not necessary that all the orders which are integral divisors would form a class. But if it is forming class it has to be an integral divisor of the original order of the group. So, I hope this is clear. So, we will take further, like the physical significance of what is a class in the next class. So that is all for today. Thank you.