Symmetry and Group Theory

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Lecture - 16
Point Group Definition and Examples

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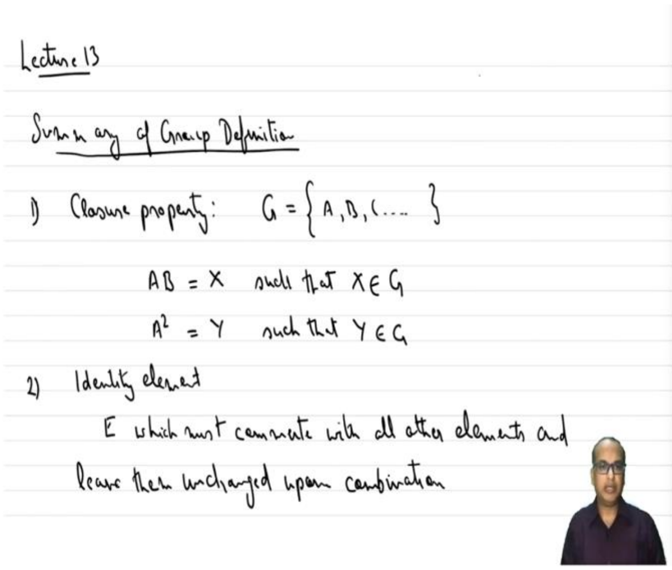

Welcome to lecture 13. Let us start looking at properties of group; point groups a little in more details. Let us start with summary of group definition. So, we said when symmetry elements or group elements, which is symmetry operations which are related by 4 properties, then these are defined as point groups.

So, the first property in that is closure property which defines that if G is a group consists of various elements, then AB = X any group element, such that X must belong to G. Similarly, if A square = Y, such that Y should also belong to G. So, that is a closure property.

Next property is identity element. So, group must have an element E, which must commute with all other elements and leave them unchanged upon combination. I am just briefing you those properties again, closure, identity.

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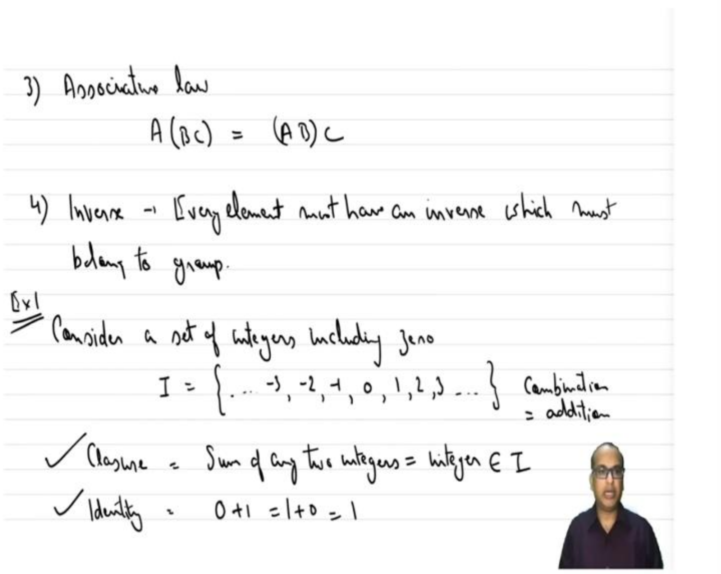

Third is, group elements must follow associative law. Associative law of combination which is ABC = AB and C. So, this is self-explanatory, we will look at certain examples to explain all of this again. Then, forth is inverse that is every element must have an inverse which must belong to group. So, these are the four properties which group elements must follow so, that they can be called as a point group.

So, let us take a few examples, let us start our examples from simple mathematics that we know already and then we will go to symmetry operations. So, let us see, this will help us understand these group properties much more. So, consider a set so, let us say call it example 1 consider a set of integers including 0. So, that means, I is a set such that you have dash, dash -3, -2, -1, 0, 1, 2, 3. So, this is a complete set now let us see if all the members of this group follow the four properties or not.

So, the closure property and in this case, for closure property, we will say that combination is equal to addition. So, we will not be considering product as a combination, we will consider addition as a combination. So, closure property, so, sum of, which tells you that sum of any 2 integers is an integer and this will belong to group I. So, you can take any integer from this and if you take a sum or combination.

The result will belong to I. So, the first property is valid. Second property is identity. So, does it have an element which combines with other elements to leave them unchanged and is also commutes with those, so that element is 0. So, for example, 0 + 1 = 1 + 0 = 1, so it leaves them unchanged and then it is also commuting with all those elements. So, identity also applies.

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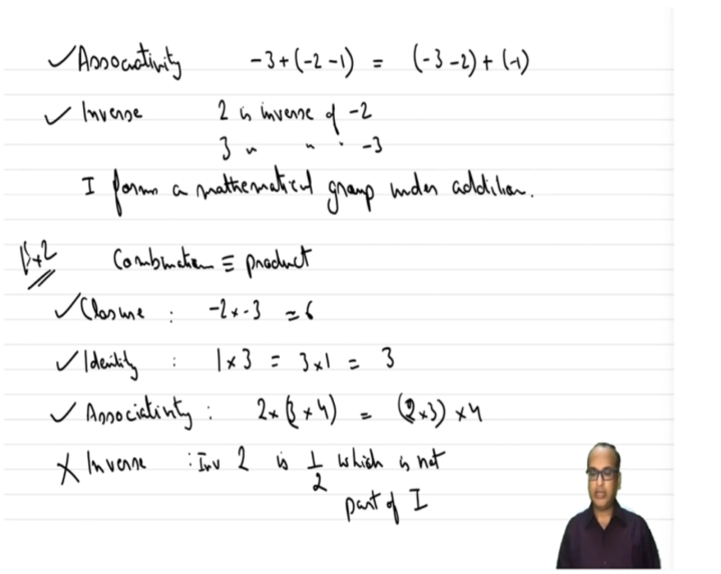

Now, next try associativity. So, when this is all in when combination is equal to addition. So, for associativity, if we say that -3 + (-2 -1), this must be equal to (-3 -2) + -1, So this holds, we all know that it will hold so associativity also applies and inverse. So inverses every integer has an inverse. So, for example, 2 is inverse of -2, remember, it is addition as a combination, so, 2 will be inverse of -2, 3 is inverse of -3.

So, they are all part of group, so inverse also applies. So that means I forms a mathematical group under addition. Now, let us say for example 2, let us see if we consider the same group, but now we say that the combination is a product or multiplication. So, in this case, let us see the closure property, does it hold true. So, -2 into -3 = 6. So, product of any 2 integers is a third integer.

So, closure property does hold true, then identity. So, 1 is an element, which leaves any other element unchanged and also comes with that. So, identity also holds. Now associativity does it hold. Let us see. So, associativity moves 2 x (3 x 4) write as (2 x 3) x 4. So that should also work associativity holds now let us look at the inverse. So, inverse of 2 is inverse of 2 is 1 / 2. In the previous case, it was -2 in this case it is 1 / 2.

Because we have changed the definition of combination. So, inverse of 2 is 1 / 2, which is not part of I. So, inverse does not hold. So that means I does not form a mathematical group under combination. So that is example 2.

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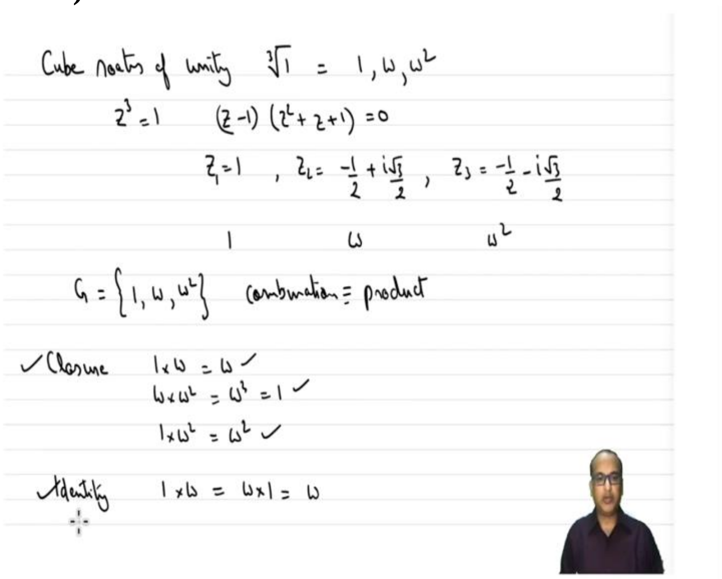

Let us look at more examples. Let us say we all know cube roots of unity, that is, if you take cube root of 1, you get 3 solutions, 1, omega, omega square. How do we get this? let us say if z cube =1, this is just a refresher and to solve for z you can factorize it as z-1 into z square + z + 1 = 0. So, you can do this factorization and this gives you first root as z = 1 which is an obvious answer and the other 2 roots are we can say z1 and z2 will be equal to – half, this is the quadratic equation, so, you can solve it + i root 3 / 2 and this is imaginary. So z3 is - half - i root 3 / 2. So, now it also, so, you can call this as 1 and this as omega and this as omega square. So, that is why I write one, omega, omega square. So, as it turns out, if you look at this, if you square this and expand this, you will get if you square this z2 will get z3 or if you square z3 you will get z2. So, if you call one of them is omega, the other one becomes omega square.

It does not matter which one you call omega, which one you mean the square both are related by square relation, you can test it yourselves. So, this is the tenth-class mathematics, which I am not going to discuss. So, let us go further. So, now let us say that this particular group, which is defined as cube root of unity, does it follow the 4 properties, so, let us test the closure property, and in this case, the combination, in the closure definition, we will consider as product.

So, now, let us see for closure, the product of every element must be an element from the group. So, 1 x omega = omega. Omega x omega square = omega cube, which is equal to 1. So, this is part of group this is part of group, and the third product is 1 x omega square which is omega square, this is also part of group, so, closure property holds. Then the second property is identity. So, for identity we know that 1 is an element which when multiplies with omega and leaves omega unchanged and also commutes with omega. So, identity also holds.

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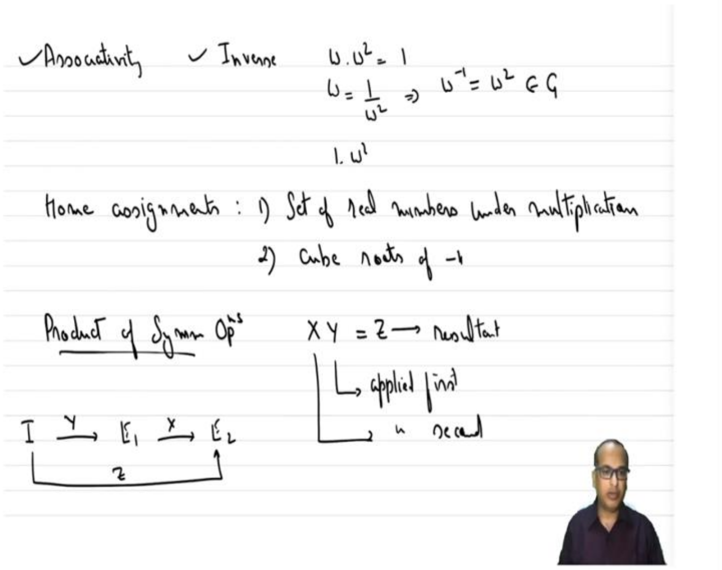

Similarly, in so, associativity will hold that is not to be shown now, you can show it and also inverse. So, we can say that omega x omega square = 1, so, that means omega = 1 / omega square. So, this implies that omega inverse = omega square. So, omega square, omega inverse has on omega square and omega square belongs to group G. Similarly, we can show for rest of the members.

So, if you take 1 into omega square in this will hold so, inverse also hold so, that means the cube root of unity form z which form some mathematical group. So, you can take some home assignments here. So, 1 is a set of real numbers under multiplication, then you also look at cube roots of -1. So, we have done it for +1 you can do it for -1, and I think these 2 examples will be sufficient for you to understand that how the 4 laws or 4 properties are used to define a particular set.

Whether that particular set will be called as a group or not. So now let us also look at certain properties. Recall some of the properties so, we have also discussed product of symmetry operations. Remember that we have done if we say X into Y = Z, we say that this operation is applied first, and this operation is applied second, and this is the result we have seen that before.

So, or in other ways, if I say that, if I start from molecule I, and I apply Y, I get let us say E1 then I apply X, I get E2 which are equivalent configurations, and this can be achieved by z this is what it means by product of symmetry operations. So, that should also be very clear. Now, let us look at a important property of a product.

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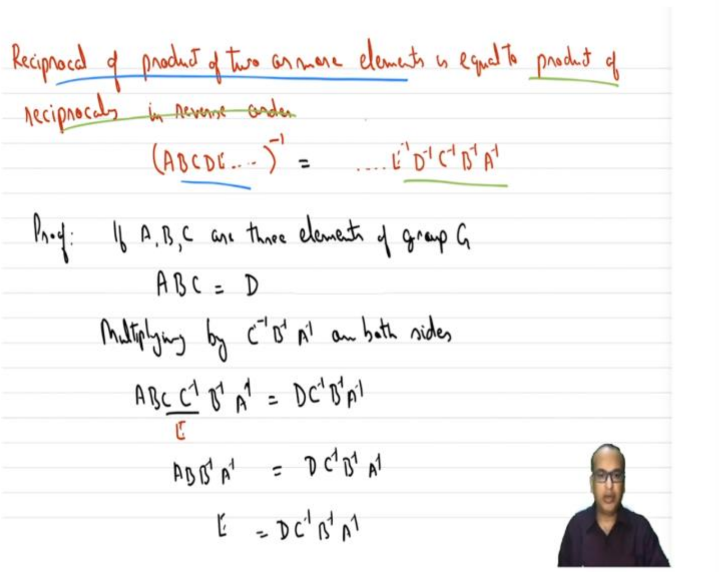

So, as it turns out reciprocal of product of 2 or more elements is equal to product of reciprocals in reverse order. So, what do I mean by that, so, mathematically you can write it as A B C D E and so on, the reciprocal of product of 2 or more elements, which is written over here is equal to a product of reciprocal in reverse order that means E inverse D inverse C inverse B inverse A inverse.

So, if I say this, product of reciprocals in reverse order will be equal to this. Now, how do I prove this, so, let us try to prove this. So, if we say, let us consider 3 elements for now, if A, B, C are 3 elements of group G, then we can write ABC = D. So, now multiplying by C inverse B inverse A inverse on both sides what do we get? Let us see. A B C C inverse B inverse A inverse gives you D C inverse B inverse A inverse.

Now, this C C inverse will become E. So, I can take this out because E commutes with everything. So, I can write it as A B B inverse A inverse and E I do not need to write = D C inverse B inverse A inverse similarly, I can write this as E again I can write A A inverse E.

So, this is nothing but E = D C inverse B inverse A inverse now I can take D that side or what I can do is.

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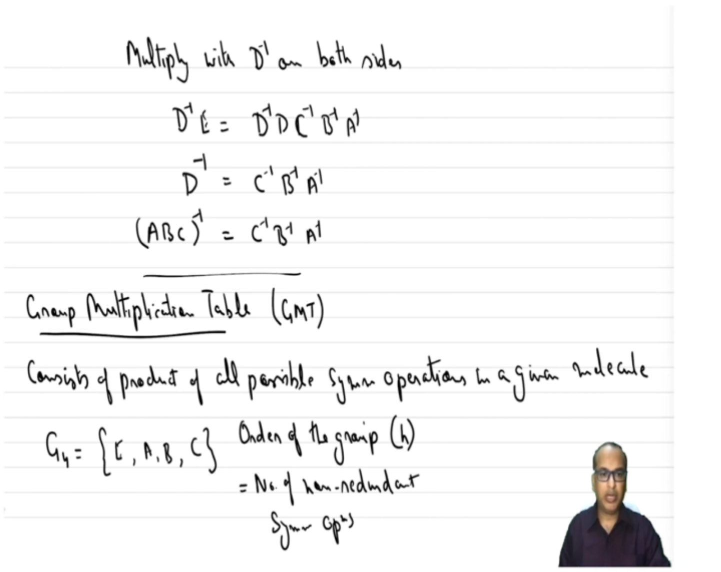

Multiply with D inverse on both sides so, what do I get. D inverse E = D inverse D C inverse B inverse A inverse. Now I can skip this thing E, I can just write D inverse D inverse D will also be equal to E. So, that also is not to be written C inverse B inverse A inverse. So, E is like mathematical one. So, which is not required if you are writing multiplication. So and we started with the assumption that ABC = D.

Product of these 3 elements is equal to D. So, we can now replace this as A B C inverse = C inverse B inverse A inverse, So, that is very easy to see. So, this is one important property that we will be using every now and then in various things. So, that is why I thought it is better to show it. So, now, let us go to something called us group multiplication table. So, why do we need to look at a group multiplication table.

So basically, what it means is it is also short formed as abbreviated as GMT. So, basically, it consists of product of all possible symmetry operations in a given molecule. So, how do you write it for example, let us say if you have a G4, so, G4 means that a group of order four which is consisting of in E, A, B, C. So, let us also define order at this point, the order of the group is denoted by letter a small letter h, is equal to number of non-redundant symmetry operations, in a particular group, that will be called as order of the group. So, now, let us see what is a group multiplication table for G 4.

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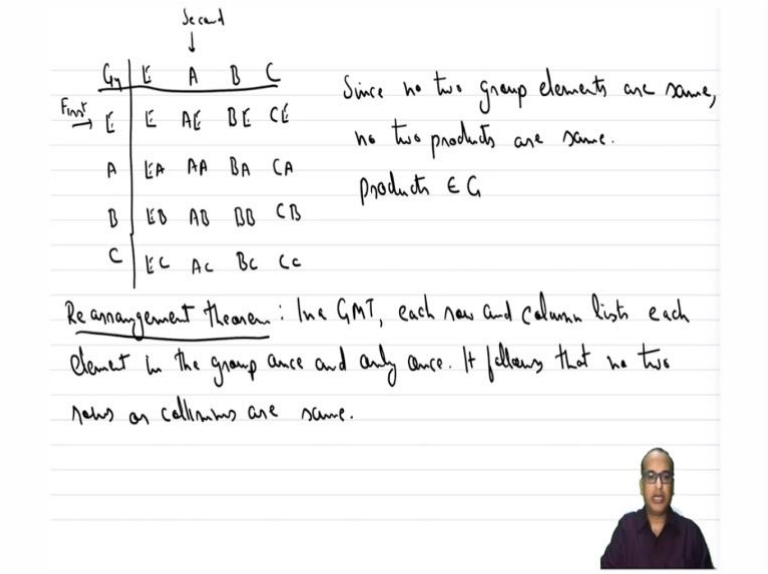

So, when I say group multiplication table, I draw it as a table. I write G4 here and then I write E, A, B, C and then in column also E, A, B, C. Now, E into E will be equal to E, in this case I multiply this as I write this as first this one will be operated first and this one will be operated second. So, then that means, it will be written as AE because this is my first operator and this is my second operator.

So, when you hear it will be written as BE, CE and here it will be written as EA EB and EC. Now, let us also write down this will be AA, this will be BA CA. We will see how to solve this and this will be AB and AC, this will be BB, BC, CB and CC. So, also one important thing since, no two group elements are same, no two products are same, and products must belong to group that we know from closure property.

So, all these products must belong to either of this E A B C, but none of this product should be repeated. So, for example, in any particular row or any particular column all the products should be unique, because all the group elements are different. So, their products should also be different. So, their product should also be unique. So, this leads to something called as re arrangement theorem.

So, what is rearrangement theorem. It says in a group multiplication table, each row and column lists each element in the group once and only once. This means it follows that no two rows or columns are same. So, both these rows and columns, all these rows and columns must be different. So, let us now try to see how to populate these group multiplication tables.

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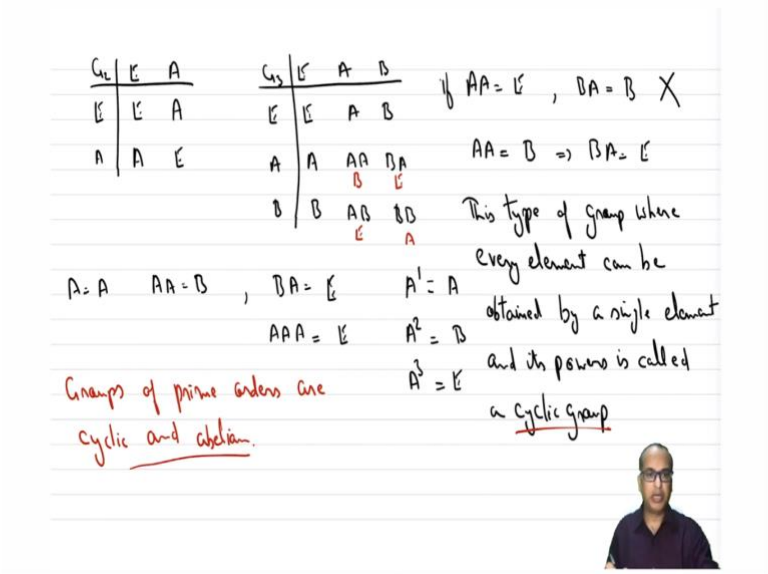

So, let us start with the simple case of G2. G2 will be order 2 that means, only 2 elements one has to be identity second can be any element. So, E A, if I multiply E with E it will always E, if I multiply E to A, it will be again A similarly, A to E will be A, A to A will be now it has to be E because it cannot go out of these 2 elements the product has to be closed product or it has to follow the closure property.

And it also complies with rearrangement theorems are they because these rows reads as this column reads as E A does this column reads as A E this is not same as this, and similarly, this row is not same as this row. So, now, let us also try G3. E, A, B, E, A, B. Now, first row will be because it has multiplied by E. So, it will be same as E A B and similarly, this column will be E A B. Now, we have to write here what is a product of AA and this will be BA this will be AB and this will be BB.

So, now, let us see if let us suppose if AA = E, so, if we replace this as E then BA this product has to be the only option is if AA becomes E, then A is already taken, E is here, then the only option that can come here is B, but now B cannot come here because B is already present in this column. So, two columns cannot have same elements or 2 rows cannot have same elements at the same column place.

So, if I put this as E, this has to be B and you cannot have two Bs in the same it is like sudoku puzzles where you cannot repeat any digit when you are playing sudoku. So very similar to that. So that means this condition is not valid. So, this leaves us you have to keep AA as B because AA now cannot be A because we already have A here. So, AA has to be B. So, if AA is B, this implies that BA has to be E.

So, then you can replace, you can write here B, AA = B, BA = E and that leaves AB this becomes here E and this becomes here A. So, now, you notice very interesting thing over here that AA = B and BA = E and B is nothing but AA. So, this becomes a triple A = E. So, if you see that A = A so, now, if you correlate A to the power of 1 = A, A to the power 2 = B A to the power cube = E.

So, this type of group, where every element can be obtained by a single element and its powers, is called a cyclic group. Also it is important to see you can verify this yourself, groups of prime orders where h = 2, 3, 5 and so on, are cyclic and abelian, abelian we have learned earlier cyclic we have learned today, so, groups of prime orders are cyclic and abelian for all such groups. So, now, let us think it is time to wrap up this part, group multiplication table.

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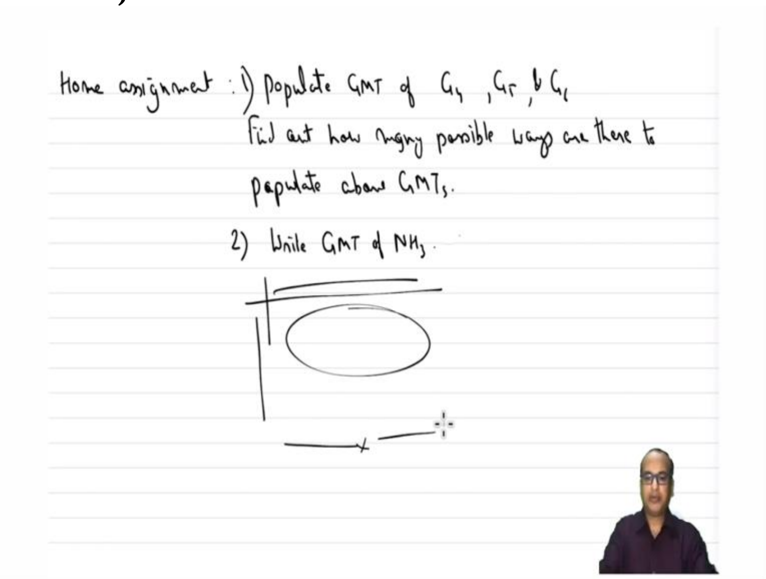

But before going let us take some home assignments. Populate GMT of G4, G5, and G6, and see for example in case of G3 we have seen or G2 we have seen that there is only one way of filling this group multiplication table. Let us see also find out how many possible ways are there to populate above GMTs. That is the first, and also do write GMT of NH3, let us you try to find out what is the point group what are the symmetry operations?

So, what you have to do is list down all the symmetry operations here list down all the symmetry operations here and then find out the all the products of the symmetry operations to populate the GMT so this will be so I am not going to tell you what is the order what are the symmetry operations so you try to exercise it, certain products will be easier to fill, while certain products you will have to actually carry out all the operations and do it.

So, this will be easier once you have the GMT of NH_3 ready with you. This will be easier to further go look at the properties of subgroups and classes and also when we take NH_3 example will be easier. So, try to do it yourself. If you have any difficulty, we can always discuss in the interaction class. I think that is all for today.