Group Theory Methods in Physics
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Lecture – 10
Young Diagram and Molecular Symmetry

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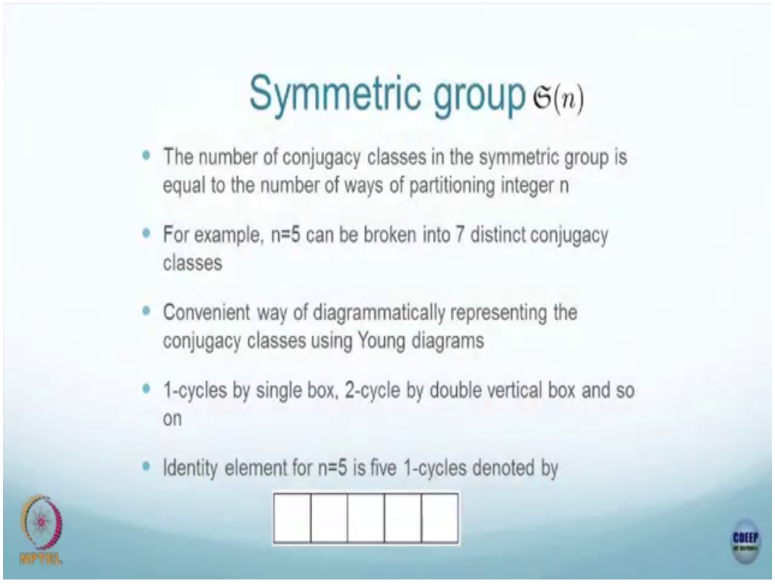

The next step is given a group how many conjugacy classes that is the next one right. So, we need to worry about how many conjugacy classes are there.

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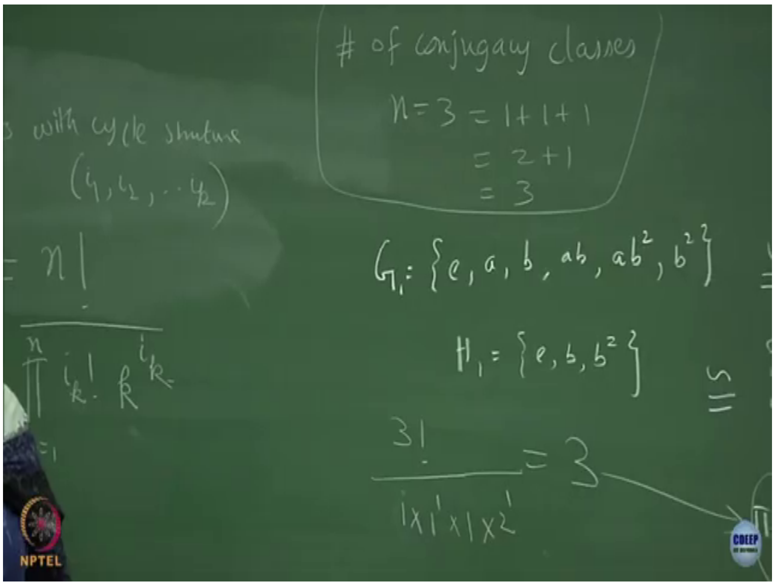

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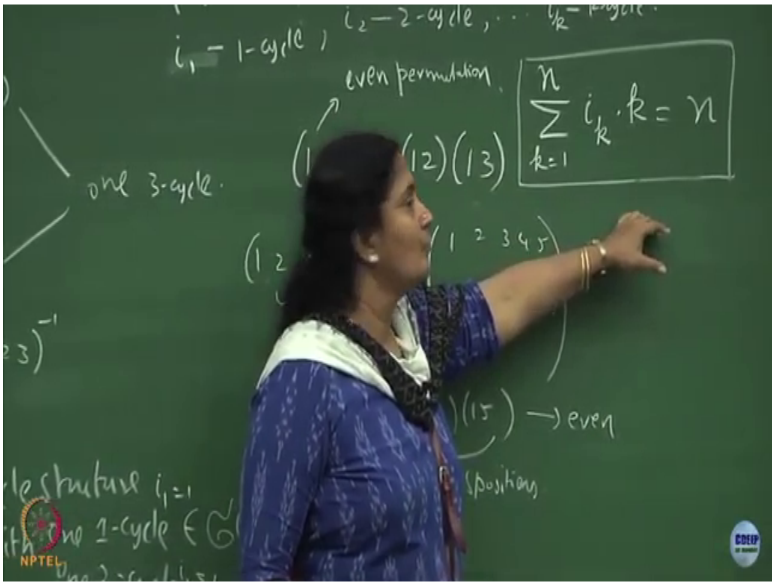

So, in this particular example, you have three conjugacy class three distinct cycle structure right. What does that tell you, what is this condition tell you? Given an integer n you have to find ways of partitioning that is all it says right. So, suppose I have n to be 3, I can partition it in various ways; I can write it as 1 plus 1 plus 1; I can write it as 2 plus 1; I can write it as 3.

This is another way of writing it essentially, you know what I mean, it is the number of 1-cycles, this is one 2-cycle, and one 1-cycle, this is one 3-cycle, right. So, this is, this number is the number of ways you can partition an integer n will tell you the number of conjugacy class, ok. And there is a nice neat way of using the Young diagram conjugacy class.

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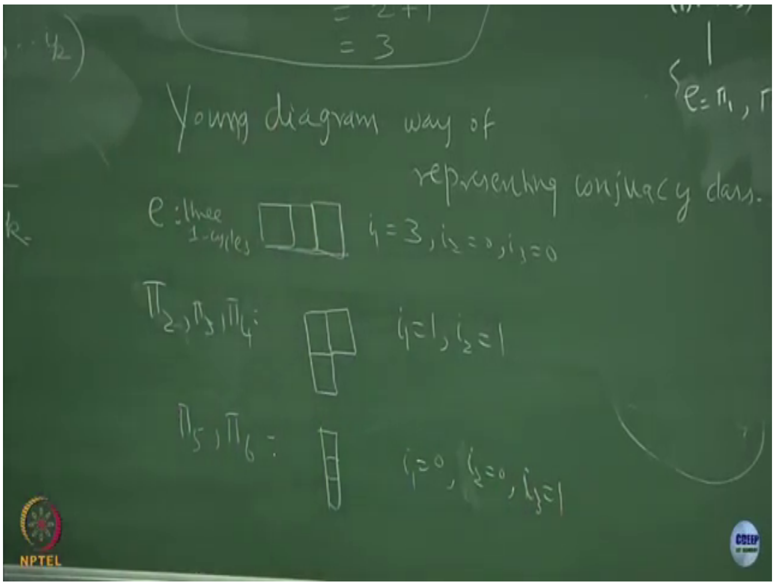

So, this partitioning as we know is nothing but three 1-cycle. For every one cycle, I am going to use a box single box ok. Three 1-cycle means I will attach to it 3 boxes. Total number of boxes will always add up to be 3, and 3 single boxes means that it is three 1-cycle, ok. So, this is your identity element which is nothing but three 1-cycles, and in the cycle structure notation I 1 is 3, number of one cycles is 3, I 2 is 0 and so on ok. This is the diagrammatic way of drawing a conjugacy class. This is a conjugacy class ok. You just look at the cycle structure.

The next conjugacy class you all know is pi, pi 2, pi 3, pi 4, it has one 2-cycle, and one 1-cycle. One cycle, I have already said you have to put a single box a, two cycle you will put always a vertical 2 box ok. So, this is I 1 is 1, I 2 is 1, total number of boxes is still 3, this is the notation.

So, tell me how will you write pi 5 and pi 6, one vertical 3 box that is it. So, this is I 1 is 0; I 2 is 0; I 3 is 1, you all with me? So, this is what is a payoff. So, each diagram is a conjugacy class ok, this conjugacy class has only one element, this diagram is the another conjugacy class, but it has three elements to determine the three elements you are going to use this formula.

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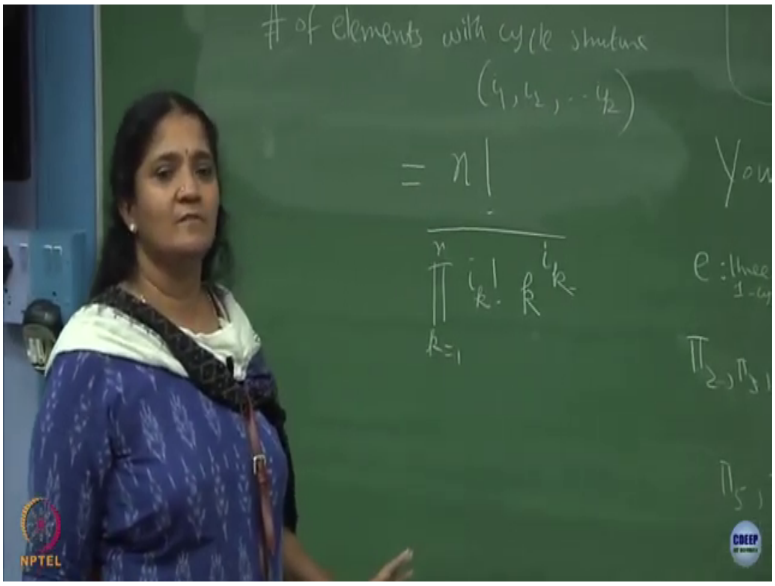

And then the way you are partitioning the integer gives you that it tells you that there are only three possible conjugacy classes. So, there are only three distinct conjugacy classes for the symmetric group of degree 3. Is that clear, no, yes, fine. So, this is a simple example, but this generalizes to arbitrary degree n whether I n factorial elements, ok. So, as an exercise, let us do symmetric group of degree 5. Can somebody enumerate for me?

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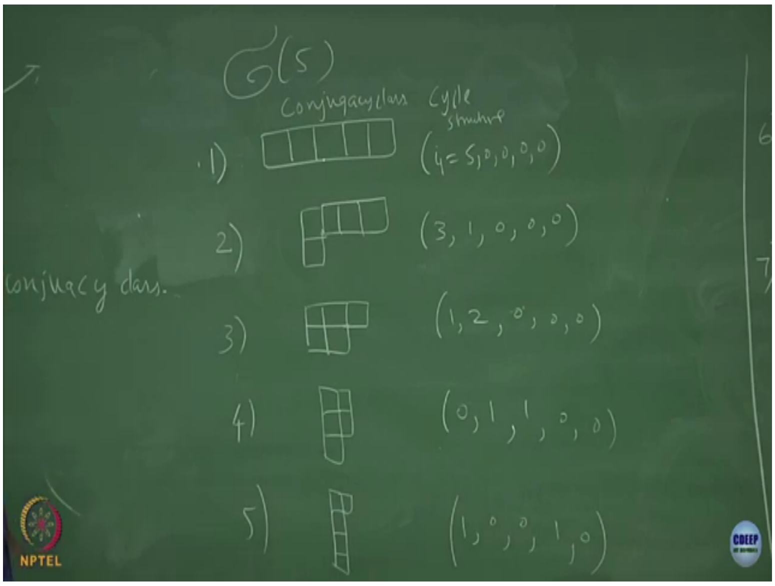

Degree 5, identity element will be, you all with me; how many elements are there? This is conjugacy class, ok. I do not even need to put it on the, so let me write it here. So, cycle structure is i 1 is 5, rest are all 0. So, let me write the cycle structure also ok. Second conjugacy class, how many conjugacy class I can write, this is allowed? Three 1-cycles and one 2-cycles, we will also add up to 5, then it is also possible. It is so easy to draw diagrams and then we will fix the things. And then one 3-cycle and one 2-cycle, then one 4-cycle and then one 3 cycle, two 1 cycle. That is it, some something more?

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Student: 5 cycle mam, cycles.

One 5-cycle. So, let me call the numbers here, first conjugacy class, second conjugacy class, third, fourth, fifth, sixth and seventh. And the cycle structure here is I am going to write it in the notation of i 1, i 2, i 3, i 4, so it is going to be, this is going to be, all with me. This one is, what about this, a numbers you can compute some of you computes using that formula, this is anyway identity element as I said will have only one element, ok.

This is I think is 5, can you check? Because you have to put i k to be 1, i 5 to be 1 and 5, 5 factorial by 5, am I right? How much is that, anyway you have to do this. So, this will be 5 into 4 right, am I right, 24, anyway I will leave it you to do it. Totally, you have to get how many total should add up to 120 elements, 5 factorial is 120. Is this right, it is correct?

So, what about here? 5 to the power of 1, so I will give you 4 factorial again 24, ok. I have not done all the elements, but I will leave it you to check it out, ok. So, I have just said for example, n equal to 5 can be broken up into 7 distinct conjugacy classes. And convenient way of diagrammatically representing conjugacy classes using young diagram, 1-cycles by single box, 2-cycle by double vertical box and so on. Only thing you have to remember is that the, you could have put double vertical box this side, the convention is that the number of boxes in the first row is always greater than or equal to the number of boxes in the second row and so on.

So, just to keep track of it, this is the convention which is followed. You stack the double vertical box to the left hand side, stack triple vertical box next to it and so on, ok. So, this is the universal conversion, sorry convention which we follow, so please do not violate this. So, you replace 1-cycle by single box, 2-cycle by double box and so on. Identity element is five 1-cycles which is denoted by 5 single boxes.

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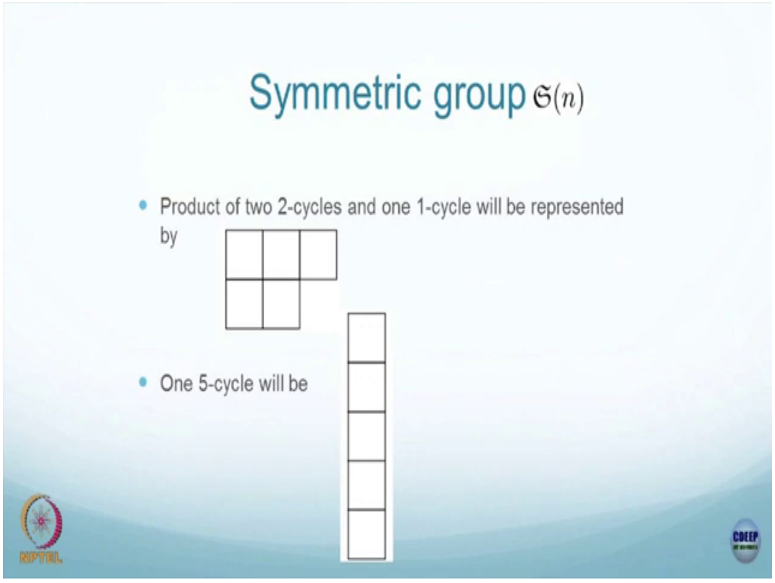

And product of two 2-cycles and one 1-cycle will be now it is clear to you, all of you, just for summary I have put it here and one 5-cycle will be this, ok.

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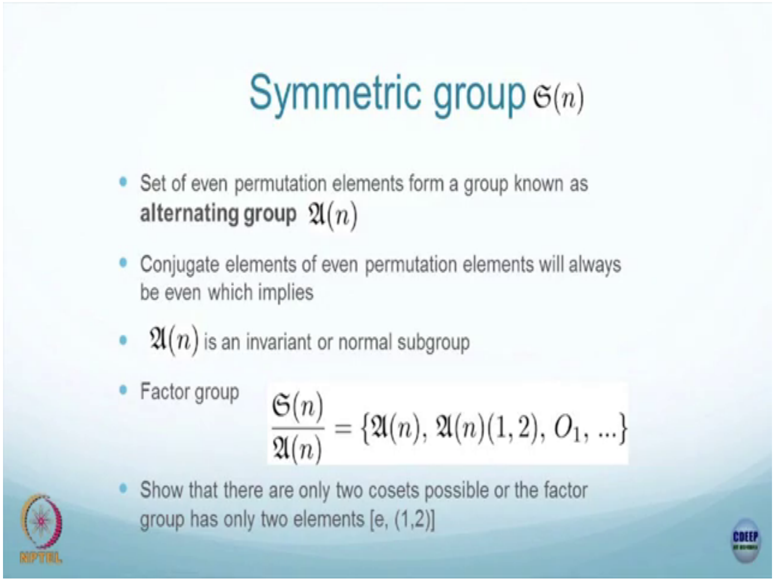

So, now I am coming back to subgroups. One of the simplest subgroups is even permutation elements ok. Any questions on this? Now, I am shifting to even permutation elements subgroups, but this is what you are going to follow for all your symmetric group of degree n, ok.

So, alternating group is the notation for symmetric group with only even permuted, subset of the symmetric group with even permutation elements, ok. So, clearly if you do conjugation with even permutation elements, so suppose you take let me call it as an even permutation element as some kind of even element here ok, if you put an order here and the inverse of that odd element.

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What do you expect, odd permutation means, how do you check whether the permutation is odd or even? You write the cycle structure as products of transposition. If there are even numbers of transposition, then it is even; if it is odd number of transposition it is odd.

Now, for an even permutation element, if I do a conjugation ok will this be even or will this be odd, what did he done this right, any odd with even is odd, right. So, what will happen here? So, this will have odd number of transposition, this will have odd number of transposition, this will have even number of transmission, totally how many are there?

Student: Even.

It is even, ok. It is even, element will be even. What does this property? So, suppose these elements are all belonging to a subgroup which I call it as an alternating group which is a subgroup of my symmetric group of degree n, if they are all elements belonging to, ok. So, let me call these elements as let us say g 1's ok or let me call it as a k 1.

Student: (Refer Time: 16:34).

I am not able to hear you. So, even permutation elements if you pull it out what will be the order is your question.

Student: Yeah.

What will be the order, half of it; half of it will be even permutation ok, odd permutations will have the remaining half, so that the total will be n factorial. So, alternating group which is the set of even permutation elements, it is a subset sitting inside symmetry group of degree n will have n factorial by 2 elements good.

Now, take an element, call it as k 1 ok, it is an element of it belongs to u 1, ok. So, let me write it as element of U n which is a subset of this. Take another element here, let me call it as t 1, which belongs to which is an element of the symmetric group of order n, of degree n sorry ok. So, take this element, but it does not belong to it is not an element of this, ok. So, t 1 is an element belonging to the symmetric group of degree n, but it is not an element of the alternating group that is why it is called odd. Interestingly, if I take t 1, k 1, t 1 inverse, you get an element which is an element of alternating group.

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What is this property? This is for arbitrary elements, what is this property, what does it tell you about the alternating group?

Student: It is a (Refer Time: 18:47).

It is an invariant group, invariant subgroup, alternating group is an invariant subgroup of the permutation group, right. I am not looking even at conjugate elements. So, even if you find a conjugate element, k 1 will give you another element we just k 2, but they all belong to the alternating group, ok. So, this is why it is an invariant subgroup.

So, you are take that example of our famous degree 3 symmetric group. What was the invariant subgroup there? Even permutations were 3-cycles, number of elements in the 3-cycle was 2, right. We did all this exercise, and we also know invariant subgroup was this was an invariant subgroup or a normal subgroup of symmetric group of degree 3, right. And this is nothing but your alternating group which has 3 factorial by 2 elements which is 3, ok.

So, I am just stressing the fact that even permutation elements which is a subgroup of the total symmetric group of degree n is also an invariant or a normal subgroup, ok. So, U n is an invariant or a normal subgroup ok, U n, and then you can play around the way we do it left coset will be same as right coset if it is an invariant subgroup. And you can look at the factor group where the kernel will be the map to an invariant, kernel will be the invariant subgroup, and you can have a list of cosets the first coset of the subgroup invariant subgroup is identity element.

The second subset will involve that invariant subgroup multiplied by an odd permutation element. You agree? It has to be the set should always have that a even may the odd will give you an odd I want to set to be involving odd permutation. So, the set can continue like this with all possible odd elements, ok clear.

But, what is interesting is that one two transposition is good enough to generate, all the odd permutation elements, ok. You do not need additional cosets, you would not need it. You will see that whatever you find will be already there in the one two transposition multiplying the alternate. This also you can rigorously prove it, but as of now you can take it as that the factor group is nothing but identity element at 1. This is probably the proof which is showing you this particular example of factor group, is this ok.

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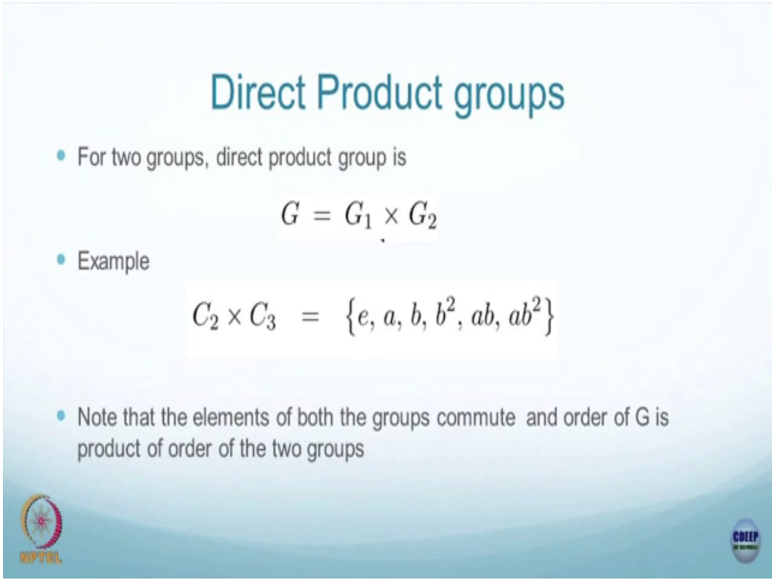

So, I just want to complete a couple of more notations that you can have products of various groups, any number of groups. This for simplicity let us take product of two groups ok; this is called as a direct product group. So, you can write G as G 1 times G 2 G 3 and so on.

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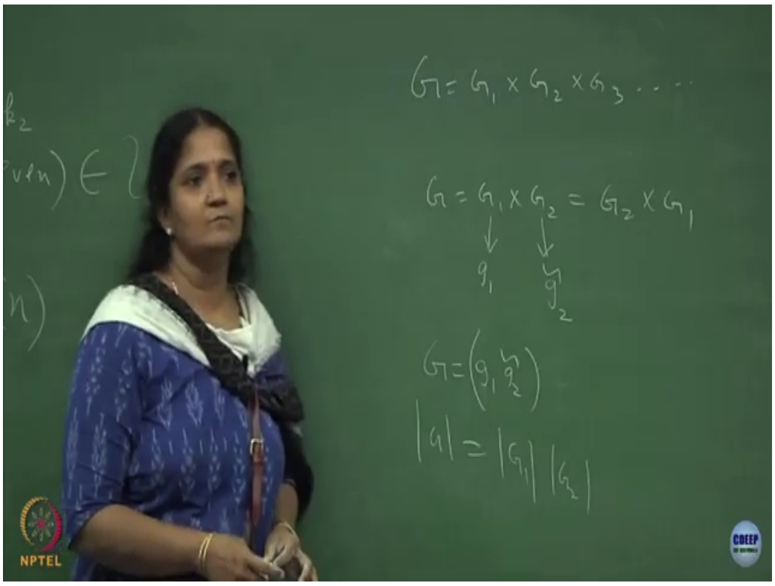

So, it could have many products. So, let us for simplicity, take G 1 cross G 2, the elements of G 1 and elements of G 2 will commute with each other, ok. So, the order really does not matter, this is same as multiplying. So, what we mean is that if you had an element here which is G 1 which belongs to this, if you have an element here which is belonging to this ok, so let me call it as g tilde 2, ok. If you take these two, you can multiply this, and write the element which belongs to this total g. So, G will be g 1 g 2 tilde does not matter whether you write g 2 before or g 1 before, ok. So, this is what is the what will be the order of this group, somebody, order of g 1 multiply the order of g 2 ok.

So, as a simple example I have given you a C 2 under C 3, C 2 was just e with a, C 3 was with e with b and b squared, it is not same as symmetric group of degree 3, ok. Why, because of this condition, if you say this group is with e and a, this group is with e, b and b squared, you can write all possible elements which is multiplying those two which is again six elements, but a b is b squared a condition is not there, a b is same as b a here clear, so that is why you will have the six elements which are listed.

Can you see the difference? This is a direct product group where the elements are composed of a and b, but this is not your symmetry group of degree 3. The order is same, but looking at it you should not say order is 6, so it should be symmetric group of degree 3, no ok.

We will come to what is the symmetric group of degree 3. Note that the elements of both the groups commute and order of G is the order of product of the orders of the groups constituting the direct product. So, this is why you call it as a direct product group. You can continue this for products of three groups and so on to build up a group of a higher order this group.

Student: Ma'am, when the group operation of (Refer Time: 27:33).

Which one? So, I am just doing it in the way where the group operation is same, but if you want to look at it as just a Cartesian product that is a different thing. But right now I am looking at it as you have two groups with the same group operations, and I want to see whether it is a direct product group or not, ok. I will come to or not with the symmetry group of degree 3, ok. So, this is a direct product group, ok.

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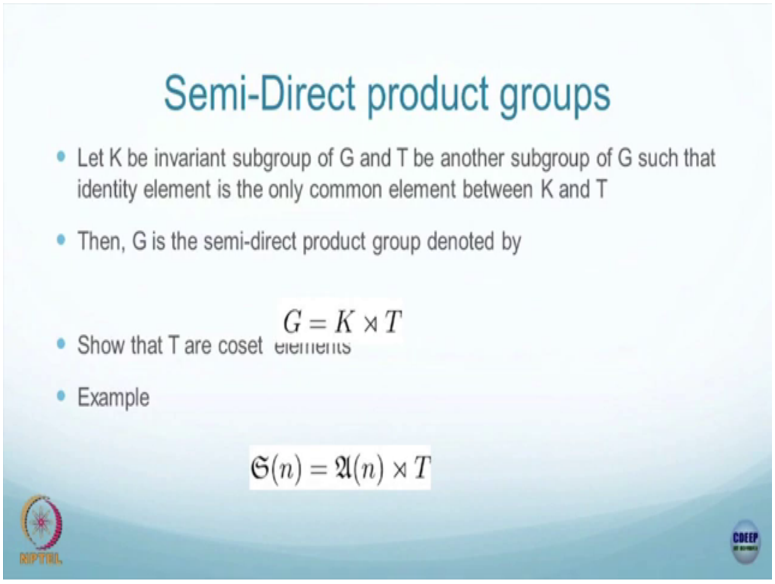

Semi-direct product; semi-direct product groups, first thing is given a group G, you see whether there is an invariant subgroup that is what happens in the case of symmetry group of degree 3 right. This is a.

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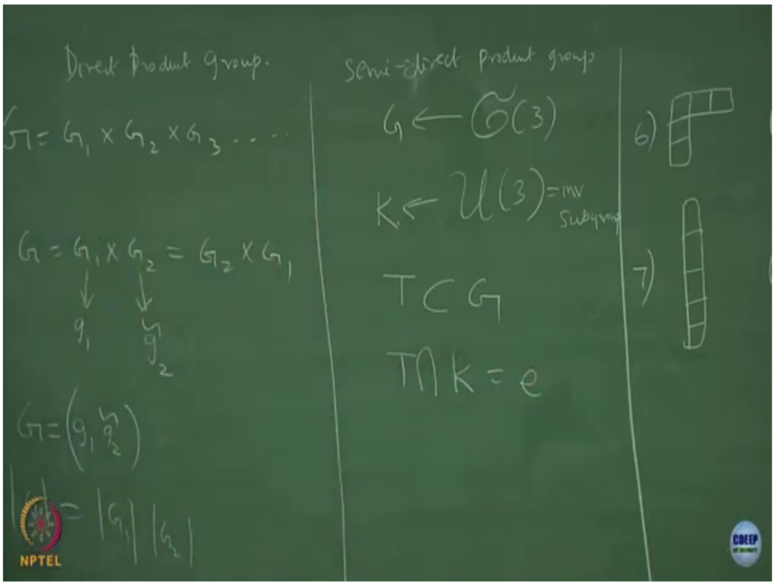

So, let us look at the symmetric group of degree 3. You have U 3, which is an invariant subgroup or a normal subgroup; we have done this now. Is that right? And now this group I call this as G, I call this as K, ok. I also have another group T, which is also subgroup of G, but T intersection K is only identity element, is that right, alternating group has identity 3-cycle and inverse of 3-cycle. And here you can say that it is identity and one transposition intersection between those two will only be identity element.

So, if you have these properties in an abstract fashion if you have a group G, but it has a invariant subgroup and you have another subgroup whose intersection with this invariant subgroup is only identity element, then we call the group G as a semi-direct product. I have shown this as a symbol on the screen.

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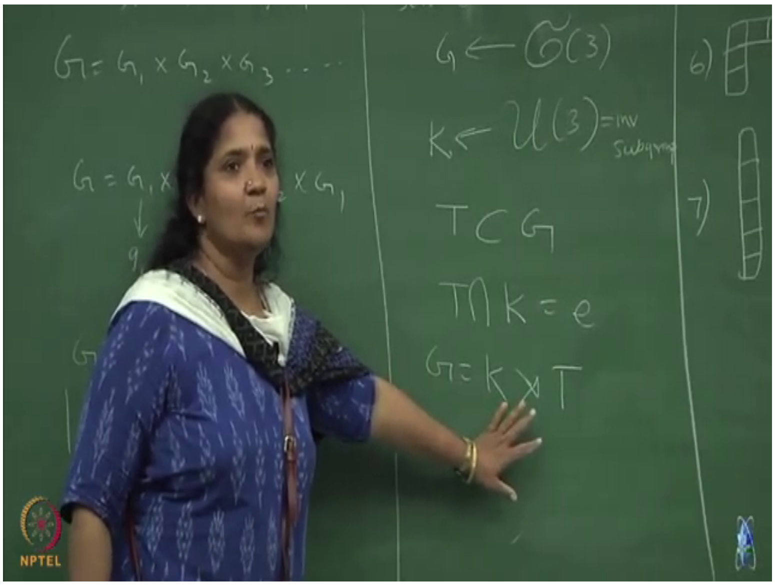

So, the group G will be K semi-direct products. So, it is written ok. So, this is the way we write the semi-direct product. It is very important the direction is very important; the first one is what we call it as an invariant subgroup with T. So, your symmetric group of degree three cannot be seen as a direct product, but can be seen as a semi-direct product ok. So, more problems, I will give it on exercises which will clarify many of these things, ok.

So, clearly for this example you know T forms the coset elements and so on. So, you have seen this. And you could write in general for a symmetric group of degree n, it is the semi-direct product of alternating group which is the group of only even permutation elements with the T, which is nothing but an identity and a one-two transposition clear.

Student: Ma’am.

Yeah.

Student: (Refer Time: 32:11).

Not necessary, I have taken an example. In an abstract case, this is an example, abstract case you can have an invariant subgroup, and you can have another subgroup such that that intersection has to be identity element that is the case, then your group can be written as a semi-direct. So, this is for an abstract group. As an example I have looked at this where the invariant subgroup is even permutation ah which is forming that alternating group ok, yeah.

And also every time when you do things you can always as I said any abstract finite group will always be isomorphic to a subgroup of this symmetric group of degree and so. In some sense ultimately you can map any finite group to some subgroups of your permutation of elements, ok. Any questions? So, now, I am going to start getting all these things look from the molecular symmetry point of view, ok.

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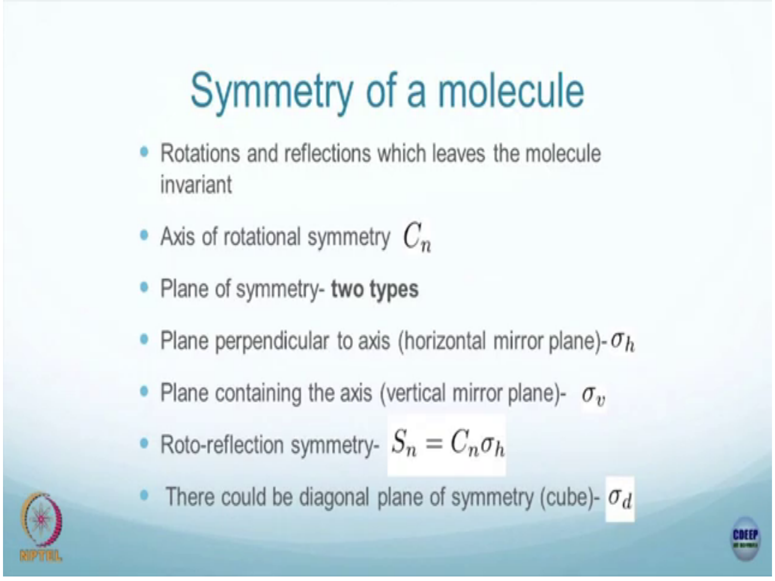

So, symmetry of a molecule; so, essentially as I said when we did the first class we had a square, take the vertices of the squares to have an atom, if you do a 90 degree rotation about an axis perpendicular to that square from through the center, you will see one atom goes into the place of the other atom and so on. But if you close your eyes and if they are identical atoms, you have not seen any change ok, so that is what is symmetry.

So, couple of symmetries which leaves the molecule, molecule is typically made of some specific arrangements of atom like water molecule or ammonia molecule. We will have a specific arrangement of the atoms and then you start looking for what is the finite group symmetry such a molecule has ok, so that is the aim.

Since we have already spent a lot of time looking at some simple examples of finite group and also properties of it, and connections to permutation group; most of the things which we are going to do here will be isomorphic to subgroups of those symmetry groups. So, in that sense, this will be giving you some visible way of looking at all these abstract discrete group elements which were see, ok. So, axis of rotational symmetry this we have already seen. If you do a rotation by 2 pi by n angle, we call that a C subscript n, and it is a cyclic group and be denoted by C n is an axis of symmetric, ok.

Then there could be planes of symmetry; plane of symmetries. One plane could be perpendicular to such an axis, I will show you some pictures, and one plane could be containing the axis, ok. The one which contains axis is what we call it as a sigma v plane, ok. So, let me just try to, so let us take this board to be where you are range atoms and then we put an axis perpendicular to it, ok.

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So, let us say that you have 3 atoms. And if you have an axis perpendicular to it, you can see that when you do a rotation perpendicular to this axis by 120 degrees, the number the atoms 1 will go to 2, 2 will go to 3. So, let us take that axis to be long the z-axis, the plane to be the xy plane. It definitely has the C 3 axis symmetry, this particular example. On top of it, I could also put a mirror ok a mirror. So, let us take this to be the y-axis, this to be the x-axis on the board put a mirror in the yz plane, ok. So, let me call the mirror by sigma yz plane, if I put a mirror passing through that contains, the z contains the axis of symmetry right, then this is what we write v is the notation which is used to say that this plane of symmetry, why it is a plane of symmetry this atom will going to this, this atom will go into this when I put a plane, ok.

So, this plane of symmetry is what we call it as a vertical plane of symmetry because the mirror contains the axis, the axis is through this, mirror is like this in the yz plane ok. There could be another mirror which is put on this plane which is the xy plane, ok. Another mirror could be in the xy plane that one is perpendicular to the axis; perpendicular, this plane mirror plane is perpendicular to the axis. So, such a plane is denoted by sigma. These are the universal notations and we are going to follow these notationsok.

So, you have an axis of symmetry. You have two types of planes of symmetry one perpendicular to the axis, another one containing the axis. Sometimes you may find that it may not have just reflection planes symmetry or a rotation plane symmetry would be a combination, rotor reflection they call it, ok. So, rotation plus a reflection and that is denoted by a symbol S n where it is a product of C n times the horizontal plane operation, ok. So, we will go through these things systematically in the next two lectures. And suppose you take a cube you can also put mirrors along the diagonal, ok. So, there could be some additional planes of symmetries which are diagonal planes.

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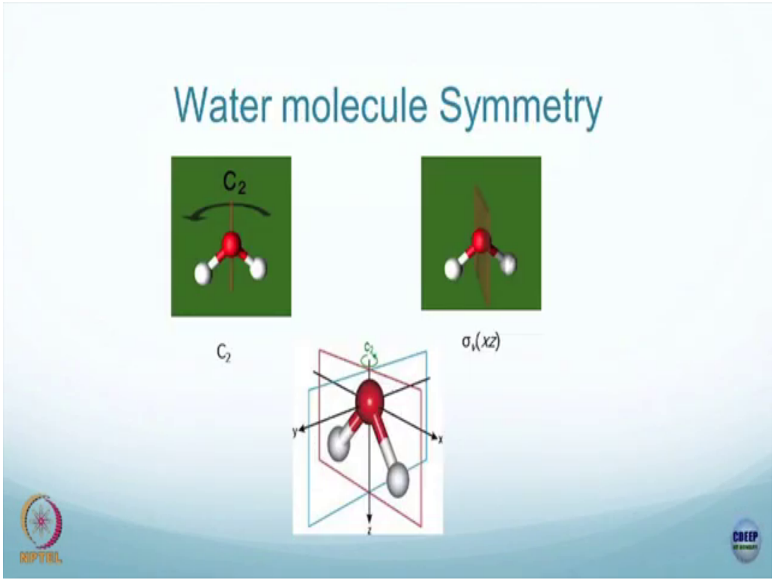

So, we will come to some of these points of symmetry. Just to show you as pictures what is being seen in various molecules if you take the water molecule which is 2-hydrogen and 1-oxygen. I have tried to put it as a 3D view by downloading some of these pictures. So, you see that there is a C 2 axis of symmetry right, and then you can also have a plane which contains the axis. So, this is what I am calling. So, x and y are conventions whichever you want to follow, but then this plane of symmetry is what we call it as a sigma v plane, ok. So, now, can you write the group elements here for a water molecule, water molecule will have, what all group elements will be there.

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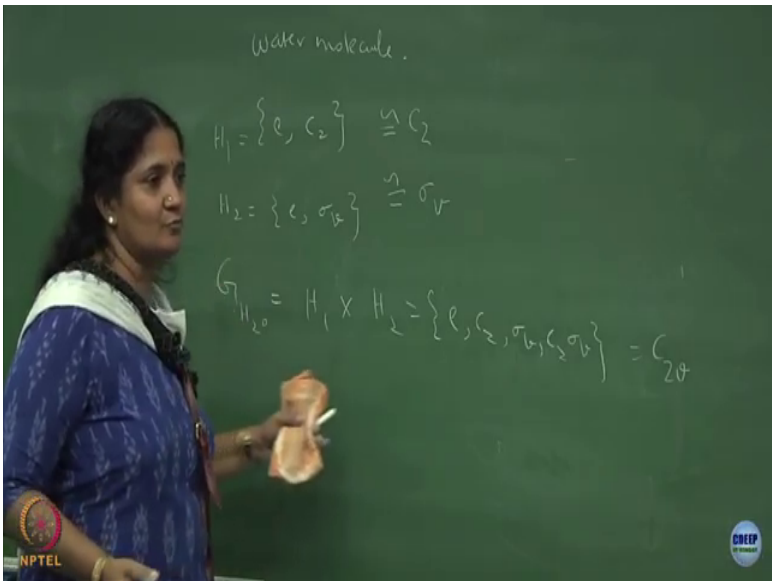

So, you can have e and C 2 ok that is one subgroup. You can have another subgroup which is e and sigma v. And your group for water molecule will be a direct product group, I am writing C 2 technically I should have called C 2 and put an element a a squared is identity, but most of the point groups now once we start doing it C 2 is considered to be the generator with 180 degree rotation. And if you want to write more elements, you will write C 2 squared, C 2 squared is also identity. So, I am trying to use it in an equivalent fashion that it is a generator of your axis of symmetry which is 180 degree axis, ok.

So, this is a direct product group, how many elements will be there, ok. And this group where you take a C 2 group and this is sometimes called as a C 2 group, this is called as a sigma v group, and this direct product is sometimes shown as C 2 v, ok.

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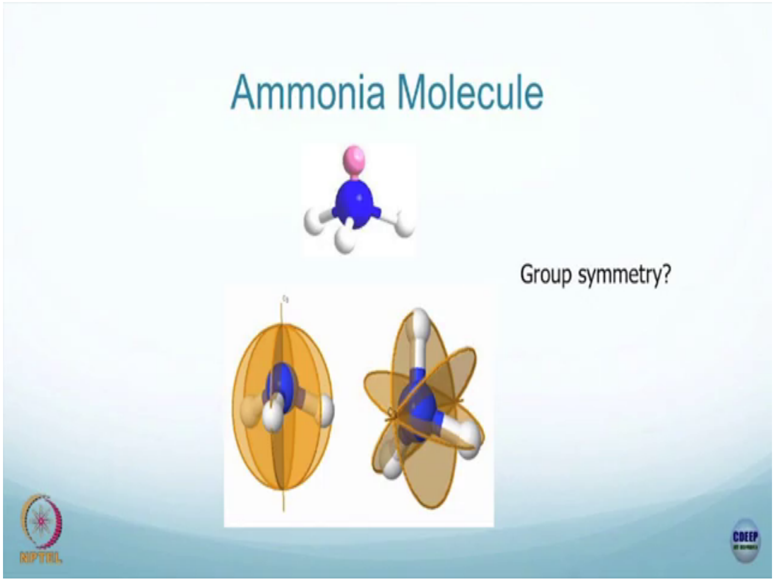

So, that is for explaining that and ammonia molecule is 1-nitrogen and 3-hydrogen. I will leave it you to check what will be the group symmetry ok, 3-hydrogens.

Student: (Refer Time: 42:35).

H 2 O, H 2 O is 2-hydrogen, yeah, what.

Student: (Refer Time: 42:41).

Yeah. So, I said it has a axis of symmetry, it is a subgroup. It also has a plane of symmetry which is also a subgroup. I showed you by picture. And then I am trying to say what is the group symmetry of this molecule, it is a direct product of these two groups that is the maximal symmetry it will have. I cannot say it has only this group; I cannot say it as only this group; it has both, so I writing it is a direct product and that I am calling it as a C 2 v, C 2 v will have four elements. Yeah, what is your confusion?

Student: (Refer Time: 43:29).

It can be interpreted as sigma v.

Student: (Refer Time: 43:48).

It is not, I am not interpreting it. I am only saying that they are four distinct symmetry operations which you can do on a water molecule. One symmetry operation where the 2-hydrogens gets exchanged is by 180 degree rotation that is a proper rotation when you do a reflection that is going to be an improper transformation that is a distinct element and it is a symmetry transmission on the water molecule, because one hydrogen goes into the other hydrogen. So, these are the maximal set of symmetry elements you can have, and they constitute a group which I am calling it as a C 2 v. Any confusion on this?

Similarly, you can show here there are 3-hydrogen atom which are you know you can take an axis through the nitrogen atom perpendicular to the plane of the hydrogen atom, and you can show that 120 degree rotation about that axis will take one to the other and so on. So, there will be a C 3 sub group right, and then you can have a mirror plane which contains this axis ok, and you can show that this mirror plane does not commute with C 2 v. It is very nice you have to play around to see what is direct product, what is semi-direct product in this language, ok.

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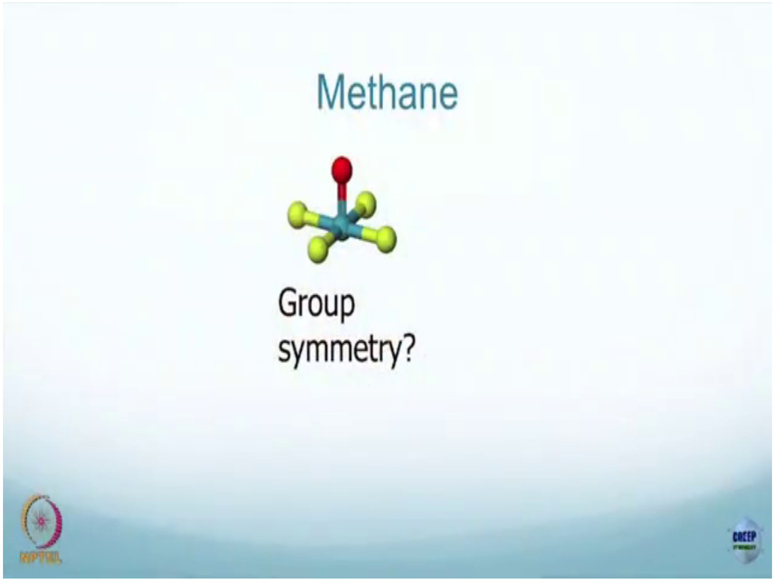

Methane is another molecule where you have 2-carbon at the center and hydrogen atoms CH 4; am I right? I am sure some all of you have done enough chemistry to at least know these molecules and how they look and so on. So, here again you can start writing what are the group elements, ok. One is four-fold axis symmetry rotation by 90 degree which will exchange all the hydrogen atoms, but there is mirror symmetry also and you have to exhaust what are the symmetries, ok.

So, we will stop here, it is already 4 and we will get on to stereographic projection in the next class.