CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

Prof. Sandeep Sangal

IIT Kanpur

Lecture 15: Point Groups - I

Continuing from the last lecture, I just want to add or emphasize certain things regarding groups: no element of the group will be repeated in a row or a column of a group multiplication table. Let us take one simple example of a group of order 3.

So, a group of order 3 would have basically 3 elements in it. One of course has to be the identity element, and 2 other elements, and it will have some combination rule. This combination rule could be anything. Let us try and build a group multiplication table for this simple group.

Now, of course, clearly, I can fill the first row and the first column: identity followed by an identity would be identity, element a followed by identity will be a, and so on. This will be the same thing that happens in the column.

This time, identity followed by element a would-be a, and then the next one would be b. Now we are left with only 4 cells to fill. Now I do not know what the combination rule is for this, whatever it is, as long as I am assured that this is actually a group.

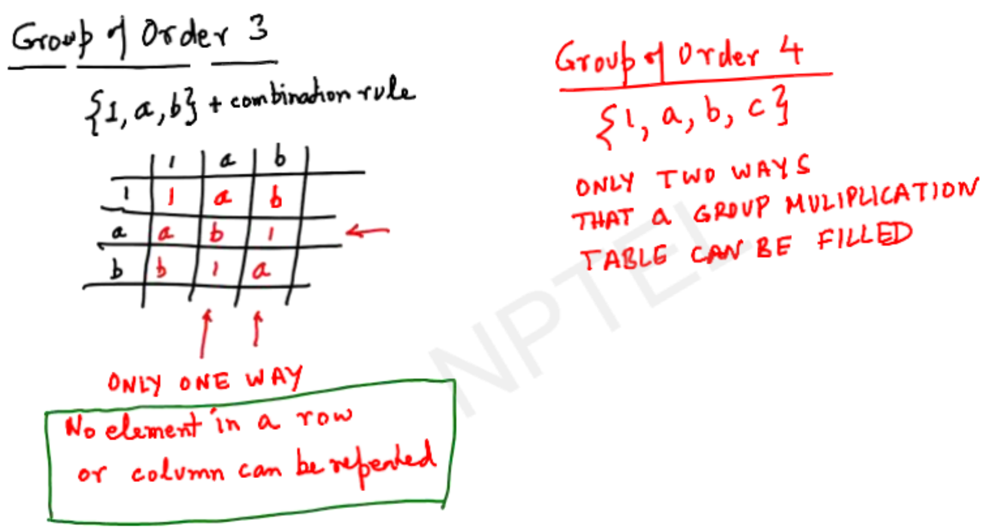
In this particular row, element a is already there; therefore, I can only put the element b or 1 in the 2 cells of this row. Now, can I put element b here? I cannot because there is already element b in the column, and hence we cannot put b here. Therefore, the only place where I can put this element is in this location. Now, only one element is left, which is the identity element. So, one has to come here.

Now, come into the second row, second column. a and b are already there; only element 1 is left. So, 1 has to come here. Similarly, if I come to this column, b is there, 1 is there, a is not there. So, a has to come here. So, there is only one way that this group multiplication table can be filled regardless of what the combination rule is.

I will just repeat that no element in a row or column can be repeated. In this case, this becomes unique. If I take a 2-element group, which is a group of order 2, the same thing will be unique. If I consider a group of order 4, I have 4 elements here. Now, there are only two ways that a group multiplication table can be filled. And of course, once you go to higher orders, there are more different ways possible for the group to operate depending on what the combination rule is.

So, the important thing is that this is what we should remember, and this will greatly facilitate us in developing different groups when we talk about symmetry groups.

(Refer Slide Time: 05:16)



Now, let me come directly to groups which have only symmetry operations in them. Let us take some groups of symmetry operations. First, let us take a simple one, or rather two of them and consider only a two-fold rotation symmetry.

Two-fold rotation symmetry would imply that it will have only two elements. All groups have to have an identity element, so it will have an identity element and a 180-degree rotation about some point A. Another group that I could consider is the presence of a mirror reflection symmetry.

This again would have only two elements: the identity element and the reflection operation, which is denoted as σ. I could very quickly geometrically visualize these two groups, and later on we will have more discussion.

Geometrical visualization could be seen like this. Let us try first of all a two-fold rotation. I have a two-fold rotation axis at some point A, and this dotted line I am just drawing as a reference. In order to geometrically visualize it, I will use an asymmetric object that I have been using earlier as well, the letter “F”. When rotated through 180 degrees, it would reposition itself here. This is a geometrical visualization of this particular group.

The second group that we can visualize is the presence of a mirror. I will denote the mirror as a solid line, and again I make use of this letter F, which is an asymmetric figure, and its reflection through the mirror. These are two different groups in which I have done this geometrical visualization, and I want to dwell a bit on why I have chosen this particular object to visualize it. This symbol F is asymmetric.

In the two-dimensional plane, we are discussing only two-dimensional symmetry at present. One property of this object is that it is chiral.

Chiral objects possess handedness; they can be either left-handed or right-handed. It is important to note that not all chiral objects are necessarily asymmetric. A chiral object is asymmetric if it lacks a plane of reflection and a center of inversion. If neither is present, the object is chiral.

The property of left-handedness or right-handedness can be illustrated using human hands. The left hand and right hand cannot be superposed on each other through any rotation; they cannot coincide in any possible way. Thus, chiral objects cannot be superposed with their mirror images. If an object has a plane of symmetry (a reflection plane), it does not exhibit handedness.

Chirality has significant implications in nature. For example, chiral molecules do not necessarily exist in equal proportions of left- and right-handed forms. Nature often shows a bias toward a particular handedness. Amino acids and sugars exist in nature with a specific handedness, and many active pharmaceutical molecules are produced with a particular handedness. Historically, this was critical in the 1960s when the drug Thalidomide caused birth defects due to the different effects of its enantiomers. The right-handed molecule had the desired effect, whereas the left-handed version produced harmful effects. This led to stricter drug testing protocols.

We now return to point groups, which are groups of symmetry operations. Consider a simple group with two elements, 1 and A_π. The group multiplication table is straightforward. The first row and first column are filled directly, and the only remaining cell is the identity. This ensures no element is repeated. The combination rule here corresponds to operations: a 180° rotation followed by another 180° rotation results in a 360° rotation, which is the identity operation. Later, these operations can be represented by matrices, and the combination rule would be matrix multiplication.

A second simple point group consists of elements 1 and the reflection operation σ. The group multiplication table is again a 2×2 table, and it appears structurally identical to the 1 and A_π two-fold rotation group.

Now consider a larger group. Let us introduce two mirrors, M_1 and M_2, perpendicular to each other. For a geometric shape with these two mirrors, consider a rectangle. Take an asymmetric or chiral object and reflect it across M_1. Denote the original object as object 1 (right-handed), and after reflection, it becomes object 2 (left-handed). Reflect object 2 across M_2, resulting in object 3 (right-handed). Reflect object 3 across M_1 to obtain object 4 (left-handed). Object 1 reflects exactly onto object 4, converting from right-handed to left-handed.

Observing this diagram, object 1 (right-handed) maps to object 2 (left-handed) and then to object 3 (right-handed). The operation that maps object 1 directly to object 3 is a 180° rotation. Similarly, object 2 maps to object 4 via a 180° rotation. This illustrates that the intersection of mirrors M_1 and M_2 at point A produces a two-fold rotational symmetry, corresponding to a rotation of π about A.

This demonstrates that combining two symmetry operations can generate a third operation, which is the basis for forming a group.

The two elements of a group, when combined through a binary operation, produce a third element, which must also be a member of the group. Therefore, A_{π} will also be a member of this group. Hence, this group consists of the identity operation 1, the reflection σ_1 from mirror 1, the reflection σ_2 from mirror 2, and a 180° rotation A_{π}. Thus, a total of four individual symmetry operations are present.

This is a group of order 4. Let us now construct the group multiplication table. First, write down the elements and fill the first row and first column as before. Next, fill the remaining cells by identifying which combinations produce the identity operation.

For instance, a reflection through mirror 1 followed by another reflection through the same mirror brings the object back to its original position. Thus, σ_1 followed by σ_1 results in the identity operation 1. Similarly, σ_2 followed by σ_2 yields 1, and A_{π} followed by A_{π} (a 180° rotation followed by another 180° rotation) also results in 1.

Next, consider combinations such as σ_2 followed by σ_1. When two perpendicular mirrors operate sequentially, the result is a 180° rotation. Therefore, $\sigma_2 * \sigma_1 = A_{\pi}$, and likewise $\sigma_1 * \sigma_2 = A_{\pi}$.

The rest of the table can now be completed systematically. For example, in the row corresponding to A_π, the elements 1 and A_π are already placed, so the remaining cell must be σ_2. Verifying with the geometric figure, a 180° rotation followed by a reflection through mirror 2 maps the object from position 1 to 3 and then to 2, which corresponds to the operation σ_1. Therefore, $A_\pi * \sigma_2 = \sigma_1$.

By continuing in this manner, all cells of the group multiplication table can be filled, completing the table for this group. This concludes the discussion for now, and we will continue exploring these concepts in the next lecture.

Thank you.

(Refer Slide Time: 25:03)