CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

Prof. Sandeep Sangal

IIT Kanpur

Lecture 16: Point Groups - II

This is the point where we had left off in the last lecture, and we had looked at this group of order 4. Now, let me take another group of order 4. This particular group had two mirrors and a two-fold rotation symmetry. Let us take a second group which has only a four-fold rotational symmetry and no mirrors.

If I list the various operations of the four-fold rotational symmetry, one is 2π or simply the identity, then the 90° rotation $\pi/2$, the 180° rotation π, and then an additional 90° rotation will take me to $-\pi/2$. So $3\pi/2$ gives a counter-clockwise rotation of 270°, and equivalently $-\pi/2$ takes me clockwise by 90°, which is the same operation. This again is a group of order 4.

Let me first geometrically visualize this group. I have a four-fold rotational symmetry, and let me draw these dotted lines as just references; these are not symmetry elements. In order to visualize this, I am going to use my asymmetric object. This is object number 1. This is taken through a counter-clockwise 90° rotation to position 2, then to position 3 and position 4, and another 90° rotation brings it back to where I started.

So, let us make a group multiplication table for this, putting the individual operations and filling the first row and the first column, 1, $A_{\pi/2}$, A_{π}, $A_{-\pi/2}$.

Now, let us see where I can put the identity operations other than the first cell that is already filled. If I look at $A_{\pi/2}$, I rotate by 90° counter-clockwise and follow it up with $A_{-\pi/2}$. So, counter-clockwise 90° followed by clockwise 90° cancels the rotation, and hence this produces the identity. The same thing applies to A_{π}: a 180° rotation followed by another 180° rotation is effectively a 360° rotation, giving the identity. For $A_{-\pi/2}$, a clockwise 90° rotation followed by $A_{\pi/2}$ again gives the identity.

The remaining elements can now be filled mechanically. Here, I cannot put $A_{\pi/2}$ in this column; if I look at this particular column, I can only place $A_{\pi/2}$ here, and what is left is A_{π}. Now, if I look at the second row, $A_{\pi/2}$, A_{π}, the element left is $A_{-\pi/2}$. Then, if I look at this column now, A_{π}, $A_{-\pi/2}$, 1, the remaining element is $A_{\pi/2}$. In this way we can fill the rest: here is $A_{\pi/2}$, and finally here is A_{π}. So, our group multiplication table is filled.

This was a slightly larger group than the previous one, but if I go back to what we had done in the last lecture. I am just going a little ahead; the logic will come later. This particular group is identified by the symbol 2. So, this is the group symbol. The mirror group is identified by the symbol m. If I look at the previous group with a two-fold rotation and two mirrors, I would call that group $2mm$, and the logic behind this notation will be explained later. Similarly, you may have guessed that this four-fold group is identified by the symbol 4. There is a certain logic to these symbols which will be discussed subsequently.

Right now, I would like to take a more elaborate example of a symmetry group, a point symmetry group. One thing I should emphasize is that these are all point groups, because in all these groups there is at least one point which remains invariant. For example, in the group m, all points on the mirror are invariant. Similarly, in the group $2mm$, there is one point in this two-dimensional group which is invariant. Likewise, in the four-fold group, the point at the rotation center remains invariant. That is why they are called point groups.

As I said, let us now consider a more elaborate example, and let me take a geometrical shape to understand this example. Let us take an equilateral triangle and examine the point symmetries associated with it. Very simply, there is a three-fold rotational symmetry present in an equilateral triangle. In addition, there are three mirror planes passing through the center of the three-fold symmetry. One can again identify the invariant point at the center.

Thus, the triangle can be rotated through a three-fold symmetry, meaning a 120° rotation, and the shape will come into self-coincidence. Similarly, the reflection planes bring the shape into self-coincidence. Let us label these mirrors as M_1, M_2, and M_3. Correspondingly, the symmetry operations will be σ_1, σ_2, and σ_3.

For reference, let the three vertices of the triangle be labeled as 1, 2, and 3. Now let me note the three operations of the three-fold rotation: the identity (doing nothing), a $+ 120^{\circ}$ rotation (counter-clockwise), and a $- 120^{\circ}$ rotation (clockwise). If I perform the identity operation, nothing changes.

So, obviously, my vertices 1, 2 and 3 are in that same position. Let us do a 120° rotation, so $A_{2\pi/3}$. This is a 120° rotation. Vertex 1 becomes this; after a 120° counter-clockwise rotation this becomes 2, this becomes 3.

Now, let us do $- 120^{\circ}$, $A_{-2\pi/3}$. So, I am doing a 120° clockwise rotation. The position of the triangle now becomes: if I rotate it clockwise, 1 will come here, 3 will move here and 2 will move here.

Now, let us do the three reflection operations. Let us do reflection operation σ_1 through mirror M_1. When I do this, vertex 3, which is on the mirror plane, remains where it is, and 1 and 2 get flipped. So, 2 will come here and 1 will come here.

Let us do the operation σ_2 through mirror plane 2. This time, 1 will remain fixed and 2 and 3 will get flipped. So, this will become this configuration.

The third one, in this case σ_3, what happens now is: this is 3, point 2 remains fixed, and 1 and 3 get flipped. So, the configuration would be like this.

So, these are all the six operations that are there in this symmetry group. So, our group elements are 1, $A_{2\pi/3}$, $A_{-2\pi/3}$, σ_1, σ_2 and σ_3. So, this is a group of order 6.

Let us try to make the group multiplication table for this. I will write down all the elements, and the first thing I do is fill the top row and the first column.

Now, let us again look at those operations which are inverses of each other, so that when combined together the result is the identity operation. If I consider $A_{-2\pi/3}$ and $A_{2\pi/3}$, then $A_{-2\pi/3}$ followed by $A_{2\pi/3}$ will obviously result in the identity, and the reverse as well. Therefore, this is identity, this one is identity. This is all that would be there for the rotations.

Let us consider the reflections: σ_1 followed by σ_1, we have already seen that the same mirror operating a second time gives the identity. σ_2 followed by σ_2 gives identity. σ_3 followed by σ_3 gives identity. So, we have realized all the identity operations here. There should be six in total, and there are six here.

Now consider the first (or rather the first–second) row, first–second column: $A_{2\pi/3}$ followed by $A_{2\pi/3}$. What would be the result of this? A 120° rotation and another 120° rotation is $4\pi/3$, which, as we have seen, is a 270° counter-clockwise rotation, or simply $A_{-2\pi/3}$ (a 120° clockwise rotation). Hence, this would be $A_{-2\pi/3}$.

Let us try to fill in some more. Let us look at $A_{2\pi/3}$, a 120° rotation counter-clockwise followed by the reflection operation σ_1. Let us refer to the figures on the left. After the 120° counter-clockwise rotation, I apply σ_1. So, what happens? 1 and 3 will get flipped while 2 remains where it is. So, instead of 2 3 1, it becomes 2 1 3. Let us look at where the 2 1 3 diagram is, and you will see it perfectly matches this, which means this should be σ_2.

Now, in the rest of the column, let me mechanically fill it. σ_2 is there; σ_3 cannot come in the last cell of this second column, so it has to come here. Now if you look at this column, the only thing left is σ_1, so σ_1 come here.

Now let me look at the second row. For σ_1 followed by $A_{2\pi/3}$, we got the result σ_2. Now let us look at the result of σ_1 followed by $A_{2\pi/3}$. So, I am here; this is where I have to fill: σ_1 followed by $A_{2\pi/3}$.

Let us look at σ_1. After a σ_1 operation, I have this triangle in the configuration 3 2 1. To this, I apply a 120° counter-clockwise rotation. So, this becomes 1 3 2 after the rotation. Where is our 1 3 2 configuration? This should be σ_3. Hence, this cell becomes σ_3.

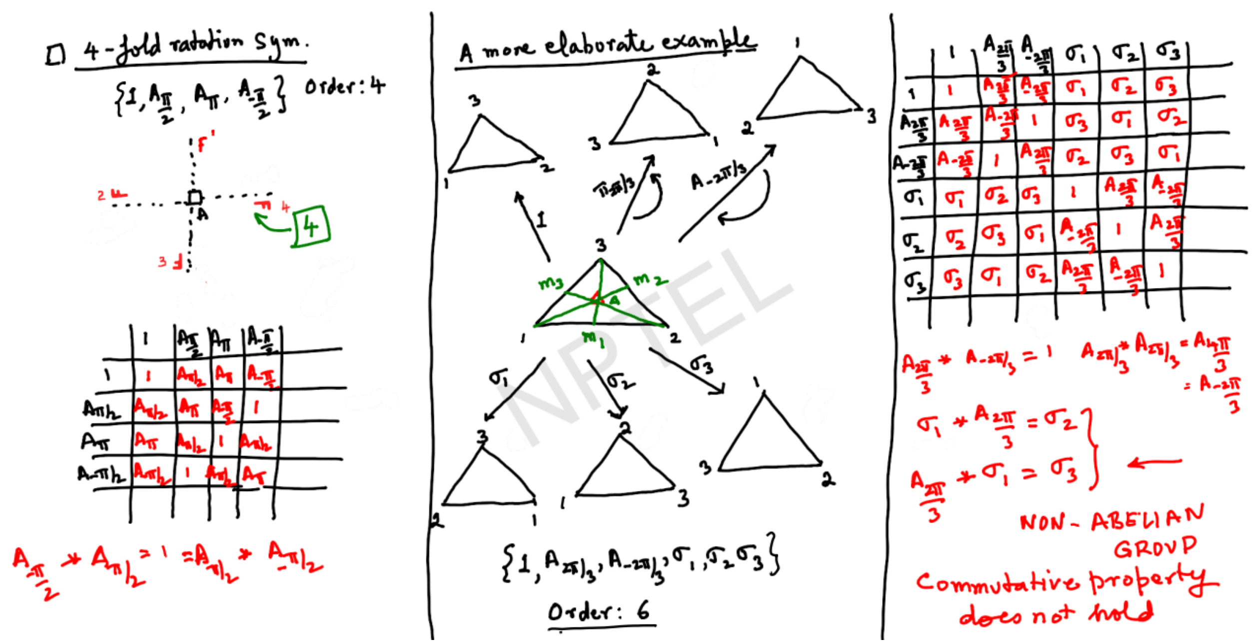
Now, the others I can quickly fill. You can also perhaps pause the video and think about how to fill the rest of the cells. But in this way, one can go ahead and fill the rest of the table.

One can observe that whenever two rotations are combined, the resulting operation is again a rotation and cannot become anything else. Likewise, when two mirror operations are applied, the outcome is a rotation, and when a mirror operation is combined with a rotation, the result must be another mirror operation. With this logic in mind, the remaining entries of the multiplication table can be completed systematically.

For example, considering the sequence $A_{2\pi/3}$, σ_2, σ_3, and σ_1, the corresponding results become σ_3, the identity, $A_{2\pi/3}$, and $A_{-2\pi/3}$. After this point, the process becomes progressively easier. Looking at a particular column where $-\ 120^{\circ}$, $+\ 120^{\circ}$, the identity, and σ_3 are already present, the remaining operations are σ_1 and σ_2. Since σ_1 already appears in the last row, it cannot occupy the final empty cell there. Therefore, σ_1 must be placed in the earlier empty position, and σ_2 fills the remaining one.

Continuing this pattern, consider the operation $A_{-2\pi/3}$. Because two mirror operations are involved, the result must convert into a rotation. This gives $A_{-2\pi/3}$, then $A_{-2\pi/3}$, and again $A_{2\pi/3}$ in the appropriate cells. Another useful observation appears when examining the operation σ_1 followed by $A_{2\pi/3}$, which gives σ_3. Importantly, reversing the order of these two operations does not produce the same result. This non-equivalence clearly indicates that the group is non-abelian, meaning that the commutative property does not hold.

(Refer Slide Time: 22:56)



Before concluding, one can visualize the group using an asymmetric motif, as done previously. Consider an object with threefold rotational symmetry and three mirror planes M_1, M_2, and M_3. Begin with the asymmetric motif labeled 1, which is right-handed.

Rotating it by 120° counterclockwise produces motif 2, which remains right-handed. Another rotation of 120° generates motif 3, also right-handed. Now apply the reflection operations to these motifs. Motif 1 becomes a left-handed configuration, denoted $1^{'}$. Motif 2 reflects to a left-handed configuration $2^{'}$, and motif 3 reflects to $3^{'}$, again left-handed.

Thus, the order of the group is 6, and this corresponds exactly to the number of asymmetric objects produced, three right-handed and three left-handed. This point group is represented by the symbol $3m$. In earlier discussions, we examined groups 2, m, $2mm$, 4, and finally the point group $3m$. In the next lecture, symmetry operations will be approached from the perspective of matrix operations, which will allow group multiplication tables to be constructed using matrix multiplication.

(Refer Slide Time: 24:52)