

CRYSTAL SYMMETRY, X-RAY DIFFRACTION, AND PHYSICAL PROPERTIES

Prof. Sandeep Sangal

IIT Kanpur

Lecture 14: What is a Group?

In this lecture I am going to talk about symmetry groups, where the individual operations associated with symmetry elements form a group. Each symmetry element possesses a number of operations, and these operations become the elements of the group. As an example, let us first consider a four-fold rotational symmetry. For a four-fold rotation, the distinct operations that can be included are precisely four. One of them is the identity operation, which in this context corresponds to a rotation of 2π (i.e., 360°), an action equivalent to doing nothing.

Let us denote the four-fold rotation axis at some point A . Around the point A , I may apply a rotation of 90° (or $\pi/2$), or 180° (or π), or 270° , or finally 360° (or 2π). A rotation of 360° is the identity operation. A rotation of 270° counter-clockwise can equivalently be described as a rotation of -90° . Thus, the four elements of the group are

$$\{1, \frac{\pi}{2}, \pi, -\frac{\pi}{2}\}.$$

Similarly, if I consider a mirror plane, then the reflection across that plane is an operation. Again, there is an identity operation, denoted by 1 , and the reflection operation, denoted by σ . Both of these examples represent point groups, and many more point groups exist. In each case, the group consists of symmetry operations that leave at least one point fixed, which is why they are called point groups.

Now, if I take such a point group and add translation symmetry to it, I obtain a space group. If this is done in two dimensions, we refer to them as two-dimensional space groups. In three dimensions, they are three-dimensional space groups, and in one-dimension, one-dimensional space groups. My preferred terminology is to call the

two-dimensional space groups “plane groups,” while for the three-dimensional groups we simply use the term “space groups.”

Up to this point, I have mentioned the term “group” but have not yet defined it. Therefore, I now need to answer the question: what is a group? In mathematics, a group is a set of elements that satisfies certain axioms under a specified binary operation. Thus, we are dealing with mathematical groups.

Let me give a working definition. Let G be a group. Then G is a set of elements together with a defined binary operation that combines any two elements of G . These two elements may be identical or different, but they must belong to the set G . Furthermore, the group G must satisfy certain axioms.

To formalize this, I denote the binary operation by the symbol $*$. If a and b are two elements of the group G , then I can combine them as $a * b$. The nature of the operation $*$ may vary: it could be addition, subtraction, multiplication, or even something more complex such as matrix multiplication (in which case matrices become the elements of the group). If the elements are numbers, then the numbers themselves constitute the group elements.

To explain the axioms clearly, let me consider a simple example: let G be the set of integers. Now I must also specify the binary operation. I choose addition as the operation. Thus G is the set of integers under addition.

Let us now look at the first axiom or property that must hold for G to form a group. This is the property of closure. For any $a, b \in G$, the result of their combination through the binary operation must also belong to G . Therefore, if the operation is addition, we require that

$$a * b = a + b \in G.$$

This is the closure property.

Closure means that for any two elements $a, b \in G$ the result of the binary operation, denoted $a * b$, must itself belong to G . In other words, if $a, b \in G$ then $a * b \in G$. As an illustrative example, consider the set of integers Z with the binary operation chosen as addition. If $a = 2$ and $b = 5$ then $a + b = 7$, and since $7 \in Z$ the closure property is satisfied. Thus, the set of integers under addition satisfies the closure axiom.

The second property is associativity. For any $a, b, c \in G$ the group operation must satisfy

$$(a * b) * c = a * (b * c),$$

so that the order of bracketing does not affect the final result. Using integers under addition as an example, let $a = 2$, $b = 3$, and $c = 5$. Then

$$(2 + 3) + 5 = 2 + (3 + 5) = 10,$$

and the result remains an element of Z . Hence associativity holds for this case.

The third axiom requires an identity element $E \in G$ such that for every $a \in G$,

$$E * a = a * E = a.$$

For the integers under addition the identity element is 0, since $0 + a = a$ and $a + 0 = a$ for all $a \in Z$.

The fourth axiom is the existence of inverses. For every $a \in G$ there must exist an inverse element $a^{-1} \in G$ such that

$$a * a^{-1} = a^{-1} * a = E,$$

where e is the identity element. In the example of integers under addition, the inverse of a is $-a$, because $a + (-a) = 0$.

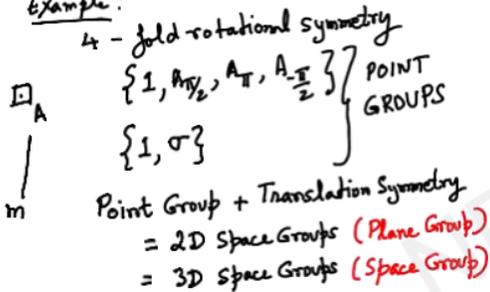
These four properties, closure, associativity, identity, and inverse are the defining axioms of a mathematical group. Some sets that might at first appear group-like fail one or more of these axioms.

(Refer Slide Time: 16:37)

Symmetry Groups

- Symmetry operations form a group

Example:



What is a Group?

- * Group (G) is a set of elements with defined binary operation for combining any two elements of the set (G)
- * Group (G) has to satisfy certain axioms

Binary Operation: *

$$a, b \in G \rightarrow a * b$$

E.g., G as a set of integers (Z) under addition '+'

Axioms

① Closure: for $a, b \in G \Rightarrow a * b = c \in G$

$$\mathbb{Z}: 2 + 5 = 7 \in \mathbb{Z}$$

② Associativity: for $a, b, c \in G$

$$a * (b * c) = (a * b) * c \in G$$

$$a=2, b=3, c=5 \Rightarrow 2 + (3+5) = (2+3) + 5 = 10 \in \mathbb{Z}$$

③ Existence of Identity element (E ∈ G)

$$a \in G, a * E = E * a = a$$

$$\mathbb{Z}: E=0, a \in \mathbb{Z}, 2+0 = 0+2 = 2$$

④ Existence of Inverse:

$$a \in G \text{ then } \exists a^{-1} \in G$$

$$a * a^{-1} = a^{-1} * a = E$$

$$\mathbb{Z}: 2 + (-2) = 0 = E$$

For instance, the set of natural numbers N (taken here to exclude 0) is closed under addition and addition is associative, but N lacks an identity element for addition, so it is not a group. The set of whole numbers (including 0) is closed under addition, associative, and has an identity element 0, but it lacks additive inverses for nonzero elements; hence the whole numbers are not a group either.

Groups may be finite. For example, the set $\{1, -1, i, -i\}$, with multiplication as the binary operation (here $i = \sqrt{-1}$), forms a group of order 4. In this context the term “multiplication table” refers to the group table for the binary operation; the word “multiplication” denotes the particular binary operation chosen and does not imply that every group operation must be the usual numerical multiplication.

All examples above conform to the four group axioms when the chosen binary operation and the element set satisfy closure, associativity, identity, and inverse; otherwise, they do not form a group.

In order to create the group multiplication table for a group of order four, construct a 4×4 array and list the group elements along the top row and the leftmost column in the same order. For the group $\{1, -1, i, -i\}$ under complex multiplication, write the header row as $1, -1, i, -i$ and repeat the same sequence down the left column. The table entries are obtained by multiplying the element from the left column by the element from the header row.

Since the operation is multiplication, the first row corresponds to $1 \cdot 1 = 1, 1 \cdot (-1) = -1, 1 \cdot i = i, 1 \cdot (-i) = -i$. Similarly, the first column entries are $1 \cdot 1 = 1, (-1) \cdot 1 = -1, i \cdot 1 = i, (-i) \cdot 1 = -i$. Consider next (-1) times each element: $(-1) \cdot (-1) = 1, i \cdot (-1) = -i, (-i) \cdot (-1) = i$. Likewise, $(-1) \cdot i = -i$. For products among i and $-i$: $i \cdot i = -1, (-i) \cdot i = 1, (-1) \cdot (-i) = i, i \cdot (-i) = 1, (-i) \cdot (-i) = -1$. Filling each cell in this manner completes the multiplication table.

One immediately observes that no element repeats in any single row or column; each row and each column is a permutation of the group elements. The identity element is 1, since multiplying any element by 1 returns the element itself. To locate inverses, identify for each element the position in the row (or column) where the product equals the identity 1. From the table, $1^{-1} = 1, (-1)^{-1} = -1, i^{-1} = -i$, and $(-i)^{-1} = i$.

As a second example, consider the additive group of integers modulo 4, often presented as “clock arithmetic” on a four-hour clock with elements $\{0, 1, 2, 3\}$. Here the binary operation is addition modulo 4: for $a, b \in \{0, 1, 2, 3\}$ define $a \oplus b \equiv (a + b) \pmod{4}$. For example, $1 \oplus 2 = 3, 3 \oplus 1 = 0$ because $3 + 1 = 4$ and $4 \pmod{4} = 0$, and $5 \pmod{4} = 1$ so that sums “wrap around” the modulus.

Constructing the table for this group, the first row (adding 0) is $0, 1, 2, 3$; adding 1 gives $1, 2, 3, 0$; adding 2 yields $2, 3, 0, 1$; and adding 3 yields $3, 0, 1, 2$. The identity element is 0, and inverses follow from the table: $0^{-1} = 0, 2^{-1} = 2, 1^{-1} = 3$, and $3^{-1} = 1$.

Both example groups are commutative: for all a, b in the group $a * b = b * a$. Such groups are called Abelian. In the context of symmetry groups, some groups are Abelian while others are not; in non-Abelian symmetry groups the order of operations matters.

The subsequent lecture will continue the discussion of group properties and their application to symmetry.

(Refer Slide Time: 32:06)

Example of sets which are not Groups

- ① Set of Natural numbers under "+"
 $N \rightarrow \{1, 2, 3, \dots\}$ NOT A Group
 \rightarrow Identity element does not exist.
- ② Set of whole number under addition "+"
 $W = \{0, 1, 2, 3, \dots\}$ NOT A Group
 Inverses do not exist

Examples of finite number of elements

Order: 4 $\{1, -1, i, -i\}$ $i = \sqrt{-1}$
 \rightarrow Under Multiplication
 Group multiplication table

Example ①

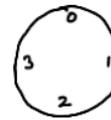
	1	-1	i	-i
1	1	-1	i	-i
-1	-1	1	-i	i
i	i	-i	1	-1
-i	-i	i	-1	1

Example ②

- Clock arithmetic

$G: \{0, 1, 2, 3\}$

Binary Operation:
 $a, b \in G \quad (a+b) \text{ mod } 4$



Identity

	0	1	2	3
0	0	1	2	3
1	1	2	3	0
2	2	3	0	1
3	3	0	1	2

Both Groups: Commutative property
 $a * b = b * a$

\Rightarrow ABELIAN GROUPS