

# Applications of group theory in spectroscopy

Igor Mazets

Atominstitut, TU Wien  
<http://atomchip.org/theory/lectures/>

WS 2024

# What is a group?

A group is a set  $\mathcal{G}$  with the following properties:

- ▶ A group operation (“multiplication”) is defined. It maps each ordered pair of group elements to another group element (called a product):

$\forall f \in \mathcal{G}, g \in \mathcal{G} \exists$  one and only one  $h = fg \in \mathcal{G}$   
(in a general case  $fg \neq gf$ )

- ▶ Associativity:

$$(g_1 g_2) g_3 = g_1 (g_2 g_3)$$

- ▶ Identity element  $e$ :

$$\exists e \in \mathcal{G} : \forall f \in \mathcal{G} \quad fe = ef = f$$

- ▶ Inverse element:

$$\forall f \in \mathcal{G} \exists f^{-1} \in \mathcal{G} :$$

$$ff^{-1} = f^{-1}f = e$$

*Try to prove the uniqueness of  $e$  and  $f^{-1}$ . Und  $(f^{-1})^{-1} = f$*

If the number  $N$  of elements of  $\mathcal{G}$  is finite, then  $\mathcal{G}$  is called finite and  $N$  is its order; otherwise  $\mathcal{G}$  is called infinite.

If the multiplication is commutative, i.e.,

$\forall f \in \mathcal{G}, g \in \mathcal{G} \quad fg = gf$ , then the group is called Abelian.

## Examples:

- ▶ Real numbers comprise a group w.r.t. addition, zero is the identity element
- ▶ Positive real numbers: arithmetic multiplication; 1 is the identity element
- ▶ Vectors (translations) in a  $D$ -dimensional space w.r.t. addition
- ▶ Rotations in a  $D$ -dimensional space
- ▶ Permutations of  $n$  objects (symmetric group  $S_n$ )

*Which of these groups are Abelian?*

Simplest non-trivial example: a group consisting of two elements  $e$  and  $f = f^{-1}$  (e.g., inversion;  $S_2$ )

## Conjugate elements

An element  $g$  is conjugate to  $h$  if  $\exists x \in \mathcal{G} : xgx^{-1} = h$

- ▶  $h$  is also conjugate to  $g$ , since  $x^{-1}hx = g$
- ▶ each element is conjugate to itself
- ▶ If  $g$  is conjugate to  $h$  then  $g^{-1}$  is conjugate to  $h^{-1}$
- ▶ If  $g$  is conjugate to  $h$  and  $h$  is conjugate to  $i$  then  $g$  is conjugate to  $i$       (*try to prove this*)

All elements of a group that are mutually conjugate comprise a class.

A group is thus partitioned into different classes.

The class containing the identity element consists of  $e$  only, since  $\forall x \ xex^{-1} = e$ .

For Abelian groups, each class consists of a single element only.

# Subgroups

If  $\mathcal{B} \subseteq \mathcal{G}$  is a group with respect to the same group operation, then  $\mathcal{B}$  is a subgroup of  $\mathcal{G}$

Examples:

- ▶  $\{e\}$  is a trivial subgroup of every group
- ▶ Integer numbers (or rational numbers) in a group of real numbers
- ▶ Rotations around a given axis in a group of all rotations in 3D
- ▶ Permutations that do not involve certain object(s)

Lagrange's theorem: If  $\mathcal{G}$  is a finite group of order  $n$  and  $\mathcal{B}$  is its subgroup of order  $m$ , then  $n/m$  is integer.

Corollary: If  $n$  is a prime number, then  $\mathcal{G}$  has no non-trivial subgroups.

# Cyclic subgroups

$$a \in \mathcal{G}$$

Elements  $e$ ,  $a^n$ ,  $(a^{-1})^n$ , where  $n = 1, 2, 3, \dots$  are all natural numbers, comprise a cyclic subgroup.

If  $\mathcal{G}$  is finite, there is a finite number of different powers of  $a$  and there is the smallest number  $p$  such that  $a^p = e$ . Then the cyclic subgroup is  $\{e, a, a^2, \dots, a^{p-1}\}$ .

1. Find examples of cyclic subgroups
2. If an order of a finite group is a prime number, what can we say about its cyclic subgroups?

# Homomorphism and isomorphism

Let  $\mathcal{G}$  be a group with a group operation  $\cdot$ .

$\mathcal{H}$  be a group with a group operation  $*$

$\varphi$  a function  $\mathcal{G} \mapsto \mathcal{H}$ .

There is a homomorphism from  $\mathcal{G}$  to  $\mathcal{H}$  if

$$\forall f \in \mathcal{G}, g \in \mathcal{G} \quad \varphi(f \cdot g) = \varphi(f) * \varphi(g).$$

If there is one-to-one correspondence between the elements of  $\mathcal{G}$  and  $\mathcal{H}$ , that is, not only  $\varphi : \mathcal{G} \mapsto \mathcal{H}$  exists, but also  $\varphi^{-1} : \mathcal{H} \mapsto \mathcal{G}$ , then these two groups are isomorphic.

Any proposition, which is true for  $\mathcal{G}$ , is also true for the isomorphic group (up to the renaming elements and the group operation).

*Find examples of isomorphic groups and of homomorphic, but not isomorphic groups.*