1.2: Operator Properties and Mathematical Groups

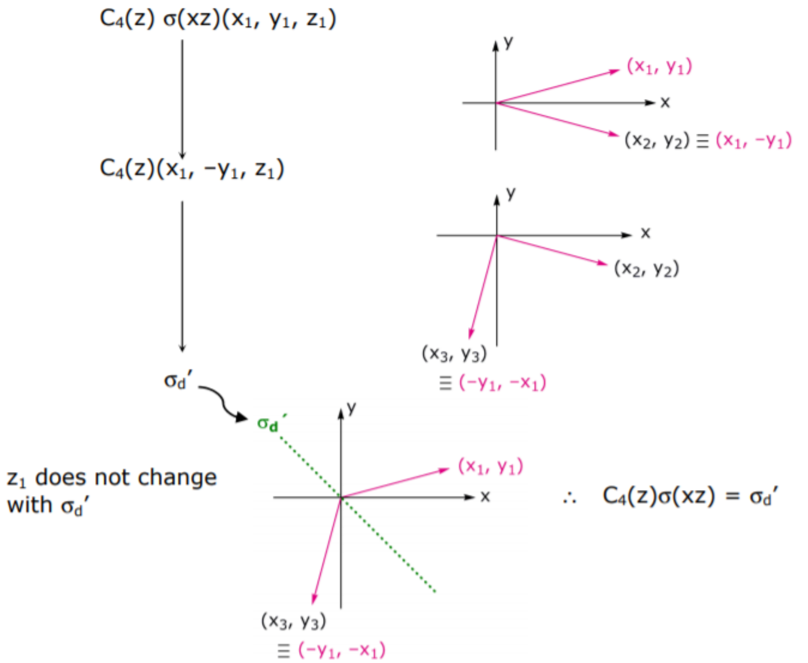
The **inverse** of A (defined as $(A)^{-1}$) is B if A · B = E

For each of the five symmetry operations:

$$(E)^{-1} = E \Longrightarrow (E)^{-1} \cdot E = E \cdot E = E$$
$$(\sigma)^{-1} = \sigma \Longrightarrow (\sigma)^{-1} \cdot \sigma = \sigma \cdot \sigma = E$$
$$(i)^{-1} = i \Longrightarrow (i)^{-1} \cdot i = i \cdot i = E$$
$$\left(C_n^m\right)^{-1} = C_n^{n-m} \Longrightarrow \left(C_n^m\right)^{-1} \cdot C_n^m = C_n^{n-m} \cdot C_n^m = C_n^n = E$$
$$\text{e.g. } \left(C_5^2\right)^{-1} = C_5^3 \text{ since } C_5^2 \cdot C_5^3 = E$$
$$\left(S_n^m\right)^{-1} = S_n^{n-m}(n \text{ even }) \Longrightarrow \left(S_n^m\right)^{-1} \cdot S_n^m = S_n^{n-m} \cdot S_n^m = S_n^n = C_n^n \cdot \sigma_h^n = E$$
$$\left(S_n^m\right)^{-1} = S_n^{2n-m}(n \text{ odd }) \Longrightarrow \left(S_n^m\right)^{-1} \cdot S_n^m = S_n^{2n-m} \cdot S_n^m = S_n^{2n} = C_n^{2n} \cdot \sigma_h^{2n} = E$$

Two operators **commute** when A · B = B · A

Example: Do $C_4(z)$ and σ(xz) commute?

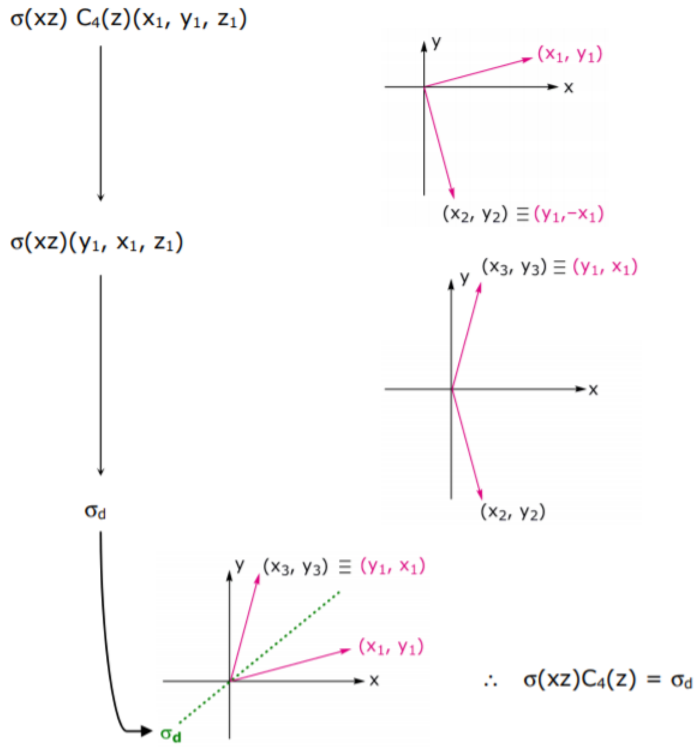


… or analyzing with matrix representations,

$$\begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$C_4(z) \cdot \sigma_{xz} = \sigma_d{}'$

Now applying the operations in the inverse order,



… or analyzing with matrix representations,

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

$$\sigma_{xz} \cdot C_4(z) = \sigma_d$$

$$\therefore \quad C_4(z)\sigma(xz) = \sigma'_d \neq \sigma(xz)C_4(z) = \sigma_d \Rightarrow \text{ so } C_4(z) \text{ does not commute with } \sigma(xz) \tag{1.2.1}$$

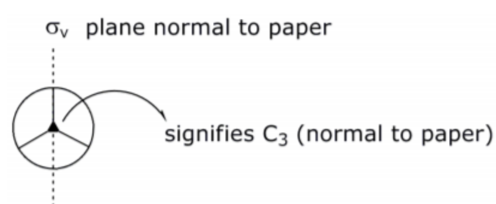
A collection of operations are a mathematical group when the following conditions are met:

- **closure**: all binary products must be members of the group
- **identity**: a group must contain the identity operator
- **inverse**: every operator must have an inverse
- **associativity**: associative law of multiplication must hold

$$(A \cdot B) \cdot C = A \cdot (B \cdot C \tag{1.2.2}$$

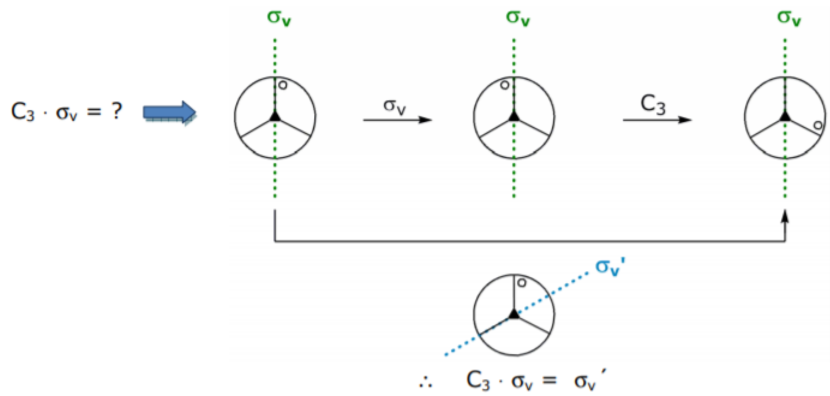
(note: commutation not required… groups in which all operators do commute are called **Abelian**)

Consider the operators C_3 and σ_v. These do not constitute a group because identity criterion is not satisfied. Do E, C_3, σ_v form a group? To address this question, a stereographic projection (featuring critical operators) will be used:



So how about closure?

$C_3 \cdot C_3 = C_3{}^2$ (so $C_3{}^2$ needs to be included as part of the group)



Thus E, C_3 and σ_v are not closed and consequently these operators do not form a group. Is the addition of $C_3{}^2$ and σ_v' sufficient to define a group? In other terms, are there any other operators that are generated by C_3 and σ_v?

… the proper rotation axis, C_3:

$$C_3$$
$$C_3 \cdot C_3 = C_3^2$$
$$C_3 \cdot C_3 \cdot C_3 = C_3^2 \cdot C_3 = C_3 \cdot C_3^2 = E$$
$$C_3 \cdot C_3 \cdot C_3 \cdot C_3 = E \cdot C_3 = C_3$$

etc.

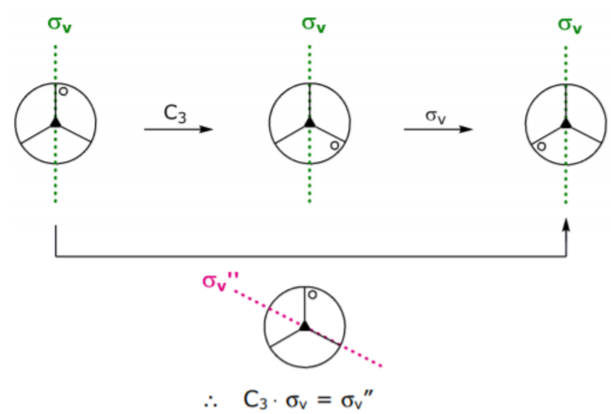
$\therefore C_3$ is the generator of E, C_3 and C_3^2, note: these three operators form a group

… for the plane of reflection, σ_v

$$\sigma_v$$
$$\sigma_v \cdot \sigma_v = E$$
$$\sigma_v \cdot \sigma_v \cdot \sigma_v = E \cdot \sigma_v = \sigma_v$$

etc.

So we obtain no new information here. But there is more information to be gained upon considering C_3 and σ_v. Have already seen that $C_3 \cdot \sigma_v = \sigma_v'$ … how about $\sigma_v \cdot C_3$



Will discover that no new operators may be generated. Moreover one finds

$$\begin{array}{ccccccc} & E^{-1} & C_3^{-1} & (C_3^2)^{-1} & \sigma_v^{-1} & (\sigma_v')^{-1} & (\sigma_v'')^{-1} \\ \text{inverses} & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow & \downarrow \\ & E & C_3^2 & C_3 & \sigma_v & \sigma_v' & \sigma_v'' \end{array}$$

The above group is closed, i.e. it contains the identity operator and meets inverse and associativity conditions. Thus the above set of operators constitutes a mathematical group (note that the group is not Abelian).

Some definitions:

Operators C_3 and σ_v are called **generators** for the group since every element of the group can be expressed as a product of these operators (and their inverses).

The **order** of the group, designated h, is the number of elements. In the above example, h = 6.

Groups defined by a single generator are called **cyclic** groups.

Example: $C_3 \rightarrow E, C_3, C_3{}^2$

As mentioned above, E, C_3, and $C_3{}^2$ meet the conditions of a group; they form a cyclic group. Moreover these three operators are a **subgroup** of E, C_3, $C_3{}^2$, σ_v, σ_v',σ_v". The order of a subgroup must be a divisor of the order of its parent group. (Example $h_{subgroup}$ = 3, h_{group} = 6 … a divisor of 2.)

A **similarity transformation** is defined as: $v^{-1} \cdot A \cdot v = B$ where B is designated the similarity transform of A by x and A and B are **conjugates** of each other. A complete set of operators that are conjugates to one another is called a **class** of the group.

Let's determine the classes of the group defined by E, C_3, $C_3{}^2$, σ_v, σ_v',σ_v"… the analysis is facilitated by the construction of a multiplication table

$$\begin{array}{c|cccccc} & E & C_3 & C_3^2 & \sigma_v & \sigma_v' & \sigma_v'' \\ \hline E & E & C_3 & C_3^2 & \sigma_v & \sigma_v' & \sigma_v'' \\ C_3 & C_3 & C_3^2 & E & \sigma_v' & \sigma_v'' & \sigma_v \\ C_3^2 & C_3^2 & E & C_3 & \sigma_v'' & \sigma_v & \sigma_v' \\ \sigma_v & \sigma_v & \sigma_v'' & \sigma_v' & E & C_3^2 & C_3 \\ \sigma_v' & \sigma_v' & \sigma_v & \sigma_v'' & C_3 & E & C_3^2 \\ \sigma_v'' & \sigma_v'' & \sigma_v' & \sigma_v & C_3^2 & C_3 & E \end{array} \tag{1.2.3}$$

may construct easily using stereographic projections

$$\begin{gathered} E^{-1} \cdot C_3 \cdot E = E \cdot C_3 \cdot E = C_3 \\ C_3^{-1} \cdot C_3 \cdot C_3 = C_3^2 \cdot C_3 \cdot C_3 = E \cdot C_3 = C_3 \\ \left(C_3^2\right)^{-1} \cdot C_3 \cdot C_3^2 = C_3 \cdot C_3 \cdot C_3^2 = C_3 \cdot E = C_3 \\ \sigma_v^{-1} \cdot C_3 \cdot \sigma_v = \sigma_v \cdot C_3 \cdot \sigma_v = \sigma_v \cdot \sigma_v' = C_3^2 \\ (\sigma_v')^{-1} \cdot C_3 \cdot \sigma_v' = \sigma_v' \cdot C_3 \cdot \sigma_v' = \sigma_v' \cdot \sigma_v'' = C_3^2 \\ (\sigma_v'')^{-1} \cdot C_3 \cdot \sigma_v'' = \sigma_v'' \cdot C_3 \cdot \sigma_v'' = \sigma_v'' \cdot \sigma_v = C_3^2 \end{gathered}$$

∴ C_3 and $C_3{}^2$ from a class

Performing a similar analysis on σ_v will reveal that σ_v, σ_v' and σ_v'' form a class and E is in a class by itself. Thus there are three classes:

$$E, \left(C_3, C_3^2\right), \left(\sigma_v, \sigma_v', \sigma_v''\right)$$

Additional properties of transforms and classes are:

- no operator occurs in more than one class
- order of all classes must be integral factors of the group's order
- in an Abelian group, each operator is in a class by itself.