Symmetry, Structure and Spectroscopy: Applications of Group Theory

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Abstract Group Theory

- Consider a set of objects $\{G\}$ and a product rule denoted $\circ$ that allows us to combine them.
- Denoted $F \circ G$, where $F, G \in \{G\}$.
- $\{G\}$ can be objects such as numbers or variables, or operators.

Examples

- The integers and any of the binary operations of arithmetic:

$$\circ = + \quad : \quad 1 + 5 = 6 \tag{1}$$

$$\circ = - \quad : \quad 1 - 5 = -4 \neq\ 5 - 1 \tag{2}$$

$$(12 - 3) - 7 = 3 \neq\ 12 - (3 - 7) = 16 \tag{3}$$

$$\circ = \div \quad : \quad 12 \div\ 3 = 4 \neq 3 \div\ 12 \text{ (not even an integer)} \tag{4}$$

- Note that so far there are no requirements that $\circ$ should obey certain rules, such as commutativity or closure.

Examples

- Translations or rotations of a physical object in two or three dimensions. Here $\circ$ denotes successive transformations.

$$\begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \circ \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

- These commute, unlike

$$\begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \circ \begin{pmatrix} \cos\phi & 0 & -\sin\phi \\ 0 & 1 & 0 \\ \sin\phi & 0 & \cos\phi \end{pmatrix}$$

Examples

- Permutations of objects: suppose we have a set $\{ABC\}$ and we have permutations defined by, e.g.,

$$(312)\{ABC\} = \{CAB\}$$

- Then

$$(312) \circ (213)\{ABC\} \; = (312)\{BAC\} = \{CBA\}$$

Closure

- Require that if $F, G \in \{G\}$, then $F \circ G \in \{G\}$ and $G \circ F \in \{G\}$.
- Note that this does not imply $F \circ G = G \circ F$.
- Such a set and closed product rule comprise a *gruppoid*.
- For example, the integers are closed under addition, multiplication, and subtraction, but not under division.
- The set of permutations of N objects is closed with respect to successive permutations.
- Successive rotations and translations in M dimensions are closed.

Imposing further rules

- Gruppoids are clearly very general things.
- Few useful properties are known for gruppoids — we have to restrict ourselves further.
- Impose restrictions on our set and product rule.

Associativity

- Require that if $F, G, H \in \{G\}$, we have

$$(F \circ G) \circ\ H = F \circ (G \circ H).$$

- For example, the addition and multiplication of integers is associative, whereas subtraction is not.
- Successive translations and rotations are associative.
- Permutations of N objects are associative.
- A set with a product rule that is closed and associative is called a *semigroup* or *monoid*.

Identity element

- Require that in $\{G\}$ there is an element E, the *identity*, such that $E \circ G = G \circ E = G$.
- For the integers, the identity for addition is 0, for multiplication it is 1; there is no identity for division.
- For translations the identity is the null operation, for rotations it is the identity rotation which is given in matrix form by a unit matrix.
- For permutations the identity is no permutation, e.g., (123).

Inverse

- For every element $G \in \{G\}$ there exists an element denoted G^{-1} such that $G^{-1} \circ G = G \circ G^{-1} = E$.
- For the integers, the inverse of k is $-k$. There is no inverse under multiplication in general. But under division every element is its own inverse!
- For a translation the inverse is -1 times the original translation. For a rotation the inverse is the same rotation in the opposite sense (matrix inverse)
- For every permutation in the set of permutations of N objects there is an inverse permutation that restores the original order.

Commutativity

- If the set $\{G\}$ has the property that for any two elements $F, G \in \{G\}$ we have $F \circ G - G \circ F = 0$, then the elements of $\{G\}$ *commute*.
- Integer addition is commutative, and so is integer multiplication; integer subtraction is not.
- Translations are commutative, and so are rotations.
- Permutations of N objects are not in general commutative except for the case $N = 2$. For instance

$$(312)\circ(213)\{ABC\} = \{CBA\} \neq (213)\circ(312)\{ABC\} = \{ACB\}$$

Groups

- A set $\{G\}$ and product rule which is associative, closed, and which contains an inverse of every element and an identity is a *group*.
- We do not *require* commutativity, but if all elements commute the group is termed an *Abelian* group.
- The integers form a group (Abelian) under addition, but not under division, multiplication, or subtraction.
- Translations of an object form a group, as do rotations, both also Abelian.
- The permutations of N objects forms a group: the *symmetric group* of N objects. The symmetric groups are not in general Abelian.

Groups

- If a set of objects and a product rule form a group we use the notation $\mathscr{G}$.
- The number of objects in the group is denoted g (this may not be a finite number).
- We will usually use the simple implied product notation FG instead of $F \circ G$.

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  - If in addition $GK - KG \; \forall \; G, K \in \mathscr{G}$, $\mathscr{G}$ is *Abelian*.

Groups

- The integers form a group under *addition*, but not under (arithmetic) *multiplication*.
- Permutations of N objects (*symmetric group*).
- *Cyclic groups*: $\{x^k; 0 \leq k \leq g-1\}$.
- Transformations that preserve the shape and size of a three-dimensional object (*point groups*).

Example: Permutations of three objects

- Consider three objects $\{XYZ\}$ and denote the permutations on these objects using the operators (ijk).
- We have six operators:

$$
\begin{array}{ll}
(123)\{XYZ\} = \{XYZ\} & (312)\{XYZ\} = \{ZXY\} \\
(231)\{XYZ\} = \{YZX\} & (132)\{XYZ\} = \{XZY\} \\
(321)\{XYZ\} = \{ZYX\} & (213)\{XYZ\} = \{YXZ\}
\end{array}
$$

- Label these operators respectively as $\{E, A, B, C, D, F\}$.
- We can write down the products of these operators and verify that they form a group, denoted $\mathscr{S}$(3).

Multiplication Table

	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	B	E	F	C	D
B	B	E	A	D	F	C
C	C	D	F	E	A	B
D	D	F	C	B	E	A
F	F	C	D	A	B	E

- Can verify that these are associative, E is identity, and all elements have an inverse. This is a (non-Abelian) group of order 6.

Multiplication Table, Subgroups

	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	B	E	F	C	D
B	B	E	A	D	F	C
C	C	D	F	E	A	B
D	D	F	C	B	E	A
F	F	C	D	A	B	E

- We can see that some elements multiply among themselves only, forming a *subgroup*. E.g., $\{E, A, B\}$.

Multiplication Table, Subgroups

- $\{E, A, B\}$ form a subgroup of order three. $\{E, C\}$ etc. form subgroups of order two. These are *proper* subgroups.
- The subgroups of order two are *isomorphic* to one another — two groups are isomorphic if they have the same multiplication table.
- The order of a subgroup must be a divisor of the order of the group (Lagrange).

Group structures

- How many groups are there of a given order g (to within an isomorphism — group structures)?
- If g is prime, the answer is *one*, isomorphic to the cyclic group of order g. Incidentally, this is Abelian.
- Hence for $g = 1, 2, 3$ there is one group structure. For $g = 4$ we have two group structures.

Groups of order four

	E	A	B	C
E	E	A	B	C
A	A	B	C	E
B	B	C	E	A
C	C	E	A	B

	E	A	B	C
E	E	A	B	C
A	A	E	C	B
B	B	C	E	A
C	C	B	A	E

- The first is isomorphic to the cylic group of order four. The second is sometimes called the *Vierergruppe*. Both are Abelian.

Groups of higher order

- There is one group structure of order five and seven, and two of order six (the symmetric group of three objects, and the cyclic group of order six).
- There are *three* groups of order eight. We will meet them later. . . .
- *Cayley's Theorem*: Any group of order g is a subgroup of the symmetric group of g objects. The latter is of order $g!$, of course.

Cosets

- If $\mathscr{H} \subset \mathscr{G}$, and $G \in \mathscr{G}$ but $G \notin \mathscr{H}$, $G\mathscr{H}$ is a *left coset* and $\mathscr{H}G$ is a *right coset*.
- Consider $\mathscr{S}$(3): say, the subgroup $\mathscr{H}$=$\{E, C\}$ and element A. We have the left coset $\{A, F\}$ and the right coset $\{A, D\}$, so left and right cosets are not in general identical.
- If we consider also the left coset from $\{E, C\}$ with B, we get $\{B, D\}$, which together with the left coset $A\{E, C\}$ and $\{E, C\}$ itself decomposes $\mathscr{S}$(3) into disjoint sets.

Cosets

- Cosets $G\mathscr{H}$ and $F\mathscr{H}$ are disjoint, and no element can occur more than once in a given coset.
- $G\mathscr{G}$ is simply $\mathscr{G}$, of course. This gives rise to the *Rearrangement Theorem*: we can replace any sum over elements G of $\mathscr{G}$ with a sum over elements HG, where H is a fixed element of $\mathscr{G}$.
- *Double cosets* $\mathscr{F}G\mathscr{H}$ also provide a partitioning of the group into disjoint sets, although an element can occur multiple times within a given double coset.

Classes

- If there is at least one $X \in \mathscr{G}$ such that

$$H = XGX^{-1}, \quad G, H \in \mathscr{G},$$

  H is *conjugate* to G.

- Clearly, if H is conjugate to G, G is conjugate to H: they are mutually conjugate.

- A subset of the elements of $\mathscr{G}$ in which all the elements are mutually conjugate is called a *conjugacy class*, or simply class.

Classes: Example

- Consider $\mathscr{S}(3)$. We have $CAC^{-1} = B$, so A and B are mutually conjugate. ($DAD^{-1} = FAF^{-1} = A$, too.)
- $ACA^{-1} = D$, $ADA^{-1} = F$, $AFA^{-1} = C$, so C, D, and F are mutually conjugate.
- E is always in a class by itself, so $\mathscr{S}(3)$ comprises three classes.
- If $\mathscr{G}$ is Abelian, $XGX^{-1} = G$, so $H = XGX^{-1}$ implies $H = G$ and each element is in a class by itself.

Representations

- Let us write the six permutations of three objects as elements of a row vector:

$$(XYZ \quad ZXY \quad YZX \quad XZY \quad ZYX \quad YXZ)$$

and consider the action of a group operator $G \in \mathscr{S}(3)$ on this vector, giving

$$\begin{aligned} &G\,(XYZ \quad ZXY \quad YZX \quad XZY \quad ZYX \quad YXZ) \\ &\qquad = (XYZ \quad ZXY \quad YZX \quad XZY \quad ZYX \quad YXZ)\,\mathbf{D}(G), \end{aligned}$$

where $\mathbf{D}(G)$ here is a 6×6 matrix.

Representations

- For example, we have

$$
\begin{aligned}
A\,(XYZ \quad ZXY \quad YZX \quad XZY \quad ZYX \quad YXZ) \\
= (ZXY \quad YZX \quad XYZ \quad YXZ \quad XZY \quad ZYX) \\
= (XYZ \quad ZXY \quad YZX \quad XZY \quad ZYX \quad YXZ)\,\mathbf{D}(A)
\end{aligned}
$$

where

$$
\mathbf{D}(A) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}
$$

Representation Matrices

$$\mathbf{D}(E) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix} \qquad \mathbf{D}(A) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

Representation Matrices

$$\mathbf{D}(B) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix} \quad \mathbf{D}(C) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

Representation Matrices

$$\mathbf{D}(D) = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix} \qquad \mathbf{D}(F) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Representations

- In this way we get six *representation matrices* denoted $\mathbf{D}(G)$, for which when

$$\begin{aligned} GH &= F, \\ \mathbf{D}(G)\mathbf{D}(H) &= \mathbf{D}(F). \end{aligned}$$

- *It is essential to understand how operators and representation matrices multiply.* The naive assumption would be that

$$\begin{aligned} GH\,(XYZ\ldots) &= G\,\{(XYZ\ldots)\,\mathbf{D}(H)\} \\ &= (XYZ\ldots)\,\mathbf{D}(H)\mathbf{D}(G) \\ &\neq (XYZ\ldots)\,\mathbf{D}(F). \end{aligned}$$

This is wrong!

Representations

- It is wrong because an operator like G or H is only defined to operate on our set of six objects, not a matrix like $\mathbf{D}(H)$. The correct form is

$$\begin{aligned} GH\,(XYZ\ldots) &= \{G\,(XYZ\ldots)\}\,\mathbf{D}(H) \\ &= (XYZ\ldots)\,\mathbf{D}(G)\mathbf{D}(H) \\ &= (XYZ\ldots)\,\mathbf{D}(F). \end{aligned}$$

- We will encounter this sort of issue again when we consider groups of transformations.

Representations

- Since

$$\mathbf{X}^{-1}\mathbf{D}(G)\mathbf{X}\mathbf{X}^{-1}\mathbf{D}(H)\mathbf{X} = \mathbf{X}^{-1}\mathbf{D}(G)\mathbf{D}(H)\mathbf{X} = \mathbf{X}^{-1}\mathbf{D}(F)\mathbf{X},$$

  representations are defined only to within a similarity transformation.

- These matrices are *unitary*. This is not required, but can always be accomplished by a similarity transformation.

Representations

- This representation is *faithful*: all six matrices are different. (Contrast with a trivial representation in which each operator is represented by a one.)
- This is termed the *regular representation*.
- Sidebar: constructing the regular representation from the multiplication table.

Representations

- Consider now a different vector denoted $(\chi_1 \;\; \chi_2 \;\; \chi_3 \;\; \chi_4 \;\; \chi_5 \;\; \chi_6)$ and constructed as

$$
\begin{aligned}
\chi_1 &= \frac{1}{\sqrt{6}}\{XYZ + ZXY + YZX + XZY + ZYX + YXZ\} \\
\chi_2 &= \frac{1}{\sqrt{6}}\{XYZ + ZXY + YZX - XZY - ZYX - YXZ\} \\
\chi_3 &= \frac{1}{\sqrt{12}}\{2XYZ - ZXY - YZX + 2XZY - ZYX - YXZ\} \\
\chi_4 &= \frac{1}{2}\{ZXY - YZX - ZYX + YXZ\} \\
\chi_5 &= \frac{1}{2}\{-ZXY + YZX - ZYX + YXZ\} \\
\chi_6 &= \frac{1}{\sqrt{12}}\{2XYZ - ZXY - YZX - 2XZY + ZYX + YXZ\}
\end{aligned}
$$

and the resulting representation matrices from

$$G(\chi_1 \;\; \chi_2 \;\; \chi_3 \;\; \chi_4 \;\; \chi_5 \;\; \chi_6) = (\chi_1 \;\; \chi_2 \;\; \chi_3 \;\; \chi_4 \;\; \chi_5 \;\; \chi_6)\mathbf{D}(G).$$

New Representation Matrices

$$\mathbf{D}(E) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

New Representation Matrices

$$\mathbf{D}(A) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

New Representation Matrices

$$\mathbf{D}(B) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

New Representation Matrices

$$\mathbf{D}(C) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \end{pmatrix}$$

New Representation Matrices

$$\mathbf{D}(D) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & 0 & -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ 0 & 0 & 0 & 0 & -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$$

New Representation Matrices

$$\mathbf{D}(F) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 & 0 \\ 0 & 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ 0 & 0 & 0 & 0 & \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$$

New Representation Matrices

- Clearly, the information contained in these new representation matrices does not require 6×6 matrices. In fact, we can present it using only scalars (1×1) and 2×2 arrays:

$$
\begin{array}{ccc}
E & A & B \\
1 & 1 & 1 \\
1 & 1 & 1 \\
\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} &
\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} &
\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \\
\\
C & D & F \\
1 & 1 & 1 \\
-1 & -1 & -1 \\
\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} &
\begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} &
\begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}
\end{array}
$$

New Representation Matrices

- Note that we have brought our original matrices to this form by a new choice of basis: i.e., by a single transformation **T**:

$$\mathbf{D}(G)_{new} = \mathbf{T}^{-1}\mathbf{D}(G)\mathbf{T}\;\forall\; G \in \mathscr{G}.$$

- It is not possible to simplify all matrices further by a *single* similarity transformation. These matrices are therefore called *irreducible*, and we thus have three *irreducible* representations of $\mathscr{S}(3)$.

- We henceforth use the term “irreducible” to mean *unitary, inequivalent, irreducible* representation or *irrep*.