Basic group theory, symmetry

“The beauty and strength of group theory applied to physics resides in the transformation of many complex symmetry operations into a fairly simple linear algebra.”

- Definition of a group
- Example of a group: $P(3)$
- $P(3)$ as the symmetry group of equilateral triangle C_{3v}
- Further terminology and properties, useful!
- Representations (efficient unified handling)
- Characters (distillation of the most important properties)
- Point groups (symmetry of molecules and crystals)

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Group

A set $\boldsymbol{G}$ of elements $A, B, \ldots$ with the binary operation (AB, called multiplication) having the following properties:

1. $AB \in \boldsymbol{G}$ (closure),
2. $(AB)C=A(BC)$ (associativity),
3. $\boldsymbol{G}$ contains E such that $EA=AE=A$ for any $A \in \boldsymbol{G}$ (E is unit element),
4. for every $A \in \boldsymbol{G}$ there exists A^{-1} such that $AA^{-1}= A^{-1}A=E$ (A^{-1} is inverse of A).

Notes:

The sequence of listing the elements does not matter.

The multiplication need not be commutative ($AB=BA$).

If it is, the group is called Abelian.

Example of a group: permutations of three symbols $P(3)$

3!=6 elements (the group *is of order* 6),

$E=(123)$ $A=(132)$ $B=(321)$ $C=(213)$ $D=(312)$ $F=(231)$

mean the final arrangement of the three symbols from the initial (123)

the multiplication means the sequential permutation of the three symbols: *AD* ... first *D*, then *A*

Multiplication table

right left	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D

$\underline{P(3)\text{ as (3x3) matrix multiplications}}$ ("row times column")

E=(123)

$$\begin{bmatrix}1\\2\\3\end{bmatrix}=\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}\begin{bmatrix}1\\2\\3\end{bmatrix}$$

A=(132)

$$\begin{bmatrix}1\\3\\2\end{bmatrix}=\begin{bmatrix}1&0&0\\0&0&1\\0&1&0\end{bmatrix}\begin{bmatrix}1\\2\\3\end{bmatrix}$$

B=(321)

$$\begin{bmatrix}3\\2\\1\end{bmatrix}=\begin{bmatrix}0&0&1\\0&1&0\\1&0&0\end{bmatrix}\begin{bmatrix}1\\2\\3\end{bmatrix}$$

C=(213)

$$\begin{bmatrix}2\\1\\3\end{bmatrix}=\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix}\begin{bmatrix}1\\2\\3\end{bmatrix}$$

D=(312)

$$\begin{bmatrix}3\\1\\2\end{bmatrix}=\begin{bmatrix}0&0&1\\1&0&0\\0&1&0\end{bmatrix}\begin{bmatrix}1\\2\\3\end{bmatrix}$$

F=(231)

$$\begin{bmatrix}2\\3\\1\end{bmatrix}=\begin{bmatrix}0&1&0\\0&0&1\\1&0&0\end{bmatrix}\begin{bmatrix}1\\2\\3\end{bmatrix}$$

$$AD=\begin{bmatrix}1&0&0\\0&0&1\\0&1&0\end{bmatrix}\begin{bmatrix}0&0&1\\1&0&0\\0&1&0\end{bmatrix}=\begin{bmatrix}0&0&1\\0&1&0\\1&0&0\end{bmatrix}=B$$

$$DA=\begin{bmatrix}0&0&1\\1&0&0\\0&1&0\end{bmatrix}\begin{bmatrix}1&0&0\\0&0&1\\0&1&0\end{bmatrix}=\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix}=C$$

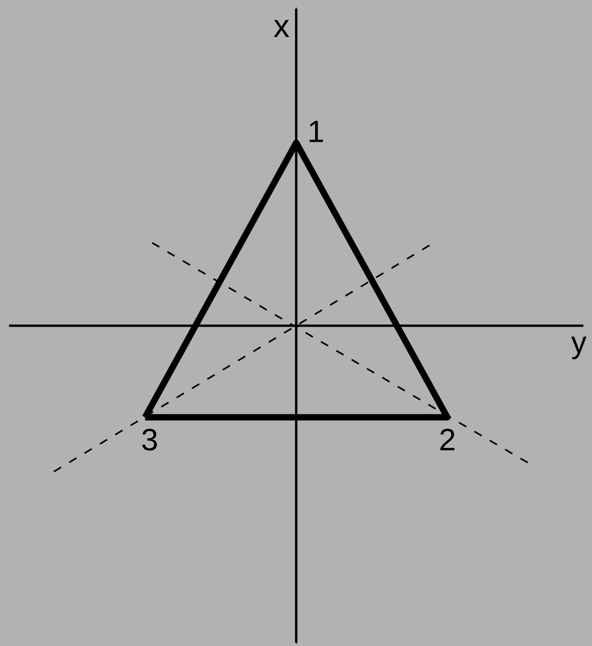
$P(3)$ as the set of (2x2) matrices (can these permute three objects?)

$$E = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad A = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \qquad B = \frac{1}{2}\begin{bmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$$

$$C = \frac{1}{2}\begin{bmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix} \qquad D = \frac{1}{2}\begin{bmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix} \qquad F = \frac{1}{2}\begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$$

$$AD = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} \frac{1}{2}\begin{bmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix} = B$$

$P(3)$ represents the symmetry operations on an equilateral triangle, the group C_{3v}



$$\begin{bmatrix} y_A \\ x_A \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} y \\ x \end{bmatrix} = \begin{bmatrix} -y \\ x \end{bmatrix}$$

$$E = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$ no change

$$A = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$ 2↔3, mirror reflection in $(x,z),(1,z)$

$$B = \frac{1}{2}\begin{bmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$$ 1↔3, mirror reflection in $(2,z)$

$$C = \frac{1}{2}\begin{bmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$$ 1↔2, mirror reflection in $(3,z)$

$$D = \frac{1}{2}\begin{bmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$$ 1,2,3→3,1,2, rotation by $2\pi/3$ about z

$$F = \frac{1}{2}\begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$$ 1,2,3→2,3,1, rotation by $4\pi/3$ about z

Further terminology and properties

1. The order of $\boldsymbol{G}$: the number of its elements; $P(3)$ is of order 6.

2. A subgroup of $\boldsymbol{G}$: a set of its elements forming a group;
   the subgroups of $P(3)$: (E), (E,A), (E,B), (E,C), (E,D,F).
   The order of a subgroup is a divisor of the order of the group.

3. The order n of $A \in \boldsymbol{G}$: the smallest value in $A^n=E$;
   in $P(3)$, E is of order 1, A,B,C are of order 2, D,F are of order 3.

4. The period of $A \in \boldsymbol{G}$ is the Abelian subgroup $(E,A, A^2 ,\ldots, A^{n-1})$, where n is the order of A; the periods of $P(3)$: (E), (E,A), (E,B), (E,C), $(E,D,D^2)=(E, F,F^2)$ $=(E,D,F)$.

Further terminology and properties, continued

5. Let $\boldsymbol{S}\equiv(E,S_1,S_2,\ldots,S_g)$ be a subgroup of $\boldsymbol{G}$ and $X\in\boldsymbol{G}$. The right coset of $\boldsymbol{S}$ is the set $(EX, S_1X,S_2X, \ldots,S_gX)$, the left coset is $(XE,XS_1,XS_2, \ldots,XS_g)$. A coset need not be a group. A coset will itself be a subgroup $\boldsymbol{S}$ if $X\in\boldsymbol{S}$. Two cosets of a given subgroup either contain the same elements, or have no elements in common.

   Examples using $P(3)$: Let $\boldsymbol{S}\equiv(E,A)$. The right cosets of $\boldsymbol{S}$ are $(E,A)E= (E,A)A=(E,A)$ which is a subgroup, and $(E,A)B= (E,A)D= (B,D)$ and $(E,A)C= (E,A)F= (C,F)$ which are not subgroups. The left cosets of (E,A) are (E,A), (C,D) and (B,F).

6. An element $B\in\boldsymbol{G}$ is called conjugate to $A\in\boldsymbol{G}$ if $B=XAX^{-1}$, where X is an arbitrary element of $\boldsymbol{G}$. If B is conjugate to A and C is conjugate to B , then C is conjugate to A.

7. A class is the set of elements of which is obtained from a given element of $\boldsymbol{G}$ by conjugation. The unit element is the only class forming a subgroup. All elements of a class have the same order. An Abelian group has as many classes as elements. There are three classes in $P(3)$: (E), (A,B,C), and (D,F).

The notion of class is very important; checking the classes of $P(3)$:

class (a helpful look at the inverses, $A^{-1}=A$, $B^{-1}=B$, $C^{-1}=C$, $D^{-1}=F$, $F^{-1}=D$):

(E) trivial, since $XEX^{-1}=E$ for any $X \in \mathbf{G}$,

(A,B,C) elements of the order of 2, red in the multiplication table,

(D,F) elements of the order of 3, green in the multiplication table;

if one product in the conjugation is outside a class, the other "brings it back"

right / left	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D

Further terminology and properties, continued

8. A subgroup $\boldsymbol{N}$ of $\boldsymbol{G}$ is called self—conjugate (or invariant, or normal) if $X\boldsymbol{N}X^{-1}=\boldsymbol{N}$, where X is an arbitrary element of $\boldsymbol{G}$.

   To obtain a self—conjugate subgroup, it is necessary to include entire classes in it. The right and left cosets of a self—conjugate subgroup are the same. The products of the elements of two right cosets of a self—conjugate subgroup form another right coset.

   For example, (E,D,F) is a self—conjugate subgroup of $P(3)$, while (E,A), (E,B), (E,C) are not; the right and left cosets $(E,D,F)A=(A,C,B)$ and $A(E,D,F)=(A,B,C)$ are the same; the products $(A,C,B)(E,D,F)$ form the right coset (A,B,C), the products $(A,B,C)(A,B,C)$ form the right coset (E,D,F).

9. A group with no self—conjugate subgroups is called simple group.

Further terminology and properties, continued

10. The factor group of $\boldsymbol{G}$ results from a self—conjugate subgroup $\boldsymbol{N}$ as the set of its cosets, i.e., each coset being considered an element of the factor group.

    $\boldsymbol{N}$ is sometimes called a normal divisor.

    Obviously, all four rules of the multiplication are satisfied:

    1. The closure: $(N_iX)(N_jY)=N_i(XN_j\,)Y=N_i(N_kX)Y=(N_iN_k)(XY)$ for $X,Y\in\boldsymbol{G}$ and $N_i,N_j,N_k\in\boldsymbol{N}$, $N_k=XN_j\,X^{-1}$.
    2. The associativity holds because it holds for the elements of $\boldsymbol{G}$.
    3. The unit element of the factor group is the coset containing $E\in\boldsymbol{G}$.
    4. The inverse element exists: $(X\boldsymbol{N})(X^{-1}\boldsymbol{N})= (\boldsymbol{N}X)(X^{-1}\boldsymbol{N})=\boldsymbol{NN}=\boldsymbol{N}$.

11. The index of a subgroup is the total number of cosets.

    The order of the factor group is the index of the self—conjugate subgroup.

Further terminology and properties, continued

For example, $\mathcal{E}$=(E,D,F) is a self—conjugate subgroup of P(3), $\mathcal{A}$=(A,B,C) is the only other (both right and left) coset. $\mathcal{E}$ and $\mathcal{A}$ form the (Abelian) factor group with the multiplication table

	$\mathcal{E}$	$\mathcal{A}$
$\mathcal{E}$	$\mathcal{E}$	$\mathcal{A}$
$\mathcal{A}$	$\mathcal{A}$	$\mathcal{E}$

This group is isomorphic (equivalent, one—to—one correspondence) with the group P(2) of the permutations of 2 objects, or with the subgroups (E,A), (E,B), (E,C) of P(3).

Representation theory

Two groups, $\boldsymbol{G}=(A,B,C,D,...)$ and $\boldsymbol{g}=(u,v,...)$ are homomorphic, if there exists a mapping (correspondence) of $\boldsymbol{G}$ into $\boldsymbol{g}$, e.g.,

$A \to u$, $(B,C) \to v$,...,

such that

$AB \to uv$, $AC \to uv$,...

If the correspondence is one—to—one (the orders of $\boldsymbol{G}$ and $\boldsymbol{g}$ are the same), the two groups are isomorphic.

For example, the mapping of $P(3)$ into $P(2)$,

$(E,D,F) \to \mathcal{E}$, $(A,B,C) \to \mathcal{A}$

is homomorphism. The correspondence of the permutation group $P(3)$ with the symmetry group of an equilateral triangle is isomorphism.

Representation theory

Homomorphism or isomorphism of a group ***G*** with a group of square matrices is called a representation of ***G***.

A matrix $D(A)$ is assigned to each $A \in \boldsymbol{G}$ such that $D(AB)=D(A)D(B)$, with the usual way of multiplication of square matrices ("row times column").

An example of a homomorphic representation of the permutation group P(3) is the group of two one—dimensional matrices [1], [-1]:

$$(E,D,F) \rightarrow [1],\ (A,B,C) \rightarrow [-1]\ .$$

The multiplication table of this matrix group is

	[1]	[-1]
[1]	[1]	[-1]
[-1]	[-1]	[1]

Representation theory

Another easily found homomorphic representation of the permutation group P(3) is the group consisting of the single one—dimensional matrix [1]:

$$(E, A, B, C, D, F) \rightarrow [1].$$

The multiplication table of this matrix group is

	[1]
[1]	[1]

The one—dimensional representation [1] is a representation of any group.

Representation theory

An isomorphic representation of the permutation group P(3) is the group of the following six three—dimensional matrices:

(they permute the elements of column or row vectors by the usual multiplication)

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

$$D(C)=\begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix}\qquad D(D)=\begin{bmatrix}0&0&1\\1&0&0\\0&1&0\end{bmatrix}\qquad D(F)=\begin{bmatrix}0&1&0\\0&0&1\\1&0&0\end{bmatrix}$$

Representation theory

Another isomorphic representation of the permutation group $P(3)$ is the group of the following six two—dimensional matrices:

(remember the transformation of the positions of vertices of the equilateral triangle)

$$D(E)=\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix} \qquad D(A)=\begin{bmatrix}-1 & 0\\ 0 & 1\end{bmatrix} \qquad D(B)=\frac{1}{2}\begin{bmatrix}1 & -\sqrt{3}\\ -\sqrt{3} & -1\end{bmatrix}$$

$$D(C)=\frac{1}{2}\begin{bmatrix}1 & \sqrt{3}\\ \sqrt{3} & -1\end{bmatrix} \qquad D(D)=\frac{1}{2}\begin{bmatrix}-1 & \sqrt{3}\\ -\sqrt{3} & -1\end{bmatrix} \qquad D(F)=\frac{1}{2}\begin{bmatrix}-1 & -\sqrt{3}\\ \sqrt{3} & -1\end{bmatrix}$$

Representation theory

In general, the representations are built from square matrices with complex elements. The symbol * denotes complex conjugation, T denotes transposition, and + denotes the adjoint:

$$D = \begin{bmatrix} d_{11} & d_{12} & \ldots \\ d_{21} & d_{22} & \ldots \\ \ldots & & \end{bmatrix}, \qquad D^T = \begin{bmatrix} d_{11} & d_{21} & \ldots \\ d_{12} & d_{22} & \ldots \\ \ldots & & \end{bmatrix}, \qquad D^+ = \begin{bmatrix} d_{11}^* & d_{21}^* & \ldots \\ d_{12}^* & d_{22}^* & \ldots \\ \ldots & & \end{bmatrix}.$$

Hermitian matrices are defined by $D^T = D^*$, or $D^+ = D$.

Unitary matrices are defined by $D^+ = D^{-1}$.

Unitary matrices preserve the norms of vectors:

$(Dv)^+ Dv = (v^+ D^+)(Dv) = v^+ v$, where v is a column vector, v^+ is the adjoint row vector.

The dimensionality of a representation is the dimensionality (the number of rows and columns) of its matrices.

Representation theory

The representations are not unique. A simple way of generating a new set of representing matrices is combining them according to

$$D(A) = \begin{bmatrix} D_n(\mathrm{A}) & O \\ O^T & D_m(\mathrm{A}) \end{bmatrix},$$

where $D_n(A)$ and $D_m(A)$ are matrices of an n— and m—dimensional representations, respectively, and O is a $n \times m$ matrix of zeros. The block form of the above $D(A)$ matrices means, that this representation is reducible (it contains at least two representations). The zero matrix "separates" the two representations in the combined matrices.

Further, performing a similarity transformation

$$UD(A)U^{-1}$$

provides a new representation, called equivalent.

Representation theory

If a similarity transformation leads to the same block form of the matrices, the representation is called reducible; otherwise it is irreducible. In other words, an irreducible representation cannot be expressed in terms of lower—dimensional representations.

Three irreducible representations of $P(3)$ are:

group element: symbol (label)	E	A	B	C	D	F
Γ_1	[1]	[1]	[1]	[1]	[1]	[1]
$\Gamma_{1'}$	[1]	[-1]	[-1]	[-1]	[1]	[1]
Γ_2	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$

Representation theory

An example of a reducible representation Γ_R of $P(3)$ is:

	E	A	B	...
Γ_R	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{-\sqrt{3}}{2} \\ 0 & 0 & \frac{-\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}$	...

The irreducible representations contained in the reducible representation Γ_R are usually listed as:

$$\Gamma_R = \Gamma_1 + \Gamma_{1'} + \Gamma_2 \, .$$

Representation theory

Among different representations, those formed by unitary matrices are of special importance. Every representation ($D(A_j)$, j=1,...,n) with nonvanishing determinants can be brought into the unitary form by a similarity transformation. This is easily seen by inspecting the Hermitian matrix

$$H = \sum_{j=1}^{n} D_j D_j^{+},$$

which can be diagonalized by the unitary transformation U formed from the set of orthonormal eigenvectors of H:

$$H_d = U^{-1} H U.$$

All elements of the diagonal matrix H_d are positive; we can therefore construct its square root and find the wanted similarity transformation as:

$$D_u(A_j) = H_d^{-1/2} U^{-1} D(A_j) U H_d^{1/2}.$$

Representation theory

It can easily be shown that the matrices D_u are unitary:

$$D_u(A_j)D_u^+(A_j) = H_d^{-1/2}U^{-1}D(A_j)UH_d^{1/2}(H_d^{-1/2}U^{-1}D(A_j)UH_d^{1/2})^+$$

$$= H_d^{-1/2}U^{-1}D(A_j)UH_dU^{-1}D^+(A_j)UH_d^{-1/2}$$

$$= H_d^{-1/2}U^{-1}D(A_j)U[\sum_{k=1}^{n}U^{-1}D(A_k)UU^{-1}D^+(A_k)U]U^{-1}D^+(A_j)UH_d^{-1/2}$$

$$= H_d^{-1/2}[\sum_{k=1}^{n}U^{-1}D(A_j)D(A_k)UU^{-1}D^+(A_k)D^+(A_j)U]H_d^{-1/2} = I,$$

where I is the unit matrix. The sum in the last row is obviously the diagonal matrix H_d, since the multiplication by the fixed matrix $D(A_j)$ merely rearranges the elements of the representation.

Representation theory

The irreducible representation has the following two properties concerning the commutation properties,

$$MD(A_j) = D(A_j)M\,,\; j = 1,\ldots,n,$$

with auxiliary matrices M (Schur's first and second lemma):

1. The only matrix commuting with all matrices of the irreducible representation is a const.$\times I$. If a non—constant commuting matrix exists, the representation is reducible.
2. If the representations ($D_a(A_j)$, j=1,...,n) and ($D_b(A_j)$, j=1,...,n) of a given group are of dimensionalities d_a and d_b, respectively, then if there is a $d_a \times d_b$ matrix M such that $$MD_a(A_j) = D_b(A_j)M\,,\; j = 1,\ldots,n,$$

then M must be the null matrix if a $d_a \neq d_b$. For a $d_a = d_b$, M is nonzero only for the two representations differing by a similarity transformation, i.e., equivalent.

Representation theory - orthogonality of irreducible representations

The irreducible representations ($D_a(A_j)$, j=1,...,n) and ($D_b(A_j)$, j=1,...,n) of a given group, of dimensionalities d_a and d_b, respectively, obey the following great orthogonality theorem:

$$\sum_{j=1}^{n} D_{a,rs}(A_j) D_{b,tu}(A_j^{-1}) = \frac{n}{d_a} \delta_{ab} \delta_{rt} \delta_{su},$$

where $D_{a,rs}$ is the element of D_a from the r-th row and s-th column, and δ_{ab} the Kronecker symbol: δ_{ab} =1 for $a=b$ and δ_{ab} =0 for $a \neq b$.

For unitary representations, the above relation simplifies to

$$\sum_{j=1}^{n} D_{a,rs}(A_j) D^{*}_{b,tu}(A_j) = \frac{n}{d_a} \delta_{ab} \delta_{rt} \delta_{su}. \qquad \text{(GOT)}$$

Representation theory- orthogonality of irreducible representations

The irreducible representations of $P(3)$:

	E	A	B	C	D	F
Γ_1	[1]	[1]	[1]	[1]	[1]	[1]
$\Gamma_{1'}$	[1]	[-1]	[-1]	[-1]	[1]	[1]
Γ_2	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$

They are orthogonal:

1. The sum in (GOT) for Γ_1 and $\Gamma_{1'}$ vanishes: as many [1]'s as [-1]'s, the sum is [0].
2. The sum in (GOT) for Γ_1 and Γ_2 vanishes:

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} + \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

Representation theory - orthogonality of irreducible representations

The irreducible representations of $P(3)$:

	E	A	B	C	D	F
Γ_1	[1]	[1]	[1]	[1]	[1]	[1]
$\Gamma_{1'}$	[1]	[-1]	[-1]	[-1]	[1]	[1]
Γ_2	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$

3. The sum in (GOT) for $\Gamma_{1'}$ and Γ_2 vanishes:

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix} - \frac{1}{2}\begin{bmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix} - \frac{1}{2}\begin{bmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

Representation theory - orthogonality of irreducible representations

The irreducible representations of $P(3)$:

	E	A	B	C	D	F
Γ_1	$[1]$	$[1]$	$[1]$	$[1]$	$[1]$	$[1]$
$\Gamma_{1'}$	$[1]$	$[-1]$	$[-1]$	$[-1]$	$[1]$	$[1]$
Γ_2	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$

The sums in (GOT) for $a=b$ are:

$$\Gamma_1: \quad [1]^2+[1]^2+[1]^2+[1]^2+[1]^2+[1]^2=[6].$$

$$\Gamma_{1'}: \quad [1]^2+[-1]^2+[-1]^2+[-1]^2+[1]^2+[1]^2=[6].$$

$$\Gamma_2: \quad \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}^2+\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}^2+\frac{1}{4}\begin{bmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}^2+\frac{1}{4}\begin{bmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}^2+\frac{1}{4}\begin{bmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}^2+\frac{1}{4}\begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}^2=\begin{bmatrix} 3 & 0 \\ 0 & 3 \end{bmatrix}.$$

Representation theory - orthogonality of irreducible representations

The irreducible representations of $P(3)$:

	E	A	B	C	D	F
Γ_1	[1]	[1]	[1]	[1]	[1]	[1]
$\Gamma_{1'}$	[1]	[-1]	[-1]	[-1]	[1]	[1]
Γ_2	$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}$	$\frac{1}{2}\begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}$

The sums in (GOT) for $a=b=\Gamma_2$ are:

$$\sum_{j=1}^{n}\sum_{m=1}^{2} D_{rm}(A_j) D_{mu}(A_j) = \frac{n}{d_a}\sum_{m=1}^{2}\delta_{rm}\delta_{mu} = \frac{n}{d_a}\delta_{ru},$$

$$\Gamma_2: \quad \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}^2 + \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}^2 + \frac{1}{4}\begin{bmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}^2 + \frac{1}{4}\begin{bmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}^2 + \frac{1}{4}\begin{bmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{bmatrix}^2 + \frac{1}{4}\begin{bmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{bmatrix}^2 = \begin{bmatrix} 3 & 0 \\ 0 & 3 \end{bmatrix}.$$

Representation theory - orthogonality of irreducible representations

The relations of (GOT) can be interpreted in the following way. The matrix elements of a unitary irreducible representation can be arranged in a set of (row or column) vectors in the space of dimensionality n (order of the group):

$$v_{a,rs} = \sqrt{d_a / n}[D_{a,rs}(A_1), D_{a,rs}(A_1), ..., D_{a,rs}(A_n)].$$

Individual vectors of this set are labeled by the symbol of the representation, a, and by the indices r and s of the row and column, respectively. All these vectors are mutually orthogonal ("projections on other members of the family vanish"). In addition, the inclusion of the normalization factor of the square root ensures the normalization (the square of the length of the vector is unity):

$$v_{a,rs} v^{+}_{a,rs} = 1.$$

The maximum number of orthogonal vectors in the n--dimensional space is n.

Representation theory - orthogonality of irreducible representations

The irreducible representations Γ_1, $\Gamma_{1'}$, and Γ_2 of $P(3)$ contain the following set of orthonormal vectors:

normalization factor	v_1	v_2	v_3	v_4	v_5	v_6
$1/\sqrt{6}$	1	1	1	1	1	1
$1/\sqrt{6}$	1	-1	-1	-1	1	1
$1/\sqrt{3}$	1	-1	1/2	1/2	-1/2	-1/2
1	0	0	-1/2	1/2	1/2	-1/2
1	0	0	-1/2	1/2	-1/2	1/2
$1/\sqrt{3}$	1	1	-1/2	-1/2	-1/2	-1/2

Representation theory - characters

The matrices $(D_a(A_j), j=1,\ldots,n)$ of a given representation are very useful in dealing with the group $\boldsymbol{G}$; however, they suffer from the arbitrariness with regard to similarity transformation , UD_aU^{-1}. Consequently, there is a reduction of information content circumventing this arbitrariness.

Let $\chi_a(A_j)$ denote the trace of the matrix $D_a(A_j)$,

$$\chi_a(A_j) = \mathrm{Tr}\left\{D_a(A_j)\right\} = \sum_{j=1}^{d_a} D_{a,jj}.$$

The set of the traces for all group elements,

$$\chi_a(A_1), \chi_a(A_2), \ldots, \chi_a(A_n),$$

is called the character of the representation (D_a). Since

$$\mathrm{Tr}\left\{UD\right\} = \sum_j \left(\sum_k U_{jk} D_{kj}\right) = \sum_k \left(\sum_j D_{kj} U_{jk}\right) = \mathrm{Tr}\left\{DU\right\},$$

the similarity transformation does not change the character of a representation:

$$\mathrm{Tr}\left\{UDU^{-1}\right\} = \mathrm{Tr}\left\{U(DU^{-1})\right\} = \mathrm{Tr}\left\{(DU^{-1})U\right\} = \mathrm{Tr}\left\{D(U^{-1}U)\right\} = \mathrm{Tr}\left\{D\right\}.$$

Equivalent representations are related to each other by a similarity transformation → they have the same character.

Representation theory - characters

The group elements within a class are related by conjugation, the corresponding representation matrices by a similarity transformation→ the corresponding entries in the character of any representation are the same.

Character table of the irreducible representations of $P(3)$:

character / representation	$\chi(E)$	$\chi(A)$	$\chi(B)$	$\chi(C)$	$\chi(D)$	$\chi(F)$
Γ_1	1	1	1	1	1	1
$\Gamma_{1'}$	1	-1	-1	-1	1	1
Γ_2	2	0	0	0	-1	-1

Its economized version (listing only the classes):

class / representation	$\boldsymbol{C}_1=(E)$	$\boldsymbol{C}_2=(A,B,C)$	$\boldsymbol{C}_3=(D,F)$
Γ_1	1	1	1
$\Gamma_{1'}$	1	-1	1
Γ_2	2	0	-1

Representation theory - characters

Characters of irreducible representations ($D_a(A_j)$, j=1,...,n) and ($D_b(A_j)$, j=1,...,n) satisfy the orthogonality relations:

$$\sum_{j=1}^{n} \chi_a(A_j)\chi_b^*(A_j) = n\delta_{ab},$$

which follow easily from the great orthogonality theorem for the matrices. The characters also satisfy the second orthogonality relation, containing a sum over classes instead of the group elements:

$$\sum_k \sqrt{\frac{n_k}{n}}\chi_a(C_k)\sqrt{\frac{n_k}{n}}\chi_b^*(C_k) = \delta_{ab},$$

where $\chi_a(C_k)$ is the (common) entry in the character of the k-th class, formed by n_k elements. The number of classes, n_c, is equal to the number of inequivalent irreducible representations , n_k. This is the maximum number of mutually orthogonal vectors in the n_c-dimensional space.

Representation theory - characters

The orthogonality of the rows of the character table of the irreducible representations of $P(3)$ can be checked by inspection:

character / representation	$\chi(E)$	$\chi(A)$	$\chi(B)$	$\chi(C)$	$\chi(D)$	$\chi(F)$
Γ_1	1	1	1	1	1	1
$\Gamma_{1'}$	1	-1	-1	-1	1	1
Γ_2	2	0	0	0	-1	-1

as well as the orthogonality of the columns of the table containing classes:

class / representation	$\boldsymbol{C}_1=(E)$	$\boldsymbol{C}_2=(A,B,C)$	$\boldsymbol{C}_3=(D,F)$
Γ_1	1	1	1
$\Gamma_{1'}$	1	-1	1
Γ_2	2	0	-1

Representation theory - constructing character tables

After finding classes, the following properties of representations are useful for the construction of character tables:

(1) The number n_r of inequivalent irreducible representations is equal to the number of classes, n_c=n_r.

(2) The sum of squares of the dimensionalities, d_j, j=1,..., n_r , is equal to the order n of the group.

(3) There is always one identity representation, showing up as a row of 1s.

(4) There is always one class composed of the identity element, showing up as a column with the traces of unity matrices, i.e., the dimensionalities.

(5) The orthogonality of characters applies, both for rows and columns.

Representation theory - constructing character tables of P(3), isomorphic with C_{3v} using the Schoenfliess notation for symmetry operations of point groups

E: identity; needed in order to form a group.

C_n: rotation by $2\pi/n$; the rotation axis is called n-fold.
The axis of highest n, called principal, is "vertical".

σ: reflection in a plane, with three kinds of suffixes.

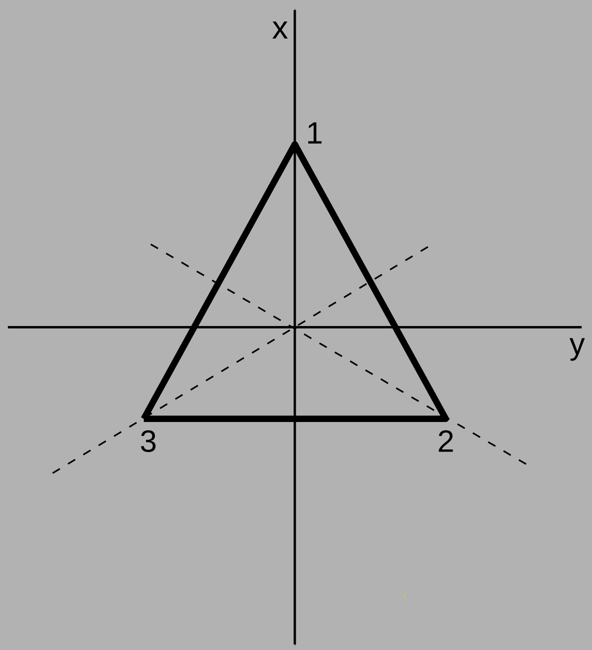
σ_h: reflection in a horizontal plane.

σ_v: reflection in a vertical plane.

σ_d: reflection in a vertical diagonal plane.

I: inversion, $x \leftrightarrow -x$, $y \leftrightarrow -y$, $z \leftrightarrow -z$.

S_n : improper rotation by $2\pi/n$, consisting of the rotation by $2\pi/n$, followed by a reflection in a horizontal plane ($\sigma_h C_n$).



class:	E	$3\sigma_v$	$2C_3$
symmetry operations:	identity	mirror plane 1 mirror plane 2 mirror plane 3	rotation by $2\pi/3$ rotation by $4\pi/3$

Representation theory - constructing character tables of P(3), isomorphic with C_{3v}

The first row and column are trivial:

class / representation	E	$3\sigma_v$	$2C_3$
Γ_1	1	1	1
$\Gamma_{1'}$	1		
Γ_2	2		

The second row has to be orthogonal to the first, with the proper value of the summed squares:

class / representation	E	$3\sigma_v$	$2C_3$
Γ_1	1	1	1
$\Gamma_{1'}$	1	-1	1
Γ_2	2		

The second and third columns have to be orthogonal to the first:

class / representation	E	$3\sigma_v$	$2C_3$
Γ_1	1	1	1
$\Gamma_{1'}$	1	-1	1
Γ_2	2	0	-1

done!

A résumé of the symmetry group C_{3v} (isomorphic with $P(3)$)

using the example of the ammonia (NH_3) molecule (N out of the plane of H_3):

6 symmetry operations, , 6-dimensional space of orthogonal vectors forming the characters

3 classes of conjugate elements, 3x3 table of characters

class / representation	E	$3\sigma_v$	$2C_3$
Γ_1	1	1	1
$\Gamma_{1'}$	1	-1	1
Γ_2	2	0	-1