Representations of crystallographic groups

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Overview.

General introduction to representation theory.

- Group actions, Group representations
- Equivalence of representations
- Invariant subspaces and reducibility
- Characters and character tables
- Theorems of orthogonality
- Direct products of irreps and their reduction into irreps

Representations of point groups.

- Representations of Abelian groups
- Character tables and irreps of point groups
- Vector and pseudovector representations of point groups
- Basis functions of irreps
- Molecular vibrations

Group action.

Definition.

A group action of a group $\mathcal{G}$ on a set Ω assigns to each pair (g, ω) an element $\omega' = g(\omega)$ of Ω such that the following hold:

(i) $g(h(\omega)) = (gh)(\omega)$;

(ii) $e(\omega) = \omega$ for the identity element e of $\mathcal{G}$.

The set $\omega^{\mathcal{G}} = \{g(\omega) \mid g \in \mathcal{G}\}$ of all elements to which ω is mapped is called the orbit of ω under $\mathcal{G}$.

Example.

A group $\mathcal{G}$ acts on itself by:

- left multiplication: $g(h) = gh$;
- right multiplication: $g(h) = hg^{-1}$;
- conjugation: $g(h) = ghg^{-1}$, the orbits are precisely the conjugacy classes of $\mathcal{G}$.

More examples.

- The symmetry group of a square acts on the corners, sides and diagonals of the square.

  Some group elements act trivially on the diagonals.
- The rotation group of a cube acts on the edge centers, face centers, space diagonals of the cube.

  The action on the space diagonals gives an isomorphism with the group S_4 of all permutations of 4 objects.
- A group $\mathcal{G}$ of real $n \times n$ matrices acts on the vectors $\mathbf{v}$ in $\mathbb{R}^n$ by the usual multiplication of matrices with column vectors: $g(\mathbf{v}) = g \cdot \mathbf{v}$.
- A point group $\mathcal{G}$ acts on the coordinates x, y, z and on functions of the coordinates, such as $xy + yz + z^2$.

Group representations.

Definition.

Let $\mathcal{G}$ be a group acting linearly on a vector space $\mathbf{V}$, i.e. such that

$$g(\mathbf{v}+\mathbf{w}) = g(\mathbf{v}) + g(\mathbf{w}) \text{ and } g(\lambda\mathbf{v}) = \lambda g(\mathbf{v}).$$

Then the mapping $\mathbf{D} : \mathcal{G} \to \mathrm{GL}(\mathbf{V})$, which assigns to each element g of $\mathcal{G}$ the linear operator $\mathbf{D}(g)$ by which it acts on $\mathbf{V}$ is called a representation of $\mathcal{G}$ on $\mathbf{V}$.

Once a basis $(\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_n)$ for $\mathbf{V}$ is chosen, the representation is realized by $n \times n$ matrices. Viewed this way, a representation is a homomorphism

$$\mathbf{D} : \mathcal{G} \to \mathrm{GL}_n(K),$$

where K is the field of scalars underlying the vector space $\mathbf{V}$.

Unless stated otherwise, we will exclusively deal with complex representations, i.e. we have $\mathbf{D} : \mathcal{G} \to \mathrm{GL}_n(\mathbb{C})$.

Definition.

For a representation $\mathbf{D}$ on a vector space $\mathbf{V}$, the dimension of $\mathbf{V}$, i.e. the size of the matrices, is called the degree or dimension of $\mathbf{D}$, denoted by $\deg(\mathbf{D})$ or $\dim(\mathbf{D})$.

Examples.

- Every group $\mathcal{G}$ has a representation of degree 1, called the trivial representation of $\mathcal{G}$, which maps every group element g to 1.
- The cyclic group $\mathcal{C}_n$ of order n generated by an element g has a 1-dimensional representation $\mathbf{D}$ given by

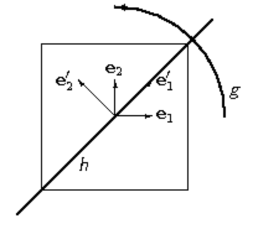
$$\mathbf{D}(g) = \exp(2\pi i/n).$$

- The group $SO_2(\mathbb{R})$ of rotations on $\mathbb{R}^2$ has a representation $\mathbf{D}$ of degree 2 which maps a rotation $\mathbf{r}_\varphi$ by the angle φ to

$$\mathbf{D}(\mathbf{r}_\varphi) = \begin{pmatrix} \cos(\varphi) & -\sin(\varphi) \\ \sin(\varphi) & \cos(\varphi) \end{pmatrix}.$$

Example.

The symmetry group *4mm* of a square can be generated by a fourfold rotation g and a diagonal reflection h in the line $x = y$.



- With respect to the basis $\mathbf{e}_1, \mathbf{e}_2$, the action of *4mm* on $\mathbb{R}^2$ gives rise to the representation $\mathbf{D}$ with

$$\mathbf{D}(g) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{D}(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

- With respect to the different basis $\mathbf{e}_1', \mathbf{e}_2'$, we obtain a different representation $\mathbf{D}'$ with

$$\mathbf{D}'(g) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{D}'(h) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Exercise 1.

In the *Klein fourgroup* $\mathcal{C}_2 \times \mathcal{C}_2 = \{e, g, h, gh\}$, the elements g, h, gh all have order 2. Is

$$\mathbf{D} : e \mapsto 1, \quad g \mapsto -1, \quad h \mapsto -1, \quad gh \mapsto -1$$

a representation of $\mathcal{C}_2 \times \mathcal{C}_2$?

Exercise 2.

A group $\mathcal{G}$ has a representation $\mathbf{D}$ such that for two elements g, h of $\mathcal{G}$ one has

$$\mathbf{D}(g) = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad \mathbf{D}(h) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Determine $\mathbf{D}(gh)$, $\mathbf{D}(g^2)$, $\mathbf{D}(h^2)$ and $\mathbf{D}(hg)$. Is $\mathcal{G}$ an Abelian group?

Exercise 3.

Show that for a point group $\mathcal{G} \leq \mathrm{GL}_3(\mathbb{R})$, the mapping $g \mapsto \det(g)$ is a representation of degree 1 of $\mathcal{G}$.
What is the kernel of this representation?

Some typical representations.

Vector representation.

If a group $\mathcal{G}$ is a group of $n \times n$ matrices (e.g. a point group $\mathcal{G} \leq \mathrm{GL}_3(\mathbb{R})$), then the identical mapping $g \mapsto g$ is a representation, called the vector representation or natural representation of $\mathcal{G}$.

Conjugate representation.

For a complex representation $\mathbf{D}$ of a group $\mathcal{G}$, replacing all matrix entries in $\mathbf{D}(g)$ by their complex conjugates yields another representation of $\mathcal{G}$, called the conjugate representation of $\mathbf{D}$ and denoted by $\mathbf{D}^*$.

Example.

$$\text{If } \mathbf{D}(g) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \text{ then } \mathbf{D}^*(g) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}.$$

Equivalence of representations.

Definition.

Two representations $\mathbf{D}$ and $\mathbf{D}'$ of a group $\mathcal{G}$ are called equivalent if there exists an invertible $n \times n$ matrix $\mathbf{X}$ such that

$$\mathbf{D}'(g) = \mathbf{X}^{-1}\mathbf{D}(g)\mathbf{X}$$

Why should we call these representations equivalent?

- Let the matrices of $\mathbf{D}$ represent the action of $\mathcal{G}$ on $\mathbf{V}$ with respect to a basis $\mathbf{v}_1, \ldots, \mathbf{v}_n$.
- Think of $\mathbf{X}$ as a basis transformation from $\mathbf{v}_1, \ldots, \mathbf{v}_n$ to a new basis $\mathbf{v}'_1, \ldots, \mathbf{v}'_n$ of $\mathbf{V}$.
- Then $\mathbf{D}'$ expresses the same action of $\mathcal{G}$ on $\mathbf{V}$ with respect to the new basis $\mathbf{v}'_1, \ldots, \mathbf{v}'_n$.

That's why!

Example.

The dihedral group $\mathcal{D}_3$ of order 6 is generated by an element g of order 3 and an element of order h such that $hgh = g^2$.

The 2-dimensional representations

$$\mathbf{D}(g) = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} = \begin{pmatrix} \cos(2\pi/3) & -\sin(2\pi/3) \\ \sin(2\pi/3) & \cos(2\pi/3) \end{pmatrix}, \quad \mathbf{D}(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\mathbf{D}'(g) = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad \mathbf{D}'(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

are equivalent via the conjugating matrix $\mathbf{X} = \begin{pmatrix} 1 & -2+\sqrt{3} \\ -2+\sqrt{3} & 1 \end{pmatrix}$.

The first representation expresses the action with respect to an orthonormal basis, the second with respect to a hexagonal basis.

Exercise 4.

Let the cyclic group $\mathcal{C}_4$ of order 4 be generated by the element g. Two of the following three representations of $\mathcal{C}_4$ are equivalent:

$$\mathbf{D}(g) = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad \mathbf{D}'(g) = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \mathbf{D}''(g) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

Determine which two are equivalent, find a conjugating matrix and give an argument why the remaining one is not equivalent.

Hint: Finding $\mathbf{X}$ such that $\mathbf{D}'(g) = \mathbf{X}^{-1}\mathbf{D}(g)\mathbf{X}$ is equivalent to finding $\mathbf{X}$ such that $\mathbf{X}\mathbf{D}'(g) = \mathbf{D}(g)\mathbf{X}$, but the latter is easier to solve.

Unitary representations.

Definition.

- A real matrix is called an orthogonal matrix if its columns form an orthonormal basis of $\mathbb{R}^n$, i.e. if $\mathbf{A}^T\mathbf{A} = \mathbf{I}_n$.
  The inverse of an orthogonal matrix is its transposed, i.e. $\mathbf{A}^{-1} = \mathbf{A}^T$.
- A complex matrix is called a unitary matrix if its columns form an orthonormal basis of $\mathbb{C}^n$, i.e. if $\mathbf{A}^T\mathbf{A}^* = \mathbf{I}_n$.
  The inverse of a unitary matrix is the transposed of the complex conjugate matrix, i.e. $\mathbf{A}^{-1} = (\mathbf{A}^*)^T = \mathbf{A}^\dagger$.
- The matrix $\mathbf{A}^\dagger = (\mathbf{A}^*)^T = (\mathbf{A}^T)^*$ is called the Hermitian conjugate of $\mathbf{A}$.
- A representation $\mathbf{D}$ such that every $\mathbf{D}(g)$ is a unitary matrix is called a unitary representation.

Theorem.

Let $\mathbf{D}$ be a representation of the finite group $\mathcal{G}$, then $\mathbf{D}$ is equivalent to a unitary representation.

A constructive proof.

Transforming an arbitrary representation into a unitary one.

Let $\mathbf{D}$ be an arbitrary representation of $\mathcal{G}$. Define

$$\mathbf{F} := \frac{1}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \mathbf{D}(g)^T \mathbf{D}(g)^*$$

then $\mathbf{F}$ is a metric tensor which is invariant under $\mathbf{D}$, i.e. one has

$$\mathbf{D}(g)^T \mathbf{F} \mathbf{D}(g)^* = \mathbf{F}.$$

Construct a matrix $\mathbf{X}$ such that

$$\mathbf{X}^T \mathbf{X}^* = \mathbf{F},$$

i.e. such that the columns of $\mathbf{X}$ form a matrix with metric tensor $\mathbf{F}$.

Then $\mathbf{X}\mathbf{D}(g)\mathbf{X}^{-1}$ is a unitary matrix.

Example.

The representation

$$\mathbf{D}(g) = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad \mathbf{D}(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

of $\mathcal{D}_3$ fixes the metric tensor $\mathbf{F} = \begin{pmatrix} 1 & -1/2 \\ -1/2 & 1 \end{pmatrix}$.
A matrix $\mathbf{X}$ for which $\mathbf{X}^T\mathbf{X} = \mathbf{F}$ is

$$\mathbf{X} = \begin{pmatrix} 1 & -1/2 \\ 0 & \sqrt{3}/2 \end{pmatrix}.$$

Conjugating with $\mathbf{X}^{-1}$ (!) gives

$$\mathbf{X}\mathbf{D}(g)\mathbf{X}^{-1} = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}, \quad \mathbf{X}\mathbf{D}(h)\mathbf{X}^{-1} = \frac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ \sqrt{3} & 1 \end{pmatrix}$$

which are orthogonal matrices (and thus also unitary).

Direct sums of representations.

Definition.

Let $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ be representations of degrees n_1 and n_2, respectively. Joining the representations $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ as diagonal blocks into matrices of size $n_1 + n_2$ gives a representation

$$\mathbf{D}^{(1)} \oplus \mathbf{D}^{(2)}(g) = \left(\begin{array}{c|c} \mathbf{D}^{(1)}(g) & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{D}^{(2)}(g) \end{array} \right)$$

of degree $n_1 + n_2$ which is called the direct sum of $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$.

The direct sum construction shows, that even up to equivalence there are infinitely many different representations of a group $\mathcal{G}$, since it allows to construct representations of arbitrary large degree.

Example.

The representation

$$\mathbf{D}^{(1)} \oplus \mathbf{D}^{(2)}(g) = \left(\begin{array}{c|cc} 1 & 0 & 0 \\ \hline 0 & 0 & -1 \\ 0 & 1 & 0 \end{array}\right), \quad \mathbf{D}^{(1)} \oplus \mathbf{D}^{(2)}(h) = \left(\begin{array}{c|cc} -1 & 0 & 0 \\ \hline 0 & 0 & 1 \\ 0 & 1 & 0 \end{array}\right)$$

is the direct sum of the 1-dimensional representation

$$\mathbf{D}^{(1)}(g) = \left(1\right), \quad \mathbf{D}^{(1)}(h) = \left(-1\right)$$

and the 2-dimensional representation

$$\mathbf{D}^{(2)}(g) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{D}^{(2)}(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

of $\mathcal{D}_4$.

Reducible representations.

Definition.

- A representation $\mathbf{D}$ is called reducible if it is equivalent to one of the form
$$\left(\begin{array}{c|c} \mathbf{D}^{(1)}(g) & \mathbf{H}^{(12)}(g) \\ \hline \mathbf{0} & \mathbf{D}^{(2)}(g) \end{array}\right).$$
In this case, $\mathbf{V}$ has an invariant subspace $\mathbf{U}$ different from $\{\mathbf{0}\}$ and $\mathbf{V}$ on which $\mathcal{G}$ acts by $\mathbf{D}^{(1)}$.
- If $\mathbf{D}$ is even equivalent to a representation of the form
$$\left(\begin{array}{c|c} \mathbf{D}^{(1)}(g) & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{D}^{(2)}(g) \end{array}\right)$$
(i.e. $\mathbf{H}^{(12)}(g) = \mathbf{0}$), then $\mathbf{D}$ is called decomposable or fully reducible. In that case, $\mathbf{V}$ has a further invariant subspace $\mathbf{W}$ on which $\mathcal{G}$ acts by $\mathbf{D}^{(2)}$ and such that $\mathbf{U} \oplus \mathbf{W} = \mathbf{V}$.
One says that $\mathbf{W}$ is a complement of $\mathbf{U}$ in $\mathbf{V}$.

Irreducible representations.

Theorem.

For representations over infinite fields like the real or complex numbers (but also the rational numbers), every reducible representation of a finite group is fully reducible.
In other words, every invariant subspace $\mathbf{U}$ of $\mathbf{V}$ has a complement $\mathbf{W}$ which is also invariant under $\mathcal{G}$.

A complement of a subspace $\mathbf{U}$ can be constructed explicitly:
For a unitary representation, the orthogonal complement $\mathbf{W} = \mathbf{U}^{\perp} = \{\mathbf{w} \in \mathbf{V} \mid \mathbf{u} \cdot \mathbf{w} = 0 \text{ for all } \mathbf{u} \in \mathbf{U}\}$ is also an invariant subspace.

Definition.

If a representation is not reducible, i.e. if the only subspaces of $\mathbf{V}$ which are invariant under $\mathbf{D}$ are the trivial subspaces $\{\mathbf{0}\}$ and $\mathbf{V}$, the representation $\mathbf{D}$ is called irreducible.

Examples.

- The representation $\mathbf{D}$ of $\mathcal{C}_2 = \{e, g\}$ with $\mathbf{D}(g) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ is reducible because it has two 1-dimensional invariant subspaces $\mathbf{U}$ and $\mathbf{W}$ spanned by the vectors $\mathbf{b}_1 = \mathbf{e}_1 + \mathbf{e}_2$ and $\mathbf{b}_2 = \mathbf{e}_1 - \mathbf{e}_2$. Transforming $\mathbf{D}$ to the basis $\mathbf{b}_1, \mathbf{b}_2$ gives the equivalent representation

$$\mathbf{D}'(g) = \left(\begin{array}{c|c} 1 & 0 \\ \hline 0 & -1 \end{array}\right).$$

- The representation

$$\mathbf{D}(g) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{D}(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

of $\mathcal{D}_4$ is irreducible, because a non-trivial invariant subspace must be 1-dimensional, i.e. spanned by a common eigenvector of the two matrices.
The eigenvectors of $\mathbf{D}(h)$ are $(1,1)^T$ and $(1,-1)^T$, but none of these vectors is an eigenvector of $\mathbf{D}(g)$.

Exercise 5.

Show that the representation

$$\mathbf{D}(g) = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad \mathbf{D}(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

of $\mathcal{D}_3$ is irreducible.

Exercise 6.

Show that the representation

$$\mathbf{D}(g) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{D}(h) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

of $\mathcal{D}_3$ is reducible.
Decompose **D** into a direct sum of irreducible representations.

Hint: Find a common eigenvector of $\mathbf{D}(g)$ and $\mathbf{D}(h)$ and show that the action on the orthogonal complement is irreducible.

Irreps.

Schur's lemma.

A complex representation $\mathbf{D}$ of degree n is irreducible if and only if only the scalar matrices (i.e. matrices of the form $\lambda \mathbf{I}_n$ for $\lambda \in \mathbb{C}$) commute with all matrices $\mathbf{D}(g)$.

Note that Schur's lemma in this form is not true for e.g. real representations.

Theorem.

- A finite group $\mathcal{G}$ has up to equivalence only a finite number of irreducible representations over $\mathbb{C}$, called irreps.
- The number of different irreps (up to equivalence) is equal to the number of conjugacy classes of $\mathcal{G}$.

From now on, we will suppress the term 'up to equivalence'. With different irreps we always mean non-equivalent irreps.

Restrictions on the degrees of irreps.

Theorem.

- Let $n_1, \ldots, n_r$ be the degrees of the different irreps of $\mathcal{G}$. Then the sum of the squares of these degrees is equal to the group order, i.e.

$$|\mathcal{G}| = n_1^2 + n_2^2 + \ldots + n_r^2.$$

  In particular, the irreps of an Abelian group all have degree 1.
- The degree of an irrep of $\mathcal{G}$ divides the group order.
- The number of irreps of degree 1 is equal to the index of the commutator subgroup $\mathcal{G}'$ in $\mathcal{G}$ (recall that the quotient group $\mathcal{G}/\mathcal{G}'$ is the largest Abelian quotient group of $\mathcal{G}$).
  In particular, the number of irreps of degree 1 is a divisor of the group order (and of course at most the number of conjugacy classes).

Example.

The octahedral group $\mathcal{O}$ (occurring e.g. as the rotation group of the cube) has order 24 and 5 conjugacy classes and thus 5 irreps.
The number of irreps of degree 1 must be 1, 2, 3 or 4.

- 4 irreps of degree 1: then $1+1+1+1+a^2=24$, but 20 is not a square $\Rightarrow$ impossible.
- 3 irreps of degree 1: then $1+1+1+a^2+b^2=24$, but 21 is not the sum of two squares $\Rightarrow$ impossible.
- 2 irreps of degree 1: then $1+1+a^2+b^2+c^2=24$ and assume that $a \leq b \leq c$.
  Try $a=3$, but then $a^2+b^2+c^2 \geq 27 \Rightarrow$ impossible.
  Try $a=2$, then $b^2+c^2=18$ and $b=c=3$ is the only possibility.
- 1 irrep of degree 1: then $1+a^2+b^2+c^2+d^2=24$. As above, a must be 2, then $b^2+c^2+d^2=19$, hence also $b=2$. But $c^2+d^2=15$ is impossible.

Thus, the degrees of the irreps of $\mathcal{O}$ are $1, 1, 2, 3, 3$.

Exercise 7.

The symmetry group $m\overline{3}$ of a tetrahedron has order 24 and 8 conjugacy classes.
Determine the degrees of the irreps of $m\overline{3}$.

Hint: Make a case distinction for the number irreps of degree 1.

Exercise 8.

Let $\mathcal{G}$ be a group of order 20.
Determine the possibilities for the degrees of the irreps of $\mathcal{G}$.

Hint: There are 3 possibilities, and all occur, e.g. for the groups $\mathcal{C}_{20}$, $\mathcal{D}_{10}$, $\mathcal{F}_{20}$.

Characters.

Definition / Lemma.

For an $n \times n$ matrix $\mathbf{A}$, the sum of the diagonal entries is called its trace, denoted by $\mathrm{tr}(\mathbf{A})$:

$$\mathrm{tr}(\mathbf{A}) = \mathbf{A}_{11} + \mathbf{A}_{22} + \ldots + \mathbf{A}_{nn}.$$

The trace of a matrix does not change under basis transformations, i.e. for an invertible matrix $\mathbf{X}$ one has $\mathrm{tr}(\mathbf{X}^{-1}\mathbf{A}\mathbf{X}) = \mathrm{tr}(\mathbf{A})$.

Definition / Lemma.

For a representation $\mathbf{D}$ of $\mathcal{G}$ the mapping $\chi_{\mathbf{D}} : \mathcal{G} \to \mathbb{C}$ given by

$$\chi_{\mathbf{D}}(g) = \mathrm{tr}(\mathbf{D}(g))$$

is called the character of $\mathbf{D}$.

Equivalent representations have the same character.

Examples.

- For the character χ of the representation $\mathbf{D}$ of $\mathcal{D}_3$ with

$$\mathbf{D}(g) = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad \mathbf{D}(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

  one has $\chi(e) = 2$, $\chi(g) = -1$, $\chi(h) = 0$.
  Since $\mathbf{D}(g^2) = \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix}$, one further has $\chi(g^2) = -1$.

- Let $\mathcal{G} \leq \mathrm{GL}_3(\mathbb{R})$ be a point group and let $\mathbf{D}$ be its vector representation with corresponding character χ.
  For a twofold rotation $\mathit{2} \in \mathcal{G}$ one has $\chi(\mathit{2}) = -1$, since $\mathbf{D}(\mathit{2})$ is equivalent to $\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$.
  Analogously, for a reflection $m \in \mathcal{G}$ one has $\chi(m) = 1$, since $\mathbf{D}(m)$ is equivalent to $\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$.

Character values.

Theorem.

Characters are constant on the conjugacy classes of $\mathcal{G}$, since for $g' = h^{-1}gh$ one has

$$\begin{aligned}\chi(g') &= \mathrm{tr}(\mathbf{D}(g')) = \mathrm{tr}(\mathbf{D}(h^{-1}gh)) \\ &= \mathrm{tr}(\mathbf{D}(h^{-1})\mathbf{D}(g)\mathbf{D}(h)) = \mathrm{tr}(\mathbf{D}(g)) = \chi(g).\end{aligned}$$

Characters are therefore completely determined by their values on representatives of the conjugacy classes and they are often specified in that way.

Theorem.

Let χ be the character of a representation $\mathbf{D}$ of $\mathcal{G}$.
Then $\chi(g^{-1}) = \chi(g)^*$ for all $g \in \mathcal{G}$.

In particular, if $\chi(g)$ is real, then g and g^{-1} have the same character value.

Criterion for equivalence.

Theorem.

Two representations **D** and **D**′ are equivalent if and only if their characters are equal.
Since characters are constant on the conjugacy classes, it is sufficient to compare two characters on representatives of the conjugacy classes.

Note that it is in general not sufficient to compare the character values on generators of the group.

Example.

Denote for the three representations

$$\mathbf{D}(g) = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad \mathbf{D}'(g) = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \mathbf{D}''(g) = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

of $\mathcal{C}_4$ the corresponding characters by χ, χ', χ''.
Then $\chi(g) = \chi'(g) = \chi''(g) = 0$, but $\chi'(g^2) = \mathrm{tr}(\mathbf{I}_2) = 2$, whereas $\chi(g^2) = \chi''(g^2) = \mathrm{tr}(-\mathbf{I}_2) = -2$.
Hence **D** and **D**″ are equivalent, but **D**′ is different.

Character table.

Definition.

Let $\mathcal{G}$ be a finite group with r conjugacy classes, represented by the elements $g_1 = e, g_2, \ldots, g_r$ and let $\mathbf{D}^{(1)}, \ldots, \mathbf{D}^{(r)}$ be the different irreps of $\mathcal{G}$.
Then the character table of $\mathcal{G}$ is the $r \times r$ matrix $\mathbf{X} = \mathbf{X}(\mathcal{G})$ with

$$\mathbf{X}_{ij} = \chi_{\mathbf{D}^{(i)}}(g_j).$$

The rows of the character table are usually labelled by names for the irreps (which may be just numbers) and the columns are labelled by representatives for the conjugacy classes.

The character table may be augmented with additional information, e.g.:

- for each column the order of the elements;
- for each column the class length of the conjugacy class;
- for the crystallographic point groups, basis functions which transform under the point group according to the irrep (to be explained).

Character table of $\mathcal{D}_3$

class length	1	2	3
element order	1	3	2
	$g_1 = e$	g_2	g_3
A_1	1	1	1
A_2	1	1	-1
E	2	-1	0

Character table of the point group *432*

class length	1	3	6	8	6
element order	1	2	2	3	4
	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
A_1	1	1	1	1	1
A_2	1	1	-1	1	-1
E	2	2	0	-1	0
T_1	3	-1	-1	0	1
T_2	3	-1	1	0	-1

Exercise 9.

Show that two irreps of an Abelian group are equivalent if and only if they are equal.

Hint: One may regard this as a trick question.

Exercise 10.

Determine the character table of the *Klein fourgroup* $\mathcal{C}_2 \times \mathcal{C}_2 = \{e, g, h, gh\}$ in which all elements $\neq e$ have order 2.

Scalar product of characters.

Definition.

For two characters χ, ψ of G, the scalar product of χ and ψ is defined as

$$(\chi, \psi)_{\mathcal{G}} = \frac{1}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \chi(g)\psi(g^{-1}) = \frac{1}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \chi(g)\psi(g)^*$$

If $g_1, \ldots, g_r$ are representatives for the conjugacy classes of $\mathcal{G}$ and if $|C_j|$ is the number of elements in the conjugacy class of g_j, then the scalar product can be written as

$$(\chi, \psi)_{\mathcal{G}} = \frac{1}{|\mathcal{G}|} \sum_{j=1}^{r} |C_j|\, \chi(g_j)\psi(g_j)^*.$$

This scalar product is one of the motivations to augment the character table with the class lengths.

Orthogonality relations.

Row orthogonality.

Let $\mathcal{G}$ be a finite group with irreducible characters $\chi_1, \ldots, \chi_r$. Then the irreducible characters of $\mathcal{G}$ form an orthonormal basis w.r.t. $(\cdot, \cdot)_{\mathcal{G}}$, i.e.:

$$(\chi_i, \chi_j)_{\mathcal{G}} = \frac{1}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \chi_i(g) \chi_j(g)^* = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j. \end{cases}$$

Column orthogonality.

The columns of the character table of $\mathcal{G}$ form an orthogonal system:

$$\sum_{i=1}^{r} \chi_i(g_j) \chi_i(g_k)^* = \begin{cases} |\mathcal{G}|/|C_j| & \text{if } j = k \\ 0 & \text{if } j \neq k \end{cases}$$

where $|C_j|$ is the class length of the conjugacy class with representative g_j.

Example.

A partially known character table can be filled with the help of the orthogonality relations.

class length	1	3	6	8	6
element order	1	2	2	3	4
	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
A_1	1	1	1	1	1
A_2	1	1	-1	1	-1
E	2				
T_1	3	-1	-1	0	1
T_2	3	-1	1	0	-1

The column orthogonality between the first and the second column gives
$1 + 1 + 2 \cdot \chi_E(2_z) - 3 - 3 = 0 \Rightarrow \chi_E(2_z) = 2$.
The same method applied to the other columns completes the table.

Example.

A partially known character table can be filled with the help of the orthogonality relations.

class length	1	3	6	8	6
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	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
A_1	1	1	1	1	1
A_2	1	1	-1	1	-1
E	2	2	0	-1	0
T_1	3	-1	-1	0	1
T_2	3	-1	1	0	-1

The column orthogonality between the first and the second column gives $1 + 1 + 2 \cdot \chi_E(2_z) - 3 - 3 = 0 \Rightarrow \chi_E(2_z) = 2$.
The same method applied to the other columns completes the table.

Exercise 11.

The following part of the character table of the *icosahedral group* $\mathcal{I}$ of order 60 is known.

class length	1	15	20	12	12
element order	1	2	3	5	5
	e	g_2	g_3	g_4	g_5
χ_1	1	1	1	1	1
χ_2	3	-1	0	$\frac{1+\sqrt{5}}{2}$	$\frac{1-\sqrt{5}}{2}$
χ_3	3	-1	0	$\frac{1-\sqrt{5}}{2}$	$\frac{1+\sqrt{5}}{2}$
χ_4	4				
χ_5	5				

Complete the character table.

Hint: You may assume that the missing entries are integers (because the incomplete characters are the only ones of their respective degrees).
Use column orthogonality and the fact that the norm of a column is $\mathcal{G}/|C_j|$.
Check your result with the row orthogonality.

The magic formula.

Irreducibility criterion.

Let χ be the character of a representation **D** of $\mathcal{G}$.
Then **D** is irreducible if and only if its character has norm 1, i.e. if

$$\frac{1}{|\mathcal{G}|}\sum_{g\in\mathcal{G}}\chi_i(g)\chi_i(g)^* = \frac{1}{|\mathcal{G}|}\sum_{g\in\mathcal{G}}|\chi_i(g)|^2 = 1.$$

Magic formula.

Let $\mathcal{G}$ be a finite group with irreducible characters $\chi_1,\ldots,\chi_r$ and let χ be an arbitrary character of $\mathcal{G}$.
Then the decomposition of χ into irreducible characters is given by

$$\chi = \sum_{i=1}^{r} m_i\chi_i \quad \text{where} \quad m_i = (\chi,\chi_i)_{\mathcal{G}} = \frac{1}{|\mathcal{G}|}\sum_{g\in\mathcal{G}}\chi(g)\chi_i(g)^*.$$

Example.

We want to decompose the character χ of $\mathcal{O}$ (appended to the character table):

$\lvert C_j \rvert$	1	3	6	8	6
	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
A_1	1	1	1	1	1
A_2	1	1	-1	1	-1
E	2	2	0	-1	0
T_1	3	-1	-1	0	1
T_2	3	-1	1	0	-1
χ	12	4	0	0	0

If we multiply the components of χ by $|C_j|$, we obtain the multiplicities as the product of the character table matrix with this vector:

$$\begin{pmatrix} m_{A_1} \\ m_{A_2} \\ m_E \\ m_{T_1} \\ m_{T_2} \end{pmatrix} = \frac{1}{24} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ 2 & 2 & 0 & -1 & 0 \\ 3 & -1 & -1 & 0 & 1 \\ 3 & -1 & 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} 12 \cdot 1 \\ 4 \cdot 3 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 2 \\ 1 \\ 1 \end{pmatrix}$$

Exercise 12.

Three characters ψ_1, ψ_2, ψ_3 of the dihedral group $\mathcal{D}_4$ of order 8 are appended to its character table:

$\lvert C_j \rvert$	1	1	2	2	2
	e	g^2	g	h	hg
χ_1	1	1	1	1	1
χ_2	1	1	1	-1	-1
χ_3	1	1	-1	-1	1
χ_4	1	1	-1	1	-1
χ_5	2	-2	0	0	0
ψ_1	6	2	0	0	0
ψ_2	10	6	-2	-2	0
ψ_3	11	7	-3	-3	-3

Determine the multiplicities with which the irreps $\chi_1, \ldots, \chi_5$ occur in ψ_1, ψ_2, ψ_3.

Orthogonality relations for matrix entries.

Definition.

An arbitrary function $\phi : \mathcal{G} \to \mathbb{C}$ is called a group function.

Theorem.

Let **D** be an irrep of degree n of $\mathcal{G}$, then

$$\frac{1}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \mathbf{D}(g)_{ij} \mathbf{D}(g^{-1})_{kl} = \begin{cases} \frac{1}{n} & \text{if } i = k \text{ and } j = l \\ 0 & \text{otherwise,} \end{cases}$$

i.e. the group functions for different positions of an irrep are orthogonal.

Moreover, if $\mathbf{D}'$ is an irrep of degree m of $\mathcal{G}$ which is different from **D**, then

$$\sum_{g \in \mathcal{G}} \mathbf{D}(g)_{ij} \mathbf{D}'(g^{-1})_{kl} = 0 \text{ for all } 1 \leq i, j \leq n, 1 \leq k, l \leq m,$$

i.e. the group functions for different irreps are orthogonal.

Projection operators.

Definition / Theorem.

If $\mathbf{\Gamma}$ is a representation of $\mathcal{G}$ and χ is the character of an irrep $\mathbf{D}$ of degree n of $\mathcal{G}$, then

- $$P_\chi = \frac{n}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \chi(g^{-1}) \mathbf{\Gamma}(g) = \frac{n}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \chi(g)^* \mathbf{\Gamma}(g)$$
  is the projection operator to the sum of the subspaces on which $\mathcal{G}$ acts by the irrep $\mathbf{D}$.
- $$P_{\mathbf{D}} = \frac{n}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \mathbf{D}(g^{-1})_{11} \mathbf{\Gamma}(g)$$
  is the projection operator to a subspace $\mathbf{U}$ of dimension m such that every basis vector of $\mathbf{U}$ can be chosen as the first basis vector of a different subspace on which $\mathcal{G}$ acts by the irrep $\mathbf{D}$.
- In case of a unitary representation $\mathbf{D}$, the projection operator $P_{\mathbf{D}}$ can be written as
  $$P_{\mathbf{D}} = \frac{n}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \mathbf{D}(g)^*_{11} \mathbf{\Gamma}(g).$$

A long example.

The dihedral group $\mathcal{D}_3$ has a representation $\mathbf{\Gamma}$ of degree 6 in which each of the irreps occurs with multiplicity equal to its degree:

$$\mathbf{\Gamma}(g) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{\Gamma}(h) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}.$$

We want to transform $\mathbf{\Gamma}$ to block diagonal form, and in order to find the corresponding subspaces we apply the projection operators.

For the trivial irrep $\mathbf{D}^{(1)}$ we get

$$P_{\mathbf{D}^{(1)}} = \frac{1}{6}(\mathbf{\Gamma}(e) + \mathbf{\Gamma}(g) + \mathbf{\Gamma}(g^2) + \mathbf{\Gamma}(h) + \mathbf{\Gamma}(gh) + \mathbf{\Gamma}(g^2h)) = \frac{1}{6} \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

It is clear that both generators fix the vector $\mathbf{v}^{(1)} = (1,1,1,1,1,1)^T$.

$$\mathbf{\Gamma}(g) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{\Gamma}(h) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

For the other 1-dimensional irrep $\mathbf{D}^{(2)}$ we get

$$P_{\mathbf{D}^{(2)}} = \frac{1}{6}(\mathbf{\Gamma}(e)+\mathbf{\Gamma}(g)+\mathbf{\Gamma}(g^2)-\mathbf{\Gamma}(h)-\mathbf{\Gamma}(gh)-\mathbf{\Gamma}(g^2h)) = \frac{1}{6}\begin{pmatrix} 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \\ -1 & -1 & -1 & 1 & 1 & 1 \end{pmatrix}.$$

One sees that $\mathbf{\Gamma}(g)$ fixes the vector $\mathbf{v}^{(2)} = (1, 1, 1, -1, -1, -1)^T$ and that $\mathbf{\Gamma}(h)$ maps it to $-\mathbf{v}^{(2)}$.

$$\mathbf{\Gamma}(g) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{\Gamma}(h) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

For the 2-dimensional irrep $\mathbf{D}^{(3)}$ we get

$$P_{\mathbf{D}^{(3)}} = \frac{1}{3}(\mathbf{\Gamma}(e) - \mathbf{\Gamma}(g) - \mathbf{\Gamma}(gh) + \mathbf{\Gamma}(g^2h)) = \frac{1}{3}\begin{pmatrix} 1 & 0 & -1 & 0 & -1 & 1 \\ -1 & 1 & 0 & -1 & 1 & 0 \\ 0 & -1 & 1 & 1 & 0 & -1 \\ 0 & -1 & 1 & 1 & 0 & -1 \\ -1 & 1 & 0 & -1 & 1 & 0 \\ 1 & 0 & -1 & 0 & -1 & 1 \end{pmatrix}$$

We take $\mathbf{v}_1^{(3)} = (1, -1, 0, 0, -1, 1)^T$ and $\mathbf{w}_1^{(3)} = (0, 1, -1, -1, 1, 0)^T$ (i.e. the first two columns of $P_{\mathbf{D}^{(3)}}$) and define

$$\mathbf{v}_2^{(3)} = \mathbf{\Gamma}(g)(\mathbf{v}_1^{(3)}) = (0, 1, -1, 1, 0, -1)^T,$$
$$\mathbf{w}_2^{(3)} = \mathbf{\Gamma}(g)(\mathbf{w}_1^{(3)}) = (-1, 0, 1, 0, -1, 1)^T.$$

Then $\mathcal{D}_3$ acts on the two subspaces with bases $\mathbf{v}_1^{(3)}$, $\mathbf{v}_2^{(3)}$ and $\mathbf{w}_1^{(3)}$, $\mathbf{w}_2^{(3)}$ by the irrep $\mathbf{D}^{(3)}$.

Summarizing, we have determined a transformation matrix

$$\mathbf{X} = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 & -1 \\ 1 & 1 & -1 & 1 & 1 & 0 \\ 1 & 1 & 0 & -1 & -1 & 1 \\ 1 & -1 & 0 & 1 & -1 & 0 \\ 1 & -1 & -1 & 0 & 1 & -1 \\ 1 & -1 & 1 & -1 & 0 & 1 \end{pmatrix}$$

which transforms

$$\mathbf{\Gamma}(g) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad \mathbf{\Gamma}(h) = \begin{pmatrix} 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}$$

to the block diagonal form

$$\mathbf{\Gamma}'(g) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{pmatrix}, \quad \mathbf{\Gamma}'(h) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

Kronecker product.

Question.

The direct sum representation $\mathbf{D}^{(1)} \oplus \mathbf{D}^{(2)}$ has as its character the sum $\chi_{\mathbf{D}^{(1)}} + \chi_{\mathbf{D}^{(2)}}$ of the corresponding characters.
Is there also a representation that has as its character the product $\chi_{\mathbf{D}^{(1)}} \cdot \chi_{\mathbf{D}^{(2)}}$ of the characters?

Definition.

For two matrices $\mathbf{A} \in \mathbb{C}^{m\times m}$ and $\mathbf{B} \in \mathbb{C}^{n\times n}$ the direct product or Kronecker product $\mathbf{A} \otimes \mathbf{B}$ of $\mathbf{A}$ and $\mathbf{B}$ is the $mn \times mn$ matrix

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} \mathbf{A}_{11}\mathbf{B} & \mathbf{A}_{12}\mathbf{B} & \cdots & \mathbf{A}_{1m}\mathbf{B} \\ \mathbf{A}_{21}\mathbf{B} & \mathbf{A}_{22}\mathbf{B} & \cdots & \mathbf{A}_{2m}\mathbf{B} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{A}_{m1}\mathbf{B} & \mathbf{A}_{m2}\mathbf{B} & \cdots & \mathbf{A}_{mm}\mathbf{B} \end{pmatrix}.$$

where $\mathbf{A}_{ij}\mathbf{B}$ is the $n \times n$ matrix obtained by multiplying all elements of $\mathbf{B}$ by $\mathbf{A}_{ij}$.

Example.

The Kronecker products $\mathbf{A} \otimes \mathbf{B}$ and $\mathbf{B} \otimes \mathbf{A}$ of the matrices

$$\mathbf{A} = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix} \text{ and } \mathbf{B} = \begin{pmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{pmatrix} \text{ are}$$

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} 0\,\mathbf{B} & (-1)\,\mathbf{B} \\ 1\,\mathbf{B} & (-1)\,\mathbf{B} \end{pmatrix} = \left(\begin{array}{ccc|ccc} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 0 & -1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 0 \end{array}\right) \text{ and}$$

$$\mathbf{B} \otimes \mathbf{A} = \begin{pmatrix} 0\,\mathbf{A} & 0\,\mathbf{A} & (-1)\mathbf{A} \\ 1\,\mathbf{A} & 0\,\mathbf{A} & 0\mathbf{A} \\ 0\,\mathbf{A} & (-1)\,\mathbf{A} & 0\mathbf{A} \end{pmatrix} = \left(\begin{array}{cc|cc|cc} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & -1 & 1 \\ \hline 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & -1 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \end{array}\right).$$

Exercise 13.

Determine the Kronecker products $\mathbf{A} \otimes \mathbf{B}$ and $\mathbf{B} \otimes \mathbf{A}$ of the matrices

$$\mathbf{A} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \text{ and } \mathbf{B} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 2 & 0 & -1 \end{pmatrix}.$$

Direct product of representations.

Lemma.

The Kronecker product has the following properties:

- $(\mathbf{A} \otimes \mathbf{B})(\mathbf{C} \otimes \mathbf{D}) = \mathbf{AC} \otimes \mathbf{BD}$.
- $\mathrm{tr}(\mathbf{A} \otimes \mathbf{B}) = \mathrm{tr}(\mathbf{A}) \cdot \mathrm{tr}(\mathbf{B})$.

Theorem / Definition.

For two representations $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ of a group $\mathcal{G}$, defining

$$\mathbf{D}(g) = \mathbf{D}^{(1)}(g) \otimes \mathbf{D}^{(2)}(g)$$

gives a representation of $\mathcal{G}$ called the direct product or tensor product of $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ and denoted by $\mathbf{D}^{(1)} \otimes \mathbf{D}^{(2)}$.
The character $\chi_{\mathbf{D}}$ is the product of the characters of $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$, i.e.

$$\chi_{\mathbf{D}}(g) = \chi_{\mathbf{D}^{(1)} \otimes \mathbf{D}^{(2)}}(g) = \chi_{\mathbf{D}^{(1)}}(g) \cdot \chi_{\mathbf{D}^{(2)}}(g).$$

Interpretation of the direct product.

Let $\mathbf{V}$ and $\mathbf{W}$ be vector spaces with basis $\mathbf{v}_1, \ldots, \mathbf{v}_n$ and $\mathbf{w}_1, \ldots, \mathbf{w}_m$, respectively.
Then the Cartesian product

$$\begin{aligned} \mathbf{v}_1\mathbf{w}_1, \mathbf{v}_1\mathbf{w}_2, \ldots, \mathbf{v}_1\mathbf{w}_m, \quad & \mathbf{v}_2\mathbf{w}_1, \mathbf{v}_2\mathbf{w}_2, \ldots, \mathbf{v}_2\mathbf{w}_m, \quad \ldots \\ \ldots \quad & \mathbf{v}_n\mathbf{w}_1, \mathbf{v}_n\mathbf{w}_2, \ldots, \mathbf{v}_n\mathbf{w}_m \end{aligned}$$

of the two bases can be taken as the basis of a new vector space, called the tensor product of $\mathbf{V}$ and $\mathbf{W}$ and denoted by $\mathbf{V} \otimes \mathbf{W}$.

If $\mathcal{G}$ acts on $\mathbf{V}$ and $\mathbf{W}$ via representations $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$, respectively, then an action on $\mathbf{V} \otimes \mathbf{W}$ can be defined by

$$g(\mathbf{v}_i\mathbf{w}_j) = g(\mathbf{v}_i)\, g(\mathbf{w}_j).$$

Taking the basis of $\mathbf{V} \otimes \mathbf{W}$ as given above, the representation corresponding to this action of $\mathcal{G}$ is precisely the direct product representation $\mathbf{D}^{(1)} \otimes \mathbf{D}^{(2)}$.

Symmetrizations.

Definition.

Let $\mathbf{V}$ be a vector space with basis $\mathbf{v}_1, \ldots, \mathbf{v}_n$, then $\{\mathbf{v}_i\mathbf{v}_j, 1 \le i, j \le n\}$ is a basis of $\mathbf{V} \otimes \mathbf{V}$.

- The symmetrized square $[\mathbf{V}]^2$ of $\mathbf{V}$ is spanned by the vectors $\mathbf{v}\mathbf{v}' \in \mathbf{V} \otimes \mathbf{V}$ for which $\mathbf{v}\mathbf{v}' = \mathbf{v}'\mathbf{v}$. A basis for this subspace is

$$\{\mathbf{v}_i\mathbf{v}_j + \mathbf{v}_j\mathbf{v}_i, 1 \le i \le j \le n\},$$

  its dimension is $\frac{1}{2}n(n+1)$.
- The antisymmetrized square $\{\mathbf{V}\}^2$ of $\mathbf{V}$ is spanned by the vectors $\mathbf{v}\mathbf{v}' \in \mathbf{V} \otimes \mathbf{V}$ for which $\mathbf{v}\mathbf{v}' = -\mathbf{v}'\mathbf{v}$. A basis for this subspace is

$$\{\mathbf{v}_i\mathbf{v}_j - \mathbf{v}_j\mathbf{v}_i, 1 \le i < j \le n\},$$

  its dimension is $\frac{1}{2}n(n-1)$.
- If $\mathcal{G}$ acts on $\mathbf{V}$ by the representation $\mathbf{D}$, then $[\mathbf{V}]^2$ and $\{\mathbf{V}\}^2$ are invariant subspaces of $\mathbf{V} \otimes \mathbf{V}$ and the corresponding representations of $\mathcal{G}$ are denoted by $[\mathbf{D}]^2$ and $\{\mathbf{D}\}^2$, respectively.

Characters of symmetrizations.

Theorem.

Let $\mathcal{G}$ act on the vector space **V** by the representation **D** with character χ.

- The character $[\chi]^2$ of the representation $[\mathbf{D}]^2$ on the symmetrized square $[\mathbf{V}]^2$ is given by

$$[\chi]^2(g) = \frac{1}{2}\left(\chi^2(g) + \chi(g^2)\right).$$

- The character $\{\chi\}^2$ of the representation $\{\mathbf{D}\}^2$ on the antisymmetrized square $\{\mathbf{V}\}^2$ is given by

$$\{\chi\}^2(g) = \frac{1}{2}\left(\chi^2(g) - \chi(g^2)\right).$$

Example.

We determine the symmetrized and antisymmetrized squares of the representations E and T_1 of the point group *432*, for which the relevant part of the character table looks as follows:

	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
E	2	2	0	-1	0
T_1	3	-1	-1	0	1

For $g = 1$, $g = 2_z$ and $g = 2_{xx0}$ we have $g^2 = 1$, furthermore $(3^+_{xxx})^2$ lies in the conjugacy class of 3^+_{xxx} and $(4^+_z)^2 = 2_z$. From that we obtain:

$$\begin{array}{lccccc}
[E]^2: & \frac{1}{2}(4+2)=3 & \frac{1}{2}(4+2)=3 & \frac{1}{2}(0+2)=1 & \frac{1}{2}(1+(-1))=0 & \frac{1}{2}(0+2)=1 \\
\{E\}^2: & \frac{1}{2}(4-2)=1 & \frac{1}{2}(4-2)=1 & \frac{1}{2}(0-2)=-1 & \frac{1}{2}(1-(-1))=1 & \frac{1}{2}(0-2)=-1
\end{array}$$

$$\begin{array}{lccccc}
[T_1]^2: & \frac{1}{2}(9+3)=6 & \frac{1}{2}(1+3)=2 & \frac{1}{2}(1+3)=2 & \frac{1}{2}(0+0)=0 & \frac{1}{2}(1+(-1))=0 \\
\{T_1\}^2: & \frac{1}{2}(9-3)=3 & \frac{1}{2}(1-3)=-1 & \frac{1}{2}(1-3)=-1 & \frac{1}{2}(0-0)=0 & \frac{1}{2}(1-(-1))=1
\end{array}$$

Exercise 14.

The character table of $\mathcal{D}_4$ is as follows:

element order	1	2	4	2	2
class length	1	1	2	2	2
	e	g^2	g	h	hg
χ_1	1	1	1	1	1
χ_2	1	1	1	-1	-1
χ_3	1	1	-1	-1	1
χ_4	1	1	-1	1	-1
χ_5	2	-2	0	0	0

Determine the symmetrized and antisymmetrized squares $[\chi_5]^2$ and $\{\chi_5\}^2$ of the 2-dimensional character χ_5 and decompose them into irreps.

Reduction of direct products into irreps.

Definition.

Let $\mathbf{D}^{(1)}, \dots, \mathbf{D}^{(r)}$ be the irreps of $\mathcal{G}$. If the direct product $\mathbf{D}^{(i)} \otimes \mathbf{D}^{(j)}$ is decomposed into irreps by

$$\mathbf{D}^{(i)} \otimes \mathbf{D}^{(j)} = \bigoplus_{k=1}^{r} c_{ij}^{k} \mathbf{D}^{(k)},$$

then the multiplicities c_{ij}^{k} are called the coefficients of the Clebsch-Gordan series or simply Clebsch-Gordan coefficients for the irreps of $\mathcal{G}$.

Note that the term Clebsch-Gordan coefficients is often used in a different meaning, especially in the context of particle physics.

Theorem.

If χ_i is the character of $\mathbf{D}^{(i)}$, then the c_{ij}^{k} can be explicitly computed by

$$c_{ij}^{k} = (\chi_i \cdot \chi_j, \chi_k)_{\mathcal{G}} = \frac{1}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \chi_i(g) \chi_j(g) \chi_k(g)^{*}.$$

Example.

The character table of the tetrahedral group $\mathcal{T}$ looks as follows:

class length	1	3	4	4
	1	2_z	3^+_{xxx}	3^-_{xxx}
A	1	1	1	1
E^1	1	1	ζ	ζ^*
E^2	1	1	ζ^*	ζ
T	3	-1	0	0

$$\zeta = \exp(2\pi i/3) = (-1 + i\sqrt{3})/2$$

The direct products with 1-dimensional representations are easy.
The only substantial effort is the decomposition of $T \otimes T$ with character $\chi_{T\otimes T} = 9 \quad 1 \quad 0 \quad 0.$
We find $c^1_{44} = c^2_{44} = c^3_{44} = \frac{1}{12}(9+3) = 1$ and $c^4_{44} = \frac{1}{12}(27-3) = 2.$

$\otimes$	A	E^1	E^2	T
A	A			
E^1	E^1	E^2		
E^2	E^2	A	E^1	
T	T	T	T	$A \oplus E^1 \oplus E^2 \oplus 2T$

Exercise 15.

Let $\mathbf{D}^{(1)}$ be an irrep of degree 1 of $\mathcal{G}$ and let $\mathbf{D}^{(2)}$ be an irrep of arbitrary degree.

Show that $\mathbf{D}^{(1)} \otimes \mathbf{D}^{(2)}$ is irreducible.

Hint: You can argue with the irreducibility criterion for characters or directly with invariant subspaces.

Irreps of direct products of groups.

Theorem.

Let $\mathcal{G} = \mathcal{H}_1 \times \mathcal{H}_2$ be a direct product of groups and write the elements of $\mathcal{G}$ as $h_1 h_2$ with $h_1 \in \mathcal{H}_1$ and $h_2 \in \mathcal{H}_2$.
Let $\mathbf{D}_1^{(i)}$ for $1 \leq i \leq r$ be the irreps of $\mathcal{H}_1$ and let $\mathbf{D}_2^{(j)}$ for $1 \leq j \leq s$ be the irreps of $\mathcal{H}_2$.

Then the irreps of $\mathcal{G}$ are given by $\mathbf{D}^{(ij)}$ with

$$\mathbf{D}^{(ij)}(h_1 h_2) = \mathbf{D}_1^{(i)}(h_1) \otimes \mathbf{D}_2^{(j)}(h_2)$$

for $1 \leq i \leq r$ and $1 \leq j \leq s$, where $\mathbf{D}_1^{(i)}(h_1) \otimes \mathbf{D}_2^{(j)}(h_2)$ denotes the Kronecker product of the matrices $\mathbf{D}_1^{(i)}(h_1)$ and $\mathbf{D}_2^{(j)}(h_2)$.

A possible proof is an application of Schur's lemma:
The only matrices commuting with the elements $h_1 e$ are block diagonal matrices and block diagonal matrices commuting with the elements $e h_2$ need to have identity matrices as blocks.

Character tables of direct products of groups.

Theorem.

Let $\mathbf{X}_1$ be the character table of $\mathcal{H}_1$ for conjugacy class representatives $h_1, \ldots, h_r$ and irreps $\mathbf{D}_1^{(1)}, \ldots, \mathbf{D}_1^{(r)}$ of $\mathcal{H}_1$ and let $\mathbf{X}_2$ be the character table of $\mathcal{H}_2$ for conjugacy class representatives $h'_1, \ldots, h'_s$ and irreps $\mathbf{D}_2^{(1)}, \ldots, \mathbf{D}_2^{(s)}$ of $\mathcal{H}_2$.

Taking the conjugacy class representatives of $\mathcal{G} = \mathcal{H}_1 \times \mathcal{H}_2$ in the order

$$h_1 h'_1, h_1 h'_2, \ldots, h_1 h'_s, \quad h_2 h'_1, h_2 h'_2, \ldots, h_2 h'_s, \quad \ldots \quad h_r h'_1, h_r h'_2, \ldots, h_r h'_s,$$

and the irreps of $\mathcal{G}$ in the order

$$\mathbf{D}^{11}, \mathbf{D}^{12}, \ldots, \mathbf{D}^{1s}, \quad \mathbf{D}^{21}, \mathbf{D}^{22}, \ldots, \mathbf{D}^{2s}, \quad \ldots \quad \mathbf{D}^{r1}, \mathbf{D}^{r2}, \ldots, \mathbf{D}^{rs},$$

the character table of $\mathcal{G}$ is the Kronecker product $\mathbf{X}_1 \otimes \mathbf{X}_2$.

In particular, if $\mathbf{X}$ is the character table of $\mathcal{H}$, then the character table of $\mathcal{C}_2 \times \mathcal{H}$ is

$$\begin{pmatrix} \mathbf{X} & \mathbf{X} \\ \mathbf{X} & -\mathbf{X} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \mathbf{X}.$$

Example.

The dihedral group $\mathcal{D}_3$ of order 6 has the character table

	e	g	h
$\chi_{\mathbf{D}^{(1)}}$	1	1	1
$\chi_{\mathbf{D}^{(2)}}$	1	-1	1
$\chi_{\mathbf{D}^{(3)}}$	2	0	-1

The direct product $\mathcal{C}_2 \times \mathcal{D}_3$ therefore has the character table

	e	g	h	$-e$	$-g$	$-h$
$\chi_{\mathbf{D}^{(11)}}$	1	1	1	1	1	1
$\chi_{\mathbf{D}^{(12)}}$	1	-1	1	1	-1	1
$\chi_{\mathbf{D}^{(13)}}$	2	0	-1	2	0	-1
$\chi_{\mathbf{D}^{(21)}}$	1	1	1	-1	-1	-1
$\chi_{\mathbf{D}^{(22)}}$	1	-1	1	-1	1	-1
$\chi_{\mathbf{D}^{(23)}}$	2	0	-1	-2	0	1

Notation: If $\mathbf{D}$ is an irrep of $\mathcal{H}$, then the corresponding irreps in the upper and lower half of the character table of $\mathcal{C}_2 \times \mathcal{H}$ are often denoted by $\mathbf{D}_g$ (for gerade) or $\mathbf{D}^+$ and $\mathbf{D}_u$ (for ungerade) or $\mathbf{D}^-$, respectively.

Exercise 16.

The dihedral group $\mathcal{D}_3$ of order 6 has the character table

	e	g	h
$\chi_{\mathbf{D}^{(1)}}$	1	1	1
$\chi_{\mathbf{D}^{(2)}}$	1	-1	1
$\chi_{\mathbf{D}^{(3)}}$	2	0	-1

Determine the character table of the direct product $\mathcal{D}_3 \times \mathcal{D}_3$.

Hint: Conjugacy class representatives of $\mathcal{D}_3 \times \mathcal{D}_3$ are the pairs

$$(e,e),(e,g),(e,h), \quad (g,e),(g,g),(g,h), \quad (h,e),(h,g),(h,h).$$

Irreps of Abelian groups.

Fundamental theorem on finite Abelian groups.

Every finite Abelian group $\mathcal{G}$ is a direct product of cyclic groups. More precisely,

$$\mathcal{G} \cong \mathcal{C}_{d_1} \times \mathcal{C}_{d_2} \times \ldots \times \mathcal{C}_{d_r}$$

such that d_i divides d_{i+1} for $1 \leq i < r$.
The orders d_i of the cyclic components of $\mathcal{G}$ in a direct product decomposition with this divisibility condition are uniquely determined and thus classify the isomorphism types of Abelian groups.

Deriving the isomorphism type.

The unique decomposition can be obtained from any direct product decomposition into cyclic groups by iteratively applying

$$\mathcal{C}_n \times \mathcal{C}_m \cong \mathcal{C}_{\mathrm{gcd}(n,m)} \times \mathcal{C}_{\mathrm{lcm}(n,m)}.$$

For example, on has

$$\mathcal{C}_2 \times \mathcal{C}_3 \times \mathcal{C}_4 \times \mathcal{C}_6 \cong \mathcal{C}_2 \times \mathcal{C}_3 \times \mathcal{C}_2 \times \mathcal{C}_{12} \cong \mathcal{C}_2 \times \mathcal{C}_6 \times \mathcal{C}_{12}.$$

Cyclic groups.

Theorem (reminder).

All irreps of an Abelian group have degree 1.

Notation.

The complex number $\exp(2\pi i/n)$ is often denoted by ζ_n and is called a primitive n-th root of unity, since $(\exp(2\pi i/n))^n = \exp(2\pi i) = 1$.

Theorem.

The irreps of the cyclic group $\mathcal{C}_n$ generated by g are of the form

$$\mathbf{D}^{(k)}(g) = \exp(2\pi i k/n) = \zeta_n^k \text{ with } 0 \leq k < n,$$

since for $\mathbf{D}^{(k)}(g) = z \in \mathbb{C}$ one requires $z^n = 1$.
For an arbitrary element $g^a \in \mathcal{C}_n$ one has

$$\mathbf{D}^{(k)}(g^a) = \exp(2\pi i(ak)/n) = \zeta_n^{ak}.$$

Direct products of cyclic groups.

Two cyclic groups.

Let $\mathcal{C}_n$ be generated by g_1 and $\mathcal{C}_m$ generated by g_2, then the irreps of $\mathcal{C}_n \times \mathcal{C}_m$ are determined by the images of g_1 and g_2:

$$\mathbf{D}^{(kl)}(g_1) = \zeta_n^k, \quad \mathbf{D}^{(kl)}(g_2) = \zeta_m^l \quad \text{with } 0 \leq k < n,\ 0 \leq l < m.$$

The representation of a general element $g_1^a g_2^b$ is given by

$$\mathbf{D}^{(kl)}(g_1^a g_2^b) = \zeta_n^{ak} \zeta_m^{bl}.$$

Two or three cyclic groups of the same order.

The irreps of $\mathcal{C}_n \times \mathcal{C}_n$ are given by

$$\mathbf{D}^{(kl)}(g_1^a g_2^b) = \zeta_n^{ak} \zeta_n^{bk} = \zeta_n^{ak+bl} \quad \text{with } 0 \leq k, l < n.$$

Analogously, the irreps of $\mathcal{C}_n \times \mathcal{C}_n \times \mathcal{C}_n$ are given by

$$\mathbf{D}^{(klm)}(g_1^a g_2^b g_3^c) = \zeta_n^{ak+bl+cm} \quad \text{with } 0 \leq k, l, m < n.$$

$\mathcal{C}_2 \times \mathcal{C}_4$.

Let $\mathcal{C}_2 = \{+1, -1\}$ and $\mathcal{C}_4$ be generated by g.
Then the irreps of $\mathcal{C}_2 \times \mathcal{C}_4$ are

$$\mathbf{D}^{(k+)}(-1) = 1,\ \mathbf{D}^{(k+)}(g) = i^k, \quad \mathbf{D}^{(k-)}(-1) = -1,\ \mathbf{D}^{(k-)}(g) = i^k$$

and the character table is as follows:

	e	g	g^2	g^3	$-e$	$-g$	$-g^2$	$-g^3$
$\mathbf{D}^{(0+)}$	1	1	1	1	1	1	1	1
$\mathbf{D}^{(1+)}$	1	i	-1	$-i$	1	i	-1	$-i$
$\mathbf{D}^{(2+)}$	1	-1	1	-1	1	-1	1	-1
$\mathbf{D}^{(3+)}$	1	$-i$	-1	i	1	$-i$	-1	i
$\mathbf{D}^{(0-)}$	1	1	1	1	-1	-1	-1	-1
$\mathbf{D}^{(1-)}$	1	i	-1	$-i$	-1	$-i$	1	i
$\mathbf{D}^{(2-)}$	1	-1	1	-1	-1	1	-1	1
$\mathbf{D}^{(3-)}$	1	$-i$	-1	i	-1	i	1	$-i$

Exercise 17.

Determine the character tables and irreps of the following two point groups:

- $mm2 \cong \mathcal{C}_2 \times \mathcal{C}_2$
  with conjugacy class representatives 1, 2_z, m_y, m_x;
- $\overline{3} \cong \mathcal{C}_3 \times \mathcal{C}_2 \cong \mathcal{C}_6$
  with conjugacy class representatives 1, 3^+, 3^-, $\overline{1}$, $\overline{3}^+$, $\overline{3}^-$.

Dihedral groups.

Definition.

The dihedral group $\mathcal{D}_n$ of order $2n$ is generated by an element g of order n and an element h of order 2 such that h conjugates g to its inverse, i.e. $h^{-1}gh = g^{-1}$.
Since h is of order 2, this means that $gh = hg^{-1}$ and $hg = g^{-1}h$.
The element g generates a cyclic normal subgroup $\mathcal{C}_n \trianglelefteq \mathcal{D}_n$ of index 2 in $\mathcal{D}_n$.

Theorem.

The dihedral group $\mathcal{D}_n$ has 2 irreps of degree 1 if n is odd and 4 irreps of degree 1 if n is even.
The 2-dimensional representations

$$\mathbf{E}_i(g) = \begin{pmatrix} \zeta_n^i & 0 \\ 0 & \zeta_n^{-i} \end{pmatrix}, \quad \mathbf{E}_i(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

are irreducible and pairwise inequivalent for $1 \leq i < n/2$.

$\mathcal{D}_6$.

The dihedral group $\mathcal{D}_6$ has conjugacy class representatives e, g, g^2, g^3, h, gh.
The commutator subgroup $\mathcal{D}_6'$ is the cyclic group generated by g^2, thus g^2 lies in the kernel of every 1-dimensional irrep of $\mathcal{D}_6$.

Using e.g. $\zeta_6 + \zeta_6^{-1} = 1$ and $\zeta_6^2 + \zeta_6^{-2} = -1$, the character table is found to be

	e	g	g^2	g^3	h	gh
χ_1	1	1	1	1	1	1
χ_2	1	-1	1	-1	-1	1
χ_3	1	-1	1	-1	1	-1
χ_4	1	1	1	1	-1	-1
$\mathbf{E}_1$	2	1	-1	-2	0	0
$\mathbf{E}_2$	2	-1	-1	2	0	0

Exercise 18.

Determine the character table and irreps of the point group *4mm* $\cong \mathcal{D}_4$ with conjugacy class representatives 1, 2_z, 4_z^+, m_{x0z}, m_{xxz}.

Exercise 19.

Determine the character table and irreps of the dihedral group $\mathcal{D}_5$ which is isomorphic to the symmetry group of a regular pentagon.

Hint: For $\mathcal{D}_n$ with n odd, the commutator subgroup $\mathcal{D}_n'$ is the cyclic group of order n generated by g, hence g lies in the kernel of both 1-dimensional irreps.

It is worthwhile to note that $\zeta_5 + \zeta_5^{-1} = (-1+\sqrt{5})/2 = 1/\tau$ and $\zeta_5^2 + \zeta_5^{-2} = (-1-\sqrt{5})/2 = -\tau$ where $\tau \approx 1.618$ is the golden ratio.

Tetrahedral group.

The tetrahedral group $\mathcal{T}$ is realized by the point group *23*.
The vector representation

$$\mathbf{D}(2_z) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{D}(3^+_{xxx}) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

of *23* is irreducible, since the eigenvectors of $\mathbf{D}(3^+_{xxx})$ are $(1,1,1)^T$, $(1,\zeta_3,\zeta_3^*)^T$ and $(1,\zeta_3^*,\zeta_3)^T$, but none of these vectors is an eigenvector for $\mathbf{D}(2_z)$.
It follows immediately that there are 3 irreps of degree 1.
From this information, the character table can be completed via the orthogonality relations:

	1	2_z	3^+_{xxx}	3^-_{xxx}
χ_1	1	1	1	1
χ_2	1			
χ_3	1			
χ_4	3	-1	0	0

Tetrahedral group.

The tetrahedral group $\mathcal{T}$ is realized by the point group *23*.
The vector representation

$$\mathbf{D}(2_z) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{D}(3^+_{xxx}) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

of *23* is irreducible, since the eigenvectors of $\mathbf{D}(3^+_{xxx})$ are $(1,1,1)^T$, $(1,\zeta_3,\zeta_3^*)^T$ and $(1,\zeta_3^*,\zeta_3)^T$, but none of these vectors is an eigenvector for $\mathbf{D}(2_z)$.
It follows immediately that there are 3 irreps of degree 1.
From this information, the character table can be completed via the orthogonality relations:

	1	2_z	3^+_{xxx}	3^-_{xxx}
χ_1	1	1	1	1
χ_2	1			
χ_3	1			
χ_4	3	-1	0	0

	1	2_z	3^+_{xxx}	3^-_{xxx}
χ_1	1	1	1	1
χ_2	1	1	ζ_3	ζ_3^*
χ_3	1	1	ζ_3^*	ζ_3
χ_4	3	-1	0	0

Octahedral group.

The octahedral group $\mathcal{O}$ is realized by the point groups *432* and $\bar{4}$*3m* which both contain *23* as a subgroup of index 2.
The vector representations of *432*

$$\mathbf{T}_1(2_{xx0}) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \mathbf{T}_1(4_z^+) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and of $\bar{4}$*3m*

$$\mathbf{T}_2(m_{x\bar{x}z}) = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{T}_2(\bar{4}_z^+) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

extend the vector representation of *23* given before.

The twofold rotations 2_x, 2_y, 2_z generate a normal subgroup of order 4 isomorphic to $\mathcal{D}_2$ and with factor group $\mathcal{O}/\mathcal{D}_2 \cong \mathcal{D}_3$.

In this factor group, the cosets of 1 and 2_z correspond to the identity element of $\mathcal{D}_3$, the coset of 3^+_{xxx} corresponds to the element g of order 3 in $\mathcal{D}_3$ and the cosets of 2_{xx0} ($m_{x\bar{x}z}$) and 4^+_z ($\bar{4}^+_z$) correspond to the element h of order 2 in $\mathcal{D}_3$.

Via this identification, the remaining three irreps of $\mathcal{O}$ are derived from the irreps of $\mathcal{D}_3$.

432	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
$\bar{4}3m$	1	2_z	$m_{x\bar{x}z}$	3^+_{xxx}	$\bar{4}^+_z$
A_1	1	1	1	1	1
A_2	1	1	-1	1	-1
E	2	2	0	-1	0
$\mathbf{T}_1$	3	-1	-1	0	1
$\mathbf{T}_2$	3	-1	1	0	-1

Pseudovectors.

Definition.

An axial vector or pseudovector $\mathbf{R}$ is transformed like the corresponding polar vector under rotations, but is invariant under inversion.
If g is an improper rotation, then $-g$ is a proper rotation and g maps $\mathbf{R}$ to $\overline{1}(-g(\mathbf{R})) = -g(\mathbf{R})$.
This means that under an improper rotation a pseudovector is mapped to the opposite of the corresponding polar vector.

Example: rotation axis.

A typical case in which axial vectors occur is the description of a rotation axis by a vector.
By convention, the vector points up the rotation axis and the rotation is counterclockwise when one looks down the axis.
Since inversion does not change the rotation, the axial vector $\mathbf{R}$ describing it has to remain the same, i.e. we require that $\overline{1}(\mathbf{R}) = \mathbf{R}$.

Two interpretations of pseudovectors.

- The pseudovector $\mathbf{R}(\mathbf{r})$ is identified with the polar vector $\mathbf{r}$, but the action of $\mathcal{G}$ is modified to

$$g(\mathbf{R}(\mathbf{r})) = \begin{cases} \mathbf{R}(g(\mathbf{r})) & \text{if } g \text{ is a proper rotation} \\ -\mathbf{R}(g(\mathbf{r})) & \text{if } g \text{ is an improper rotation.} \end{cases}$$

  For the standard basis $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ of $\mathbb{R}^3$, the corresponding pseudovectors are simply denoted by $\mathbf{R}_x, \mathbf{R}_y, \mathbf{R}_z$ (instead of $\mathbf{R}(\mathbf{e}_x), \mathbf{R}(\mathbf{e}_y), \mathbf{R}(\mathbf{e}_z)$).

- The pseudovectors are realized as vector products, i.e. for the standard basis $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ of $\mathbb{R}^3$ we define the vectors

$$\mathbf{R}_x = \mathbf{e}_y \times \mathbf{e}_z, \quad \mathbf{R}_y = \mathbf{e}_z \times \mathbf{e}_x, \quad \mathbf{R}_z = \mathbf{e}_x \times \mathbf{e}_y.$$

  Then the action of $\mathcal{G}$ on the pseudovectors is obtained by applying the elements of $\mathcal{G}$ to the components of the vector products.

Example.

The rotoinversion $\overline{4}_z^+ = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ maps the standard basis as follows:

$$\mathbf{e}_x \mapsto -\mathbf{e}_y, \quad \mathbf{e}_y \mapsto \mathbf{e}_x, \quad \mathbf{e}_z \mapsto -\mathbf{e}_z.$$

Since $\overline{4}_z^+$ is an improper rotation, its action on the pseudovectors in the first interpretation is given by

$$\mathbf{R}_x \mapsto \mathbf{R}_y, \quad \mathbf{R}_y \mapsto -\mathbf{R}_x, \quad \mathbf{R}_z \mapsto \mathbf{R}_z.$$

In the second interpretation we get the same result:

$$\begin{aligned}
\mathbf{R}_x &= \mathbf{e}_y \times \mathbf{e}_z \mapsto \mathbf{e}_x \times (-\mathbf{e}_z) = \mathbf{e}_z \times \mathbf{e}_x = \mathbf{R}_y, \\
\mathbf{R}_y &= \mathbf{e}_z \times \mathbf{e}_x \mapsto (-\mathbf{e}_z) \times (-\mathbf{e}_y) = -(\mathbf{e}_y \times \mathbf{e}_z) = -\mathbf{R}_x, \\
\mathbf{R}_z &= \mathbf{e}_x \times \mathbf{e}_y \mapsto (-\mathbf{e}_y) \times \mathbf{e}_x = \mathbf{e}_x \times \mathbf{e}_y = \mathbf{R}_z.
\end{aligned}$$

Exercise 20.

Determine the action of the following two point group elements g and h on the pseudovectors $\mathbf{R}_x$, $\mathbf{R}_y$, $\mathbf{R}_z$:

$$g = \begin{pmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad h = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}.$$

Hint: You may want to find out, whether an element is a proper or improper rotation.

Pseudovector representation.

Definition.

For a subgroup $\mathcal{G}$ of $\mathrm{GL}_3(\mathbb{R})$ with vector representation $\mathbf{D}^t$, the representation $\mathbf{D}^r$ on the pseudovectors of $\mathbb{R}^3$ is called the pseudovector representation of $\mathcal{G}$.

Theorem.

The pseudovector representation $\mathbf{D}^r$ of $\mathcal{G}$ can be described as follows:

- $\mathbf{D}^r$ equivalent to the antisymmetrized square of the vector representation, i.e.
$$\mathbf{D}^r = \{\mathbf{D}^t\}^2.$$
- $\mathbf{D}^r$ is obtained by multiplying the vector representation by the determinant of the respective matrix, i.e.
$$\mathbf{D}^r(g) = \det(g)\mathbf{D}^t(g).$$

Example.

The point group $\mathcal{G} = \overline{4}3m$ has the character table

	1	2_z	$m_{x\overline{x}z}$	3^+_{xxx}	$\overline{4}^+_z$
A_1	1	1	1	1	1
A_2	1	1	-1	1	-1
E	2	2	0	-1	0
T_1	3	-1	-1	0	1
T_2	3	-1	1	0	-1

T_2 is the vector representation of $\overline{4}3m$ and A_2 is the irrep obtained by taking the determinants of the vector representation of $\mathcal{G}$.
Since $A_2 \otimes T_2 = T_1$, we see that T_1 is the pseudovector representation of $\overline{4}3m$.

Alternatively, we have already seen earlier that T_1 is the antisymmetrized square $\{T_2\}^2$ of the vector representation of $\mathcal{G}$.

Exercise 21.

The character table of the point group $m\bar{3}m$ is

	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z	$\bar{1}$	m_z	$m_{x\bar{x}z}$	$\bar{3}^+_{xxx}$	$\bar{4}^+_z$
χ_1	1	1	1	1	1	1	1	1	1	1
χ_2	1	1	−1	1	−1	1	1	−1	1	−1
χ_3	2	2	0	−1	0	2	2	0	−1	0
χ_4	3	−1	−1	0	1	3	−1	−1	0	1
χ_5	3	−1	1	0	−1	3	−1	1	0	−1
χ_6	1	1	1	1	1	−1	−1	−1	−1	−1
χ_7	1	1	−1	1	−1	−1	−1	1	−1	1
χ_8	2	2	0	−1	0	−2	−2	0	1	0
χ_9	3	−1	−1	0	1	−3	1	1	0	−1
χ_{10}	3	−1	1	0	−1	−3	1	−1	0	1

Determine which irrep is the vector representation of $m\bar{3}m$ and which is the pseudovector representation.

Should we vote?

Functions of coordinates.

A subgroup $\mathcal{G}$ of $\mathrm{GL}_3(\mathbb{R})$ acts naturally on the coordinates x, y, z of a vector $\mathbf{v} = x\mathbf{e}_x + y\mathbf{e}_y + z\mathbf{e}_z$. But then, it also acts on functions in the coordinates, i.e. on expressions like x^2, yz^2 or $xy + xz + yz$.

The coordinates x, y, z may be regarded as

- commuting variables: in this case xy and yx are the same function;
- non-commuting variables: in this case xy and yx are different functions.

Example.

The rotation $2_{xx0} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ maps the coordinates as follows:

$$x \mapsto y, \quad y \mapsto x, \quad z \mapsto -z.$$

This means that $x^2 \mapsto y^2$, $yz^2 \mapsto xz^2$ and $xy + xz + yz \mapsto yx - yz - xz$.

Basis functions of irreps.

Definition.

Let **F** be a linear space of functions in the coordinates x, y, z which is closed under the action of $\mathcal{G} \leq \mathrm{GL}_3(\mathbb{R})$ and denote the representation obtained from the action of $\mathcal{G}$ on **F** by **D**.
Then the functions of a subspace $\mathbf{F}^{(i)}$ of **F** on which $\mathcal{G}$ acts by the irrep $\mathbf{D}^{(i)}$ are called basis functions of that irrep.
This means that the basis functions of an irrep transform exactly according to the irrep under the action of $\mathcal{G}$.

Example.

For the cyclic group of order 2 generated by the rotation
$2_{xx0} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$, the functions xy, z^2, $x^2 + y^2$ and $xz - yz$ are fixed by 2_{xx0} and thus are basis functions for the trivial irrep of $\mathcal{C}_2$.
The functions $xz + yz$ and $x^2 - y^2$ are mapped to their negatives and thus are basis functions for the non-trivial irrep of $\mathcal{C}_2$.

Typical spaces of functions.

- Linear functions of the form $ax + by + cz$. A natural basis for this space are the functions x, y, z which of course transform according to the vector representation of $\mathcal{G}$.
- Quadratic functions of the form $ax^2 + by^2 + cz^2 + dxy + exz + fyz$. A natural basis for this space are the functions $x^2, y^2, z^2, xy, xz, yz$ which transform according to the symmetrized square of the vector representation of $\mathcal{G}$.
- If we do not assume that x, y, z are commuting variables, we have $xy \neq yx$. The above case then corresponds to the symmetric quadratic functions $x^2, y^2, z^2, (xy + yx), (xz + zx), (yz + zy)$.
- The complement of the symmetric quadratic functions are the antisymmetric quadratic functions with basis $\mathbf{J}_x = yz - zy$, $\mathbf{J}_y = zx - xz$, $\mathbf{J}_z = xy - yx$. These transform according to the antisymmetrized square of the vector representation of $\mathcal{G}$, i.e. according to the pseudovector representation of $\mathcal{G}$.

Exercise 22.

The point group *mm2* is generated by

$$2_z = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad m_y = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and has character table

	1	2_z	m_y	m_x
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1

Determine the basis functions for the action of *mm2* on the quadratic functions $x^2, y^2, z^2, xy, xz, yz$.

A worked example.

The point group $\overline{4}2m \cong \mathcal{D}_4$ is generated by the elements $\overline{4}_z$ and 2_x, its vector representation $\mathbf{\Gamma}$ is given by

$$\mathbf{\Gamma}(\overline{4}_z) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad \mathbf{\Gamma}(2_x) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The action on the quadratic functions $x^2, y^2, z^2, xy, xz, yz$ is the symmetrized square $[\mathbf{\Gamma}]^2$:

$$[\mathbf{\Gamma}]^2(\overline{4}_z) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}, \quad [\mathbf{\Gamma}]^2(2_x) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

From the character table of $\mathcal{D}_4$ we deduce that

$$[\mathbf{\Gamma}]^2 = 2\mathbf{D}^{(1)} \oplus \mathbf{D}^{(3)} \oplus \mathbf{D}^{(4)} \oplus \mathbf{D}^{(5)}.$$

For the occurring irreps, compute the projection operators

$$P_{\chi_i} = \frac{\chi_i(1)}{8} \sum_{g \in \bar{4}2m} \chi_i(g)^* [\mathbf{\Gamma}]^2(g)$$

$$P_{\chi_1} = \frac{1}{2}\begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad P_{\chi_3} = \frac{1}{2}\begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$P_{\chi_4} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, \quad P_{\chi_5} = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix},$$

which have ranks 2, 1, 1, 1, as required.

Conclusion.

- the functions $x^2 + y^2$ and z^2 are basis functions for $\mathbf{D}^{(1)}$,
- $x^2 - y^2$ is a basis function for $\mathbf{D}^{(3)}$,
- xy is a basis function for $\mathbf{D}^{(4)}$,
- the functions xz, yz are basis functions for the irrep $\mathbf{D}^{(5)}$.

Augmented character table

The character table of $\overline{4}2m$, augmented with the basis functions, looks as follows:

	1	2_z	$\overline{4}_z$	2_x	m_{xxz}	basis functions
χ_1	1	1	1	1	1	$x^2 + y^2, z^2$
χ_2	1	1	1	-1	-1	$\mathbf{J}_z$
χ_3	1	1	-1	1	-1	$x^2 - y^2$
χ_4	1	1	-1	-1	1	z, xy
χ_5	2	-2	0	0	0	$(x, y), (\mathbf{J}_x, \mathbf{J}_y), (xz, yz)$

Molecular vibrations.

Take a molecule consisting of N atoms and install in the position of each atom a local coordinate system (x_i, y_i, z_i).
The action of the symmetry group $\mathcal{G}$ of the molecule on these $3N$ local coordinates gives rise to a representation $\mathbf{\Gamma}$ of degree $3N$ of $\mathcal{G}$, which is sometimes called the mechanical representation.

Since global translations and global rotations can be expressed in the local coordinates, the space of local coordinates contains a subspace on which $\mathcal{G}$ acts by the vector representation $\mathbf{\Gamma}^t$ and a subspace on which $\mathcal{G}$ acts by the pseudovector representation $\mathbf{\Gamma}^r$. Thus,

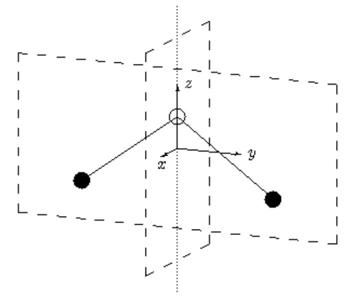
$$\mathbf{\Gamma} = \mathbf{\Gamma}^t \oplus \mathbf{\Gamma}^r \oplus \mathbf{\Gamma}^v$$

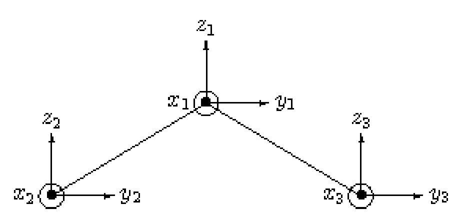
where $\mathbf{\Gamma}^v$ is the action on vibrational modes we are interested in.

Molecule of water type.

The molecule is situated in the yz-plane. The non-trivial elements of its symmetry group *mm2* $\cong \mathcal{D}_2$ are a twofold rotation 2_z around the z-axis, a reflection m_y in the xz-plane and a reflection m_x in the yz-plane.

Local coordinates are installed in each of the atoms.





The action of *mm2* on the atoms gives rise to a permutation representation

$$\mathbf{\Pi}(2_z) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \ \mathbf{\Pi}(m_y) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \ \mathbf{\Pi}(m_x) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

indicating that 2_z and m_y fix atom 1 and swap atoms 2 and 3 and that m_x fixes all three atoms.
Since the local coordinate systems are all set up in the same way, the representation $\mathbf{\Gamma}$ is the direct product of this permutation representation $\mathbf{\Pi}$ with the vector representation $\mathbf{\Gamma}^t$ of $\mathcal{G}$:

$$\mathbf{\Gamma} = \mathbf{\Pi} \otimes \mathbf{\Gamma}^t.$$

The character $\chi_{\mathbf{\Gamma}}$ can be determined by

$$\chi_{\mathbf{\Gamma}}(g) = (\text{number of atoms fixed by } g) \cdot \chi_{\mathbf{\Gamma}^t}(g)$$

because only atoms which are fixed by an element g correspond to a block on the diagonal in $\mathbf{\Gamma}$.

$$
\mathbf{\Gamma}(2_z) = \mathbf{\Pi}(2_z) \otimes \mathbf{\Gamma}^t(2_z) = \left(\begin{array}{ccc|ccc|ccc}
-1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\hline
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0
\end{array}\right)
$$

$$
\mathbf{\Gamma}(m_y) = \mathbf{\Pi}(m_y) \otimes \mathbf{\Gamma}^t(m_y) = \left(\begin{array}{ccc|ccc|ccc}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
\hline
0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0
\end{array}\right)
$$

$$
\mathbf{\Gamma}(m_x) = \mathbf{\Pi}(m_x) \otimes \mathbf{\Gamma}^t(m_x) = \left(\begin{array}{ccc|ccc|ccc}
-1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1
\end{array}\right)
$$

Exercise 23.

The non-trivial elements of the symmetry group *mm2* of the water-type molecule are

$$2_z = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad m_y = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad m_x = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

2_z and m_y swap atoms 2 and 3 and fix atom 1, m_x fixes all three atoms.

The character table of *mm2* with the characters of the vector representation $\mathbf{\Gamma}^t$ and of the pseudovector representation $\mathbf{\Gamma}^r$ is

$mm2$	1	2_z	m_y	m_x
A_1	1	1	1	1
A_2	1	1	−1	−1
B_1	1	−1	1	−1
B_2	1	−1	−1	1
$\mathbf{\Gamma}^t$	3	−1	1	1
$\mathbf{\Gamma}^r$	3	−1	−1	−1

Determine the character of the representation $\mathbf{\Gamma}$.
Decompose $\mathbf{\Gamma}$, $\mathbf{\Gamma}^t$ and $\mathbf{\Gamma}^r$ into irreps and determine from this the irreps occurring in the vibrational part $\mathbf{\Gamma}^v$ of $\mathbf{\Gamma}$.

From the character table

	1	2_z	m_y	m_x
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	1	-1
B_2	1	-1	-1	1
$\mathbf{\Gamma}$	9	-1	1	3
$\mathbf{\Gamma}^t$	3	-1	1	1
$\mathbf{\Gamma}^r$	3	-1	-1	-1

we derive that

$$\mathbf{\Gamma} = 3A_1 \oplus A_2 \oplus 2B_1 \oplus 3B_2, \quad \mathbf{\Gamma}^t = A_1 \oplus B_1 \oplus B_2, \quad \mathbf{\Gamma}^r = A_2 \oplus B_1 \oplus B_2$$

from which we conclude that the vibrational part $\mathbf{\Gamma}^v$ of $\mathbf{\Gamma}$ is

$$\mathbf{\Gamma}^v = 2A_1 \oplus B_2.$$

We thus require the projection operators P_{A_1} and P_{B_2}.

$$P_{A_1} = \frac{1}{4}(\mathbf{\Gamma}(e) + \mathbf{\Gamma}(2_z) + \mathbf{\Gamma}(m_y) + \mathbf{\Gamma}(m_x)) = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}$$

projects to vectors of the form $(0, 0, a, 0, b, c, 0, -b, c)^T$.

The vector $\mathbf{t}_z = (0, 0, 1, 0, 0, 1, 0, 0, 1)^T = z_1 + z_2 + z_3$ corresponds to a global translation along the z-axis.

The vibrational modes are chosen orthogonal to the translational vector, e.g. as

$$\mathbf{v}_1 = (0, 0, 2, 0, 0, -1, 0, 0, -1)^T = 2z_1 - z_2 - z_3,$$
$$\mathbf{v}_2 = (0, 0, 0, 0, 1, 0, 0, -1, 0)^T = y_2 - y_3.$$

$$P_{B_2} = \frac{1}{4}(\mathbf{\Gamma}(e) - \mathbf{\Gamma}(2_z) - \mathbf{\Gamma}(m_y) + \mathbf{\Gamma}(m_x)) = \frac{1}{2}\begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 \end{pmatrix}$$

projects to vectors of the form $(0, a, 0, 0, b, c, 0, b, -c)^T$.

The vector $\mathbf{t}_y = (0, 1, 0, 0, 1, 0, 0, 1, 0)^T = y_1 + y_2 + y_3$ corresponds to a global translation along the y-axis.
The vector $\mathbf{r}_x = (0, -1, 0, 0, 0, 0, 0, -1, 1)^T = -y_1 - z_2 + z_3$ corresponds to a global rotation around the x-axis.

The vibrational mode is chosen orthogonal to these two vectors:

$$\mathbf{v}_3 = (0, 2, 0, 0, -1, -1, 0, -1, 1)^T = 2y_1 - y_2 - z_2 - y_3 + z_3.$$

Vibrational modes of the water type molecule.