Representations of crystallographic groups

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Contents

Some useful literature

Books providing the basic theory of group representations, but aimed at applications in physics or chemistry:

- D.M. Bishop, *Group Theory and Chemistry*, Clarendon Press, Oxford, 1973.
- A.D. Boardman, D.E. O'Connor, P.A. Young, *Symmetry and its Applications in Science*, McGraw-Hill, London, 1973.
- M. Burrow, *Representation Theory of Finite Groups*, Academic Press, New York, 1971.
- C.J. Bradley, A.P. Cracknell, *The Mathematical Theory of Symmetry in Solids*, Clarendon Press, Oxford, 2010.
- M.S. Dresselhaus, G. Dresselhaus, A. Jorio, *Group Theory. Applications to the Physics of Condensed Matter*, Springer, Berlin, 2008.
- T. Hahn (ed.), *International Tables for Crystallography, Vol. A, 5^{th} ed.*, Springer, Dordrecht, 2005.
- T. Janssen, *Crystallographic Groups*, North-Holland, Amsterdam, 1973.
- P. Jacobs, *Group Theory with Applications in Chemical Physics*, Cambridge University Press, Cambridge, 2005.

Mathematical books providing a full coverage of the required representation theory (including proofs):

- J.L. Alperin, R.B. Bell: *Groups and Representations.* Springer, New York, 1995.
- W. Burnside: *Theory of Groups of Finite Order.* Dover Phoenix Editions, 2004
- M. Burrow: *Representation Theory of Finite Groups.* Dover, 1993.
- C.W. Curtis, I. Reiner: *Methods of Representation Theory.* Wiley, New York, 1981.
- L.C. Grove: *Groups and Characters.* Wiley, New York, 1997.
- B. Huppert: *Endliche Gruppen I (Chapter V).* Springer, 1967.
- I.M. Isaacs: *Character Theory of Finite Groups.* American Mathematical Society, 2006.
- G. James, M. Liebeck: *Representations and Characters of Groups.* Cambridge University Press, Cambridge, 2001.
- J.-P. Serre: *Linear Representations of Finite Groups.* Springer, New York, 1977.

List of symbols

$\mathbf{U}$, $\mathbf{V}$, $\mathbf{W}$	vector spaces
$\mathbf{a}$, $\mathbf{b}$, $\mathbf{e}$, $\mathbf{r}$, $\mathbf{v}$, $\mathbf{w}$	vectors
$\mathbf{e}_1, \ldots, \mathbf{e}_n$	standard basis of an n-dimensional vector space
x, y, z	point coordinates, coordinate functions
$\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{X}$	$(n \times n)$ matrices
$\boldsymbol{A}_{ij}$	entry in position (i, j) of the matrix $\boldsymbol{A}$
$\boldsymbol{A}^T$	transposed matrix
$\boldsymbol{A}^*$	complex conjugate matrix
$\boldsymbol{A}^\dagger = (\boldsymbol{A}^T)^*$	Hermitian conjugate matrix
$\mathrm{tr}(\boldsymbol{A})$	trace of the matrix $\boldsymbol{A}$
$\det(\boldsymbol{A})$	determinant of the matrix $\boldsymbol{A}$
$\mathcal{G}$, $\mathcal{H}$	groups
g, h, x, e	group elements, identity element of a group
$\mathcal{H} \leq \mathcal{G}$	$\mathcal{H}$ is a subgroup of $\mathcal{G}$
$\mathcal{N} \trianglelefteq \mathcal{G}$	$\mathcal{N}$ is a normal subgroup of $\mathcal{G}$
$\mathcal{G}/\mathcal{N}$	factor group
$\ker(\varphi)$, $\mathrm{im}(\varphi)$	kernel and image of a homomorphism
$\mathcal{G}'$	commutator subgroup of $\mathcal{G}$
$\mathcal{G} \times \mathcal{H}$	direct product of groups
$\mathcal{C}_n$, $\mathcal{D}_n$	cyclic group of order n, dihedral group of order $2n$
$\mathcal{T}$, $\mathcal{O}$	tetrahedral group, octahedral group
$\mathbf{D}$	group representation
$\deg(\mathbf{D})$	degree of the representation $\mathbf{D}$
$\mathbf{D}(g)$	matrix of the group element g in the representation $\mathbf{D}$
$\mathbf{D}^{(i)}$	i-th irrep
$\mathbf{D}^*$	complex conjugate representation
$\chi_{\mathbf{D}}$	character of the representation $\mathbf{D}$
$\chi_{\mathbf{D}^{(i)}}$, χ_i	character of the irrep $\mathbf{D}^{(i)}$
$\mathbf{X}$, $\mathbf{X}(\mathcal{G})$	character table of $\mathcal{G}$
$\mathbf{D}^{(i)} \oplus \mathbf{D}^{(j)}$	direct sum of the irreps $\mathbf{D}^{(i)}$ and $\mathbf{D}^{(j)}$
$\mathbf{D}^{(i)} \otimes \mathbf{D}^{(j)}$	direct product of the irreps $\mathbf{D}^{(i)}$ and $\mathbf{D}^{(j)}$
$[\mathbf{D}]^2$, $\{\mathbf{D}\}^2$	symmetrized and antisymmetrized square of the representation $\mathbf{D}$
m_i	multiplicity of the i-th irrep in a representation
P_χ, $P_{\mathbf{D}}$	projection operators
$\zeta_n = \exp(2\pi i/n)$	primitive n-th root of unity
$\mathbf{R}_x$, $\mathbf{R}_y$, $\mathbf{R}_z$	pseudo- or axial vectors
$\mathbf{J}_x$, $\mathbf{J}_y$, $\mathbf{J}_z$	coordinate functions of pseudovectors

1 General introduction to representation theory

In the first part of this course we will cover the general concepts of representation theory, before applying them to crystallographic point groups in the second part. Since representations are a specific kind of actions of groups, we start with a short overview of the relevant concepts of group theory and discuss briefly the basic idea of group actions. We then develop the required theory for group representations.

1.1 Basic concepts from group theory

Definition 1.1.1 A *group* $\mathcal{G}$ is a set of elements on which a binary operation is defined, usually written as a product $g \cdot h$ or simply gh, which fulfills the following conditions:

(1) The operation is *associative*, i.e. $(gh)k = g(hk)$.

(2) $\mathcal{G}$ contains a *unity* or *identity element* e for which $ge = eg = g$ for all $g \in \mathcal{G}$.

(3) Every element $g \in \mathcal{G}$ has an inverse element g^{-1} for which $gg^{-1} = g^{-1}g = e$.

If a group $\mathcal{G}$ contains finitely many elements, it is called a *finite group* and the number of elements is called the *order* of the group, denoted by $|\mathcal{G}|$.
A group with infinitely many elements is called a group of *infinite order* or an *infinite group*.

The group operation is not required to be commutative, i.e. in general one will have $gh \neq hg$. However, the case that all elements of a group commute is an important special case.

Definition 1.1.2 A group $\mathcal{G}$ is called a *commutative* or *Abelian group* if $gh = hg$ for all $g, h \in \mathcal{G}$.

Note that for Abelian groups the group operation is often written as addition $g + h$, e.g. if the group elements are vectors.

Since checking associativity is often quite tedious, it is very convenient to circumvent it by noting that the elements of a (candidate) group actually are elements of a larger group in which the product is already known to be associative.

Definition 1.1.3 A subset $\mathcal{H} \subseteq \mathcal{G}$ is called a *subgroup* of $\mathcal{G}$, denoted by $\mathcal{H} \leq \mathcal{G}$, if its elements form a group with respect to the restriction of the binary operation of $\mathcal{G}$ to $\mathcal{H}$.
In order for a subset $\mathcal{H}$ of $\mathcal{G}$ to be a subgroup, it is necessary and sufficient to check that $\mathcal{H}$ is closed under the group operation and under taking inverses, i.e. that for $h, h' \in \mathcal{H}$ one has $hh' \in \mathcal{H}$ and $h^{-1} \in \mathcal{H}$.

Group elements can be classified according to several properties. An obvious one is the *order* of a group element, but there are more informative classifications.

Definition 1.1.4 Let $\mathcal{G}$ be a group.

(i) An element g in $\mathcal{G}$ has *order* n if n is the smallest positive integer such that $g^n = e$ is the identity element of $\mathcal{G}$.

(ii) Two elements g and g' of $\mathcal{G}$ are called *conjugate* (in $\mathcal{G}$) if $g' = x^{-1}gx$ for some element $x \in \mathcal{G}$. The element x is called a *conjugating element*.

Conjugate elements have the same order, but also share geometrical properties, e.g. being a rotation, reflection etc.

(iii) The elements of $\mathcal{G}$ which are conjugate to g form the *conjugacy class* of g, denoted by $g^{\mathcal{G}}$.

The number of elements in the conjugacy class of g is called the *class length* of g.

> The class lengths can actually be derived from the orders of certain subgroups and in particular have to be divisors of the group order: The elements h in $\mathcal{G}$ which commute with g form a subgroup $C_{\mathcal{G}}(g)$ of $\mathcal{G}$, called the *centralizer* of g in $\mathcal{G}$:
>
> $$C_{\mathcal{G}}(g) = \{h \in \mathcal{G} \mid gh = hg\}.$$
>
> The product of the class length with the order of the centralizer equals the order of $\mathcal{G}$, i.e. $|g^{\mathcal{G}}| \cdot |C_{\mathcal{G}}(g)| = |\mathcal{G}|$.

Homomorphisms and normal subgroups

In order to relate two groups, mappings between the groups which are compatible with the group operations are very useful.

Definition 1.1.5 For two groups $\mathcal{G}, \mathcal{H}$, a mapping φ from $\mathcal{G}$ to $\mathcal{H}$ is called a *group homomorphism* or *homomorphism* for short, if it is compatible with the group operations of $\mathcal{G}$ and $\mathcal{H}$, i.e. if

$$\varphi(gg') = \varphi(g)\varphi(g') \text{ for all } g, g' \in \mathcal{G}.$$

In the schematic description of a homomorphism in Figure 1 this means that the two curved arrows give the same result.

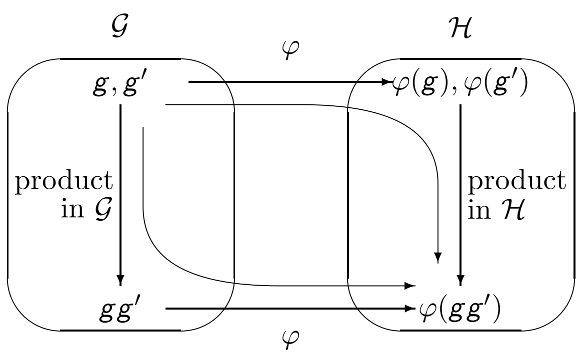

Figure 1: Schematic description of a homomorphism

It follows from the definition of a homomorphism that the identity element of $\mathcal{G}$ has to be mapped to the identity element of $\mathcal{H}$. In general, however, also other elements than the identity element may be mapped to the identity element of $\mathcal{H}$.

Definition 1.1.6 Let φ be a group homomorphism from $\mathcal{G}$ to $\mathcal{H}$ and let e be the identity element of $\mathcal{H}$.

(i) The set $\{g \in \mathcal{G} \mid \varphi(g) = e\}$ is called the *kernel* of φ, denoted by $\ker(\varphi)$.

(ii) The set $\varphi(\mathcal{G}) = \{\varphi(g) \mid g \in \mathcal{G}\}$ is called the *image* of φ, denoted by $\mathrm{im}(\varphi)$.

(iii) A homomorphism for which $\ker(\varphi) = \{e\}$ is called *injective* or a *monomorphism*, a homomorphism for which $\mathrm{im}(\varphi) = \mathcal{H}$ is called *surjective* or an *epimorphism*.

A homomorphism which is both injective and surjective is called *bijective* or an *isomorphism*.

Definition 1.1.7 Groups $\mathcal{G}$ and $\mathcal{H}$ for which an isomorphism from $\mathcal{G}$ to $\mathcal{H}$ exists are called *isomorphic*, denoted by $\mathcal{G} \cong \mathcal{H}$.
Isomorphic groups are basically the same group with different names for the group elements.

Homomorphisms allow to restrict the attention to relevant information about a group by ignoring the information about the elements in the kernel of a homomorphism. For example, if we are only interested whether elements of a group $\mathcal{G} \leq O_3(\mathbb{R})$ are rotations or not, we map the element g to $\det(g)$. The image of this homomorphism is the group of order 2 consisting only of the elements $\{+1, -1\}$, the kernel are the rotations in $\mathcal{G}$ and the non-rotations are the elements mapped to -1.

Definition 1.1.8 For a subgroup $\mathcal{H}$ of $\mathcal{G}$ the set $g\mathcal{H} = \{gh \mid h \in \mathcal{H}\}$ is called a *left coset* relative to $\mathcal{H}$, the element g is called the *coset representative* of $g\mathcal{H}$.
Analogously, $\mathcal{H}g = \{hg \mid h \in \mathcal{H}\}$ is called a *right coset* relative to $\mathcal{H}$.

In the case of a finite group $\mathcal{H}$, all cosets have cardinality $|\mathcal{H}|$. Cosets form a partition of $\mathcal{G}$, i.e. two cosets are either disjoint or equal. In particular, every element of a coset can be chosen as coset representative.

Definition 1.1.9 If the number of cosets of $\mathcal{G}$ relative to a subgroup $\mathcal{H}$ is finite, the number of cosets is called the *index* of $\mathcal{H}$ in $\mathcal{G}$, denoted by $[\mathcal{G} : \mathcal{H}]$.

Let $\mathcal{N} = \ker(\varphi)$ be the kernel of a homomorphism φ from $\mathcal{G}$ to $\mathcal{H}$, then every element gn of a left coset $g\mathcal{N}$ is mapped to the element $\varphi(gn) = \varphi(g)\varphi(n) = \varphi(g)e = \varphi(g)$ of $\mathcal{H}$. Elements from different cosets relative to $\mathcal{N}$ are mapped to different elements of $\mathcal{H}$.
But by the same argument also the elements of the *right coset* $\mathcal{N}g$ are mapped to $\varphi(g)$. Therefore the left and right cosets of $\mathcal{N}$ coincide, thus $\mathcal{N}g = g\mathcal{N}$, i.e. $\mathcal{N} = g^{-1}\mathcal{N}g$ for all $g \in \mathcal{G}$.

Definition 1.1.10 A subgroup $\mathcal{N}$ of $\mathcal{G}$ for which $g^{-1}\mathcal{N}g = \mathcal{N}$ for all g in $\mathcal{G}$ is called a *normal subgroup* or *invariant subgroup* of $\mathcal{G}$. One writes $\mathcal{N} \trianglelefteq \mathcal{G}$.
The kernels of homomorphisms are normal subgroups and every normal subgroup can be obtained as the kernel of a suitable homomorphism.

The crucial feature of normal subgroups is that they allow to define a group structure on the cosets relative to $\mathcal{N}$. If g, h are elements of $\mathcal{G}$ then the product of the (left) cosets $g\mathcal{N}$ and $h\mathcal{N}$ is defined to be the coset with representative gh, i.e.

$$(g\mathcal{N})(h\mathcal{N}) = (gh)\mathcal{N}.$$

Since left and right cosets coincide, one usually omits these attributes for the cosets relative to a normal subgroup.

The above definition only gives a valid group operation because the left and right cosets of $\mathcal{N}$ coincide. For a subgroup $\mathcal{H}$ that is not normal, the coset $(gh)\mathcal{H}$ depends on the choice of representatives g and h and the group operation would not be well-defined.

Definition 1.1.11 Let $\mathcal{N}$ be a normal subgroup of $\mathcal{G}$. Then the set $\{g\mathcal{N} \mid g \in \mathcal{G}\}$ of cosets of $\mathcal{G}$ relative to $\mathcal{N}$ form a group with the group operation

$$(g\mathcal{N})(h\mathcal{N}) = (gh)\mathcal{N}.$$

This group is denoted by $\mathcal{G}/\mathcal{N}$ and is called the *quotient group* or *factor group* of $\mathcal{G}$ by $\mathcal{N}$.

The following theorem, stating that the image of a homomorphism is isomorphic to a factor group relative to its kernel, is of invaluable importance.

Theorem 1.1.12 (*Homomorphism theorem*) If φ is a homomorphism from $\mathcal{G}$ to $\mathcal{H}$ and if $\mathcal{N} = \ker(\varphi)$ is the kernel of φ, then the image $\varphi(\mathcal{G}) = \mathrm{im}(\varphi)$ is isomorphic to the factor group $\mathcal{G}/\mathcal{N}$.
The isomorphism is explicitly given by $g\mathcal{N} \mapsto \varphi(g)$.

A group contains some normal subgroups which are of special significance.

Definition 1.1.13 Let $\mathcal{G}$ be a group.

(i) The set $Z(\mathcal{G}) = \{h \in \mathcal{G} \mid gh = hg \text{ for all } g \in \mathcal{G}\}$ of elements of $\mathcal{G}$ commuting with all elements of $\mathcal{G}$ is a normal subgroup called the *center* of $\mathcal{G}$.

The center of a group contains precisely those elements which form conjugacy classes on their own, i.e. conjugacy classes of class length 1.

(ii) For two elements g, h, the element $[g, h] = g^{-1}h^{-1}gh$ is called the *commutator* of g and h.

The smallest subgroup containing all commutators is a normal subgroup called the *commutator subgroup* of $\mathcal{G}$, denoted by $\mathcal{G}'$.

The factor group $\mathcal{G}/\mathcal{G}'$ is the largest factor group of $\mathcal{G}$ which is Abelian, i.e. for each normal subgroup $\mathcal{N} \trianglelefteq \mathcal{G}$ for which $\mathcal{G}/\mathcal{N}$ is Abelian one has $\mathcal{G}' \subseteq \mathcal{N}$.

There are various ways to construct larger groups from small ones. The easiest and most important one is the direct product of two groups.

Definition 1.1.14 For two groups $\mathcal{G}$ and $\mathcal{H}$, a group structure on the pairs (g, h) with $g \in \mathcal{G}$ and $h \in \mathcal{H}$ is obtained by defining the product componentwise, i.e. by

$$(g, h)(g', h') = (gg', hh').$$

The group obtained from $\mathcal{G}$ and $\mathcal{H}$ in this way is called the *direct product* of $\mathcal{G}$ and $\mathcal{H}$ and is denoted by $\mathcal{G} \times \mathcal{H}$.
If $\mathcal{G}$ and $\mathcal{H}$ are finite groups, then $|\mathcal{G} \times \mathcal{H}| = |\mathcal{G}| \cdot |\mathcal{H}|$. Moreover, $\mathcal{G}$ and $\mathcal{H}$ can be regarded as being embedded in the direct product as the elements with one component the identity element: $\mathcal{G} \equiv \{(g, e_{\mathcal{H}}) \mid g \in \mathcal{G}\}$ and $\mathcal{H} \equiv \{(e_{\mathcal{G}}, h) \mid h \in \mathcal{H}\}$. With this identification, $\mathcal{G}$ and $\mathcal{H}$ are normal subgroups of $\mathcal{G} \times \mathcal{H}$ with $\mathcal{G} \cap \mathcal{H} = \{e\}$ and all elements of $\mathcal{G}$ commute with all elements of $\mathcal{H}$.

In many situations it is both cumbersome and superfluous to look at all elements of a group. Instead, one only considers a small subset of the group elements from which all other elements can be obtained by forming products.

Definition 1.1.15 A subset $\mathcal{S} \subseteq \mathcal{G}$ is called a set of *generators* or *generating set* for $\mathcal{G}$ if every element of $\mathcal{G}$ can be obtained as a finite product of elements from $\mathcal{S}$ or their inverses.

Definition 1.1.16 A group that is generated by a single element is called a *cyclic group*.
Up to isomorphism there exists only a single cyclic group of order n, which is denoted by $\mathcal{C}_n$.

Cyclic groups together with the direct product construction give a complete overview of finite Abelian groups.

Theorem 1.1.17 (*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.

If the assumption that d_i divides d_{i+1} is dropped, an Abelian group can be written in different ways. For example, one has $\mathcal{C}_6 \cong \mathcal{C}_2 \times \mathcal{C}_3$. However, the unique decomposition can be easily read off from any direct product decomposition into cyclic groups using the *greatest common divisor* (gcd) and *least common multiple* (lcm) of the group orders. The crucial observation is that

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

Applying this isomorphism as long as there are cyclic groups with orders not dividing each other finally yields the unique decomposition described above. For example, on has

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

1.2 Group actions

The concept of a group is the essence of an abstraction process which distilled the common features of various examples of groups. On the other hand, although abstract groups are mathematical objects in their own right, they are interesting because the group elements can be applied to certain objects. Examples are:

- The symmetry group of a square permutes the corners of the square, but also its sides.
- A crystallographic space group moves the atoms in direct space.
- A crystallographic point group can be applied to the face normals of a macroscopic crystal.

In fact, in crystallography the abstract groups play only a minor role, one is much more familiar with e.g. the point groups. For example, the abstract group $\mathcal{C}_2$ with two elements occurs in three versions, differing by their action on $\mathbb{R}^3$:

(1) In the group m, the element of order 2 has a 2-dimensional plane of points which are fixed.

(2) In the group *2*, the element of order 2 has a 1-dimensional line of points which are fixed.

(3) In the group $\overline{1}$, the element of order 2 has just a single point which is fixed.

The formal definition of a group action is as follows:

Definition 1.2.1 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) $g(h(\omega)) = (gh)(\omega)$, i.e. successively applying two group elements is the same as applying their product;

(ii) $e(\omega) = \omega$ for the identity element e of $\mathcal{G}$, i.e. the identity element does not alter anything.

Often, two elements ω and ω' are regarded as equivalent if there is a group element moving ω to ω'.

Definition 1.2.2 Two elements $\omega, \omega' \in \Omega$ lie in the same *orbit* under $\mathcal{G}$ if there exists $g \in \mathcal{G}$ such that $\omega' = g(\omega)$.
The set $\omega^{\mathcal{G}} := \{g(\omega) \mid g \in \mathcal{G}\}$ of all elements in the orbit of ω is called the *orbit* of ω under $\mathcal{G}$.

Example 1.2.3 A group $\mathcal{G}$ acts on itself by left and right multiplication:

(i) $g(h) = gh$ is the action of $\mathcal{G}$ on itself by *left multiplication*. Note that the compatibility of the action with the group product is just the associativity of the group product.

(ii) $g(h) = hg^{-1}$ is the action of $\mathcal{G}$ on itself by *right multiplication*. In this case the inverse of g is required in the action, because $(g_1 g_2)(h) = h(g_1 g_2)^{-1} = h g_2^{-1} g_1^{-1} = g_1(h g_2^{-1}) = g_1(g_2(h))$.

Example 1.2.4 A group $\mathcal{G}$ acts on the set of its elements by conjugation: $g(h) = ghg^{-1}$. The orbits for this action are precisely the *conjugacy classes* of $\mathcal{G}$.

Example 1.2.5

(i) The symmetry group of a square acts on the *corners*, *sides* and *diagonals* of the square.

Note that some group elements fix both diagonals, i.e. these elements act *trivially* on the diagonals.

(ii) The rotation group of a cube acts on the *edge centers*, *face centers* and *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.

Example 1.2.6 A group $\mathcal{G} \leq \mathrm{GL}_n(\mathbb{R})$ 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: $g(\mathbf{v}) = g \cdot \mathbf{v}$.
Analogously, a group $\mathcal{G} \leq \mathrm{GL}_n(\mathbb{C})$ of complex $n \times n$ matrices acts on the vectors $\mathbf{v}$ in $\mathbb{C}^n$.

Example 1.2.7 Let $\mathcal{G}$ be a group of real or complex $n \times n$ matrices.

(i) $\mathcal{G}$ acts on the $n \times n$ matrices (corresponding to the linear operators of $\mathbb{R}^n$ or $\mathbb{C}^n$) by $g(\boldsymbol{A}) = g\boldsymbol{A}g^{-1}$.

(ii) $\mathcal{G}$ acts on the metric tensors by $g(\boldsymbol{M}) = (g^{-1})^T \boldsymbol{M} (g^{-1})^*$, where g^* denotes the complex conjugate of the matrix g.

These actions describe the effect of the basis transformation g on the matrices of a linear operator and of a metric tensor, respectively.

Example 1.2.8 A point group $\mathcal{G} \leq \mathrm{GL}_3(\mathbb{R})$ acts on the coordinates x, y, z and on functions of the coordinates, such as $xy + yz + z^2$.

1.3 Group representations

A particularly useful action of groups is their action on vector spaces. On the one hand, often such an action comes into play naturally, since groups describe symmetries of objects in 3-dimensional space. On the other hand, vector spaces can be dealt with by the powerful methods of linear algebra.

Definition 1.3.1 Let $\mathcal{G}$ be a group acting linearly on a vector space $\mathbf{V}$, i.e. such that

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

(i) 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 $\mathbf{V}$.

(ii) If $\mathbf{V}$ is a vector space of dimension n, then n is called the *degree* or *dimension* of the representation $\mathbf{D}$, denoted by $\deg(\mathbf{D})$ or $\dim(\mathbf{D})$.

(iii) 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 $\mathbf{V}$. This is sometimes called a *matrix representation* of $\mathcal{G}$, but usually also simply a *representation*.

The entries in the matrices of a representation are scalars from the field underlying the vector space $\mathbf{V}$. In this course, unless explicitly stated otherwise, we will always assume that $\mathbf{V}$ is a *complex* vector space, hence the representation consists of matrices over the complex numbers $\mathbb{C}$, i.e. we have

$$\mathbf{D} : \mathcal{G} \to \mathrm{GL}_n(\mathbb{C}).$$

Such representations are verbosely called *complex representations*, but for simplicity we will usually omit the attribute 'complex'.

Besides complex representations one may also encounter the following types of representations:

Real representations: If the group $\mathcal{G}$ describes some phenomenon in a physical space like $\mathbb{R}^3$, the vector space is often a real vector space and the representation consists of matrices over $\mathbb{R}$.

Rational representations: In the case of groups acting on discrete periodic structures (like crystals), the rational vector space $\mathbb{Q}^n$ is often more appropriate than $\mathbb{R}^n$, since only fractions are required.

Integral representations: Although the integers do not form a field (as required for the scalars of a vector space), a group may act on a linear space over the integers, which is called a $\mathbb{Z}$-*module*. This is for example the case for groups acting on lattices. Then the representation consists of integral matrices.

Definition 1.3.2 Every group $\mathcal{G}$ has a 1-dimensional representation obtained by mapping every group element g to 1.
This representation is called the *trivial representation* or *identity representation* of $\mathcal{G}$, sometimes also the *totally symmetric representation* of $\mathcal{G}$.

Example 1.3.3 The cyclic group $\mathcal{C}_n$ of order n generated by an element g has a 1-dimensional representation $\mathbf{D}$ given by

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

Example 1.3.4 The group $SO_2(\mathbb{R})$ of rotations on $\mathbb{R}^2$ has (with respect to the standard basis $\mathbf{e}_1 = (1,0)^T, \mathbf{e}_2 = (0,1)^T$ of $\mathbb{R}^2$) a 2-dimensional representation $\mathbf{D}$ which maps a rotation $\boldsymbol{r}_\varphi$ by the angle φ to

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

Example 1.3.5 The symmetry group *4mm* of a square can be generated by a fourfold rotation g and a diagonal reflection h in the line $x = y$ (see Figure 2).

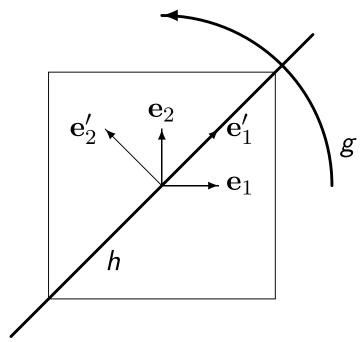

Figure 2: Symmetry group of a square

With respect to the basis $\mathbf{e}_1 = (1,0), \mathbf{e}_2 = (0,1)$, the action of *4mm* on $\mathbb{R}^2$ gives rise to the representation $\mathbf{D}$ with

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

However, with respect to the different basis $\mathbf{e}_1' = (1,1), \mathbf{e}_2' = (-1,1)$, we obtain a 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?

Definition 1.3.6 If a group $\mathcal{G}$ happens to be given as a group of $n \times n$ matrices, the identical mapping $g \mapsto g$ is a representation, called the *vector representation* or *natural representation* of $\mathcal{G}$.

Definition 1.3.7 For a complex representation $\mathbf{D}$ of a group $\mathcal{G}$, replacing all entries by their complex conjugates yields another representation of $\mathcal{G}$, called the *complex conjugate representation* or simply *conjugate representation* of $\mathbf{D}$ and denoted by $\mathbf{D}^*$.
If a representation happens to consist of real matrices, one has of course $\mathbf{D} = \mathbf{D}^*$.

Example 1.3.8 If $\mathbf{D}(g) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$, then one has $\mathbf{D}^*(g) = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}$. in the conjugate representation.

Example 1.3.9 For the representation $\mathbf{D}(g) = \exp(2\pi i/n)$ of a cyclic group of order n, the conjugate representation is $\mathbf{D}^*(g) = \exp(-2\pi i/n) = \exp(2\pi i(n-1)/n)$.

An important representation is obtained from the action of $\mathcal{G}$ on itself by left or right multiplication.

Definition 1.3.10 Let $\mathcal{G}$ be a group of order n and let $g_1, g_2, \ldots, g_n$ be the elements of $\mathcal{G}$. If we choose a basis $\mathbf{v}_{g_1}, \mathbf{v}_{g_2}, \ldots, \mathbf{v}_{g_n}$ of $\mathbb{C}^n$, then the action

$$g(\mathbf{v}_{g_i}) = \mathbf{v}_{gg_i}$$

gives a representation of degree $|\mathcal{G}|$ of $\mathcal{G}$, called the *(left) regular representation* $\boldsymbol{\Gamma}_l$ of $\mathcal{G}$.
The right multiplication gives rise to the *(right) regular representation* $\boldsymbol{\Gamma}_r$ with the action

$$g(\mathbf{v}_{g_i}) = \mathbf{v}_{g_i g^{-1}}.$$

Note that the matrices of the (left and right) regular representation are *permutation matrices*, i.e. in every row and column there is precisely one entry 1 and the others are 0.

Example 1.3.11 The symmetry group $\mathcal{D}_4$ of a square is generated by a fourfold rotation g and a reflection h (e.g. in the x-axis) and contains the elements $e, g, g^2, g^3, h, hg, hg^2, hg^3$. Conjugating the rotation g by the reflection h gives the inverse rotation g^3, i.e. we have $hgh = g^3$ and thus $gh = hg^3$.
For the action by left multiplication we get

$$ge = g, gg = g^2, gg^2 = g^3, gg^3 = e, gh = hg^3, ghg = h, ghg^2 = hg, ghg^3 = hg^2 \text{ and}$$
$$he = h, hg = hg, hg^2 = hg^2, hg^3 = hg^3, hh = e, hhg = g, hhg^2 = g^2, hhg^3 = g^3$$

from which we get the left regular representation

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

Action on function spaces

If $\mathcal{G}$ acts on some set Ω, then it also acts on the functions $f : \Omega \to \mathbb{C}$, namely by

$$g(f)(\omega) = f(g^{-1}(\omega)).$$

In particular, if $\mathcal{G}$ acts on some vector space $\mathbf{V}$ via the representation $\mathbf{D}$, it also acts on the functions from $\mathbf{V}$ to $\mathbb{C}$ by

$$g(f)(\mathbf{v}) = f(\mathbf{D}(g^{-1})(\mathbf{v})).$$

By this construction, $\mathcal{G}$ can be regarded as a group of operators on the functions on $\mathbf{V}$.

1.4 Equivalence of representations

Since a representation by matrices depends on the choice of a basis for $\mathbf{V}$, one identifies representations which only differ by the chosen basis. Since a basis transformation can be expressed by a transformation matrix $\boldsymbol{X}$, the transition from one basis to another corresponds to a conjugation by an invertible matrix.

Definition 1.4.1 Two representations $\mathbf{D}$ and $\mathbf{D}'$ of a group $\mathcal{G}$ are called *equivalent* if there exists an invertible $n \times n$ matrix $\boldsymbol{X}$ such that

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

The reasoning behind calling representations equivalent which are conjugate to each other is as follows:

- 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 $\boldsymbol{X}$ 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 $\mathbf{v}'_1, \ldots, \mathbf{v}'_n$.

Example 1.4.2 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 $hgh = g^2$.
This group has the 2-dimensional representations

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

$$\mathbf{D}'(g) = \begin{pmatrix} \exp(2\pi i/3) & 0 \\ 0 & \exp(2\pi i/3) \end{pmatrix}, \quad \mathbf{D}'(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

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

These three representations are equivalent, because $\boldsymbol{X}' = \begin{pmatrix} 1 & -i \\ -i & 1 \end{pmatrix}$ conjugates $\mathbf{D}$ to $\mathbf{D}'$ and $\boldsymbol{X}'' = \begin{pmatrix} 1 & -2+\sqrt{3} \\ -2+\sqrt{3} & 1 \end{pmatrix}$ conjugates $\mathbf{D}$ to $\mathbf{D}''$.

The representation $\mathbf{D}$ expresses the action with respect to an *orthonormal basis*, the representation $\mathbf{D}''$ 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 $\boldsymbol{X}$ such that $\mathbf{D}'(g) = \boldsymbol{X}^{-1}\mathbf{D}(g)\boldsymbol{X}$ is equivalent to finding $\boldsymbol{X}$ such that $\boldsymbol{X}\mathbf{D}'(g) = \mathbf{D}(g)\boldsymbol{X}$, but the latter is easier to solve.

A real representation can of course always be regarded as a complex representation (in which by chance only real numbers occur). Conversely, a complex representation $\mathbf{D}$ can be turned into a real representation $\mathbf{D}_{\mathbb{R}}$ of twice the degree as follows:

Replace every entry $z = x + iy$ by the 2×2 matrix $\begin{pmatrix} x & y \\ -y & x \end{pmatrix}$, then the resulting representation $\mathbf{D}_{\mathbb{R}}$ is equivalent to the direct sum representation $\mathbf{D} \oplus \mathbf{D}^*$, i.e. the representation in block diagonal form

$$\left(\begin{array}{c|c} \mathbf{D}(g) & \mathbf{0} \\ \hline \mathbf{0} & \mathbf{D}^*(g) \end{array}\right).$$

To see this, let $(\mathbf{a}_1, \mathbf{b}_1, \ldots, \mathbf{a}_n, \mathbf{b}_n)$ be the basis of the $2n$-dimensional real representation $\mathbf{D}_{\mathbb{R}}$, then the basis transformation to the basis $(\mathbf{a}_1 + i\mathbf{b}_1, \ldots, \mathbf{a}_n + i\mathbf{b}_n, \mathbf{a}_1 - i\mathbf{b}_1, \ldots, \mathbf{a}_n - i\mathbf{b}_n)$ gives precisely the representation $\mathbf{D} \oplus \mathbf{D}^*$.

1.5 Unitary representations

On the n-dimensional real space $\mathbb{R}^n$ the *scalar product* of two vectors $\mathbf{a} = (a_1, \ldots, a_n)^T$ and $\mathbf{b} = (b_1, \ldots, b_n)^T$ is given by

$$\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^{n} a_i b_i.$$

Analogously, on the n-dimensional complex space $\mathbb{C}^n$ the *Hermitian product* of two vectors $\mathbf{a} = (a_1, \ldots, a_n)^T$ and $\mathbf{b} = (b_1, \ldots, b_n)^T$ is given by

$$\mathbf{a} \cdot \mathbf{b} = \sum_{i=1}^{n} a_i b_i^*$$

where $z^* = x - iy$ is the complex conjugate of $z = x + iy$. The complex conjugate is required to ensure that $\mathbf{a} \cdot \mathbf{a} > 0$ for $\mathbf{a} \neq \mathbf{0}$. In both cases, the Euclidean length of a vector is given by $\|\mathbf{a}\| = \sqrt{\mathbf{a} \cdot \mathbf{a}}$.

Definition 1.5.1

(i) A real matrix is called an *orthogonal* matrix if its columns form an orthonormal basis of $\mathbb{R}^n$, i.e. if $\boldsymbol{A}^T \boldsymbol{A} = \boldsymbol{I}_n$.

The inverse of an orthogonal matrix thus is just its transposed matrix, i.e. $\boldsymbol{A}^{-1} = \boldsymbol{A}^T$.

(ii) A complex matrix is called a *unitary* matrix if its columns form an orthonormal basis of $\mathbb{C}^n$, i.e. if $\boldsymbol{A}^T \boldsymbol{A}^* = \boldsymbol{I}_n$.

The inverse of a unitary matrix thus is the transposed of the complex conjugate matrix, i.e. $\boldsymbol{A}^{-1} = (\boldsymbol{A}^*)^T = \boldsymbol{A}^\dagger$.

(iii) The matrix $\boldsymbol{A}^\dagger = (\boldsymbol{A}^*)^T = (\boldsymbol{A}^T)^*$ is called the *Hermitian conjugate* of $\boldsymbol{A}$.

Definition 1.5.2 A representation D of $\mathcal{G}$ such that $\mathsf{D}(g)$ is a unitary matrix for every $g \in \mathcal{G}$ is called a *unitary representation* of $\mathcal{G}$.

For elements of a point group it is clear that an orthonormal basis is mapped to an orthonormal basis again, since point group elements are isometries. Thus, point group representations that are written with respect to an orthonormal basis are unitary representations.
However, also for an arbitrary finite group, any representation is equivalent to a unitary representation. Note that this statement is in general not true for infinite groups.

Theorem 1.5.3 Let D be a representation of the finite group $\mathcal{G}$, then D is equivalent to a unitary representation.

The proof of this theorem is actually constructive: Define

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

then $\boldsymbol{F}$ is a metric tensor which is invariant under D, i.e. one has $\mathsf{D}(g)^T \boldsymbol{F} \mathsf{D}(g)^* = \boldsymbol{F}$. Construct a matrix $\boldsymbol{X}$ such that $\boldsymbol{X}^T \boldsymbol{X}^* = \boldsymbol{F}$, i.e. such that the columns of $\boldsymbol{X}$ form a matrix with metric tensor $\boldsymbol{F}$. Then $\boldsymbol{X} \mathsf{D}(g) \boldsymbol{X}^{-1}$ is a unitary matrix.

Example 1.5.4 The representation

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

of $\mathcal{D}_3$ fixes the metric tensor $\boldsymbol{F} = \begin{pmatrix} 1 & -1/2 \\ -1/2 & 1 \end{pmatrix}$.

A matrix $\boldsymbol{X}$ for which $\boldsymbol{X}^T\boldsymbol{X} = \boldsymbol{F}$ is

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

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

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

which are orthogonal matrices (and thus also unitary).

> Note that the transition of a complex representation to a real representations discussed after Example 1.4.2 turns unitary matrices into orthogonal matrices.

1.6 Invariant subspaces and reducibility

It is easy to build a new representation from given representations by joining the matrices into a block diagonal matrix.

Definition 1.6.1 Let $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ be representations of degrees n_1 and n_2, respectively. Then joining the representations $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$ as diagonal blocks into matrices of size n_1+n_2 gives a representation $\mathbf{D}^{(1)} \oplus \mathbf{D}^{(2)}$ of degree $n_1 + n_2$ with

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

which is called the *direct sum* of the representations $\mathbf{D}^{(1)}$ and $\mathbf{D}^{(2)}$.

Example 1.6.2 We have seen in Example 1.3.5 that

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

is a representation of the symmetry group $\mathcal{D}_4$ of a square. A 1-dimensional representation $\mathbf{D}^{(1)}$ is obtained by taking the determinant of the matrices of $\mathbf{D}^{(2)}$, this gives

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

The direct sum of these two representations is given by

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

The direct sum construction shows, that even up to equivalence there are infinitely many representations, since there are representations of arbitrary large degree. However, if one restricts to representations which can not be written in the form of block diagonal matrices, the situation becomes different.

Definition 1.6.3

(i) A representation $\mathbf{D}$ is called *reducible* if there is a subspace $\mathbf{U}$ of $\mathbf{V}$ different from $\{\mathbf{0}\}$ and $\mathbf{V}$ such that $\mathbf{U}$ is invariant under $\mathbf{D}$, i.e. for which $\mathbf{D}(g)(\mathbf{u}) \in \mathbf{U}$ for all $\mathbf{u}$ in $\mathbf{U}$ and all g in $\mathcal{G}$.

By choosing the basis of $\mathbf{V}$ such that the first vectors are a basis of $\mathbf{U}$, a reducible representation $\mathbf{D}$ is equivalent to one of the form

$$\left(\begin{array}{c|c} \mathbf{D}^{(1)}(g) & \mathbf{H}^{(12)}(g) \\ \hline \mathbf{0} & \mathbf{D}^{(2)}(g) \end{array}\right).$$

(ii) If for a reducible representation $\mathbf{D}$ the basis of $\mathbf{V}$ can be chosen such that $\mathbf{H}^{(12)}(g) = \mathbf{0}$ for all g, i.e. such that $\mathbf{D}$ is equivalent to a representation of the form

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

then $\mathbf{D}$ is called *decomposable* or *fully reducible*. In that case, the basis vectors extending the basis of $\mathbf{U}$ to a basis of $\mathbf{V}$ span a subspace $\mathbf{W}$ on which $\mathcal{G}$ acts by the representation $\mathbf{D}^{(2)}$. One says that $\mathbf{W}$ is a *complement* of $\mathbf{U}$ in $\mathbf{V}$.

(iii) 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*.

(iv) If $\mathbf{V}$ allows no decomposition $\mathbf{V} = \mathbf{U} \oplus \mathbf{W}$ into nontrivial subspaces $\mathbf{U}$ and $\mathbf{W}$ which are invariant under $\mathbf{D}$, the representation is called *indecomposable*.

Terminology: Because the term *irreducible representation* is fairly long and will occur very often, we will use the short form *irrep* for irreducible representations.

A priori, one may expect that decomposability is a stronger property than reducibility and that irreducibility is a stronger property than indecomposability. In a more general context, this is indeed the case, but in the case of complex or real representations, reducibility and decomposability is actually the same.

Lemma 1.6.4 For vector spaces $\mathbf{V}$ over infinite fields like $\mathbb{R}$ or $\mathbb{C}$, but also over the rational numbers $\mathbb{Q}$, every reducible representation 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: If we assume that the representation is given by unitary matrices, the complement is simply the orthogonal complement $\mathbf{W} = \mathbf{U}^{\perp} = \{\mathbf{v} \mid \mathbf{u} \cdot \mathbf{v} = 0 \text{ for all } \mathbf{u} \in \mathbf{U}\}$ of the subspace $\mathbf{U}$. This space is invariant under $\mathbf{D}$, since the scalar product is unaffected by the application of $\mathbf{D}(g)$.

The statement of Lemma 1.6.4 is not true over finite fields with p^f elements, for which p divides the group order, and it is also not true over the integers.

Example 1.6.5 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 the two 1-dimensional invariant subspaces $\mathbf{U}$ and $\mathbf{W}$ spanned by the vectors $\mathbf{b}_1 = \mathbf{e}_1 + \mathbf{e}_2$ and $\mathbf{b}_2 = \mathbf{e}_1 - \mathbf{e}_2$. However, over the integers, the subspace

> $\mathbf{U}$ has no $\mathbf{D}$-invariant complement in $\mathbb{Z}^2$, since $\mathbf{b}_1, \mathbf{b}_2$ span a sublattice of index 2. The basis transformation to $\mathbf{D}'(g) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ is only possible over $\mathbb{Q}$, but not over $\mathbb{Z}$.
>
> This example actually lies at the core of the subdivision of geometric classes into arithmetic classes.

Clearly, 1-dimensional representations are always irreducible. For 2- and 3-dimensional representations, a reducible representation necessarily has a 1-dimensional invariant subspace. This can be found as a common eigenvector for the generators (for possibly different eigenvalues).

Example 1.6.6 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

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

Example 1.6.7 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 $\mathbf{D}$ 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.

For representations of degrees beyond 3 the problem of deciding whether a representation is irreducible or not becomes more complicated, since invariant subspaces of dimension ≥ 2 are harder to find. However, there is a clear criterion to distinguish between irreducible and reducible representations.

Theorem 1.6.8 (*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 $\lambda \boldsymbol{I}_n$ for $\lambda \in \mathbb{C}$) commute with all matrices $\mathbf{D}(g)$.

The proof of this crucial result is actually quite simple: The characteristic polynomial of a matrix $\boldsymbol{X}$ commuting with all $\mathbf{D}(g)$ has a complex root λ, hence $\boldsymbol{X} - \lambda \boldsymbol{I}_n$ has a nontrivial kernel. Since the kernel of such a matrix is invariant under $\mathbf{D}$, it follows that the kernel is $\mathbb{C}^n$ and hence $\boldsymbol{X} = \lambda \boldsymbol{I}_n$.

For real representations, the situation is slightly more complicated. In that case, the matrices commuting with all $\mathbf{D}(g)$ form a space of dimension 1, 2 or 4:

dim 1 : If $\mathbf{D}$ remains irreducible when regarded as a complex representation, then only the scalar matrices commute with all $\mathbf{D}(g)$.

dim 2 : If $\mathbf{D}$ splits into two complex conjugate irreps when regarded as a complex representation, then the commuting matrices can be identified with $\mathbb{C}$.

dim 4 : It can also happen that $\mathbf{D}$ splits into two copies of the same irreps when regarded as a complex representation. In this case the commuting matrices can be identified with the Hamilton quaternions $\mathbb{H}$.

If we now combine the concept of irreducible representations with that of equivalent representations, we finally arrive at a finite set of representations for a finite group $\mathcal{G}$.

Theorem 1.6.9 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 is equal to the number of conjugacy classes of the group $\mathcal{G}$.

Terminology: From now on, we will suppress the term 'up to equivalence'. With *different irreps* we always mean (unless stated otherwise) *non-equivalent irreps*.

The possible degrees of irreps are restricted by certain conditions. The first follows from a structure theorem about fairly general abstract structures, called *semisimple algebras*. Its application to finite groups leads to the following result.

Theorem 1.6.10 Let $\mathbf{D}^{(1)}, \ldots, \mathbf{D}^{(r)}$ be the irreps of the finite group $\mathcal{G}$ and let $n_1, \ldots, n_r$ be their degrees. Then the regular representation of $\mathcal{G}$ contains the irrep $\mathbf{D}^{(i)}$ with multiplicity n_i, i.e. the regular representation is equivalent to

$$\underbrace{\mathbf{D}^{(1)} \oplus \ldots \oplus \mathbf{D}^{(1)}}_{n_1} \bigoplus \underbrace{\mathbf{D}^{(2)} \oplus \ldots \oplus \mathbf{D}^{(2)}}_{n_2} \bigoplus \cdots \bigoplus \underbrace{\mathbf{D}^{(r)} \oplus \ldots \oplus \mathbf{D}^{(r)}}_{n_r}$$

A consequence of the above theorem is that the matrices of an irrep of degree n span the full space of $n \times n$ matrices.

Corollary 1.6.11 Let $\mathbf{D}$ be an irrep of $\mathcal{G}$ of degree n. Then the matrices $\mathbf{D}(g)$ contain a basis of the space of $n \times n$ matrices, i.e. every $n \times n$ matrix $\boldsymbol{A}$ can be written as a linear combination $\boldsymbol{A} = \sum_{g \in \mathcal{G}} a_g g$ for certain (not uniquely determined) coefficients $a_g \in \mathbb{C}$.

This result also implies Schur's lemma, since a matrix commuting with all group elements, also commutes with all linear combinations of group elements and thus has to commute with all $n \times n$ matrices. But only scalar matrices have this property.
Furthermore, we obtain a (fairly generous) upper bound for the degrees of the irreps, since a basis of the $n \times n$ matrices consists of n^2 elements, thus we have $|\mathcal{G}| \geq n^2$. But a much stronger result can be derived from the above theorem.

Corollary 1.6.12 The sum of the squares of the degrees of the different irreps of a finite group $\mathcal{G}$ is equal to the group order, i.e.

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

Corollary 1.6.13 All irreps of an Abelian group $\mathcal{G}$ have degree 1, since every group element forms a conjugacy class on its own and the only possibility to write $|\mathcal{G}|$ as a sum of $|\mathcal{G}|$ nonzero squares is to have all degrees equal to 1.

The result of Corollary 1.6.12 is actually sufficient to determine the degrees of the irreps for all isomorphism types of crystallographic point groups in dimension 3, except for the group $\mathcal{O}_h$. However, a couple of further restrictions on the degrees of the irreps are useful.
The following result requires some non-trivial number theoretic considerations.

Lemma 1.6.14 The degree of an irrep of $\mathcal{G}$ divides the group order.

> Using some deeper insights, one can even sharpen this result. Ito's theorem states that the degrees of the irreps divide the order of the factor group $\mathcal{G}/\mathcal{A}$ if $\mathcal{A}$ is an Abelian normal subgroup of $\mathcal{G}$. In particular, the degrees divide the index $[\mathcal{G} : Z(\mathcal{G})]$ of the center $Z(\mathcal{G})$ of $\mathcal{G}$ in $\mathcal{G}$.

The number of 1-dimensional irreps can be determined from purely group properties.

Lemma 1.6.15 The 1-dimensional irreps of a group $\mathcal{G}$ are in bijection with the irreps of the commutator factor group $\mathcal{G}/\mathcal{G}'$. This means that the number of 1-dimensional irreps is equal to the index of the commutator subgroup $\mathcal{G}'$ in $\mathcal{G}$.
In particular, the number of 1-dimensional irreps is a divisor of the group order.

With these results, one can actually determine the degrees of the irreps of all crystallographic point groups, knowing their order, their number of conjugacy classes and (only for the group $\mathcal{O}_h$) the commutator subgroup.

Example 1.6.16 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 $1, 1, 2, 3, 3$.

Example 1.6.17 The group $\mathcal{O}_h$ of order 48 has 10 conjugacy classes. Since one irrep is the trivial representation of degree 1, 47 has to be written as the sum of nine squares. Since $47/9 > 5$ and $\sqrt{47-8} < 7$ the highest degree of an irrep is at least 3 and at most 6. Working out the different possibilities, one gets the following solutions:

- $48 = 6^2 + 2^2 + 1 + 1 + 1 + 1 + 1 + 1 + 1 + 1$
- $48 = 5^2 + 3^2 + 2^2 + 2^2 + 1 + 1 + 1 + 1 + 1 + 1$
- $48 = 4^2 + 4^2 + 3^2 + 1 + 1 + 1 + 1 + 1 + 1 + 1$
- $48 = 4^2 + 3^2 + 2^2 + 2^2 + 2^2 + 2^2 + 2^2 + 1 + 1 + 1$
- $48 = 3^2 + 3^2 + 3^2 + 3^2 + 2^2 + 2^2 + 1 + 1 + 1 + 1$

The second solution is ruled out, since 5 does not divide 48. The third solution is ruled out, since it has 7 1-dimensional irreps and 7 does not divide 48.
In order to rule out other solutions, one needs some knowledge about the group. E.g., $\mathcal{O}_h$ contains $\mathcal{T}$ as a normal subgroup of index 4, thus the commutator subgroup is a subgroup of $\mathcal{T}$ and has index at least 4. This rules out the fourth solution. Furthermore, since the octahedral group acts irreducibly on 3-dimensional space, there has to be an irrep of degree 3. This leaves only the last solution and the degrees of the irreps are $1, 1, 1, 1, 2, 2, 3, 3, 3, 3$. Alternatively, one might know that the commutator group of $\mathcal{O}_h$ is actually equal to $\mathcal{T}$, which shows that there have to be four 1-dimensional irreps.

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 $\mathcal{C}_{20}$, $\mathcal{D}_{10}$, $\mathcal{F}_{20}$.

If the structure of a group $\mathcal{G}$ is known, in particular its normal subgroups, then part of the information about the irreps of $\mathcal{G}$ can be derived from the factor groups of $\mathcal{G}$.

Theorem 1.6.18 If $\mathcal{N} \trianglelefteq \mathcal{G}$ is a normal subgroup of $\mathcal{G}$ and if $\mathbf{D}_{\mathcal{N}}$ is a representation of the factor group $\mathcal{G}/\mathcal{N}$, then $\mathbf{D}(g) = \mathbf{D}_{\mathcal{N}}(g\mathcal{N})$ is a well-defined representation of $\mathcal{G}$ with $\mathcal{N}$ in its kernel.
If $\mathbf{D}_{\mathcal{N}}$ is irreducible, then also $\mathbf{D}$ is irreducible.

1.7 Characters of representations and character tables

Since we regard equivalent representations as not essentially different, it would be useful to have a simple criterion to determine whether two representations are equivalent. Finding a conjugating matrix is tedious and showing that none exists is even more difficult. However, a very simple concept comes to our rescue, distilling a matrix in a single number.

Definition 1.7.1 For an $n \times n$ matrix $\boldsymbol{A}$, the sum of the diagonal entries is called its *trace*, denoted by $\mathrm{tr}(\boldsymbol{A})$:

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

Like the determinant, the trace of a matrix does not change under basis transformations, i.e. for an invertible matrix $\boldsymbol{X}$ one has

$$\mathrm{tr}(\boldsymbol{X}^{-1}\boldsymbol{A}\boldsymbol{X}) = \mathrm{tr}(\boldsymbol{A}).$$

In particular, for equivalent representations D and D', the matrices $\mathsf{D}(g)$ and $\mathsf{D}'(g)$ have the same traces. This gives rise to the concept of *characters*.

Definition 1.7.2 For a representation D of $\mathcal{G}$ the mapping $\chi_{\mathsf{D}} : \mathcal{G} \to \mathbb{C}$ given by

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

is called the *character* of D.
A character is called *reducible*, *decomposable*, *irreducible*, *indecomposable* etc. if the corresponding representation has the respective property. Also, the *character degree* is the degree of the corresponding representation.

Corollary 1.7.3 Equivalent representations have the same character.

Example 1.7.4 For the character χ of the representation D of $\mathcal{D}_3$ with

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

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

Example 1.7.5 Let $\mathcal{G} \leq \mathrm{GL}_3(\mathbb{R})$ be a point group and let D be its vector representation with corresponding character χ.

For a twofold rotation $2 \in \mathcal{G}$ one has $\chi(2) = -1$, since $\mathsf{D}(2)$ is equivalent to $\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$
(choosing the basis $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ such that $\mathbf{b}_1$ is along the rotation axis and $\mathbf{b}_2$ and $\mathbf{b}_3$ are perpendicular to it).

Analogously, for a reflection $m \in \mathcal{G}$ one has $\chi(m) = 1$, since $\mathsf{D}(m)$ is equivalent to $\begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$
(choosing the basis $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ such that $\mathbf{b}_1$ is normal to the reflection plane and $\mathbf{b}_2$ and $\mathbf{b}_3$ lie in the reflection plane).

Over $\mathbb{C}$, every matrix $\boldsymbol{A}$ of finite order (i.e. for which $\boldsymbol{A}^m = \boldsymbol{I}_n$ for some m) can be diagonalized and must have complex numbers of absolute value 1 on the diagonal. For such a diagonalized matrix $\boldsymbol{A}$ one has $\boldsymbol{A}^{-1} = \boldsymbol{A}^*$ and hence $\mathrm{tr}(\boldsymbol{A}^{-1}) = \mathrm{tr}(\boldsymbol{A})^*$. We thus have derived the following useful result.

Lemma 1.7.6 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.

We have already stated that equivalent representations have the same character. The crucial point is now that also the converse is true, i.e. characters actually characterize the equivalence classes of representations.

Theorem 1.7.7 Two representations $\mathbf{D}$ and $\mathbf{D}'$ are equivalent if and only if their characters are equal.

Note: It is in general not enough to compare the character values on generators of the group, but we will see below (see Lemma 1.7.10) that it is sufficient to compare two characters on representatives of the conjugacy classes.

We have seen that replacing all entries in a representation $\mathbf{D}$ by their complex conjugates yields another representation $\mathbf{D}^*$. This representation is equivalent to $\mathbf{D}$ precisely when the character $\chi_{\mathbf{D}}$ of $\mathbf{D}$ has only real values.

Whether a character is real or not gives rise to a classification of irreps into three types:

- ∘ If the character has non-real values, then the representation can certainly not be realized over $\mathbb{R}$ and the irrep is said to be of *complex type*.
  This case corresponds to an irrep over $\mathbb{R}$ that splits into a pair of complex conjugate irreps over $\mathbb{C}$.
- \+ If the character has only real values and the irrep is equivalent to a representation over $\mathbb{R}$, the irrep is said to be of *real type*.
  This case corresponds to an irrep over $\mathbb{R}$ that remains irreducible over $\mathbb{C}$.
- − If the character has only real values but the irrep is not equivalent to a representation over $\mathbb{R}$, the irrep is said to be of *symplectic type*.
  This case corresponds to an irrep over $\mathbb{R}$ that splits into a pair of equivalent irreps over $\mathbb{C}$.

Note that irreps of symplectic type do not occur amongst the irreps of point groups in dimensions 2 and 3. The smallest example of an irrep of symplectic type occurs for the *quaternion group* Q_8 of order 8 which has an irrep of degree 2 that can only be realized as an irrep of degree 4 over $\mathbb{R}$.

Example 1.7.8 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 $\chi'(g^2) = \mathrm{tr}(\boldsymbol{I}_2) = 2$, whereas $\chi(g^2) = \chi''(g^2) = \mathrm{tr}(-\boldsymbol{I}_2) = -2$.
Hence $\mathbf{D}$ and $\mathbf{D}''$ are equivalent, but $\mathbf{D}'$ is different.

It is remarkable, that looking at a single number for each matrix, one can decide whether there exists an $n \times n$ matrix conjugating one representation into another. This is even more remarkable, since characters are constant on conjugacy classes, i.e. a character is actually determined by its r values on representatives of the conjugacy classes.

Definition 1.7.9 A mapping $\phi : \mathcal{G} \to \mathbb{C}$ is called a *group function* of $\mathcal{G}$.
If a group function ϕ is constant on the conjugacy classes of $\mathcal{G}$, i.e. if $\phi(g) = \phi(h^{-1}gh)$ for all h in $\mathcal{G}$, then ϕ is called a *class function* of $\mathcal{G}$.

Lemma 1.7.10 Characters are class functions, since for $g' = h^{-1}gh$ one has

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

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

If we order the elements of a finite group $\mathcal{G}$ of order n in some way, $g_1, \ldots, g_n$ say, we can represent a group function ϕ by the vector $(\phi(g_1), \ldots, \phi(g_n))$. With this identification, the standard basis of $\mathbb{C}^n$ (consisting of the vectors with a 1 in one component and 0 else) correspond to the *characteristic functions* of the group elements, i.e. with the functions

$$\phi_g(h) = \begin{cases} 1 & \text{if } h = g \\ 0 & \text{if } h \neq g. \end{cases}$$

For a group $\mathcal{G}$ with r conjugacy classes, the class functions of $\mathcal{G}$ form a vector space of dimension r. The r characters of the irreps of $\mathcal{G}$ are contained in this space and could be linearly dependent or independent. In fact, they are always independent and thus form a basis for the space of class functions.

Lemma 1.7.11 Every class function of $\mathcal{G}$ is a linear combination of the irreps of $\mathcal{G}$.

Since we have seen that up to equivalence there are as many irreps as there are conjugacy classes and now can describe equivalence classes of representations by their characters, the crucial information about the irreps of a group can be stored in an $r \times r$ matrix containing the characters of the irreps, given by their values on the conjugacy classes.

Definition 1.7.12 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.
However, sometimes the character table is 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 each row an indication of the type of irrep to which the character gives rise (see the remarks after Theorem 1.6.8 and Theorem 1.7.7);

- for the crystallographic point groups, basis functions which transform under the point group according to the irrep (see section 2.5).

Example 1.7.13 The dihedral group $\mathcal{D}_3$ of order 6 (realized by the point groups *32* and *3m* has two 1-dimensional and one 2-dimensional irreps (as will be derived in section 2.3). The character table looks as follows:

class length	1	2	3
element order	1	3	2
	$g_1 = e$	g_2	g_3
χ_1	1	1	1
χ_2	1	1	-1
χ_3	2	-1	0

Example 1.7.14 The point group *432* of order 24 (isomorphic to the octahedral group $\mathcal{O}$) has the following character table:

class length	1	3	6	8	6
element order	1	2	2	3	4
	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
χ_1	1	1	1	1	1
χ_2	1	1	-1	1	-1
χ_3	2	2	0	-1	0
χ_4	3	-1	-1	0	1
χ_5	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.

1.8 Theorems of orthogonality

We have seen that the irreducible characters form a basis of the class functions of a group. This basis has many further useful properties, which are usually formulated via a scalar product for the functions on a group.

Definition 1.8.1 For two group functions ϕ, ψ of G, the *scalar product* of ϕ and ψ is defined as

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

If ϕ and ψ are class functions and $g_1, \ldots, g_r$ 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

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

This version is particularly useful when characters are taken from the character table of a group (in particular if the class length is displayed in the character table).
If there is no doubt about the group $\mathcal{G}$, the index indicating it is often omitted and we write (ϕ, ψ) for the scalar product of ϕ and ψ.

The crucial observation is now that the irreducible characters form an orthonormal basis with respect to this scalar product.

Theorem 1.8.2 (*Orthogonality relation for characters*) 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 with respect to the scalar product on the class functions of $\mathcal{G}$, i.e.:

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

In particular, the irreducible characters are precisely those which have norm 1 with respect to the scalar product on class functions.

Corollary 1.8.3 Let χ be the character of a representation $\mathbf{D}$ of $\mathcal{G}$. Then $\mathbf{D}$ is irreducible if and only if

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

An immediate consequence of the orthonormality of the irreducible characters is the *'magic formula'* which gives the decomposition of an arbitrary character into irreps.

Corollary 1.8.4 (*Magic formula*) Let $\mathcal{G}$ be a finite group, let χ be an arbitrary character of $\mathcal{G}$ and let $\chi_1, \ldots, \chi_r$ be the irreducible characters of $\mathcal{G}$. Then the decomposition of χ into irreducible characters is given by

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

Since the characters determine the representations up to equivalence, computing the scalar products with the irreducible characters is sufficient to determine the block diagonal form of an arbitrary representation (in case the irreps are known).

Example 1.8.5 We want to decompose the character χ of *432* (appended to the character table):

$\|C_j\|$	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 11.
Three characters ψ_1, ψ_2, ψ_3 of the dihedral group $\mathcal{D}_4$ of order 8 are appended to its character table:

$\|C_j\|$	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.

Since the *rows* of the character table from a system of orthonormal vectors (taking the sizes of the conjugacy classes into account), one may also ask about the *columns* of the character table. Indeed, there is also an orthogonality relation for the columns.

Theorem 1.8.6 (*Column orthogonality*) Let $\mathcal{G}$ be a finite group with irreducible characters $\chi_1, \ldots, \chi_r$ and let $g_1, \ldots, g_r$ be conjugacy class representatives. Denote by $|C_j|$ the class length of the conjugacy class of g_j. Then

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

This means that different columns of the character table are orthogonal to each other and that the norm of a column is related to the corresponding class length.

Applying the column orthogonality theorem to the first column we rediscover that the sum of the squares of the degrees of the irreps equals the group order (since the identity element forms a class of length 1).

Example 1.8.7 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:

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 12.
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 by applying the row orthogonality relations.

Let $\mathbf{D}$ be an irrep of degree n of $\mathcal{G}$. If we fix a position (i,j) in the matrices and look at the group function obtained by picking from $\mathbf{D}(g)$ the entry in position (i,j), we get n^2 group functions. Since the squares of the degrees of the irreps add up to the group order, looking at these group functions for all irreps gives precisely $|\mathcal{G}|$ group functions. These group functions not only turn out to be linearly independent, they are even orthogonal with respect to the scalar product for group functions.

Theorem 1.8.8 (*Orthogonality relation for irreps*) Let $\mathbf{D}$ 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 $\mathbf{D}$, then

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

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

Projection operators

If a representation $\mathbf{\Gamma}$ of $\mathcal{G}$ is given, the 'magic formula' of Corollary 1.8.4 allows to compute the multiplicities m_i with which the different irreps of $\mathcal{G}$ occur in Γ, using only the character values. However, if bases for the subspaces on which $\mathcal{G}$ acts by the irreps are explicitly required, some more work has to be done.

Theorem 1.8.9 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 $\mathbf{D}$.

This projection yields a basis for the sum of the subspaces on which $\mathcal{G}$ acts by the irrep $\mathbf{D}$. If $\mathbf{D}$ occurs with multiplicity $m=1$ this is precisely what we desire. However, if $m>1$ the theorem in general does not allow to easily extract bases for single subspaces on which $\mathcal{G}$ acts by the irrep $\mathbf{D}$. For this task we actually require a group function.

Theorem 1.8.10 If $\mathbf{\Gamma}$ is a representation of $\mathcal{G}$ and $\mathbf{D}$ is an irrep of degree n of $\mathcal{G}$, then

$$P_{\mathbf{D}} = \frac{n}{|\mathcal{G}|}\sum_{g\in\mathcal{G}} \mathbf{D}(g^{-1})_{11}\mathbf{\Gamma}(g)$$

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 D, we have $\mathsf{D}(g^{-1}) = \mathsf{D}(g)^\dagger = (\mathsf{D}(g)^T)^*$. This means that $\mathsf{D}(g^{-1})_{11} = \mathsf{D}(g)^*_{11}$ and thus the projection operator can be written as

$$P_{\mathsf{D}} = \frac{n}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \mathsf{D}(g)^*_{11} \mathbf{\Gamma}(g).$$

Applying the elements of $\mathbf{\Gamma}$ to the basis elements of U simultaneously gives bases for m different subspaces on which $\mathcal{G}$ acts by the irrep D.

Example 1.8.11 We demonstrate this procedure on the regular representation of the 2-dimensional point group *3m*. This point group is generated by the matrices

$$3 = g = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \quad m = h = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and the group elements are e, g, g^2, h, gh, g^2h. The left regular representation $\mathbf{\Gamma}$ of *3m* on the elements in this order is given by

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

From the theory we know that each of the irreps occurs with multiplicity equal to its degree. For the 1-dimensional irreps, Theorems 1.8.9 and 1.8.10 actually coincide. For the trivial irrep $\mathsf{D}^{(1)}$ we get

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

It is clear that both generators fix the vector $\mathbf{v}^{(1)} = (1,1,1,1,1,1)^T$.
The other 1-dimensional irrep $\mathsf{D}^{(2)}$ of *3m* is given by the determinant of the matrices. We get

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

Again one sees immediately 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 $-\mathbf{v}^{(2)}$.

The most interesting case is that of the 2-dimensional irrep $\mathbf{D}^{(3)}$ of *3m*, which is simply the vector representation by which the group is given. Picking out the $(1,1)$ entries of the matrices gives

$$\begin{aligned} &\mathbf{D}^{(3)}(e)_{11} = 1, \quad \mathbf{D}^{(3)}(g)_{11} = 0, \qquad \mathbf{D}^{(3)}(g^2)_{11} = -1, \\ &\mathbf{D}^{(3)}(h)_{11} = 0, \quad \mathbf{D}^{(3)}(gh)_{11} = -1, \quad \mathbf{D}^{(3)}(g^2h)_{11} = 1 \end{aligned}$$

and we get

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

which is a matrix of rank 2, as it should be.
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

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

One sees that $\mathbf{\Gamma}(h)(\mathbf{v}_1^{(3)}) = \mathbf{v}_2^{(3)}$ and $\mathbf{\Gamma}(h)(\mathbf{w}_1^{(3)}) = \mathbf{w}_2^{(3)}$ and moreover that $\mathbf{\Gamma}(g)(\mathbf{v}_2^{(3)}) = -\mathbf{v}_1^{(3)} - \mathbf{v}_2^{(3)}$ and $\mathbf{\Gamma}(g)(\mathbf{w}_2^{(3)}) = -\mathbf{w}_1^{(3)} - \mathbf{w}_2^{(3)}$. Thus, *3m* 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

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

with columns $\mathbf{v}^{(1)}, \mathbf{v}^{(2)}, \mathbf{v}_1^{(3)}, \mathbf{v}_2^{(3)}, \mathbf{w}_1^{(3)}, \mathbf{w}_2^{(3)}$ 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

$$\Gamma'(g) = \left(\begin{array}{c|c|cc|cc} 1 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{array}\right), \quad \Gamma'(h) = \left(\begin{array}{c|c|cc|cc} 1 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & -1 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \end{array}\right).$$

1.9 Direct products of irreps and their reductions into irreps

An obvious way to build representations from irreps is to form the direct sum, which means to combine two or more irreps as blocks on the diagonal of a larger matrix. The character belonging to a direct sum representation is clearly the sum of the characters of its components. We will now see that also the product of two characters corresponds to a representation built from the representations corresponding to the characters.

It is a priori not clear that the product of two characters yields the character of a representation at all. Of course, it is a class function and thus a linear combination of the irreps, but it is not guaranteed that all the coefficients are non-negative.

Definition 1.9.1 For two matrices $\boldsymbol{A} \in \mathbb{C}^{m\times m}$ and $\boldsymbol{B} \in \mathbb{C}^{n\times n}$ the *direct product* or *Kronecker product* $\boldsymbol{A} \otimes \boldsymbol{B}$ of $\boldsymbol{A}$ and $\boldsymbol{B}$ is the $mn \times mn$ matrix

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

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

Example 1.9.2 The Kronecker products $\boldsymbol{A} \otimes \boldsymbol{B}$ and $\boldsymbol{B} \otimes \boldsymbol{A}$ of the matrices

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

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

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

Exercise 13.
Determine the Kronecker products $\boldsymbol{A} \otimes \boldsymbol{B}$ and $\boldsymbol{B} \otimes \boldsymbol{A}$ of the matrices

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

Lemma 1.9.3 The Kronecker product has the following properties:

(i) $(\boldsymbol{A} \otimes \boldsymbol{B})(\boldsymbol{C} \otimes \boldsymbol{D}) = \boldsymbol{AC} \otimes \boldsymbol{BD}$.

(ii) $\mathrm{tr}(\boldsymbol{A} \otimes \boldsymbol{B}) = \mathrm{tr}(\boldsymbol{A}) \cdot \mathrm{tr}(\boldsymbol{B})$.

The first property shows that if we take two representations $\mathsf{D}^{(1)}$ and $\mathsf{D}^{(2)}$ of a group $\mathcal{G}$, then defining

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

gives again a representation of $\mathcal{G}$, since

$$
\mathsf{D}(gh) = \mathsf{D}^{(1)}(gh) \otimes \mathsf{D}^{(2)}(gh) = (\mathsf{D}^{(1)}(g) \otimes \mathsf{D}^{(2)}(g))(\mathsf{D}^{(1)}(h) \otimes \mathsf{D}^{(2)}(h)) = \mathsf{D}(g)\mathsf{D}(h).
$$

From the second property we then see that the character of D is the product of the characters of $\mathsf{D}^{(1)}$ and $\mathsf{D}^{(2)}$.

Definition 1.9.4 For two representations $\mathsf{D}^{(1)}$ and $\mathsf{D}^{(2)}$ of a group $\mathcal{G}$, defining

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

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

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

The vector space on which $\mathcal{G}$ acts by the direct product representation can be constructed as follows: Let V and 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

$$
\mathbf{v}_1\mathbf{w}_1, \mathbf{v}_1\mathbf{w}_2, \ldots, \mathbf{v}_1\mathbf{w}_m, \quad \mathbf{v}_2\mathbf{w}_1, \mathbf{v}_2\mathbf{w}_2, \ldots, \mathbf{v}_2\mathbf{w}_m, \quad \ldots \quad \mathbf{v}_n\mathbf{w}_1, \mathbf{v}_n\mathbf{w}_2, \ldots, \mathbf{v}_n\mathbf{w}_m
$$

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

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

In the special case that $\mathbf{V}=\mathbf{W}$, the vector space $\mathbf{V}\otimes\mathbf{V}$ can be split into two subspaces which are invariant under the action of $\mathcal{G}$.

Definition 1.9.5 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 $\mathbf{V}\otimes\mathbf{V}$.

(i) 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 $\frac{1}{2}n(n+1)$.

(ii) 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 $\frac{1}{2}n(n-1)$.

(iii) 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.

The characters for the action of $\mathcal{G}$ on the symmetrized and antisymmetrized squares of $\mathbf{V}$ can be determined from the character of $\mathbf{D}$.

Theorem 1.9.6 Let $\mathcal{G}$ act on the vector space $\mathbf{V}$ by the representation $\mathbf{D}$ with character χ.

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

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

(ii) 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 1.9.7 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:

	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
$[E]^2$	$\frac{1}{2}(4+2)=3$	$\frac{1}{2}(4+2)=3$	$\frac{1}{2}(0+2)=1$	$\frac{1}{2}(1+(-1))=0$	$\frac{1}{2}(0+2)=1$
$\{E\}^2$	$\frac{1}{2}(4-2)=1$	$\frac{1}{2}(4-2)=1$	$\frac{1}{2}(0-2)=-1$	$\frac{1}{2}(1-(-1))=1$	$\frac{1}{2}(0-2)=-1$
$[T_1]^2$	$\frac{1}{2}(9+3)=6$	$\frac{1}{2}(1+3)=2$	$\frac{1}{2}(1+3)=2$	$\frac{1}{2}(0+0)=0$	$\frac{1}{2}(1+(-1))=0$
$\{T_1\}^2$	$\frac{1}{2}(9-3)=3$	$\frac{1}{2}(1-3)=-1$	$\frac{1}{2}(1-3)=-1$	$\frac{1}{2}(0-0)=0$	$\frac{1}{2}(1-(-1))=1$

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 into irreps

The direct product of two irreps is in general not irreducible, but it can be decomposed into irreps (e.g. by the 'magic formula' 1.8.4). The multiplicities that occur in this special situation are usually called the *coefficients of the Clebsch-Gordan series*.

Definition 1.9.8 Let $\mathbf{D}^{(1)}, \ldots, \mathbf{D}^{(r)}$ be the irreps of $\mathcal{G}$ and let $\chi_1, \ldots, \chi_r$ be the corresponding characters. 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: The term *Clebsch-Gordan coefficients* is often used in a different meaning, especially in the context of particle physics.

Because the direct product of representations is symmetric, we clearly have $c_{ij}^k = c_{ji}^k$. Furthermore, if $\mathbf{D}^{(1)}$ is the trivial representation, then $c_{i1}^i = 1$ and $c_{i1}^k = 0$ for $k \neq i$, since $\mathbf{D}^{(i)} \otimes \mathbf{D}^{(1)} = \mathbf{D}^{(i)}$.

The following explicit formula for the coefficients of the Clebsch-Gordan series follows immediately from the 'magic formula' and the fact that the character of the direct product representation is the product of the characters of its components.

Lemma 1.9.9 If χ_i is the character of $\mathbf{D}^{(i)}$, then the c_{ij}^k can be explicitly computed by

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

A compact way to display the coefficients of the Clebsch-Gordan series is an $r \times r$ matrix in which the (i, j) entry is the vector $(c_{ij}^1, c_{ij}^2, \ldots, c_{ij}^r)$. However, it is more common that the (i, j) entry explicitly gives the decomposition of $\mathbf{D}^{(i)} \otimes \mathbf{D}^{(j)}$ into irreps. Note that this matrix is symmetric, hence only the elements for $i \le j$ (upper triangular matrix) or $i \ge j$ (lower triangular matrix) have to be displayed.

Example 1.9.10 The character table of the tetrahedral group $\mathcal{T}$ looks as follows:

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

where $\zeta_3 = \exp(2\pi i/3) = (-1 + i\sqrt{3})/2$ is a third root of unity.
Of course $\chi_i \cdot \chi_1 = \chi_i$, further one immediately sees that $\chi_2 \cdot \chi_2 = \chi_3$, $\chi_3 \cdot \chi_2 = \chi_1$, $\chi_3 \cdot \chi_3 = \chi_2$ and that $\chi_4 \cdot \chi_2 = \chi_4 \cdot \chi_3 = \chi_4$.
The only substantial effort is the decomposition of $\mathbf{D}^{(4)} \otimes \mathbf{D}^{(4)}$ with character $\chi_4 \cdot \chi_4 = [9 \quad 1 \quad 0 \quad 0]$.
We find $c_{44}^1 = c_{44}^2 = c_{44}^3 = \frac{1}{12}(9+3) = 1$ and $c_{44}^4 = \frac{1}{12}(27-3) = 2$, i.e.

$$\chi_4 \cdot \chi_4 = \chi_1 + \chi_2 + \chi_3 + 2\chi_4.$$

The matrix containing the coefficients of the Clebsch-Gordan series for $\mathcal{T}$ therefore looks as follows:

$\otimes$	$\mathbf{D}^{(1)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(4)}$
$\mathbf{D}^{(1)}$	$(1,0,0,0)$			
$\mathbf{D}^{(2)}$	$(0,1,0,0)$	$(0,0,1,0)$		
$\mathbf{D}^{(3)}$	$(0,0,1,0)$	$(1,0,0,0)$	$(0,1,0,0)$	
$\mathbf{D}^{(4)}$	$(0,0,0,1)$	$(0,0,0,1)$	$(0,0,0,1)$	$(1,1,1,2)$

or with the explicit decomposition into irreps:

$\otimes$	$\mathbf{D}^{(1)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(4)}$
$\mathbf{D}^{(1)}$	$\mathbf{D}^{(1)}$			
$\mathbf{D}^{(2)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(3)}$		
$\mathbf{D}^{(3)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(1)}$	$\mathbf{D}^{(2)}$	
$\mathbf{D}^{(4)}$	$\mathbf{D}^{(4)}$	$\mathbf{D}^{(4)}$	$\mathbf{D}^{(4)}$	$\mathbf{D}^{(1)} \oplus \mathbf{D}^{(2)} \oplus \mathbf{D}^{(3)} \oplus 2\mathbf{D}^{(4)}$

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.

1.10 Irreps of direct products of groups

Since many point groups are direct products of the form $\mathcal{G} = \mathcal{H}_1 \times \mathcal{H}_2$, and in particular of the form $\mathcal{G} = \mathcal{H} \times \mathcal{C}_2$, we take a closer look at this situation.
Note that the elements g of $\mathcal{G} = \mathcal{H}_1 \times \mathcal{H}_2$ can be written as $g = h_1 h_2$ with $h_1 \in \mathcal{H}_1$ and $h_2 \in \mathcal{H}_2$.

Theorem 1.10.1 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 $1 \le i \le r$ be the irreps of $\mathcal{H}_1$ and let $\mathbf{D}_2^{(j)}$ for $1 \le j \le s$ 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 $1 \le i \le r$ and $1 \le j \le s$, 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 $\mathbf{D}_2^{(j)}(h_2)$ (see Definition 1.9.1).

That $\mathcal{G}$ has rs irreps follows from the fact that if $h_1, \ldots, h_r$ are conjugacy class representatives of $\mathcal{H}_1$ and $h'_1, \ldots, h'_s$ are conjugacy class representatives of $\mathcal{H}_2$ then the elements $h_i h'_j$ for $1 \le i \le r$ and $1 \le j \le s$ are conjugacy class representatives of $\mathcal{G}$.

Moreover, the inner product for class functions shows that the given characters are indeed irreducible, since

$$\begin{aligned}
&\frac{1}{|\mathcal{G}|} \sum_{g \in \mathcal{G}} \chi_{\mathbf{D}^{(ij)}}(g) \chi_{\mathbf{D}^{(ij)}}(g)^* \\
=&\frac{1}{|\mathcal{H}_1|\,|\mathcal{H}_2|} \sum_{h_1 \in \mathcal{H}_1} \sum_{h_2 \in \mathcal{H}_2} \chi_{\mathbf{D}_1^{(i)}}(h_1) \chi_{\mathbf{D}_2^{(j)}}(h_2) \chi_{\mathbf{D}_1^{(i)}}(h_1)^* \chi_{\mathbf{D}_j^{(j)}}(h_2)^* \\
=&\frac{1}{|\mathcal{H}_1|} \sum_{h_1 \in \mathcal{H}_1} \chi_{\mathbf{D}_1^{(i)}}(h_1) \chi_{\mathbf{D}_1^{(i)}}(h_1)^* \underbrace{\left(\frac{1}{|\mathcal{H}_2|} \sum_{h_2 \in \mathcal{H}_2} \chi_{\mathbf{D}_2^{(j)}}(h_2) \chi_{\mathbf{D}_2^{(j)}}(h_2)^* \right)}_{=1 \text{ (since } \mathbf{D}_2^{(j)} \text{ is irreducible)}} \\
=&\frac{1}{|\mathcal{H}_1|} \sum_{h_1 \in \mathcal{H}_1} \chi_{\mathbf{D}_1^{(i)}}(h_1) \chi_{\mathbf{D}_1^{(i)}}(h_1)^* = 1 \text{ (since } \mathbf{D}_1^{(i)} \text{ is irreducible).}
\end{aligned}$$

It only remains to show that the characters are indeed all different, but that is not difficult.

An alternative 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.

As a consequence, we can obtain the character table of a direct product $\mathcal{G} = \mathcal{H}_1 \times \mathcal{H}_2$ as the Kronecker product of the character tables of $\mathcal{H}_1$ and $\mathcal{H}_2$. For that, we have to sort the conjugacy classes and the irreps in a suitable way.

Corollary 1.10.2 Let $\mathbf{X}_1$ be the character table of $\mathcal{H}_1$ such that $(\mathbf{X}_1)_{ij} = \chi_{\mathbf{D}_1^{(i)}}(h_j)$ 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 $h'_1, \dots, h'_s$ and irreps $\mathbf{D}_2^{(1)}, \dots, \mathbf{D}_2^{(s)}$ of $\mathcal{H}_2$.
Then taking the conjugacy class representatives of $\mathcal{G} = \mathcal{H}_1 \times \mathcal{H}_2$ in the order

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

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

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

the character table of $\mathcal{G}$ is given by 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 given by

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

since $\mathcal{C}_2$ has character table

	e	g
χ_1	1	1
χ_2	1	−1

.

Example 1.10.3 The dihedral group $\mathcal{D}_3$ of order 6 (realized by the point groups *3m* and *32*) has the character table

	1	2	3
$\chi_{\mathbf{D}^{(1)}}$	1	1	1
$\chi_{\mathbf{D}^{(2)}}$	1	−1	1
$\chi_{\mathbf{D}^{(3)}}$	2	0	−1

(where we label the conjugacy classes by elements in *32*).
The direct product $\mathcal{C}_2 \times \mathcal{D}_3$ (realized by the point groups $\overline{3}m$, *622*, *6mm*, $\overline{6}2m$) therefore has the character table

	1	2	3	$\overline{1}$	m	$\overline{3}$
$\chi_{\mathbf{D}^{(11)}}$	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

Terminology: 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

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

2 Representations of point groups

In this part of the course we will derive the irreps and character tables of the (3-dimensional) crystallographic point groups by applying the general theory of the first part. Since the irreps depend only on the isomorphism type of the point group, it is sufficient to derive the irreps for the 18 isomorphism types of point groups. The assignment of point groups to abstract groups is given in Table 1.

abstract group	order	point groups
$\mathcal{C}_1$	1	*1*
$\mathcal{C}_2$	2	*2*, *m*, $\overline{1}$
$\mathcal{C}_3$	3	*3*
$\mathcal{C}_4$	4	*4*, $\overline{4}$
$\mathcal{C}_6 \cong \mathcal{C}_3 \times \mathcal{C}_2$	*6*	$\overline{3}$, *6*, $\overline{6}$
$\mathcal{C}_{4h} \cong \mathcal{C}_4 \times \mathcal{C}_2$	8	*4/m*
$\mathcal{C}_{6h} \cong \mathcal{C}_6 \times \mathcal{C}_2$	12	*6/m*
$\mathcal{D}_2 \cong \mathcal{C}_2 \times \mathcal{C}_2$	4	*2/m*, *222*, *mm2*
$\mathcal{D}_3$	6	*32*, *3m*
$\mathcal{D}_4$	8	*422*, *4mm*, $\overline{4}2m$
$\mathcal{D}_6 \cong \mathcal{D}_{3h} \cong \mathcal{D}_3 \times \mathcal{C}_2$	12	$\overline{3}m$, *622*, *6mm*, $\overline{6}2m$
$\mathcal{D}_{2h} \cong \mathcal{D}_2 \times \mathcal{C}_2 \cong \mathcal{C}_2 \times \mathcal{C}_2 \times \mathcal{C}_2$	8	*mmm*
$\mathcal{D}_{4h} \cong \mathcal{D}_4 \times \mathcal{C}_2$	16	*4/mmm*
$\mathcal{D}_{6h} \cong \mathcal{D}_6 \times \mathcal{C}_2$	24	*6/mmm*
$\mathcal{T}$	12	*23*
$\mathcal{T}_h \cong \mathcal{T} \times \mathcal{C}_2$	24	$m\overline{3}$
$\mathcal{O}$	24	*432*, $\overline{4}3m$
$\mathcal{O}_h \cong \mathcal{O} \times \mathcal{C}_2$	48	$m\overline{3}m$

Table 1: Isomorphism classes of point groups as abstract groups

We start with a general analysis of the irreps of Abelian and dihedral groups (of arbitrary order), since these groups and their direct products with $\mathcal{C}_2$ cover all point groups except for the tetrahedral and octahedral groups.

2.1 Irreps of Abelian groups

The irreps of Abelian groups are particularly easy, because (as we have already seen), they all have to have degree 1. This is due to the fact that on the one hand in an Abelian group every element forms a conjugacy class on its own so that there are as many irreps as group elements. On the other hand the squares of the degrees of the irreps add up to the group order, hence all the degrees have to be 1.

Theorem 2.1.1 All irreps of an Abelian group have degree 1.

As a consequence, irreps and their characters coincide for Abelian groups. In particular, irreps can only be equivalent if they are equal.

Cyclic groups

Let $\mathcal{G} = \mathcal{C}_n = \{e, g, g^2, \ldots, g^{n-1}\}$ be the cyclic group of order n, generated by the element g. On the one hand, every (1-dimensional) irrep $\mathbf{D}$ is determined by $\mathbf{D}(g) = z \in \mathbb{C}$. On the other hand, $1 = \mathbf{D}(e) = \mathbf{D}(g^n) = (\mathbf{D}(g))^n = z^n$. Hence, z has to be an *n-th root of unity*, i.e. a complex number of the form $\exp(2\pi i\theta) = \cos(2\pi\theta) + i\sin(2\pi\theta)$ such that $n\theta$ is an integer. Since $\exp(2\pi i) = 1$, we furthermore can restrict θ to the interval $[0, 1)$ (with 1 excluded). Thus the only possibilities for z are $z_k = \exp(2\pi ik/n) = \exp(2\pi i/n)^k$ with $0 \leq k < n$. Since these are n different irreps, this gives indeed all irreps of $\mathcal{C}_n$.

The following notation is useful and often used.

Definition 2.1.2 The element $\zeta_n = \exp(2\pi i/n) = \cos(2\pi/n)+i\sin(2\pi/n)$ is called a *primitive n-th root of unity.*

Example 2.1.3 We have $\zeta_2 = -1$, $\zeta_3 = \frac{-1+i\sqrt{3}}{2}$, $\zeta_4 = i$, $\zeta_6 = \frac{1+i\sqrt{3}}{2} = \zeta_3^2$ and $\zeta_8 = \frac{1+i}{\sqrt{2}}$.

Summarizing the above discussion, we get the following important result.

Theorem 2.1.4 The irreps of the cyclic group $\mathcal{C}_n$ generated by g are given by

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

For an arbitrary element $g^a \in \mathcal{C}_n$ we thus have $\mathbf{D}^{(k)}(g^a) = \exp(2\pi i(ak)/n) = \zeta_n^{ak}$.

Direct products of cyclic groups

Since we know by Theorem 1.1.17 that every Abelian group is the direct product of cyclic groups, we can now obtain the irreps of any Abelian group from the irreps of cyclic groups via Theorem 1.10.1. Equivalently, we can construct the character table of any Abelian group from the character tables of cyclic groups via Corollary 1.10.2.

Corollary 2.1.5 The irreps of $\mathcal{C}_n \times \mathcal{C}_m$ with $\mathcal{C}_n$ generated by g_1 and $\mathcal{C}_m$ generated by g_2 are determined by the images of the generators g_1 and g_2 and are given by

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

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

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

Corollary 2.1.6 Specializing $m = n$ in Corollary 2.1.5, the irreps of $\mathcal{C}_n \times \mathcal{C}_n$ are given by

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

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

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

The above result on the irreps of $\mathcal{C}_n \times \mathcal{C}_n \times \mathcal{C}_n$ is actually the starting point for the construction of the irreps of *space groups*. If $\mathcal{T}$ is the translation subgroup of a space group $\mathcal{G}$, then one starts with an irrep of the factor group $\mathcal{T}/\mathcal{T}^n \cong \mathcal{C}_n \times \mathcal{C}_n \times \mathcal{C}_n$. From there, the irreps of $\mathcal{G}$ are determined by an *induction process* which is a general procedure to build representations of supergroups from those of subgroups.

Example 2.1.7 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	$-i$

Note that due to the special case of a direct product with $\mathcal{C}_2$ we have adopted a naming scheme with superscripts $k+$ and $k-$ instead of the general kl superscripts.

Exercise 17.
Determine the character tables and irreps of the following two point groups:

(i) $mm2 \cong \mathcal{C}_2 \times \mathcal{C}_2$ with conjugacy class representatives 1, 2_z, m_y, m_x;

(ii) $\overline{3} \cong \mathcal{C}_3 \times \mathcal{C}_2 \cong \mathcal{C}_6$ with conjugacy class representatives 1, 3^+, 3^-, $\overline{1}$, $\overline{3}^+$, $\overline{3}^-$.

2.2 Irreps of dihedral groups

In a certain sense, the easiest class of non-Abelian groups are the *dihedral groups* $\mathcal{D}_n$, because they contain a cyclic group $\mathcal{C}_n$ as normal subgroup of index 2. The dihedral group $\mathcal{D}_n$ occurs e.g. as the symmetry group of a regular n-gon or of a regular n-sided prism.

Definition 2.2.1 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 $\mathcal{D}_n$.
Alternatively, the group $\mathcal{D}_n$ can be generated by two elements k, h of order 2 such that the product kh has order n. In fact, this set of generators is obtained from the previous by defining $k = gh$.

In order to determine the irreps of the dihedral groups, it is convenient to distinguish between the cases that n is even and that n is odd.

Lemma 2.2.2 Let n be even and let $\mathcal{D}_n$ be the dihedral group of order $2n$ generated by an element g of order n and an element h of order 2 with $hg = g^{-1}h$.

(i) Representatives for the conjugacy classes are given by

$$e, \{g^i, 1 \le i \le n/2\}, h, gh$$

i.e. there are $n/2 + 3$ conjugacy classes.

(ii) The commutator group $\mathcal{D}_n{}'$ is generated by g^2 and has index 4 in $\mathcal{D}_n$, hence there are four 1-dimensional irreps. Consequently, there must be $n/2-1$ further irreps of degree at least 2 and since $4+(n/2-1)\cdot 2^2 = 2n$ all other irreps indeed must have degree 2.

(iii) The 2-dimensional irreps can be realized as follows, using a primitive n-th root of unity $\zeta_n = \exp(2\pi i/n)$:

$$\mathbf{E}_i(g) = \begin{pmatrix} \zeta_n^i & 0 \\ 0 & \zeta_n^{-i} \end{pmatrix}, \quad \mathbf{E}_i(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \text{ for } 1 \le i < n/2$$

are all irreducible and pairwise inequivalent.

Lemma 2.2.3 Let n be odd and let $\mathcal{D}_n$ be the dihedral group of order $2n$ generated by an element g of order n and an element h of order 2 with $hg = g^{-1}h$.

(i) Representatives for the conjugacy classes are given by

$$e, \{g^i, 1 \le i \le (n-1)/2\}, h$$

i.e. there are $(n-1)/2+2$ conjugacy classes.

(ii) The commutator group $\mathcal{D}_n{}'$ is generated by g and has index 2 in $\mathcal{D}_n$, hence there are two 1-dimensional irreps. Consequently, there must be $(n-1)/2$ further irreps of degree at least 2 and since $2+(n-1)/2\cdot 2^2 = 2n$ all other irreps indeed must have degree 2.

(iii) The 2-dimensional irreps can be realized in the same way as for the case of n even, using again a primitive n-th root of unity $\zeta_n = \exp(2\pi i/n)$:

$$\mathbf{E}_i(g) = \begin{pmatrix} \zeta_n^i & 0 \\ 0 & \zeta_n^{-i} \end{pmatrix}, \quad \mathbf{E}_i(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \text{ for } 1 \le i < n/2$$

are all irreducible and pairwise inequivalent.

Note that in Lemma 2.2.2 and 2.2.3 we adopted the convention to label 2-dimensional irreps by the letter $\mathbf{E}$.

Example 2.2.4 The dihedral group $\mathcal{D}_6$ of order 12 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.

2.3 Character tables and irreps of point groups

In this section we give the character tables and irreps of the point groups (as abstract groups). For the Abelian groups and the dihedral groups and their products with $\mathcal{C}_2$ we apply the results from sections 2.1 and 2.2 combined with the theory for direct products developed in section 1.10. The remaining point groups, i.e. the tetrahedral and octahedral groups and their direct products with $\mathcal{C}_2$ will be treated separately.

Abelian groups

For Abelian groups the irreps coincide with their characters, hence giving the character tables provides a full description of the irreps. Since the class lengths are all 1, they are omitted from the character tables.

Cyclic group $\mathcal{C}_1$ — point group *1*

element order	1
	e
χ_1	1

Cyclic group $\mathcal{C}_2$ — point groups $\bar{1}$, *2*, *m*

element order	1	2
	e	g
χ_1	1	1
χ_2	1	-1

Cyclic group $\mathcal{C}_3$ — point group *3*

element order	1	3	3
	e	g	g^2
χ_1	1	1	1
χ_2	1	ζ_3	ζ_3^*
χ_3	1	ζ_3^*	ζ_3

where $\zeta_3 = \exp(2\pi i/3) = (-1 + i\sqrt{3})/2$ and $\zeta_3^* = \zeta_3^2$.

Cyclic group $\mathcal{C}_4$ point groups *4*, $\overline{4}$

element order	1	4	2	4
	e	g	g^2	g^3
χ_1	1	1	1	1
χ_2	1	i	-1	$-i$
χ_3	1	-1	1	-1
χ_4	1	$-i$	-1	i

where $i = \exp(2\pi i/4)$.

Cyclic group $\mathcal{C}_6$ point groups $\overline{3}$, *6*, $\overline{6}$

element order	1	6	3	2	3	6
	e	g	g^2	g^3	g^4	g^5
χ_1	1	1	1	1	1	1
χ_2	1	ζ_6	ζ_3	-1	ζ_3^*	ζ_6^*
χ_3	1	ζ_3	ζ_3^*	1	ζ_3	ζ_3^*
χ_4	1	-1	1	-1	1	-1
χ_5	1	ζ_3^*	ζ_3	1	ζ_3^*	ζ_3
χ_6	1	ζ_6^*	ζ_3^*	-1	ζ_3	ζ_6

where $\zeta_6 = \exp(2\pi i/6) = (1 + i\sqrt{3})/2$, $\zeta_6^* = \zeta_6^5$ and $\zeta_3 = \zeta_6^2 = \exp(2\pi i/3) = (-1 + i\sqrt{3})/2$.
Note that since $\mathcal{C}_6 \cong \mathcal{C}_2 \times \mathcal{C}_3$, this character table can also be obtained as the Kronecker product of the character tables of $\mathcal{C}_2$ and $\mathcal{C}_3$. To identify the character tables, one has to permute some rows and columns and to apply the identity $\zeta_6 = -\zeta_3^2$.

Direct product $\mathcal{C}_2 \times \mathcal{C}_2$ point groups *222*, *mm2*, *2/m*

For labelling the columns, we take the first component $\mathcal{C}_2$ of the direct product to be the group $\{\pm 1\}$ and the second component to be generated by g.

element order	1	2	2	2
	e	g	$-e$	$-g$
χ_1	1	1	1	1
χ_2	1	-1	1	-1
χ_3	1	1	-1	-1
χ_4	1	-1	-1	1

Direct product $\mathcal{C}_2 \times \mathcal{C}_4$ point group *4/m*

For labelling the columns, we take the first component $\mathcal{C}_2$ of the direct product to be the group $\{\pm 1\}$ and the second component to be generated by g.

element order	1	4	2	4	2	4	2	4
	e	g	g^2	g^3	$-e$	$-g$	$-g^2$	$-g^3$
χ_1	1	1	1	1	1	1	1	1
χ_2	1	i	-1	$-i$	1	i	-1	$-i$
χ_3	1	-1	1	-1	1	-1	1	-1
χ_4	1	$-i$	-1	i	1	$-i$	-1	i
χ_5	1	1	1	1	-1	-1	-1	-1
χ_6	1	i	-1	$-i$	-1	$-i$	1	i
χ_7	1	-1	1	-1	-1	1	-1	1
χ_8	1	$-i$	-1	i	-1	i	1	$-i$

where $i = \exp(2\pi i/4)$.

Direct product $\mathcal{C}_2 \times \mathcal{C}_6$ point group *6/m*

For labelling the columns, we take the first component $\mathcal{C}_2$ of the direct product to be the group $\{\pm 1\}$ and the second component to be generated by g.

element order	1	6	3	2	3	6	2	6	6	2	6	6
	e	g	g^2	g^3	g^4	g^5	$-e$	$-g$	$-g^2$	$-g^3$	$-g^4$	$-g^5$
χ_1	1	1	1	1	1	1	1	1	1	1	1	1
χ_2	1	ζ_6	ζ_3	-1	ζ_3^*	ζ_6^*	1	ζ_6	ζ_3	-1	ζ_3^*	ζ_6^*
χ_3	1	ζ_3	ζ_3^*	1	ζ_3	ζ_3^*	1	ζ_3	ζ_3^*	1	ζ_3	ζ_3^*
χ_4	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1
χ_5	1	ζ_3^*	ζ_3	1	ζ_3^*	ζ_3	1	ζ_3^*	ζ_3	1	ζ_3^*	ζ_3
χ_6	1	ζ_6^*	ζ_3^*	-1	ζ_3	ζ_6	1	ζ_6^*	ζ_3^*	-1	ζ_3	ζ_6
χ_7	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1
χ_8	1	ζ_6	ζ_3	-1	ζ_3^*	ζ_6^*	-1	ζ_3^*	ζ_6^*	1	ζ_6	ζ_3
χ_9	1	ζ_3	ζ_3^*	1	ζ_3	ζ_3^*	-1	ζ_6^*	ζ_6	-1	ζ_6^*	ζ_6
χ_{10}	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1
χ_{11}	1	ζ_3^*	ζ_3	1	ζ_3^*	ζ_3	-1	ζ_6	ζ_6^*	-1	ζ_6	ζ_6^*
χ_{12}	1	ζ_6^*	ζ_3^*	-1	ζ_3	ζ_6	-1	ζ_3	ζ_6	1	ζ_6^*	ζ_3^*

where $\zeta_6 = \exp(2\pi i/6) = (1 + i\sqrt{3})/2$, $\zeta_6^* = \zeta_6^5$ and $\zeta_3 = \zeta_6^2 = \exp(2\pi i/3) = (-1 + i\sqrt{3})/2$.

Direct product $\mathcal{C}_2 \times \mathcal{C}_2 \times \mathcal{C}_2$ point group *mmm*

For labelling the columns, we take the first component $\mathcal{C}_2$ of the direct product to be the group $\{\pm 1\}$ and the second and third components to be generated by g and h, respectively.

element order	1	2	2	2	2	2	2	2
	e	g	h	gh	$-e$	$-g$	$-h$	$-gh$
χ_1	1	1	1	1	1	1	1	1
χ_2	1	−1	1	−1	1	−1	1	−1
χ_3	1	1	−1	−1	1	1	−1	−1
χ_4	1	−1	−1	1	1	−1	−1	1
χ_5	1	1	1	1	−1	−1	−1	−1
χ_6	1	−1	1	−1	−1	1	−1	1
χ_7	1	1	−1	−1	−1	−1	1	1
χ_8	1	−1	−1	1	−1	1	1	−1

Dihedral groups

From the analysis in Lemma 2.2.2 and 2.2.3 we can read off the irreps and character tables of the dihedral groups occurring as point groups.

The dihedral group $\mathcal{D}_2 \cong \mathcal{C}_2 \times \mathcal{C}_2$ is Abelian and was already treated above.

Dihedral group $\mathcal{D}_3$ point groups *32*, *3m*

class length	1	2	3
element order	1	3	2
	e	g	h
χ_1	1	1	1
χ_2	1	1	−1
χ_3	2	−1	0

The element h is a twofold rotation in *32* and a reflection in *3m*.

The 2-dimensional irrep with character χ_3 is given by

$$\mathbf{D}^{(3)}(g) = \begin{pmatrix} \zeta_3 & 0 \\ 0 & \zeta_3^2 \end{pmatrix}, \quad \mathbf{D}^{(3)}(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which is equivalent to

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

This is the vector representation of the 2-dimensional point group $3m$.

Dihedral group $\mathcal{D}_4$ point groups *422*, *4mm*, $\overline{4}m$

class length	1	2	1	2	2
element order	1	4	2	2	2
	e	g	g^2	h	gh
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	0	−2	0	0

The elements h and gh are twofold rotations in *422* (with axes making an angle of $\pi/4$), reflections in *4mm* (with normal vectors making an angle of $\pi/4$) and a twofold rotation and a reflection in $\overline{4}2m$.

The 2-dimensional irrep with character χ_5 is given by

$$\mathbf{D}^{(5)}(g) = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}, \quad \mathbf{D}^{(5)}(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which is equivalent to

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

This is the vector representation of the 2-dimensional point group $4mm$.

Dihedral group $\mathcal{D}_6$ point groups *622*, *6mm*, $\overline{6}2m$, $\overline{3}m$

class length	1	2	2	1	3	3
element order	1	6	3	2	2	2
	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
χ_5	2	1	−1	−2	0	0
χ_6	2	−1	−1	2	0	0

Note that since $\mathcal{D}_6 \cong \mathcal{C}_2 \times \mathcal{D}_3$, this character table can also be obtained as the Kronecker product of the character tables of $\mathcal{C}_2$ and $\mathcal{D}_3$. To identify the character tables, one has to permute some rows and columns.

The elements h and gh are twofold rotations in *622* (with axes making an angle of $\pi/6$), reflections in *6mm* (with normal vectors making an angle of $\pi/6$) and a twofold rotation and a reflection in $\overline{6}2m$ and $\overline{3}m$.

The 2-dimensional irrep with character χ_5 is given by

$$\mathbf{D}^{(5)}(g) = \begin{pmatrix} \zeta_6 & 0 \\ 0 & \zeta_6^5 \end{pmatrix}, \quad \mathbf{D}^{(5)}(h) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which is equivalent to

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

This is the vector representation of the 2-dimensional point group $6mm$.

The 2-dimensional irrep with character χ_6 has g^3 in its kernel and is thus an irrep of the factor group $\mathcal{D}_6/\mathcal{C}_2 \cong \mathcal{D}_3$. The matrices for g and h are precisely the same as those for g and h in $\mathcal{D}_3$ given above.

The irreps and character tables of direct products $\mathcal{C}_2 \times \mathcal{D}_n$ are obtained easily via Theorem 1.10.1 and Corollary 1.10.2. For the irreps, the situation is summarized in the following lemma.

Lemma 2.3.1 Let $\mathcal{C}_2 = \{1, -1\}$ be a cyclic group of order 2 and let $\mathcal{D}_n$ be a dihedral group generated by elements g and h. Then the direct product $\mathcal{C}_2 \times \mathcal{D}_n$ is generated by $-1, g, h$. Let $\mathbf{D}^{(i)}$ be an irrep of degree m of $\mathcal{D}_n$. Then $\mathbf{D}^{(i)}$ gives rise to two irreps $\mathbf{D}^{(i+)}$ and $\mathbf{D}^{(i-)}$ of $\mathcal{C}_2 \times \mathcal{D}_n$ which are obtained by extending $\mathbf{D}^{(i)}$ to $\mathcal{C}_2 \times \mathcal{D}_n$ via $\mathbf{D}^{(i+)}(-1) = \boldsymbol{I}_m$ and $\mathbf{D}^{(i-)}(-1) = -\boldsymbol{I}_m$. The irreps $\mathbf{D}^{(i+)}$ and $\mathbf{D}^{(i-)}$ are therefore determined by

$$\begin{aligned} \mathbf{D}^{(i+)}(-1) &= \boldsymbol{I}_m, & \mathbf{D}^{(i+)}(g) &= \mathbf{D}^{(i)}(g), & \mathbf{D}^{(i+)}(h) &= \mathbf{D}^{(i)}(h), \\ \mathbf{D}^{(i-)}(-1) &= -\boldsymbol{I}_m, & \mathbf{D}^{(i-)}(g) &= \mathbf{D}^{(i)}(g), & \mathbf{D}^{(i-)}(h) &= \mathbf{D}^{(i)}(h). \end{aligned}$$

Because obtaining the irreps in this way is straightforward, we will only give the character tables for the direct products of $\mathcal{D}_n$ with $\mathcal{C}_2$.

Direct product $\mathcal{C}_2 \times \mathcal{D}_4$ point group *4/mmm*

For labelling the columns, we take the first component $\mathcal{C}_2$ of the direct product to be the group $\{\pm 1\}$ and the second component to be generated by g and h.

class length	1	2	1	2	2	1	2	1	2	2
element order	1	4	2	2	2	2	4	2	2	2
	e	g	g^2	h	gh	$-e$	$-g$	$-g^2$	$-h$	$-gh$
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	1	−1	1	1	−1	1	−1	1	1	−1
χ_4	1	1	1	−1	−1	1	1	1	−1	−1
χ_5	2	0	−2	0	0	2	0	−2	0	0
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	1	−1	1	1	−1	−1	1	−1	−1	1
χ_9	1	1	1	−1	−1	−1	−1	−1	1	1
χ_{10}	2	0	−2	0	0	−2	0	2	0	0

Direct product $\mathcal{C}_2 \times \mathcal{D}_6$ point group *6/mmm*

For labelling the columns, we take the first component $\mathcal{C}_2$ of the direct product to be the group $\{\pm 1\}$ and the second component to be generated by g and h.

class length	1	2	2	1	3	3	1	2	2	1	3	3
element order	1	6	3	2	2	2	2	6	6	2	2	2
	e	g	g^2	g^3	h	gh	$-e$	$-g$	$-g^2$	$-g^3$	$-h$	$-gh$
χ_1	1	1	1	1	1	1	1	1	1	1	1	1
χ_2	1	−1	1	−1	−1	1	1	−1	1	−1	−1	1
χ_3	1	−1	1	−1	1	−1	1	−1	1	−1	1	−1
χ_4	1	1	1	1	−1	−1	1	1	1	1	−1	−1
χ_5	2	1	−1	−2	0	0	2	1	−1	−2	0	0
χ_6	2	−1	−1	2	0	0	2	−1	−1	2	0	0
χ_7	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1
χ_8	1	−1	1	−1	−1	1	−1	1	−1	1	1	−1
χ_9	1	−1	1	−1	1	−1	−1	1	−1	1	−1	1
χ_{10}	1	1	1	1	−1	−1	−1	−1	−1	−1	1	1
χ_{11}	2	1	−1	−2	0	0	−2	−1	1	2	0	0
χ_{12}	2	−1	−1	2	0	0	−2	1	1	−2	0	0

Tetrahedral group $\mathcal{T}$

For the tetrahedral group $\mathcal{T}$ we know that the 3-dimensional vector representation of the point group *23* $\cong \mathcal{T}$ is irreducible, since the group elements do not have a common eigenvector (none of the threefold axes is left invariant by one of the twofold rotations). This representation is given by

$$\mathbf{D}^{(4)}(2_z) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{D}^{(4)}(3^+_{xxx}) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}.$$

Because $|\mathcal{T}| = 12$, this immediately implies that $\mathcal{T}$ has three 1-dimensional irreps, since then $12 = 1 + 1 + 1 + 3^2$ is the only way of writing 12 as a sum of squares.
The twofold rotations $2_x, 2_y, 2_z$ generate a normal subgroup of order 4 (isomorphic to $\mathcal{D}_2$) and this is the commutator subgroup $\mathcal{T}'$ of $\mathcal{T}$. Since the commutator subgroup is in the kernel of every 1-dimensional irrep, the character table of $\mathcal{T}$ is completely determined.

Tetrahedral group $\mathcal{T}$ point group *23*

class length	1	3	4	4
element order	1	2	3	3
	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

where $\zeta_3 = \exp(2\pi i/3) = (-1 + i\sqrt{3})/2$ and $\zeta_3^* = \zeta_3^2$.

For the irreps of the direct product $\mathcal{C}_2 \times \mathcal{T}$, we again simply have to extend an irrep of degree m of $\mathcal{T}$ to the generator -1 of $\mathcal{C}_2$ by either $-1 \mapsto \boldsymbol{I}_m$ or $-1 \mapsto -\boldsymbol{I}_m$. The character table of $\mathcal{C}_2 \times \mathcal{T}$ is obtained via Corollary 1.10.2.

Direct product $\mathcal{C}_2 \times \mathcal{T}$ point group $\overline{3}m$

class length	1	3	4	4	1	3	4	4
element order	1	2	3	3	2	2	6	6
	1	2_z	3^+_{xxx}	3^-_{xxx}	$\overline{1}$	m_z	$\overline{3}^+_{xxx}$	$\overline{3}^-_{xxx}$
χ_1	1	1	1	1	1	1	1	1
χ_2	1	1	ζ_3	ζ_3^*	1	1	ζ_3	ζ_3^*
χ_3	1	1	ζ_3^*	ζ_3	1	1	ζ_3^*	ζ_3
χ_4	3	-1	0	0	3	-1	0	0
χ_5	1	1	1	1	-1	-1	-1	-1
χ_6	1	1	ζ_3	ζ_3^*	-1	-1	$-\zeta_3$	$-\zeta_3^*$
χ_7	1	1	ζ_3^*	ζ_3	-1	-1	$-\zeta_3^*$	$-\zeta_3$
χ_8	3	-1	0	0	-3	1	0	0

Octahedral group $\mathcal{O}$

The octahedral group is only slightly more involved than the tetrahedral group. First of all, we know that the 3-dimensional vector representation of the point group $432 \cong \mathcal{O}$ is irreducible. Moreover, $\mathcal{O}' = \mathcal{T}$, hence the commutator subgroup has index 2 in $\mathcal{O}$, thus there are exactly two 1-dimensional irreps. Furthermore, we know that the twofold rotations 2_x, 2_y, 2_z generate a normal subgroup of order 4 (isomorphic to $\mathcal{D}_2$), and the factor group $\mathcal{O}/\mathcal{D}_2 \cong \mathcal{D}_3$. Since an irrep of the factor group gives rise to an irrep of the full group, $\mathcal{O}$ also has a 2-dimensional irrep. We have thus found 4 irreps with degrees 1, 1, 2, 3, and since $\mathcal{O}$ has 5 conjugacy classes, the last irrep necessarily also has degree 3.
Since $\mathcal{O}$ has two realizations as a point group, namely 432 and $\overline{4}3m$, we give two sets of representatives for the conjugacy classes:

432	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
$\overline{4}3m$	1	2_z	$m_{x\overline{x}z}$	3^+_{xxx}	$\overline{4}^+_z$

Note that $m_{x\overline{x}z}$ and $\overline{4}^+_z$ are just the products of 2_{xx0} and 4^+_z with the inversion $\overline{1}$.
The nontrivial 1-dimensional irrep is easy to construct, since it has $\mathcal{T}$ in its kernel, therefore the conjugacy class representatives of $\mathcal{O}$ contained in $\mathcal{T}$ (i.e. 1, 2_z, 3^+_{xxx}) are mapped to 1, the other elements are mapped to -1.
The vector representation of 432 is given by extending the 3-dimensional representation of $\mathcal{T}$ given above by

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

The vector representation of $\overline{4}3m$ is given by extending the 3-dimensional representation of

$\mathcal{T}$ given above by

$$\mathbf{D}^{(5)}(m_{x\bar{x}z}) = \begin{pmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{D}^{(5)}(\overline{4}_z^+) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Note that $\mathbf{D}^{(5)}$ is simply the tensor product of $\mathbf{D}^{(4)}$ with the non-trivial 1-dimensional irrep of $\mathcal{O}$.

Finally, in the factor group $\mathcal{O}/\mathcal{D}_2 \cong \mathcal{D}_3$ 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 $(\overline{4}^+_z)$ correspond to the element h of order 2 in $\mathcal{D}_3$.

Octahedral group $\mathcal{O}$ — point groups 432, $\overline{4}3m$

class length	1	3	6	8	6
element order	1	2	2	3	4
432	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
$\overline{4}3m$	1	2_z	$m_{x\bar{x}z}$	3^+_{xxx}	$\overline{4}^+_z$
χ_1	1	1	1	1	1
χ_2	1	1	−1	1	−1
χ_3	2	2	0	−1	0
χ_4	3	−1	−1	0	1
χ_5	3	−1	1	0	−1

For the irreps of the direct product $\mathcal{C}_2 \times \mathcal{O}$, we again simply have to extend an irrep of degree m of $\mathcal{O}$ to the generator -1 of $\mathcal{C}_2$ by either $-1 \mapsto \boldsymbol{I}_m$ or $-1 \mapsto -\boldsymbol{I}_m$. The character table of $\mathcal{C}_2 \times \mathcal{O}$ is obtained via Corollary 1.10.2.

Direct product $\mathcal{C}_2 \times \mathcal{O}$ — point group $m\overline{3}m$

class length	1	3	6	8	6	1	3	6	8	6
element order	1	2	2	3	4	2	2	2	6	4
	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z	$\overline{1}$	m_z	$m_{x\bar{x}z}$	$\overline{3}^+_{xxx}$	$\overline{4}^+_z$
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

2.4 Vector and pseudovector representations of point groups

If a finite subgroup $\mathcal{G}$ of $GL_3(\mathbb{R})$ is given, its elements are either *proper rotations* (in case $\det(g) = 1$) or *improper rotations* (in case $\det(g) = -1$). The action of $\mathcal{G}$ on $\mathbb{R}^3$ is an action on *polar vectors*. However, using the 1-dimensional irrep given by $g \mapsto \det(g)$, we can also obtain an action on *axial vectors* or *pseudovectors*.

Definition 2.4.1 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 2.4.2 A typical case in which pseudovectors occur is the description of a rotation axis by a vector (which also explains the alternative term 'axial vector').
By convention, the vector points up the rotation axis and the rotation is counterclockwise when one looks down the axis, see Figure 3.
Since inversion neither changes the rotation axis nor the sense of rotation, the axial vector $\mathbf{R}$ describing it has to remain the same, i.e. we require that $\overline{1}(\mathbf{R}) = \mathbf{R}$.

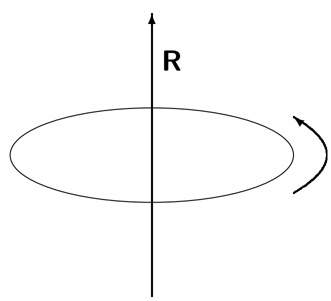

Figure 3: Axial vector describing a rotation axis

There are two common ways of looking at pseudovectors:

(1) 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 $\mathbf{R}(\mathbf{e}_x), \mathbf{R}(\mathbf{e}_y), \mathbf{R}(\mathbf{e}_z)$).

(2) 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.

Note that the second interpretation of pseudovectors is restricted to $\mathbb{R}^3$, since it requires the vector product. The first interpretation can be applied for every vector space on which $\mathcal{G}$ acts.

Example 2.4.3

(i) The rotation $2_{xx0} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$ 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 2_{xx0} is a proper rotation, its action on the pseudovectors in the first interpretation is simply given by

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

In the second interpretation we get

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

which indeed coincides with the first interpretation.

(ii) The reflection $m_{xxz} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ 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 m_{xxz} is an improper rotation, its action on the pseudovectors in the first interpretation is given by

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

since the pseudovectors have to be mapped to the opposites of the corresponding polar vectors.

In the second interpretation we get

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

hence again the two interpretations coincide.

(iii) 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

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

In the second interpretation we get

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

as expected.

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.

Starting with a representation of a subgroup $\mathcal{G} \leq \mathrm{GL}_3(\mathbb{R})$ which gives the action of $\mathcal{G}$ on the polar vectors of some vector space $\mathbf{V}$, it is straightforward to determine the representation obtained for the action of $\mathcal{G}$ on the elements of $\mathbf{V}$ interpreted as pseudovectors.

Definition 2.4.4 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 2.4.5 Let $\mathcal{G}$ be a subgroup of $\mathrm{GL}_3(\mathbb{R})$ and denote by $\mathbf{D}^t$ its vector representation and by $\mathbf{D}^r$ its pseudovector representation.

(i) The pseudovector representation is obtained by multiplying the vector representation by the determinant of the respective matrix, i.e.

$$\mathbf{D}^r(g) = \det(g)\mathbf{D}^t(g).$$

In other words, if we denote by $\mathbf{D}^{(0)}$ the 1-dimensional irrep of $\mathcal{G}$ given by $\mathbf{D}^{(0)}(g) = \det(g)$, then the pseudovector representation is the direct product representation

$$\mathbf{D}^r = \mathbf{D}^{(0)} \otimes \mathbf{D}^t,$$

because the improper rotations of $\mathcal{G}$ are precisely those elements of $\mathcal{G}$ with $\det(g) = -1$ and for these the matrices have to be multiplied by -1.

(ii) The pseudovector representation is equivalent to the antisymmetrized square of the vector representation, i.e.

$$\mathbf{D}^r = \{\mathbf{D}^t\}^2.$$

Note that for a group of proper rotations, the irrep $\mathbf{D}^{(0)}$ is the trivial representation of $\mathcal{G}$ and the representations of $\mathcal{G}$ on polar vectors and pseudovectors coincide (as they should).

Example 2.4.6 The point group $\mathcal{G} = \overline{4}3m$ has the character table

	1	2_z	$m_{x\overline{x}z}$	3^+_{xxx}	$\overline{4}^+_z$
χ_1	1	1	1	1	1
χ_2	1	1	−1	1	−1
χ_3	2	2	0	−1	0
χ_4	3	−1	−1	0	1
χ_5	3	−1	1	0	−1

The vector representation of $\overline{4}3m$ has the character χ_5 and χ_2 is the character obtained by taking the determinants of the vector representation of $\mathcal{G}$. Since $\chi_2 \cdot \chi_5 = \chi_4$, we see that χ_4 is the character of the pseudovector representation of $\overline{4}3m$.
Alternatively, one easily sees that χ_4 is the antisymmetrized square $\{\chi_5\}^2$ of the character χ_5 of the vector representation of $\mathcal{G}$.

Note that for the 2-dimensional irrep of $\overline{4}3m$ the actions on polar vectors and pseudovectors coincide, since $\chi_2 \cdot \chi_3 = \chi_3$.

Exercise 21.
The character table of the point group $m\overline{3}m$ is

	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z	$\overline{1}$	m_z	$m_{x\overline{x}z}$	$\overline{3}^+_{xxx}$	$\overline{4}^+_z$
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 $m\overline{3}m$ and which is the pseudovector representation.

Hint: Remember what you know about the traces of reflections and twofold rotations.

2.5 Basis functions of irreps

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 2.5.1 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 $xy + xz + yz \mapsto yx - yz - xz$.

If one selects a linear space of functions in the coordinates which is closed under the group action, one obtains a representation of $\mathcal{G}$ on these functions.

Definition 2.5.2 Let $\mathbf{F}$ 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 $\mathbf{F}$ by $\mathbf{D}$.
Let the i-the irrep $\mathbf{D}^{(i)}$ of $\mathcal{G}$ occur with multiplicity m_i in $\mathbf{D}$, i.e. let $\mathbf{D} = m_1\mathbf{D}^{(1)} \oplus \ldots \oplus m_r\mathbf{D}^{(r)}$ be the decomposition of $\mathbf{D}$ into irreps.
Then the functions of a subspace $\mathbf{F}^{(i)}$ of $\mathbf{F}$ 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 2.5.3 For the cyclic group 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 $\mathcal{C}_2$.

Common choices for the linear space of functions are:

(1) 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 $\mathcal{G}$.

(2) 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 $\mathcal{G}$.

(3) If we do not assume that x, y, z are commuting variables, we have $xy \neq yx$. Case (2) above then corresponds to the symmetric quadratic functions $x^2, y^2, z^2, (xy+yx), (xz+zx), (yz+zy)$.

(4) 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
χ_1	1	1	1	1
χ_2	1	1	−1	−1
χ_3	1	−1	1	−1
χ_4	1	−1	−1	1

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

In order to elucidate the concept of basis functions, we give a detailed derivation of the linear and quadratic basis functions of the point group $\overline{4}2m$.

Example 2.5.4 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

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

and its character table is

	1	2_z	$\overline{4}_z$	2_x	m_{xxz}
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

From the character table we immediately conclude that $\mathbf{\Gamma} = \mathbf{D}^{(4)} \oplus \mathbf{D}^{(5)}$. Hence we know that from the 3-dimensional space of functions spanned by the coordinates x, y, z, one function transforms with $\mathbf{D}^{(4)}$ and a 2-dimensional space transforms with $\mathbf{D}^{(5)}$. Since both $\overline{4}_z$ and 2_x map z to $-z$, the coordinate function z transforms with $\mathbf{D}^{(4)}$ and the space spanned by the functions x, y transforms with $\mathbf{D}^{(5)}$.

For the action on the pseudovector coordinates $\mathbf{J}_x, \mathbf{J}_y, \mathbf{J}_z$ we note that χ_3 is the character corresponding to the determinant of the vector representation, hence the pseudovector representation of $\overline{4}2m$ is given by

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

Since we already know that the coordinate function z transforms with $\mathbf{D}^{(4)}$, we can conclude that the pseudovector coordinate $\mathbf{J}_z$ transforms with $\mathbf{D}^{(3)} \otimes \mathbf{D}^{(4)} = \mathbf{D}^{(2)}$. By the same argument, the space spanned by the pseudovector coordinates $\mathbf{J}_x, \mathbf{J}_y$ transforms with $\mathbf{D}^{(5)}$, since $\mathbf{D}^{(3)} \otimes \mathbf{D}^{(5)} = \mathbf{D}^{(5)}$.

In order to deal with the quadratic functions, we need to decompose the symmetrized square of the vector representation. However, in order to get the functions which transform with the different irreps (without guessing), we actually have to apply the projection operators to the irreps.
The action of $\overline{4}_z$ and 2_x on the functions $x^2, y^2, z^2, xy, xz, yz$ is given by

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

From the character table we deduce that $[\mathbf{\Gamma}]^2 = 2\mathbf{D}^{(1)} \oplus \mathbf{D}^{(3)} \oplus \mathbf{D}^{(4)} \oplus \mathbf{D}^{(5)}$.
We now compute the projection operators

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

in order to explicitly find the functions on which $\overline{4}2m$ acts according to the different irreps. We get

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

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

which have ranks 2, 1, 1, 1, as required.
From this we conclude:

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

The character table of $\overline{4}2m$, augmented with the basis functions, therefore 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	$(x,y), (\mathbf{J}_x, \mathbf{J}_y), (xz, yz)$

Note that with the basis functions added, the character table depends on the point group and not only on the abstract isomorphism type of the point group.

From the character table including the basis functions, the vector and pseudovector representation of the group can of course immediately be read off:

- The vector representation is equivalent to the sum of the irreps in which the linear coordinate functions x, y, z (or linear combinations of these) occur.
- The pseudovector representation is equivalent to the sum of the irreps in which the pseudovector coordinates $\mathbf{J}_x, \mathbf{J}_y, \mathbf{J}_z$ (or linear combinations of these) occur.

The basis functions are also crucial in spectroscopy analysis. If a molecule has symmetry group $\mathcal{G}$, then the infrared (IR) active modes are those which have linear coordinate functions as basis functions, i.e. which occur in the vector representation of $\mathcal{G}$. The Raman active modes are those which have quadratic coordinate functions as basis functions, i.e. which occur in the symmetrized square of the vector representation of $\mathcal{G}$.

2.6 Molecular vibrations

In this final section we illustrate the use of various of the concepts discussed so far by applying them to the analysis of vibrational modes of a molecule.

We look at a molecule consisting of N atoms. In the position of each atom, we install 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*.
The action of $\mathcal{G}$ on global translations is given by the vector representation $\mathbf{\Gamma}^t$ of $\mathcal{G}$. Since a global translation can be expressed in the local coordinates, we see that the space of local coordinates contains a subspace on which $\mathcal{G}$ acts by $\mathbf{\Gamma}^t$.
Further, the action of $\mathcal{G}$ on global rotations is given by the pseudovector representation $\mathbf{\Gamma}^r$ of $\mathcal{G}$ i.e. by the antisymmetrized square of the vector representation of $\mathcal{G}$. Since also a global rotation can be expressed in the local coordinates, the space of local coordinates also contains a subspace on which $\mathcal{G}$ acts by $\mathbf{\Gamma}^r$.
If one is interested in vibrational modes, global translations and global rotations are usually neglected and the interesting subspace containing the vibrational modes is just the complement of the two spaces on which $\mathcal{G}$ acts by $\mathbf{\Gamma}^t$ and $\mathbf{\Gamma}^r$. In particular it is a subspace of dimension $3N-6$ (ignoring the special case of linear molecules).

Summarizing, the representation $\mathbf{\Gamma}$ giving the action of $\mathcal{G}$ on the local coordinates can be written as

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

where $\mathbf{\Gamma^t}$ is the vector representation of $\mathcal{G}$, $\mathbf{\Gamma^r}$ is the pseudovector representation of $\mathcal{G}$ and $\mathbf{\Gamma}^v$ is the action on vibrational modes.

In order to get a concrete description of the vibrational modes, we have to obtain explicit bases for the irreps occurring in $\mathbf{\Gamma}^v$. This is achieved by applying the projection operators of the irreps (see 1.8.9 and 1.8.10) to $\mathbf{\Gamma}$ and filtering out the parts belonging to $\mathbf{\Gamma}^v$.

Example 2.6.1 As a worked example we discuss a molecule of water type as displayed in Figure 4. The molecule is situated in the yz-plane. The non-trivial elements of its symmetry group $\mathcal{G} = mm2 \cong \mathcal{D}_2$ 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.

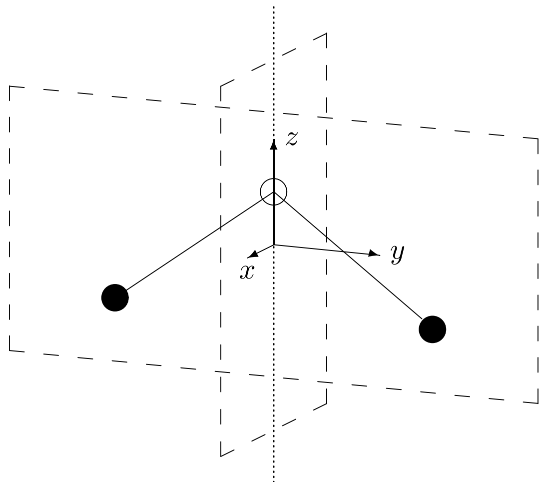

Figure 4: Molecule of water type

In order to describe the effect of the symmetry operations on the single atoms, we install local coordinate systems in each of the atoms as shown in Figure 5. Note that the molecule is now displayed in the yz-plane, the x-axis points out of the plane.

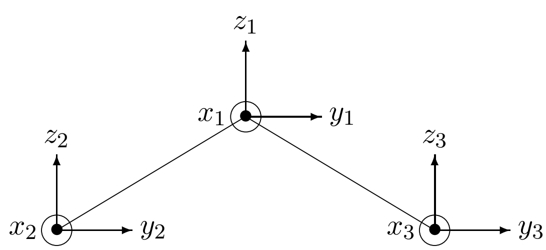

Figure 5: Local coordinate systems

The action of $\mathcal{G}$ on the local coordinates is

2_z	m_y	m_x
$(x_1, y_1, z_1) \mapsto (-x_1, -y_1, z_1)$	$(x_1, y_1, z_1) \mapsto (x_1, -y_1, z_1)$	$(x_1, y_1, z_1) \mapsto (-x_1, y_1, z_1)$
$(x_2, y_2, z_2) \mapsto (-x_3, -y_3, z_3)$	$(x_2, y_2, z_2) \mapsto (x_3, -y_3, z_3)$	$(x_2, y_2, z_2) \mapsto (-x_2, y_2, z_2)$
$(x_3, y_3, z_3) \mapsto (-x_2, -y_2, z_2)$	$(x_3, y_3, z_3) \mapsto (x_2, -y_2, z_2)$	$(x_3, y_3, z_3) \mapsto (-x_3, y_3, z_3)$

from which we could immediately write down the matrices of $\mathbf{\Gamma}$.

However, it is easier and also enlightening to notice that the elements of $\mathcal{G}$ permute the atoms of the molecule. Identifying the atoms with the indices of their local coordinate systems, we see that 2_z and m_y fix atom 1 and swap atoms 2 and 3 and that m_x fixes all three atoms. This gives rise to a *permutation representation* $\mathbf{\Pi}$ of $\mathcal{G}$ on the atoms, also called the *equivalence representation*, which is given by

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

Since the local coordinate systems are all set up in the same way, it now follows that the representation $\mathbf{\Gamma}$ is the direct product of this permutation representation $\mathbf{\Pi}$ with the vector representation of $\mathcal{G}$, i.e.

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

The character $\chi_{\mathbf{\Gamma}}$ can be easily determined, because only atoms which are fixed by an element g correspond to a block on the diagonal in $\mathbf{\Gamma}$. Since each block on the diagonal has trace $\chi_{\mathbf{\Gamma}^t}(g)$, one has

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

Exercise 23.
The non-trivial elements of the symmetry group *mm2* of the water-type molecule are

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

The elements 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 $\mathbf{\Gamma}^r$ appended, 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

(i) Determine the character of the representation $\mathbf{\Gamma}$.

(ii) 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 $\mathbf{\Gamma}$.

In order to decompose this representation it is useful to display the character table of $\mathcal{G}$. We append the characters $\chi_{\mathbf{\Gamma}}$ of $\mathbf{\Gamma}$, $\chi_{\mathbf{\Gamma}^t}$ of the vector representation of $\mathcal{G}$ (acting on usual polar vectors) and $\chi_{\mathbf{\Gamma}^r}$ of the pseudovector representation of $\mathcal{G}$ (acting on axial vectors).

	1	2_z	m_y	m_x
$A_1 = \chi_1$	1	1	1	1
$A_2 = \chi_2$	1	1	-1	-1
$B_1 = \chi_3$	1	-1	1	-1
$B_2 = \chi_4$	1	-1	-1	1
$\chi_{\mathbf{\Gamma}}$	9	-1	1	3
$\chi_{\mathbf{\Gamma}^t}$	3	-1	1	1
$\chi_{\mathbf{\Gamma}^r}$	3	-1	-1	-1

Using the 'magic formula' Corollary 1.8.4 to determine the multiplicities of the irreps in the different representations, we derive that

$$\mathbf{\Gamma} = 3A_1 \oplus A_2 \oplus 2B_1 \oplus 3B_2,$$

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

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

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

In order to find an explicit basis for the vibrational modes, we compute the projection operators P_{A_1} and P_{B_2} and for that we finally require the explicit matrices for the representation $\mathbf{\Gamma}$:

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

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

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

For the projection operator P_{A_1} to the sum of the subspaces on which $\mathbf{\Gamma}$ acts by the trivial representation A_1, we get

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

which is a matrix of rank 3 (as expected) and projects to vectors of the form

$$(0, 0, a, 0, b, c, 0, -b, c)^T.$$

We know that there must be a translational subspace of dimension 1, since A_1 occurs with multiplicity 1 in $\mathbf{\Gamma}^t$ and easily see that such a vector is $\mathbf{t}_z = (0, 0, 1, 0, 0, 1, 0, 0, 1)^T = z_1 + z_2 + z_3$, corresponding to a global translation along the z-axis.
Now the vibrational modes should be chosen orthogonal to the translational vector, and an easy choice is

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

These two vibrational modes can be visualized as follows:

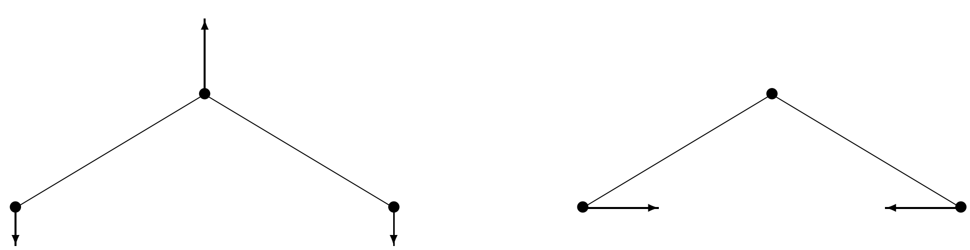

Figure 6: Vibrational modes $\mathbf{v}_1$ (left) and $\mathbf{v}_2$ (right) for the irrep A_1

For the projection operator P_{B_2} to the sum of the subspaces on which $\mathbf{\Gamma}$ acts by the representation B_2, we get

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

which is a matrix of rank 3 (as it should) and projects to vectors of the form

$$(0, a, 0, 0, b, c, 0, b, -c)^T.$$

Again there must be a translational subspace of dimension 1, and we see that such a vector is $\mathbf{t}_y = (0, 1, 0, 0, 1, 0, 0, 1, 0)^T = y_1 + y_2 + y_3$, corresponding to a global translation along the y-axis.
We also know that there must be a rotational subspace of dimension 1 since B_2 occurs with multiplicity 1 in $\mathbf{\Gamma}^r$.
Choosing the origin in the middle of the base of the molecule, we see that a rotation $\mathbf{R}_z$ around the z-axis corresponds to $x_2 - x_3$, a rotation $\mathbf{R}_y$ around the y-axis corresponds to x_1 and a rotation $\mathbf{R}_x$ around the x-axis corresponds to $-y_1 - z_2 + z_3$.
The vibrational vector should be orthogonal to $\mathbf{t}_y$ and to $\mathbf{r}_x = (0, -1, 0, 0, 0, 0, 0, -1, 1)^T$ and we find that such a vector is

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

This vibrational mode can be visualized as follows:

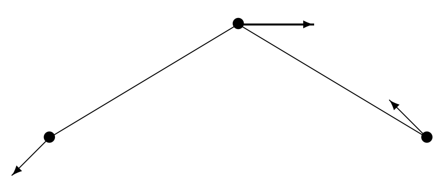

Figure 7: Vibrational mode $\mathbf{v}_3$ for the irrep B_2

Review exercises

Exercise 1.
Let $\mathcal{D}_4$ be the dihedral group of order 8 generated by an element g of order 4 and an element h of order 2 with $gh = hg^{-1}$.
Show that the representations $\mathbf{D}$ and $\mathbf{D}'$ given by

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

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

are equivalent.
Find an explicit matrix $\boldsymbol{X}$ conjugating $\mathbf{D}$ to $\mathbf{D}'$.

Exercise 2.
The character table of the tetrahedral group $\mathcal{T}$ is

$\mathcal{T}$	1	2_z	3^+_{xxx}	3^-_{xxx}
χ_1	1	1	1	1
χ_2	1	1	ζ	ζ^*
χ_3	1	1	ζ^*	ζ
χ_4	3	−1	0	0

where $\zeta = \exp(2\pi i/3)$.
Let $\mathbf{D}$ be the 3-dimensional irrep of $\mathcal{T}$.
Determine the multiplicities with which the irreps of $\mathcal{T}$ occur in the representation $\mathbf{D}\otimes\mathbf{D}\otimes\mathbf{D}$ (which has character χ_4^3).

Exercise 3.
Let $\mathcal{G}$ be a finite group and assume that the irreps $\mathbf{D}^{(1)}, \ldots, \mathbf{D}^{(r)}$ are known.
Show that the direct product $\mathcal{G} \times \mathcal{C}_2$ has precisely two irreps which coincide with $\mathbf{D}^{(i)}$ on $\mathcal{G}$ (viewed as a subgroup of $\mathcal{G} \times \mathcal{C}_2$). Describe these irreps.

Exercise 4.
Assume that the coefficients c_{ij}^k of the Clebsch-Gordan series of a group $\mathcal{G}$ are known.
Express the coefficients of the Clebsch-Gordan series of the direct product $\mathcal{C}_2 \times \mathcal{G}$ in terms of the c_{ij}^k.

Exercise 5.
Determine the coefficients of the Clebsch-Gordan series for the dihedral groups $\mathcal{D}_3$ and $\mathcal{D}_4$ and for the octahedral group $\mathcal{O}$. The character tables of these groups are:

$\mathcal{D}_3$	e	g	h
χ_1	1	1	1
χ_2	1	1	−1
χ_3	2	−1	0

$\mathcal{D}_4$	e	g	g^2	h	gh
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	0	−2	0	0

$\mathcal{O}$	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
χ_1	1	1	1	1	1
χ_2	1	1	−1	1	−1
χ_3	2	2	0	−1	0
χ_4	3	−1	−1	0	1
χ_5	3	−1	1	0	−1

Exercise 6.
Let $\mathcal{D}_3$ be the dihedral group of order 6 generated by an element g of order 3 and an element h of order 2. The character table of $\mathcal{D}_3$ is displayed in the previous exercise. The 2-dimensional irrep is given by

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

(i) Determine the character table of the direct product $\mathcal{D}_3 \times \mathcal{D}_3$ (which does not occur as a crystallographic point group).

(ii) Determine the irreps of degree > 1 of $\mathcal{D}_3 \times \mathcal{D}_3$ explicitly (it is enough to give the matrices for generators).

Exercise 7.
Let $\mathbf{D}$ be a 2-dimensional representation of a group $\mathcal{G}$.
Show that the antisymmetrized square $\{\mathbf{D}\}^2$ of $\mathbf{D}$ is given by $\{\mathbf{D}\}^2(g) = \det(\mathbf{D}(g))$.
Hint: Let $\mathbf{D}(g) = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$ be the action of g on the basis $\mathbf{v}_1, \mathbf{v}_2$. Determine the action of g on $\mathbf{v}_1\mathbf{v}_2$, $\mathbf{v}_2\mathbf{v}_1$ and thus on $\mathbf{v}_1\mathbf{v}_2 - \mathbf{v}_2\mathbf{v}_1$.

Exercise 8.
Let $\mathcal{G}$ be a subgroup of $\mathrm{GL}_3(\mathbb{R})$ and let $\mathbf{D}^t$ be its vector representation with character χ^t. Show that the pseudovector representation $\mathbf{D}^r$ of $\mathcal{G}$ is equivalent to the antisymmetrized square $\{\mathbf{D}^t\}^2$ of $\mathbf{D}^t$.
Hint: The character χ^r of the pseudovector representation is given by $\chi^r(g) = \det(g)\chi^t(g)$. It is sufficient to check that χ^r coincides with the character $\{\chi^t\}^2$. For that, assume that g is a diagonal matrix of the form $\begin{pmatrix} \pm 1 & 0 & 0 \\ 0 & z & 0 \\ 0 & 0 & z^* \end{pmatrix}$ where z^* is the complex conjugate of z.

Exercise 9.
The point group $4mm$ is generated by the elements

$$4_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad m_x = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

(i) Determine the representation $\mathbf{\Gamma}$ of $4mm$ on the coordinate functions $x^2, y^2, z^2, xy, xz, yz$.

(ii) Decompose $\mathbf{\Gamma}$ into irreps and determine the basis functions corresponding to the occurring irreps.

Hint: The trivial irrep occurs with multiplicity 2 and the irrep of degree 2 occurs with multiplicity 1.

Solutions to review exercises

Exercise 1.
Let $\mathcal{D}_4$ be the dihedral group of order 8 generated by an element g of order 4 and an element h of order 2 with $gh = hg^{-1}$.
Show that the representations $\mathbf{D}$ and $\mathbf{D}'$ given by

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

are equivalent.
Find an explicit matrix $\boldsymbol{X}$ conjugating $\mathbf{D}$ to $\mathbf{D}'$.

Solution: Let $\boldsymbol{X} = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$. We require

$$\boldsymbol{X}^{-1}\mathbf{D}(g)\boldsymbol{X} = \mathbf{D}'(g) \text{ and } \boldsymbol{X}^{-1}\mathbf{D}(h)\boldsymbol{X} = \mathbf{D}'(h) \text{ which is equivalent to}$$
$$\mathbf{D}(g)\boldsymbol{X} = \boldsymbol{X}\mathbf{D}'(g) \text{ and } \mathbf{D}(h)\boldsymbol{X} = \boldsymbol{X}\mathbf{D}'(h).$$

Evaluating the condition for g gives

$$\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} a & c \\ b & d \end{pmatrix} = \begin{pmatrix} -b & -d \\ a & c \end{pmatrix} = \begin{pmatrix} ia & -ic \\ ib & -id \end{pmatrix} = \begin{pmatrix} a & c \\ b & d \end{pmatrix}\begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix}$$

from which we conclude that $b = -ia$ and $d = ic$. Inserting this in $\boldsymbol{X}$ and evaluating the condition for h gives

$$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} a & c \\ -ia & ic \end{pmatrix} = \begin{pmatrix} a & c \\ ia & -ic \end{pmatrix} = \begin{pmatrix} c & a \\ ic & -ia \end{pmatrix} = \begin{pmatrix} a & c \\ -ia & ic \end{pmatrix}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

from which we conclude that $c = a$. Choosing $a = 1$ we get the conjugating matrix

$$\boldsymbol{X} = \begin{pmatrix} 1 & 1 \\ -i & i \end{pmatrix}.$$

Exercise 2.
The character table of the tetrahedral group $\mathcal{T}$ is

$\mathcal{T}$	1	2_z	3^+_{xxx}	3^-_{xxx}
χ_1	1	1	1	1
χ_2	1	1	ζ	ζ^*
χ_3	1	1	ζ^*	ζ
χ_4	3	-1	0	0

where $\zeta = \exp(2\pi i/3)$.
Let $\mathbf{D}$ be the 3-dimensional irrep of $\mathcal{T}$.

Determine the multiplicities with which the irreps of $\mathcal{T}$ occur in the representation $\mathbf{D}\otimes\mathbf{D}\otimes\mathbf{D}$ (which has character χ_4^3).

Solution: The character $\chi = \chi_4^3$ is $(27, -1, 0, 0)$ (written like the rows in the character table). In order to evaluate the 'magic formula', i.e. the scalar product of the class functions, we require the class lengths, which are 1, 3, 4, 4 for the conjugacy classes with representatives 1, 2_z, 3^+_{xxx}, 3^-_{xxx}, respectively.
From this we see that

$$\begin{aligned} m_1 &= (\chi,\chi_1) = \frac{1}{12}(27 + 3\cdot(-1)) = 2 \\ m_2 &= (\chi,\chi_2) = \frac{1}{12}(27 + 3\cdot(-1)) = 2 \\ m_3 &= (\chi,\chi_3) = \frac{1}{12}(27 + 3\cdot(-1)) = 2 \\ m_4 &= (\chi,\chi_3) = \frac{1}{12}(81 + 3\cdot 1) = 7 \end{aligned}$$

and we convince ourselves that $2+2+2+7\cdot 3 = 27$, i.e. the decomposition obtained has the correct degree.

Exercise 3.
Let $\mathcal{G}$ be a finite group and assume that the irreps $\mathbf{D}^{(1)}, \ldots, \mathbf{D}^{(r)}$ are known.
Show that the direct product $\mathcal{G}\times\mathcal{C}_2$ has precisely two irreps which coincide with $\mathbf{D}^{(i)}$ on $\mathcal{G}$ (viewed as a subgroup of $\mathcal{G}\times\mathcal{C}_2$). Describe these irreps.

Solution: Let the cyclic group $\mathcal{C}_2$ be $\{+1,-1\}$. The irreps of $\mathcal{C}_2$ are given by $\mathbf{D}^{(+)}(-1) = 1$ and $\mathbf{D}^{(-)}(-1) = 1$.
The elements of $\mathcal{G}\times\mathcal{C}_2$ are of the form $(g,1)$ and $(g,-1)$ with $g\in\mathcal{G}$.
We know that the irreps of $\mathcal{G}\times\mathcal{C}_2$ are obtained as the Kronecker products of the irreps of $\mathcal{G}$ with those of $\mathcal{C}_2$.
The Kronecker product of the irrep $\mathbf{D}^{(i)}$ of $\mathcal{G}$ with $\mathbf{D}^{(+)}$ gives an irrep $\mathbf{D}^{(i+)}$ of $\mathcal{G}\times\mathcal{C}_2$ with

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

If we identify the generator -1 of $\mathcal{C}_2$ with the element $(1,-1)$ of $\mathcal{G}\times\mathcal{C}_2$, the representation is actually determined by the image of -1, since together with the elements of $\mathcal{G}$, -1 generates $\mathcal{G}\times\mathcal{C}_2$. This image is simply $\mathbf{D}^{(i+)}(-1) = \boldsymbol{I}$.
The Kronecker product of $\mathbf{D}^{(i)}$ with $\mathbf{D}^{(-)}$ gives an irrep $\mathbf{D}^{(i-)}$ of $\mathcal{G}\times\mathcal{C}_2$ with

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

It is already determined by $\mathbf{D}^{(i-)}(-1) = -\boldsymbol{I}$.

Exercise 4.
Assume that the coefficients c_{ij}^k of the Clebsch-Gordan series of a group $\mathcal{G}$ are known.
Express the coefficients of the Clebsch-Gordan series of the direct product $\mathcal{C}_2\times\mathcal{G}$ in terms of the c_{ij}^k.

Solution: Let $\mathbf{X}$ be the character table of $\mathcal{G}$. We know that the character table of $\mathcal{C}_2\times\mathcal{G}$ is given by

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

Assume that $\mathcal{G}$ has r irreps with characters $\chi_1, \ldots, \chi_r$. Let $\psi_1, \ldots, \psi_r, \psi_{r+1}, \ldots, \psi_{2r}$ be the characters of the irreps of $\mathcal{C}_2 \times \mathcal{G}$. Then for $1 \leq i \leq r$, ψ_i is of the form (χ_i, χ_i) and ψ_{i+r} is of the form $(\chi_i, -\chi_i)$.
To get the coefficients of the Clebsch-Gordan series of $\mathcal{C}_2 \times \mathcal{G}$, we have to distinguish the following four cases with $1 \leq i, j \leq r$:

$$\begin{aligned}
\psi_i \cdot \psi_j &= (\chi_i \cdot \chi_j, \chi_i \cdot \chi_j) \\
\psi_i \cdot \psi_{j+r} &= (\chi_i \cdot \chi_j, -\chi_i \cdot \chi_j) \\
\psi_{i+r} \cdot \psi_j &= (\chi_i \cdot \chi_j, -\chi_i \cdot \chi_j) \\
\psi_{i+r} \cdot \psi_{j+r} &= (\chi_i \cdot \chi_j, \chi_i \cdot \chi_j)
\end{aligned}$$

Denoting the coefficients of the Clebsch-Gordan series for $\mathcal{C}_2 \times \mathcal{G}$ by d_{ij}^k we conclude that for $1 \leq k \leq r$ we have

$$\begin{array}{ll}
d_{ij}^k = c_{ij}^k, & d_{ij}^{k+r} = 0 \\
d_{i,j+r}^k = 0, & d_{i,j+r}^{k+r} = c_{ij}^k \\
d_{i+r,j}^k = 0, & d_{i+r,j}^{k+r} = c_{ij}^k \\
d_{i+r,j+r}^k = c_{ij}^k, & d_{i+r,j+r}^{k+r} = 0.
\end{array}$$

Exercise 5.
Determine the coefficients of the Clebsch-Gordan series for the dihedral groups $\mathcal{D}_3$ and $\mathcal{D}_4$ and for the octahedral group $\mathcal{O}$. The character tables of these groups are:

$\mathcal{D}_3$	e	g	h
χ_1	1	1	1
χ_2	1	1	-1
χ_3	2	-1	0

$\mathcal{D}_4$	e	g	g^2	h	gh
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	0	-2	0	0

$\mathcal{O}$	1	2_z	2_{xx0}	3^+_{xxx}	4^+_z
χ_1	1	1	1	1	1
χ_2	1	1	-1	1	-1
χ_3	2	2	0	-1	0
χ_4	3	-1	-1	0	1
χ_5	3	-1	1	0	-1

Solution: We display the coefficients of the Clebsch-Gordan series as a lower triangular matrix containing as (i, j) entry the vector $(c_{ij}^1, \ldots, c_{ij}^r)$ and with the explicit decomposition into irreps:

$\mathcal{D}_3$	$\mathbf{D}^{(1)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(3)}$
$\mathbf{D}^{(1)}$	$(1,0,0)$		
$\mathbf{D}^{(2)}$	$(0,1,0)$	$(1,0,0)$	
$\mathbf{D}^{(3)}$	$(0,0,1)$	$(0,0,1)$	$(1,1,1)$

$\mathcal{D}_3$	$\mathbf{D}^{(1)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(3)}$
$\mathbf{D}^{(1)}$	$\mathbf{D}^{(1)}$		
$\mathbf{D}^{(2)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(1)}$	
$\mathbf{D}^{(3)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(1)} \oplus \mathbf{D}^{(2)} \oplus \mathbf{D}^{(3)}$

$\mathcal{D}_4$	$\mathbf{D}^{(1)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(4)}$	$\mathbf{D}^{(5)}$
$\mathbf{D}^{(1)}$	$(1,0,0,0,0)$				
$\mathbf{D}^{(2)}$	$(0,1,0,0,0)$	$(1,0,0,0,0)$			
$\mathbf{D}^{(3)}$	$(0,0,1,0,0)$	$(0,0,0,1,0)$	$(1,0,0,0,0)$		
$\mathbf{D}^{(4)}$	$(0,0,0,1,0)$	$(0,0,1,0,0)$	$(0,1,0,0,0)$	$(1,0,0,0,0)$	
$\mathbf{D}^{(5)}$	$(0,0,0,0,1)$	$(0,0,0,0,1)$	$(0,0,0,0,1)$	$(0,0,0,0,1)$	$(1,1,1,1,0)$

$\mathcal{D}_4$	$\mathbf{D}^{(1)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(4)}$	$\mathbf{D}^{(5)}$
$\mathbf{D}^{(1)}$	$\mathbf{D}^{(1)}$				
$\mathbf{D}^{(2)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(1)}$			
$\mathbf{D}^{(3)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(4)}$	$\mathbf{D}^{(1)}$		
$\mathbf{D}^{(4)}$	$\mathbf{D}^{(4)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(1)}$	
$\mathbf{D}^{(5)}$	$\mathbf{D}^{(5)}$	$\mathbf{D}^{(5)}$	$\mathbf{D}^{(5)}$	$\mathbf{D}^{(5)}$	$\mathbf{D}^{(1)} \oplus \mathbf{D}^{(2)} \oplus \mathbf{D}^{(3)} \oplus \mathbf{D}^{(4)}$

$\mathcal{O}$	$\mathbf{D}^{(1)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(4)}$	$\mathbf{D}^{(5)}$
$\mathbf{D}^{(1)}$	$(1,0,0,0,0)$				
$\mathbf{D}^{(2)}$	$(0,1,0,0,0)$	$(1,0,0,0,0)$			
$\mathbf{D}^{(3)}$	$(0,0,1,0,0)$	$(0,0,1,0,0)$	$(1,1,1,0,0)$		
$\mathbf{D}^{(4)}$	$(0,0,0,1,0)$	$(0,0,0,0,1)$	$(0,0,0,1,1)$	$(1,0,1,1,1)$	
$\mathbf{D}^{(5)}$	$(0,0,0,0,1)$	$(0,0,0,1,0)$	$(0,0,0,1,1)$	$(0,1,1,1,1)$	$(1,0,1,1,1)$

$\mathcal{O}$	$\mathbf{D}^{(1)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(4)}$	$\mathbf{D}^{(5)}$
$\mathbf{D}^{(1)}$	$\mathbf{D}^{(1)}$				
$\mathbf{D}^{(2)}$	$\mathbf{D}^{(2)}$	$\mathbf{D}^{(1)}$			
$\mathbf{D}^{(3)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(3)}$	$\mathbf{D}^{(1)} \oplus \mathbf{D}^{(2)} \oplus \mathbf{D}^{(3)}$		
$\mathbf{D}^{(4)}$	$\mathbf{D}^{(4)}$	$\mathbf{D}^{(5)}$	$\mathbf{D}^{(4)} \oplus \mathbf{D}^{(5)}$	$\mathbf{D}^{(1)} \oplus \mathbf{D}^{(3)} \oplus \mathbf{D}^{(4)} \oplus \mathbf{D}^{(5)}$	
$\mathbf{D}^{(5)}$	$\mathbf{D}^{(5)}$	$\mathbf{D}^{(4)}$	$\mathbf{D}^{(4)} \oplus \mathbf{D}^{(5)}$	$\mathbf{D}^{(2)} \oplus \mathbf{D}^{(3)} \oplus \mathbf{D}^{(4)} \oplus \mathbf{D}^{(5)}$	$\mathbf{D}^{(1)} \oplus \mathbf{D}^{(3)} \oplus \mathbf{D}^{(4)} \oplus \mathbf{D}^{(5)}$

Exercise 6.
Let $\mathcal{D}_3$ be the dihedral group of order 6 generated by an element g of order 3 and an element h of order 2. The character table of $\mathcal{D}_3$ is displayed in the previous exercise. The 2-dimensional irrep is given by

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

(i) Determine the character table of the direct product $\mathcal{D}_3 \times \mathcal{D}_3$ (which does not occur as a crystallographic point group).

(ii) Determine the irreps of degree > 1 of $\mathcal{D}_3 \times \mathcal{D}_3$ explicitly (it is enough to give the matrices for generators).

Solution: The elements of $\mathcal{D}_3 \times \mathcal{D}_3$ are pairs (g_1, g_2) with $g_1 \in \mathcal{D}_3$ and $g_2 \in \mathcal{D}_3$.

(i) Representatives of the conjugacy classes of $\mathcal{D}_3 \times \mathcal{D}_3$ are (e,e), (e,g), (e,h), (g,e), (g,g), (g,h), (h,e), (h,g), (h,h) and with respect to this ordering of the conjugacy classes the character table of $\mathcal{D}_3 \times \mathcal{D}_3$ is the Kronecker product of the character table of $\mathcal{D}_3$ with itself. We thus obtain the following character table:

$\mathcal{D}_3 \times \mathcal{D}_3$	(e,e)	(e,g)	(e,h)	(g,e)	(g,g)	(g,h)	(h,e)	(h,g)	(h,h)
χ_{11}	1	1	1	1	1	1	1	1	1
χ_{12}	1	1	−1	1	1	−1	1	1	−1
χ_{13}	2	−1	0	2	−1	0	2	−1	0
χ_{21}	1	1	1	1	1	1	−1	−1	−1
χ_{22}	1	1	−1	1	1	−1	−1	−1	1
χ_{23}	2	−1	0	2	−1	0	−2	1	0
χ_{31}	2	2	2	−1	−1	−1	0	0	0
χ_{32}	2	2	−2	−1	−1	1	0	0	0
χ_{33}	4	−2	0	−2	1	0	0	0	0

(ii) Generators for $\mathcal{D}_3 \times \mathcal{D}_3$ are the pairs (e,g), (e,h), (g,e), (h,e).

Kronecker products with 1-dimensional irreps are straightforward, we get

$$\mathbf{D}^{(13)} : (e,g) \mapsto \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \; (e,h) \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; (g,e) \mapsto \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; (h,e) \mapsto \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\mathbf{D}^{(23)} : (e,g) \mapsto \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \; (e,h) \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \; (g,e) \mapsto \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; (h,e) \mapsto \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\mathbf{D}^{(31)} : (e,g) \mapsto \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; (e,h) \mapsto \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; (g,e) \mapsto \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \; (h,e) \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

$$\mathbf{D}^{(32)} : (e,g) \mapsto \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \; (e,h) \mapsto \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \; (g,e) \mapsto \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}, \; (h,e) \mapsto \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

Finally, for the 4-dimensional irrep $\mathbf{D}^{(33)}$ we see precisely how the Kronecker product works:

$$(e,g) \mapsto \left(\begin{array}{cc|cc} 0 & -1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ \hline 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & -1 \end{array}\right), \quad (e,h) \mapsto \left(\begin{array}{cc|cc} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{array}\right),$$

$$(g,e) \mapsto \left(\begin{array}{cc|cc} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ \hline 1 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{array}\right), \quad (h,e) \mapsto \left(\begin{array}{cc|cc} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ \hline 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{array}\right).$$

Exercise 7.
Let $\mathbf{D}$ be a 2-dimensional representation of a group $\mathcal{G}$.
Show that the antisymmetrized square $\{\mathbf{D}\}^2$ of $\mathbf{D}$ is given by $\{\mathbf{D}\}^2(g) = \det(\mathbf{D}(g))$.

Hint: Let $\mathbf{D}(g) = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$ be the action of g on the basis $\mathbf{v}_1, \mathbf{v}_2$. Determine the action of g on $\mathbf{v}_1\mathbf{v}_2$, $\mathbf{v}_2\mathbf{v}_1$ and thus on $\mathbf{v}_1\mathbf{v}_2 - \mathbf{v}_2\mathbf{v}_1$.

Solution: $\mathbf{D}(g) = \begin{pmatrix} a & c \\ b & d \end{pmatrix}$ maps $\mathbf{v}_1$ to $a\mathbf{v}_1 + b\mathbf{v}_2$ and $\mathbf{v}_2$ to $c\mathbf{v}_1 + d\mathbf{v}_2$. Hence it maps $\mathbf{v}_1\mathbf{v}_2$ and $\mathbf{v}_2\mathbf{v}_1$ as follows:

$$\begin{aligned}
\mathbf{v}_1\mathbf{v}_2 &\mapsto (a\mathbf{v}_1 + b\mathbf{v}_2)(c\mathbf{v}_1 + d\mathbf{v}_2) = ac\mathbf{v}_1\mathbf{v}_1 + ad\mathbf{v}_1\mathbf{v}_2 + bc\mathbf{v}_2\mathbf{v}_1 + cd\mathbf{v}_2\mathbf{v}_2, \\
\mathbf{v}_2\mathbf{v}_1 &\mapsto (c\mathbf{v}_1 + d\mathbf{v}_2)(a\mathbf{v}_1 + b\mathbf{v}_2) = ac\mathbf{v}_1\mathbf{v}_1 + bc\mathbf{v}_1\mathbf{v}_2 + ad\mathbf{v}_2\mathbf{v}_1 + cd\mathbf{v}_2\mathbf{v}_2.
\end{aligned}$$

From this we see that

$$\begin{aligned}
\mathbf{v}_1\mathbf{v}_2 - \mathbf{v}_2\mathbf{v}_1 &\mapsto ad\mathbf{v}_1\mathbf{v}_2 + bc\mathbf{v}_2\mathbf{v}_1 - bc\mathbf{v}_1\mathbf{v}_2 + ad\mathbf{v}_2\mathbf{v}_1 = (ad - bc)\mathbf{v}_1\mathbf{v}_2 - (ad - bc)\mathbf{v}_2\mathbf{v}_1 \\
&= (ad - bc)(\mathbf{v}_1\mathbf{v}_2 - \mathbf{v}_2\mathbf{v}_1) = \det(\mathbf{D}(g))(\mathbf{v}_1\mathbf{v}_2 - \mathbf{v}_2\mathbf{v}_1).
\end{aligned}$$

Exercise 8.
Let $\mathcal{G}$ be a subgroup of $\mathrm{GL}_3(\mathbb{R})$ and let $\mathbf{D}^t$ be its vector representation with character χ^t. Show that the pseudovector representation $\mathbf{D}^r$ of $\mathcal{G}$ is equivalent to the antisymmetrized square $\{\mathbf{D}^t\}^2$ of $\mathbf{D}^t$.
Hint: The character χ^r of the pseudovector representation is given by $\chi^r(g) = \det(g)\chi^t(g)$. It is sufficient to check that χ^r coincides with the character $\{\chi^t\}^2$. For that, assume that g is a diagonal matrix of the form $\begin{pmatrix} \pm 1 & 0 & 0 \\ 0 & z & 0 \\ 0 & 0 & z^* \end{pmatrix}$ where z^* is the complex conjugate of z.

Solution: Since g is a matrix of finite order, it can be diagonalized over $\mathbb{C}$ and the entries on the diagonal are roots of unity. On the other hand, since g is a real matrix, either all diagonal entries are real, i.e. 1 or -1, or one is real and the other two are complex conjugates. Thus, g is equivalent to a matrix of the form $\begin{pmatrix} a & 0 & 0 \\ 0 & z & 0 \\ 0 & 0 & z^* \end{pmatrix}$ with $z \in \mathbb{C}$ and $a = \pm 1$.
If $a = 1$, g is a proper rotation and in this case we have $\chi^r(g) = 1 + z + z^*$.
If $a = -1$, g is an improper rotation and in this case we have $\chi^r(g) = -(-1 + z + z^*) = 1 - z - z^*$.
On the other hand, the character value of the antisymmetrized square is $\{\chi^t\}^2(g) = \frac{1}{2}(\chi^t(g)^2 - \chi^t(g^2))$.
We have $\chi^t(g) = a + z + z^*$ and thus $\chi^t(g)^2 = 1 + z^2 + (z^*)^2 + 2az + 2az^* + 2$ and $\chi^t(g^2) = 1 + z^2 + (z^*)^2$. This gives $\{\chi^t\}^2(g) = 1 + az + az^*$, as required.

Exercise 9.
The point group *4mm* is generated by the elements

$$4_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad m_x = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

(i) Determine the representation $\boldsymbol{\Gamma}$ of *4mm* on the coordinate functions $x^2, y^2, z^2, xy, xz, yz$.

(ii) Decompose $\mathbf{\Gamma}$ into irreps and determine the basis functions corresponding to the occurring irreps.

Hint: The trivial irrep occurs with multiplicity 2 and the irrep of degree 2 occurs with multiplicity 1.

Solution: The actions of 4_z and m_x on the coordinate functions is given by

$$\begin{array}{lllllll} 4_z: & x^2 \mapsto y^2, & y^2 \mapsto x^2, & z^2 \mapsto z^2, & xy \mapsto -xy, & xz \mapsto yz, & yz \mapsto -xz \\ m_x: & x^2 \mapsto x^2, & y^2 \mapsto y^2, & z^2 \mapsto z^2, & xy \mapsto -xy, & xz \mapsto -xz, & yz \mapsto yz \end{array}$$

hence the representation $\mathbf{\Gamma}$ is given by

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

Two 1-dimensional and two 2-dimensional blocks are indicated on the diagonal, showing that z^2 is a basis function for the trivial irrep and that xy is a basis function for the irrep $4_z \mapsto -1$, $m_x \mapsto -1$. Further, the lower 2×2 block shows that xz, yz are basis functions for the 2-dimensional irrep of *4mm*.

What remains is the upper 2×2 block. This block is not irreducible, since the matrix $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ is equivalent to $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ via the basis transformation $\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$. In other words, 4_z maps $x^2 + y^2$ to $x^2 + y^2$ and $x^2 - y^2$ to $-(x^2 - y^2)$. Thus, $x^2 + y^2$ is also a basis function for the trivial irrep and $x^2 - y^2$ is a basis function for the irrep $4_z \mapsto -1$, $m_x \mapsto 1$.

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