Symmetry in Physics

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These lecture notes on Symmetry in Physics evolved out of lecture notes of a course at the VU Amsterdam on Group Theory in Physics written by B.L.G. Bakker and D. Boer.

Contents

Chapter 1

Mathematics of symmetry: groups and group theory

[Topics in this chapter are covered in the book of Jones in chapters 1 and 2.]

1.1 Introduction

Symmetry plays an important role in the description of physical systems, ranging from tangible objects like crystals to more abstract notions like the laws of Nature. A system displays symmetry when it is invariant under a set of operations. This set of operations forms an algebraic structure called a group. Very broadly, groups can be divided into two types: discrete groups which have a countable number of elements, and continuous (Lie) groups for which the elements depend continuously (analytically) on a set of parameters. Both types appear frequently in physics. Examples of discrete groups are the symmetry groups of molecules and crystals, and the permutation groups. Examples of continuous groups are the group of rotations in three dimensions and the Lorentz group.

Groups have abstract definitions independent of the many different meanings that may be assigned to the elements. In order to apply group theory in physics one has to consider the quantities on which the group elements act, such as vectors in a three-dimensional space or wave functions in a Hilbert space. By acting on a particular space the group elements will take on a particular form which is called a *representation*. The topic of representations will be explored in Chapters 2 and 3.

In a nutshell this is what this course is about: to discuss and analyze 1) discrete and continuous groups of relevance to physics and 2) their representations needed

for applications in physics.

This first chapter is about the structure of groups from a mathematical viewpoint. In addition, it discusses several groups of importance to physics, with emphasis on groups of isometries (transformations that preserve distances) and their subgroups.

1.2 Abstract Groups

Groups can be defined and discussed independent of the *meaning* of the elements.

Definition *group*
A group G is the pair $(G; \circ)$ where G is a set of elements and $\circ$ is a composition (multiplication) law, such that

(i) $g_1, g_2 \in G \Rightarrow g_1 \circ g_2 \in G$ [closure]

(ii) $g_1, g_2, g_3 \in G \Rightarrow g_1 \circ (g_2 \circ g_3) = (g_1 \circ g_2) \circ g_3$ [associative law]

(iii) $\exists e \in G \; \forall g \in G : e \circ g = g \circ e = g$ [existence of neutral/unit/identity element]

(iv) $\forall g \in G \; \exists g^{-1} \in G : g \circ g^{-1} = g^{-1} \circ g = e$ [existence of inverse]

Definition *order*
The number of elements of a group is called the order of the group and is denoted by $[g]$.

Example 1
The integers with addition form the group $G = (\mathsf{Z}; +)$. Q: what is the neutral element and the order of this group?

Example 2
The integers with addition modulo n form the group $\mathsf{Z}_n = (\{0, 1, 2, \ldots, n-1\}, +(\mathrm{mod}\, n))$. Recall that two integers are equal modulo n if their difference is an integer multiple of n, e.g. $5(\mathrm{mod}\, 2) = 1$ and $-2(\mathrm{mod}\, 7) = 5$.

Example 3
The real numbers excluding 0 form the group $G = (\mathsf{R}\backslash\{0\}; \times)$ with multiplication as the composition law. Q: what is its neutral element?

Example 4 D_2
The symmetry group of a non-square rectangle in two dimensions has the following group table (abbreviating $g \circ h$ by gh):

$\circ$	e	v	h	r
e	e	v	h	r
v	v	e	r	h
h	h	r	e	v
r	r	h	v	e

, where

$\circ$	h
g	gh

Note that a group table is a Latin square: each element appears only once in each row and column. This is because the inverse element g^{-1} exists, so $g^{-1}gh = h$ should give the original set of elements h back. Note that a Latin square is not automatically a group, it may not satisfy the associative law. In physics usually gh means: first apply h and then g. The associative law is then automatically satisfied. This in particular applies to matrix multiplication, i.e. when the elements of a group are matrices.

Theorem
Let $h \in G$. Consider the set $hG = \{hg | g \in G\}$. Then $hG = G$.
Proof

(i) $G \subseteq hG$. Take $g \in G$ then $h^{-1}g \in G$, so $g = hh^{-1}g \in hG$.

(ii) $hG \subseteq G$. This is evident from the definition of a group.

As $G \subseteq hG$ and $hG \subseteq G$, $hG = G$.

□

In other words, acting with any group element h on the group just permutes the elements in the group.

Definition *Abelian*
A group G is said to be Abelian if the composition law is commutative:
$g_1 \circ g_2 = g_2 \circ g_1$, $\forall g_1, g_2 \in G$. Otherwise the group is called non-Abelian.

For an Abelian group the group table is symmetric under reflection in the diagonal. The smallest non-Abelian group is of order six: D_3 (see section 1.4). At order eight there are two distinct non-Abelian groups: D_4 and the quaternion group Q.

Example 5 Quaternions
Here is the multiplication table (not group table) that defines the quaternions 1, i, j and k:

	1	i	j	k
1	1	i	j	k
i	i	-1	k	-j
j	j	-k	-1	i
k	k	j	-i	-1

If one includes $-1, -i, -j, -k$ as elements one obtains the quaternion group Q discussed in Jones, exercise 4.6. As said, it is a non-Abelian group of order 8.

The following 2×2 matrices can be used as quaternions:

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & -i \\ -i & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}.$$

This links the quaternions with the Pauli matrices and spin-1/2 particles in quantum mechanics (see chapters 3 & 4).

1.3 Subgroups

Definition *subgroup, proper subgroup*
Let $(G; \circ)$ be a group. If $H \subseteq G$ and $(H; \circ)$ is also a group, then H is said to be a subgroup of G. If $H \neq G$ and $H \neq \{e\}$, then the subgroup H is said to be a proper subgroup of G. Notation: $H < G$ for H a proper subgroup.

Example 6
For any group G with identity e, $(\{e\}; \circ)$ is a subgroup of G, but not a proper subgroup.

Example 7
Consider $G = (\mathsf{C}\backslash\{0\}; \times)$, the group of nonzero complex numbers with multiplication as the composition law. The group $H = (\{z \in \mathsf{C} \,|\, |z| = 1\}; \times)$ of complex phases forms a subgroup of G. The group H is also often interpreted as the group $U(1)$ of all unitary 1×1 "matrices" consisting of elements $(e^{i\varphi})$ with $\varphi \in [0, 2\pi]$.

Example 8
Let $\{z_0, \ldots, z_{n-1}\}$ be the n distinct roots of unity, i.e. solutions of the equation $z^n = 1$, so $z_m = \exp(2m\pi i/n)$. Then $G = (\{z_0, \ldots, z_{n-1}\}; \times)$ forms a finite subgroup of $(\mathsf{C}\backslash\{0\}; \times)$ and of its subgroup $U(1)$. Since $z_m z_k = z_{(m+k) \bmod n}$, G has the same structure as the group of the integers under addition modulo n, denoted by Z_n.

1.4 Important finite groups

Thus far we have mostly discussed groups of numbers, not connected to symmetry in physics in an immediately obvious way. However, many finite groups can be viewed as groups of symmetry transformations of rigid bodies in Euclidean space,

such as polygons, or more generally polyhedra, and for example molecules. This applies even to a group like Z_n that may seem nothing more than a mathematical toy. This is illustrated in this section which discusses four classes of groups that are frequently encountered in physics.

The cyclic groups C_n
Consider a plane rotation over an angle $2\pi/n$, say c. Then c, c^2, ..., c^{n-1} are all different rotations. However, $c^n = e$ as a rotation over 2π is equivalent to no rotation at all. If we now define $c^p \circ c^q = c^{(p+q) \bmod n}$ then the rotations c, c^2, ..., $c^n = e$ form a group. This group is called the *cyclic group of order n*. It is said to be *generated* by the element c: $\mathrm{gp}\{c\}$. An application of this group is the symmetry of a *directed* n-sided polygon.

Clearly C_n and Z_n have the same structure.

The dihedral groups D_n
Consider again a plane regular n-sided polygon. If the sides of this polygon are not directed and we consider it embedded in three-dimensional space, we can in addition to the rotation in the plane of the polygon consider also rotations about a line in the plane over an angle π: a '2-fold' rotation about a '2-fold' axis. If we combine those with the rotations belonging to C_n we get the group D_n.

Groups of this type are often specified via so-called presentations (a set of generators whose powers and products generate the group subject to specified relations or conditions), not to be confused with *re*presentations to be discussed in chapter 2. For example, the presentation of the cyclic groups is:

$$C_n = \mathrm{gp}\{c\} \text{ with } c^n = e$$

and of the dihedral groups:

$$D_n = \mathrm{gp}\{c, b\} \text{ with } c^n = b^2 = (bc)^2 = e$$

Q: How to know that the latter specifies the group D_n?
Aim to write all elements in the form $b^k c^m$, which means one needs to figure out how to commute cb. For D_n: $bcbc = e$, s.t. $cb = b^{-1}c^{-1} = bc^{n-1}$. Explicit investigation of powers and products of generators and products thereof, then quickly terminates (quickly in case of D_n means after one has found $2n$ elements). It yields: $\{e, c, \ldots, c^{n-1}, b, bc, \ldots, bc^{n-1}\}$.

D_2 is a special (Jones: 'degenerate') case: $C_2 \times C_2$, since what does a polygon with 2 sides mean? It is better viewed as the symmetry of a rectangle as we

have seen, and also of the symbol $\leftrightarrow$. It is also called the 4-group (in German "Vierergruppe"): $\{e, c, b, bc\}$.

C_n and D_n are examples of *point groups*: symmetry groups of finite bodies (which must leave at least one point of the body fixed). C_n and D_n are the point groups whose elements are all pure rotations, which are well realizable symmetries of a rigid body. This is as opposed to reflections. We can not perform in nature the reflection of a rigid body physically. That is the reason why molecules that are each other's mirror image (so-called enantiomers) may have different properties. They are not simply rotated versions of each other.

The symmetric groups S_n

Consider ordered n-tuples, say $(a_1, \ldots, a_n)$. A permutation of this n-tuple changes it into another n-tuple. If we consider the permutation p_1 followed by the permutation p_2 by $p = p_1 \circ p_2$, we see immediately that p is also a permutation of this n-tuple. It is easy to see that all permutations have an inverse and that all the axioms of a group are fulfilled by the permutations of $(a_1, \ldots, a_n)$. The set of all permutations of n objects forms a group of order $n!$ called the *symmetric group* S_n.

A permutation p of n objects is a mapping $p : i \mapsto p(i),\ i = 1, \ldots, n$, such that p is invertible. An explicit matrix-like notation is often used:

$$p = \begin{pmatrix} 1 & 2 & \ldots & n \\ p(1) & p(2) & \ldots & p(n) \end{pmatrix}.$$

Note that the permutation is defined by the relation between the two entries in the same column of the $2 \times n$ "matrix". Therefore, the order of the columns does not matter. The product of two permutations is then

$$\begin{aligned} p_2 \circ p_1 &= \begin{pmatrix} 1 & \ldots & n \\ p_2(1) & \ldots & p_2(n) \end{pmatrix} \begin{pmatrix} 1 & \ldots & n \\ p_1(1) & \ldots & p_1(n) \end{pmatrix} \\ &= \begin{pmatrix} p_1(1) & \ldots & p_1(n) \\ p_2(p_1(1)) & \ldots & p_2(p_1(n)) \end{pmatrix} \begin{pmatrix} 1 & \ldots & n \\ p_1(1) & \ldots & p_1(n) \end{pmatrix} \\ &= \begin{pmatrix} 1 & \ldots & n \\ p_2(p_1(1)) & \ldots & p_2(p_1(n)) \end{pmatrix} \end{aligned}$$

where the columns of the first permutation are put in such an order that the second row of the first permutation is identical to the first row of the second permutation. If we define the composition law $\circ$ by

$$p_2 \circ p_1 : i \mapsto p_2(p_1(i))$$

then we see that $p_2 \circ p_1$ is also a permutation.

The identity is the permutation where both rows are identical, i.e. the permutation $p(i) = i$. It can be written in $n!$ ways, e.g.,

$$e = \begin{pmatrix} 1 & \dots & n \\ 1 & \dots & n \end{pmatrix} = \begin{pmatrix} p(1) & \dots & p(n) \\ p(1) & \dots & p(n) \end{pmatrix},$$

where p is an arbitrary permutation.
The inverse to a permutation p can be written as

$$p^{-1} = \begin{pmatrix} p(1) & \dots & p(n) \\ 1 & \dots & n \end{pmatrix}$$

The composition law is associative:

$$\begin{aligned} (p_2 \circ p_1) &: k \mapsto p_2(p_1(k)) \\ p_3 &: k \mapsto p_3(k) \\ p_3 &: p_2(p_1(k)) \mapsto p_3(p_2(p_1(k))) \end{aligned}$$

so we find

$$p_3 \circ (p_2 \circ p_1) : k \mapsto p_3(p_2(p_1(k))).$$

On the other hand

$$\begin{aligned} p_3 \circ p_2 &: k \mapsto p_3(p_2(k)) \\ p_1 &: k \mapsto p_1(k) \\ p_3 \circ p_2 &: p_1(k) \mapsto p_3(p_2(p_1(k))) \end{aligned}$$

so

$$(p_3 \circ p_2) \circ p_1 : k \mapsto p_3(p_2(p_1(k))).$$

We see that $p_3 \circ (p_2 \circ p_1) = (p_3 \circ p_2) \circ p_1$, so the composition law is indeed associative.
Conclusion: *S_n is a group*

It is often more convenient to write permutations in terms of *cycles*.

(i) A **transposition** or 2-cycle is a permutation p such that $p(i_1) = i_2$, $p(i_2) = i_1$ and $p(i) = i,\ i \notin \{i_1, i_2\}$.

(ii) An m-cycle is a permutation such that $p(i_1) = i_2$, $p(i_2) = i_3$, …, $p(i_{m-1}) = i_m$, $p(i_m) = i_1$ and $p(i) = i,\ i \notin \{i_1, \dots, i_m\}$. This m-cycle will be denoted by

$(i_1, \ldots, i_m)$.

(iii) If the two cycles $(i_1, \ldots, i_{m_1})$ and $(j_1, \ldots, j_{m_2})$ have no elements in common, then they commute.

(iv) Every m-cycle can be written (not uniquely) as a product of $m-1$ (overlapping) transpositions, e.g.,

$$(i_1, \ldots, i_m) = (i_1, i_2)(i_2, i_3) \ldots (i_{m-1}, i_m) = (i_1, i_m)(i_1, i_{m-1}) \ldots (i_1, i_2)$$

(v) Every permutation p can be factorized *uniquely* into disjoint cycles: $p = (i_1, \ldots, i_{m_1}) \ldots (k_1, \ldots, k_{m_p})$, where the elements not permuted are written as 1-cycles, e.g., $(l_1) \ldots (l_\omega)$, or not written at all. So the identity can be written in cycle notation as $(1) \ldots (n)$ or simply as (1).

Example: $(23)(132) = (12)$ corresponds to

$$\begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix} \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}$$

Also, $(132) = (23)(12)$ which is not one of the two forms written above in point (iv): $(132) = (13)(32)$ and $(132) = (12)(13)$.

The alternating groups A_n

One can separate the permutations into two categories, said to be *even* and *odd*, respectively. A permutation p is said to be even if it can be written as a product of an even number of permutations that interchange two elements of the n-tuple, i.e. *transpositions*. A permutation that is not even is said to be odd. One can immediately draw the conclusion that the product of two even permutations is even. As the identity can be considered a permutation that contains no transpositions at all, it is also even. The inverses of even permutations are also even. The even permutations form a subgroup of S_n called the *alternating group* A_n. Q: how about the odd permutations? Do they form a group as well?

The *sign* or *parity* of a permutation q is $+1$ if q is even (can be written as the product of an even number of transpositions), otherwise it is -1.

These finite groups are important to know because they occur frequently in physics. One encounters them in solid state physics, crystallography, molecular physics (spectroscopy), quantum mechanics (n-particle wave functions), and particle physics (investigating finite symmetries in the neutrino sector is a hot topic currently for example).

The rotational symmetry groups of the Platonic solids are: A_4 - tetrahedron; S_4 - cube and octahedron; A_5 - dodecahedron and icosahedron. Including reflections these three groups become S_4, $S_4 \times \mathsf{Z}_2$ and $A_5 \times \mathsf{Z}_2$, resp. Here the product is defined as ordered pairs of group elements (see Jones for more details).

1.5 Conjugacy Classes

If we consider different symmetry transformations, we sense intuitively that some of them are related, they are of the same 'type' or not. For instance, reflections share the property that they change the "handedness" of a motion or a geometric figure from left- to right-handed and vice versa, whereas rotations do not. This intuition can be made into a precise notion, that of conjugacy of operations. This leads to the definition of conjugacy classes.

Definition *conjugate*
Two elements g_1, $g_2 \in G$ are called conjugate if there exists an element $h \in G$ such that $g_1 = hg_2h^{-1}$.

The property of being conjugate is an equivalence relation. If two elements a and b of some set S are equivalent, we write $a \sim b$. For an equivalence relation the following holds:

reflexive	$a \sim a \quad \forall a \in S$,
symmetric	$a \sim b$ implies $b \sim a \quad \forall a, b \in S$,
transitive	if $a \sim b$ and $b \sim c$ then $a \sim c \quad \forall a, b, c \in S$

Definition *class*
A class K of a group G is a subset of G such that all elements of K are conjugate to each other and no elements of $G \setminus K$ are conjugate to any element of K. Notation of Jones:

$$(a) = \{b | b = gag^{-1} \text{ for some } g \in G\}$$

Conjugacy as an equivalence relation ($a \sim b$ if $a \in (b)$) provides a 'partition' of G into disjoint classes (see Jones for further details).

Knowing the number of classes of a group helps in classifying the representations of that group (next chapter).

Theorem
Let G be a group, $\{K_i\}$ the set of its classes. Then the following properties hold
(i) Any element of G belongs to exactly one class.

(ii) $\{e\}$ is a class.
(iii) If G is Abelian then all classes consist of single elements of G.

Definition *center*
The center of a group G is the set of elements of G that commute with all other elements of G:

$$Z(G) = \{z \in G | zg = gz \ \forall g \in G\}.$$

The center is an Abelian subgroup that consists of all elements that form a class by themselves.

Example The group D_3
Consider the equilateral triangle ABC. Its vertices are located in points a, b and c. As a plane triangle, it has the following symmetries:

(i) rotations over an angle of $0°, 120°, 240°$ about an axis through its center of gravity and perpendicular to the plane of the triangle. The rotation over $120°$ will be denoted by R, such that R^2 is the rotation over $240°$ and $R^3 \equiv E$ over $360°$, or equivalently $0°$.

(ii) reflections in a bisectrix of any of the vertices, denoted by S_A, S_B, S_C, with $S_\alpha^2 = E$, $(\alpha = A, B, C)$

The operations S_α can also be viewed as rotations over an angle π in 3-dimensional space. In this case one deals with a (point) group of pure rotations in three dimensions, which turns out to be D_3.

We take the passive point of view, i.e., the triangle is kept fixed, the frame of reference is transformed. Denote the original triangle as (Aa, Bb, Cc), then the effect of the operations S_A and R is depicted in the figure.

Applying the operations consecutively, one finds the following group table

$\circ$	R	R^2	S_A	S_B	S_C
R	R^2	E	S_C	S_A	S_B
R^2	E	R	S_B	S_C	S_A
S_A	S_B	S_C	E	R	R^2
S_B	S_C	S_A	R^2	E	R
S_C	S_A	S_B	R	R^2	E

This is the group table of D_3, with for instance $c = R$ and $b = S_A$. Indeed one has $S_\alpha^2 = E$ (i.e. $S_\alpha^{-1} = S_\alpha$) and $R^3 = E$ (i.e. $R^{-1} = R^2$).

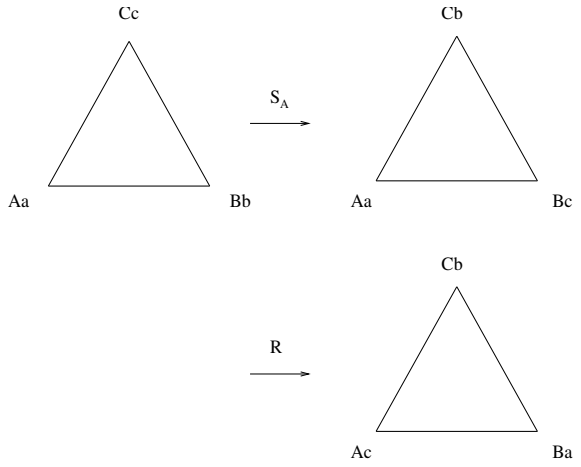


Figure 1.1: Symmetries of the plane equilateral triangle. The depicted operations are both on the original triangle.

Proper subgroups
$\mathcal{R} = \{E, R, R^2\}, \quad \mathcal{S}_A = \{E, S_A\}, \quad \mathcal{S}_B = \{E, S_B\}, \quad \mathcal{S}_C = \{E, S_C\}.$

Although D_3 is not Abelian, these subgroups are.

Classes
The classes are $(E) = \{E\}$, $(R) = \{R, R^2\}$ and $(S) = \{S_A, S_B, S_c\}$.

Note that the rotations over the same angle are conjugate to each other (both R and R^2 are rotations over 120°, just in opposite directions). This can be understood as follows. Consider the action of any such operation b on a general vector $\vec{v}$: $b\vec{v} = \vec{v}'$, then $(gbg^{-1})(g\vec{v}) = gb\vec{v} = g\vec{v}'$, that is, if b takes $\vec{v}$ to $\vec{v}'$, then gbg^{-1} takes the transformed vector $g\vec{v}$ to the similarly transformed vector $g\vec{v}'$. So they represent the same operation (same angles and invariant axes stay invariant). See figure 2.1 of Jones, page 21. This allows for a geometrical understanding of conjugacy.

Remarks

(i) Any transformation $T \in D_3$ permutes the coordinates of the vertices. So we can consider D_3 as the group of permutations of three objects (S_3) as well. It must have 3!=6 elements. For higher n S_n contains more elements than D_n ($n! > 2n$ for $n > 3$). Consider for example a square and permute $ABCD \to BACD$. This is not an operation that leaves the square invariant. D_n is a proper subgroup of S_n.

(ii) Classes of a subgroup H do not necessarily coincide with the intersections

of the classes of G with H. E.g. consider the subgroup $\mathcal{R} = \{E, R, R^2\}$ and its intersection with the class $(R) = \{R, R^2\}$ of D_3: (R), but since $\mathcal{R}$ is Abelian, its classes are $(E), (R)$ and (R^2). Also, the classes of D_n for $n > 3$ are not simply the ones of S_n restricted to the elements that are in D_n. For example, consider D_4. The rotations around the diagonal of a square are not conjugate to the rotations around the lines that intersect two opposing sides. The element that would relate them is a rotation around $\pi/4$ which is not in the group.

1.6 Isometries

Isometries are transformations that leave distances unchanged. In this section we discuss the group of isometries in three dimensional space R^3.

Definition *isometry*
A transformation T is said to be an isometry if for any two vectors $\vec{x}, \vec{y} \in \mathsf{R}^3$, T preserves the length of their difference: $\|T\vec{x} - T\vec{y}\| = \|\vec{x} - \vec{y}\|$.

Definition *Euclidean Group*
The set of all isometries of R^3 is called the Euclidean Group in 3 dimensions, denoted by $E(3)$ (also sometimes by $ISO(3)$).

A vector in R^3 can be expanded in an orthonormal basis $\{\hat{e}_1, \hat{e}_2, \hat{e}_3\}$ of R^3: $\vec{x} = \sum_{i=1}^{3} x_i \hat{e}_i$, where the coefficients or *vector components* x_i are real numbers. The group $O(3)$ is the set of all transformations of the basis vectors that leave their length *and* the origin invariant. It is the continuous analogue of the point groups discussed before.

In the vector space R^3 basis transformations R take the form

$$\hat{e}'_j = R\hat{e}_j = \sum_{i=1}^{3} \hat{e}_i R_{ij}$$

Upon a basis transformation the components of the vector $\vec{x}$ with respect to the new basis are also transformed. We find

$$\vec{x} = \sum_{i=1}^{3} x_i \hat{e}_i = \sum_{j=1}^{3} x'_j \hat{e}'_j = \sum_{i=1}^{3} \sum_{j=1}^{3} x'_j \hat{e}_i R_{ij}.$$

So we see that

$$x_i = \sum_{j=1}^{3} R_{ij} x'_j.$$

R belongs to $O(3)$ if the length of $\vec{x}$ is invariant, i.e., $\sum_i x_i^2 = \sum_j x_j'^2$, from which we find $RR^\mathsf{T} = \mathbf{1}$, where R^T is the transpose of the matrix R, or in components

$$\sum_{i=1}^{3} R_{ij}R_{ik} = \delta_{jk}, \quad (j,k = 1,2,3).$$

Matrices that have this property are said to be *orthogonal* and form the group $O(3)$ of orthogonal 3×3 matrices. Matrices in $O(3)$ have $\det R = \pm 1$, since $\det RR^\mathsf{T} = \det R \det R^\mathsf{T} = (\det R)^2 = 1$. If $\det R = 1$, T is said to belong to $SO(3)$, the *special* orthogonal group in three dimensions.

Definition *Space inversion P*
The space inversion P is the transformation that reverses the direction of all basis vectors

$$P\hat{e}_i = -\hat{e}_i.$$

This operation has the property $P^2 = I$ so $P^{-1} = P$.

Let $R' \in O(3)$ with determinant $\det R' = -1$. Then $R = R'P \in SO(3)$. Consequently, $R' = RP$, so we can conclude that the elements of $O(3)$ can be written as either a rotation, in which case they belong to $SO(3)$, or as a rotation times the inversion.

Definition *translation*
The operator $T_{\vec{a}}$ is said to be a translation, iff

$$T_{\vec{a}}\vec{x} = \vec{x} + \vec{a}, \quad (\vec{x}, \vec{a} \in \mathsf{R}^3).$$

Remark
Rotations are linear transformations, translations are not. The translations form an Abelian subgroup of $E(3)$.

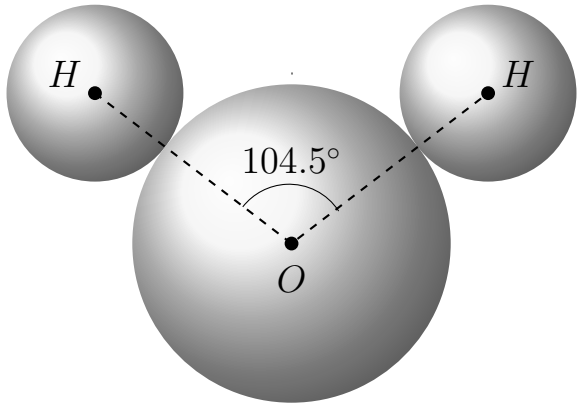
Every $T \in E(3)$ can be uniquely written as a rotation/reflection followed by a translation, i.e.

$$T = T_{\vec{a}}O \equiv (O|\vec{a}), \quad \text{with } \vec{a} \in \mathsf{R}^3, O \in O(3).$$

1.7 Space groups

Symmetries of molecules and crystals can be viewed as discrete subgroups of $E(3)$. The term "molecule" is used here in a geometrical sense: it is an ordered set M

of points in R^3. These points may not all be equivalent: they may be occupied by different "atoms". The symmetry group of a molecule M is the subset of $E(3)$ that leaves the molecule invariant: $G = \{T \in E(3) | TM = M\}$. As an example, consider the water molecule H_2O:



To find all symmetry transformations (rotations *and* reflections in three dimensions) that leave the water molecule invariant, consider the centers of the atoms to be in the x-y plane, with the x direction parallel to the H centers and the y axis orthogonal to it, running through the O center. Apart from the trivial operation e, the molecule is invariant under a rotation c around the y axis over 180°, a reflection b in the x-y plane, and a reflection (which is equal to bc) in the y-z plane. These operations mathematically form the group D_2 ($gp\{b, c\}$ with $c^2 = b^2 = (bc)^2 = e$), but since it includes reflections which cannot be performed physically, the symmetry group of the water molecule is usually called C_{2v}, which is isomorphic to D_2. Here we will not worry about the naming scheme of such finite subgroups of $O(3)$.

If atoms are ordered in a *lattice*, we have, besides the symmetry group that is necessarily a subgroup of $O(3)$, also translation symmetry.

An infinite three-dimensional lattice is defined by

(i) basic lattice vectors $\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$,

(ii) lattice coordinate vectors $\vec{n} = (n_1, n_2, n_3)$ with integer components.

The vectors $\vec{a}_i$ define the orientations of the lattice. Any element (atom) of the lattice is characterized by a coordinate vector $\vec{n}$ such that its position is given by

$$\vec{r} = \vec{r}_0 + \vec{t}_n = \vec{r}_0 + n_1\vec{a}_1 + n_2\vec{a}_2 + n_3\vec{a}_3$$

for some $\vec{n}$ and $\vec{r}_0$. The latter is connected to the choice of the origin of the coordinate system, so it can be set to $\vec{0}$ by a translation of the origin.

The subgroup T^∞ of $E(3)$, given by

$$T^\infty = \{(E|\vec{t}_n)\},$$

is said to be the group of *primitive translations* of the lattice, where E is the identity in $O(3)$. T^∞ is an Abelian subgroup of $E(3)$, it is of infinite order. In three dimensions there are 14 different types of lattices, the so-called Bravais lattices. We shall not discuss them here in detail.

Symmetry groups of crystals can be divided into two types: crystallographic point groups and space groups, subgroups of $O(3)$ and $E(3)$, respectively. Recall that point groups are finite groups of isometries that leave at least one point invariant (a center of rotation). If one applies this to a crystal and requires translational periodicity (in other words, more than one center of rotation), then there 32 possibilities: the crystallographic point groups. This is a consequence of the crystallographic restriction theorem (proven at the end of chapter 2): if a discrete group of displacements has more than one center of rotation, then there can only be 2, 3, 4, or 6-fold symmetry.

The set $\{(R|\vec{0}\,)\},\ R \in O(3)$, such that for all $\vec{t}_n$ the vector $R\vec{t}_n$ is again a lattice vector, is said to be the *maximal point group* of the lattice. Lattices with the same maximal point group are said to belong to the same lattice system. In three dimensions there are 7 lattice systems.

If one extends the crystallographic point groups by including in the group the translations that leave the crystal invariant, then one arrives at the *space groups*. In any number of dimensions there are a finite number of space groups. It is not a goal of this course to examine or count all crystallographic point groups and space groups (consult for example S. Sternberg, Group Theory and Physics, 1994). It may be clear though that not every Bravais lattice is compatible with all crystallographic point groups (e.g. every lattice is symmetric under $-\mathbf{1}$, but not all point groups contain $-\mathbf{1}$), such that the number of space groups in three dimensions is expected to be smaller than 14 times 32. In fact, in three dimensions there are 230 space groups. In two dimensions there are 5 Bravais lattices, 10 crystallographic point groups (C_n and D_n for $n = 1, 2, 3, 4, 6$), and 17 space groups. These 17 so-called wallpaper patterns exhibit four types of isometries: translations, rotations, reflections, and glide reflections (combinations of a reflection in a line L and a translation along L by a distance d).

Background information: There exist no crystals with a 5-fold symmetry, but so-called quasi-crystals with this pentagonal symmetry have been found. A quasi(periodic)-crystal is a structure that is ordered but not periodic. It can fill a whole plane or volume but has no translational

symmetry. The Nobel prize in Chemistry 2011 (and the Wolf prize in Physics in 1999) was awarded to Dan Shechtman for the discovery of quasi-crystals. He had discovered an alloy of aluminum and manganese that turned out to be an icosahedral quasi-crystal showing a pentagonal symmetry. Aperiodic tilings of the plane form a two-dimensional analogue of quasi-crystals. In 1966 the mathematician Robert Berger came up with the first aperiodic tiling using a set of 20,426 distinct tile shapes. In 1974 Roger Penrose produced an aperiodic tiling of the plane with just two tiles (modulo rotations).

Quasiperiodic crystals can be viewed as projections of a higher-dimensional periodic lattice, where the projected or intersecting (hyper)plane makes an irrational angle w.r.t. the higher dimensional lattice. This insight stems from the field of almost-periodic functions, which was started in 1925 by the mathematician Harald Bohr (brother of Niels Bohr). This topic is beyond the scope of these lectures.

1.8 Non-Euclidean symmetry

In physics very often one also deals with non-Euclidean spaces. For instance, four-dimensional space-time is not a Euclidean R^4, rather it is Minkowski space. There is a non-Euclidean metric $g_{\mu\nu} = \mathrm{diag}(1, -1, -1, -1)$ that specifies how distances are measured. If x^μ is a four-vector (coordinate vector in Minkowski space), then $x^2 = \sum_{\mu,\nu=0}^{3} g_{\mu\nu} x^\mu x^\nu = x_0^2 - \sum_{i=1}^{3} x_i^2$. The group of isometries of Minkowski space is the Poincaré group, also sometimes referred to as the inhomogeneous Lorentz group. An element of the Poincaré group P is a pair $(\Lambda|t)$, where Λ represents a Lorentz transformation and t a translation. The action of an element of P on an arbitrary four vector x is $(\Lambda|t)x = \Lambda x + t$, or in components $((\Lambda|t)x)^\mu = \Lambda^\mu{}_\nu x^\nu + t^\mu$.

The composition law of elements of the Poincaré group is

$$(\Lambda_1|t_1)(\Lambda_2|t_2) = (\Lambda_1\Lambda_2|\Lambda_1 t_2 + t_1).$$

The Lorentz group $L = \{\Lambda\}$ can be identified with the subgroup of elements $(\Lambda|\mathbf{0})$ of P. The translations form a subgroup, T, of P. Every element of the Poincaré group can be uniquely written as

$$(\Lambda|t) = (\mathbf{1}|t)(\Lambda|\mathbf{0}).$$

1.9 Homomorphisms and isomorphisms

Before, we have stated that the group $(\{z \in \mathsf{C} | z^n = 1\}; \times)$ consisting of the n distinct roots of unity has the "same structure" as the group Z_n of integers with

addition modulo n. In this section we make this statement precise via a 1-1 mapping between the groups. We introduce special types of mappings, homomorphisms and isomorphisms, which are tools to compare groups, i.e. to decide whether two groups are the same.

Definition *homomorphism, isomorphism*
A mapping $\phi : G \to G'$ of a group G with composition law $\circ$ into a group G' with composition law $\cdot$ is said to be homomorphic (a homomorphism), iff $\forall g_1, g_2 \in G : \ \phi(g_1 \circ g_2) = \phi(g_1) \cdot \phi(g_2)$. In general, a homomorphism is a many-to-one mapping. The mapping ϕ is said to be isomorphic (an isomorphism) if besides being a homomorphism it is bijective (1-1 and onto). If G and G' are isomorphic, we will write $G \cong G'$.

Definition *kernel*
Let G and G' be groups, ϕ a homomorphism $\phi : G \to G'$. The set $K = \{g \in G | \phi(g) = e'\}$, with e' the identity in G', is said to be the kernel (ker) of ϕ.

One can always restrict G' to the image of ϕ (which is a group itself), such that the mapping becomes onto. In addition, one can always make the mapping 1-1 by "dividing out" the kernel. For details (that are beyond the scope of this lecture) we refer to Jones, p. 31-33.

Example
The group $(\{z \in \mathsf{C} | z^n = 1\}; \times)$ consisting of the n distinct roots of unity is isomorphic to the group Z_n of the integers under addition modulo n. The isomorphism is provided by the mapping $m \mapsto \exp(2\pi i m/n)$.

Example
Consider the mapping ϕ from $E(3)$ to $(\{1, -1\}; \times)$, ϕ: $(O|\vec{a}) \mapsto \det O$. This map is a homomorphism. Its kernel, called $E^+(3)$, is a subgroup of $E(3)$. $E^+(3)$ is the *proper Euclidean group* or the group of *rigid motions*. It consists of translations, rotations around an axis, and the latter combined with translations along that axis, called a screw displacement or screw operation.

Cayley's theorem
Every finite group of order n is isomorphic to a subgroup of S_n. The action of any element g_j of a group G on all other elements $\{g_1, \ldots, g_n\}$ can be viewed as a permutation: $\{g_j g_1, \ldots, g_j g_n\} = \{g_{p_j(1)}, \ldots, g_{p_j(n)}\}$. In this way g_j can be associated in a 1-1 way to the permutation p_j, it will follow the group multiplication (which is invertible). In this way it forms a subgroup of S_n. See Jones for further details.

Background information: All finite groups have been classified. This classification refers to

so-called simple groups, which are groups that have no subgroups that stay invariant under conjugation. In a sense the simple groups are the "atoms" from which all other groups can be built. The classification theorem (completed in 2004) states that every finite simple group is isomorphic to one of the following groups: a cyclic group C_p of prime order; an alternating group A_n with $n \geq 5$; a simple group of Lie type; or, one of the 26 "sporadic" groups. We will not elaborate on what these latter two types of groups are, except mention that the largest sporadic group is called the Monster group. It is a group of approximately $8 \cdot 10^{53}$ elements and was first constructed in 1982 by Robert Griess.

Chapter 2

Applying group theory: representations

[Topics in this chapter are covered in the book of Jones in chapters 3, 4, 5.1.]

Thus far, we have discussed groups and their properties. Groups have abstract definitions independent of the many different meanings that may be assigned to the elements. In this chapter we will look at how to apply this theory of algebraic structures to physical situations. In order to apply group theory in physics one has to consider the quantities on which the group elements act, such as vectors in a three-dimensional space or wave functions in a Hilbert space. These quantities form a *carrier space* for a *representation* of the group. If the carrier space is a vector space, then the action of the group on this space can be represented by matrices, forming a matrix representation of the group. In other words, it is the assignment of a matrix to every element of the group. In this way one obtains a group of matrices, which may be smaller than the original group, because the same matrix may be assigned to more than one element of the original group.

A matrix representation is thus a mapping of a group onto a group of matrices and the matrices of the representation (rep) can be viewed as linear transformations acting on a vector space of the same dimension as that of the matrices. So in order to apply group theory one not only needs to identify the relevant symmetry group of the physical system but also the vector space of states, in order to determine the relevant representation. For example, if one deals with vectors in three dimensional space, one naturally considers three-dimensional matrix representations. If one deals with quantum mechanical wave functions $|n, l, m\rangle$ for given n and l, then a $(2l+1)$-dimensional representation is the natural choice. As the number of applications for any given group can *in principle* be infinite, one

would like to know all representations a group can have. This may seem like an impossible goal to achieve, given the infinite number of groups and infinite number of representations per group. Nevertheless, the task can be made manageable by the following two insights. The first insight is that for a given dimension we are actually only interested in representations that do not just differ by a basis transformation in the vector space, the so-called inequivalent representations. The second insight is that one can always build a new representation from two other ones by considering their direct sum or direct product. Turning this around one can distinguish, on the one hand, reducible representations that can be composed from smaller representations, and, on the other hand, irreducible representations that cannot. The latter are the building blocks of all other representations. Once one knows all inequivalent irreps of a group, one can find or construct any representation required for a particular application.

2.1 Representations

The starting point is the group $GL(d, \mathsf{K})$, the General Linear group of invertible $d \times d$ matrices with elements taken from the field K. In most cases of interest to physicists K is either the field of real (R) or complex (C) numbers. The composition law is ordinary matrix multiplication. Invertible means that the determinant of the matrices does not vanish, i.e. it is non-singular.

Definition *(matrix) representation*
A (matrix) representation (rep) of dimension d of a group G is defined as a homomorphism $D : G \to GL(d, \mathsf{K})$. That is, it is a homomorphism from the group G onto a subgroup $D(G)$ of $GL(d, \mathsf{K})$ such that for all $g \in G$ the determinant of $D(g)$ does not vanish and ordinary matrix multiplication is the composition law in $D(G)$.

One may generalize the definition of a rep to cases where $GL(d, \mathsf{K})$ is replaced by a group $GL(V)$ of invertible linear operators on some vector space V. This is quite typical for Quantum Mechanics or Quantum Field Theory. Upon a choice of basis for V, one establishes an isomorphism between $GL(V)$ and $GL(n, \mathsf{K})$ (i.e., $GL(\mathsf{R}^n)$ or $GL(\mathsf{C}^n)$). In this way the group multiplication becomes matrix multiplication.

Definition *faithful*
If a rep D is an isomorphism, it is said to be faithful.

Example 1 *Trivial rep*

Let G be any group. The mapping $\phi(g) = 1,\ \forall g \in G$ is a rep, the 1-dimensional trivial rep. $D(G) = (1; \times)$. Even though it does not seem like an informative rep, it actually arises frequently in applications as we will see. It is used for quantities that do not transform at all under the action of the group.

Example 2
Let $G = GL(d, \mathsf{K})$. Define the mapping $\phi : G \to (\mathsf{R}\backslash\{0\}; \times)$ by $\phi(g) = \det(g) \neq 0$. Then ϕ is a rep. Hence, $D' = \det D$ is a rep for any rep D of any group. Sometimes D' is equal to the trivial rep, sometimes it is a nontrivial 1-dimensional rep.

Example 3 The group D_3
Consider again the equilateral triangle ABC. Its vertices are located in points a, b and c, that are transformed under the symmetry operations E, R, R^2 (rotations over an angle of $0°, 120°, 240°$ about an axis through its center of gravity and perpendicular to the plane of the triangle) and S_A, S_B, S_C (reflections in or rotations over π about a bisectrix of any of the vertices). Denote the original triangle as (Aa, Bb, Cc), then the effect of the operations S_A and R is depicted in the figure.

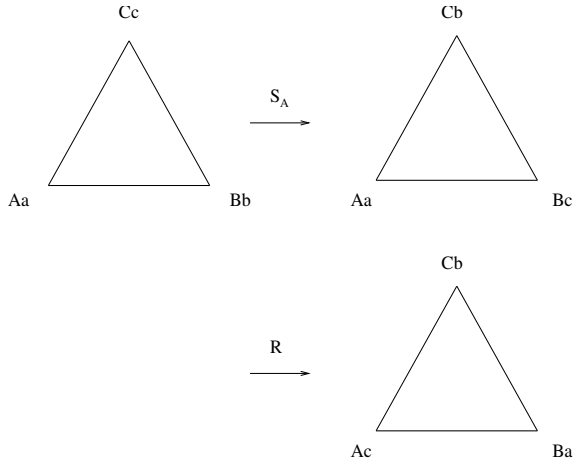


Figure 2.1: Symmetries of the plane equilateral triangle. The depicted operations are both on the original triangle.

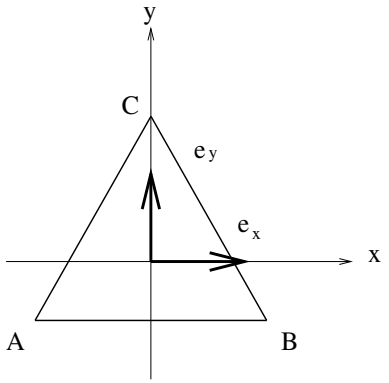
For convenience, we also recall the group table, which is the one of D_3:

$\circ$	R	R^2	S_A	S_B	S_C
R	R^2	E	S_C	S_A	S_B
R^2	E	R	S_B	S_C	S_A
S_A	S_B	S_C	E	R	R^2
S_B	S_C	S_A	R^2	E	R
S_C	S_A	S_B	R	R^2	E

Now let us consider several reps of D_3. First of all, there is the trivial rep, which we will denote here as $D^{(1)}$: $D^{(1)}(g) = (1)\ \forall g \in G$.

There is another 1-dimensional rep. Recall that $D_3 \cong S_3$, so one can consider the sign or parity of the permutations corresponding to the elements: $S_A = (23), S_B = (13), S_C = (12), R = (123), R^2 = (132)$, which have signs $-1, -1, -1, 1, 1$, respectively. This forms a non-trivial rep called $D^{(2)}$.

A two-dimensional rep $D^{(3)}$ can be obtained from an embedding of the triangle ABC in R^2. The coordinates of A, B and C in the coordinate frame $(\hat{e}_x, \hat{e}_y)$ are



A: $\left(-\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \equiv a$, B: $\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}\right) \equiv b$, C: $(0,1) \equiv c$. A rotation about the origin over an angle ϕ takes $\hat{e}_x$ and $\hat{e}_y$ to

$$\begin{aligned} R_\phi \hat{e}_x \equiv \hat{e}'_x &= \cos\phi\, \hat{e}_x + \sin\phi\, \hat{e}_y, \\ R_\phi \hat{e}_y \equiv \hat{e}'_y &= -\sin\phi\, \hat{e}_x + \cos\phi\, \hat{e}_y. \end{aligned}$$

The *components* of vectors transform according to the inverse transformations. We find for the matrices ($\cos(120^\circ) = \cos(2\pi/3) = -\frac{1}{2}, \sin(2\pi/3) = \frac{\sqrt{3}}{2}$)

$$D^{(3)}(R) = R^{-1}_{120^\circ} = \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix},$$

$$D^{(3)}(R^2) = R^{-1}_{240^\circ} = D^{(3)}(R)^{-1} = D^{(3)}(R)^T = \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}.$$

A reflection in the y-axis, S_C, takes $\hat{e}_x$ to $-\hat{e}_x$, but $\hat{e}_y$ is not changed. The corresponding coordinate transformation matrix is

$$D^{(3)}(S_C) = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}.$$

The other transformations, S_A and S_B, are easily deduced using the group table: $S_A = R^2 S_C$ for instance. Then one finds for the transformation matrices

$$D^{(3)}(S_A) = \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}, \quad D^{(3)}(S_B) = \begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{bmatrix}.$$

Clearly, one must have $S_A a = a$ etc, and $S_A b = c$, $S_A c = b$ etc. These relations are easy to check. Also, note that the determinant of the matrices is exactly what one expects: $+1$ for rotations and -1 for reflections.

We can also use an embedding of the triangle ABC in R^3 to obtain a three-dimensional rep called D^V, where V stands for vector. The coordinates of A, B and C in the coordinate frame $(\hat{e}_x, \hat{e}_y, \hat{e}_z)$ are A: $\left(-\frac{\sqrt{3}}{2}, -\frac{1}{2}, 0\right) \equiv a$, B: $\left(\frac{\sqrt{3}}{2}, -\frac{1}{2}, 0\right) \equiv b$, C: $(0, 1, 0) \equiv c$. This yields the matrices:

$$D^V(R) = \begin{bmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad D^V(R^2) = \begin{bmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

The transformations S_α are now viewed as rotations over an angle π, yielding:

$$D^V(S_C) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix},$$

$$D^V(S_A) = \begin{bmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}, \quad D^V(S_B) = \begin{bmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

The determinant of all these matrices is exactly what one expects for rotations: $+1$. [The rep D^V in Jones is not identical to the one here, but it is equivalent (see below), just differing in the choice of basis]

The above reps will be discussed further later on, so please keep them in mind.

Let us now generalize the above procedure of obtaining reps of different dimensions by considering carrier spaces V of different dimensions. Let V be a linear vector space with a basis $\{\hat{e}_1, \ldots, \hat{e}_d\}$. It is supposed to be orthonormal: $\hat{e}_m^\dagger \hat{e}_n = (\hat{e}_m, \hat{e}_n) = \delta_{mn}$. The last expression denotes the inner product in V. Define for all $g \in G$ an operator $T(g)$ on V as follows

$$T(g)\hat{e}_n = \sum_{m=1}^{d} \hat{e}_m D_{mn}(g)$$

Note the order of the indices on D. The reverse order would not correspond to a representation.

The operator T is clearly linear

$$T(g) \sum_j b_j \hat{e}_j = \sum_j b_j T(g)\hat{e}_j.$$

We can express the matrix elements of $D(g)$ in terms of those of $T(g)$

$$D_{mn}(g) = \hat{e}_m^\dagger T(g)\hat{e}_n = (\hat{e}_m, T(g)\hat{e}_n).$$

For D to be a homomorphism, the operator T must satisfy: $T(g_1 g_2) = T(g_1)T(g_2)$. A vector space in which a group G acts in this way is called a G-module.

Definition *equivalent reps*
Let D be a d-dim rep of a group G and let S be a non-singular $d \times d$ matrix. The mapping D': $G \to GL(d, \mathsf{K})$ with $D'(g) = SD(g)S^{-1}$ is said to be equivalent to D. Notation: $D' \sim D$.

Remark
Note that D' is also a rep. A *similarity transformation* $SD(g)S^{-1}$ is merely a change of basis, because if

$$T(g)\hat{e}_n = \sum_m \hat{e}_m D_{mn}(g),$$

then

$$T(g)\hat{e}'_n = \sum_m \hat{e}'_m D'_{mn}(g),$$

provided $D'_{mn}(g) = S_{mk} D_{kl}(g)(S^{-1})_{ln}$ and $\hat{e}_m = \hat{e}'_k S_{km}$. So one sees that the set of linear operators $\{T(g)\}$ corresponds to an entire equivalence class of matrix representations.

For one-dimensional reps it holds that two reps are equivalent iff they are equal. Hence, for the D_3 example above, one observes that $D^{(1)} \not\sim D^{(2)}$.

Definition *unitary rep*
A rep D is said to be unitary if $D(g)$ is a unitary matrix for all $g \in G$, i.e., $D^\dagger(g)D(g) = D(g)D^\dagger(g) = I$, the identity in $GL(d, \mathsf{K})$.

Without proof we state the following theorem (interested students can find the proof in Jones).

Theorem
If G is a group of finite order $[g]$, then every rep of G is equivalent to a unitary rep.

It means that whenever we have a rep D of a finite group that is not a unitary rep (i.e. $D_{ij}(g) = (\hat{e}_i, T(g)\hat{e}_j)$, such that $D_{ij}(g)^\dagger D_{jk}(g) \neq \delta_{ik}$), then there is always a different basis that is orthonormal w.r.t. a different scalar product, $\{\hat{e}'_i, \hat{e}'_j\} = \delta_{ij}$, such that $D'_{ij}(g) = \{\hat{e}'_i, T(g)\hat{e}'_j\}$ *is* unitary.

2.2 Reducible and irreducible representations

Definition *reducible, irreducible*
A rep D of a group G is said to be reducible if it is equivalent to a rep D' for which every matrix (i.e. $\forall g \in G$) has the form

$$D'(g) = \begin{pmatrix} D_1(g) & B(g) \\ \emptyset & D_2(g) \end{pmatrix}.$$

The matrix S that establishes this, should itself be g-independent. If D is not reducible it is said to be irreducible (an irrep).

Remarks

(i) The matrices D_i, $(i = 1, 2)$ form reps. If D_i are not irreps, then they can be brought into the same form as D' itself, until the reps D_i on the diagonal are irreps.

(ii) The space V has an *invariant subspace* V_1 under the group G with dimension equal to d_1, the dimension of D_1. In order to see this, let $\{\hat{e}_n\}$ be a basis in V. Then

$$\begin{aligned} T(g)\hat{e}_n &= \sum \hat{e}_m D_{mn}(g) \\ &= \sum_{m=1}^{d_1} \hat{e}_m D_{mn}(g) + \sum_{m=d_1+1}^{d} \hat{e}_m D_{mn}(g). \end{aligned}$$

Now take n between 1 and d_1, then we have

$$T(g)\hat{e}_n = \sum_{m=1}^{d_1} \hat{e}_m D_{mn}(g) = \sum_{m=1}^{d_1} \hat{e}_m \left[D_1(g)\right]_{mn} .$$

Hence D_1 is a rep. The invariant subspace, also called a submodule, is $V_1 = \text{Span}\{\hat{e}_1, \ldots, \hat{e}_{d_1}\}$. It is a subspace of V that is itself closed under the action of the group: $\vec{u} \in V_1 \Rightarrow T(g)\vec{u} \in V_1 \ \forall g \in G$. Its orthonormal complement $V_2 = \text{Span}\{\hat{e}_{d_1+1}, \ldots, \hat{e}_{d_1+d_2}\}$ is, however, not invariant under G.

(iii) If D' would be unitary, then reducibility is equivalent to *full reducibility* or *decomposability*:

$$D' = \begin{bmatrix} D_1 & \emptyset \\ \emptyset & D_2 \end{bmatrix} .$$

In this case both V_1 and V_2 are invariant subspaces. Notation: $V = V_1 \oplus V_2$. If D_i are not irreps, then one can decompose them as well, until all reps on the diagonal are irreps.

Just to reiterate the most important point, the presence of an invariant subspace in the carrier space V of a rep D means that D cannot be an irrep.

Maschke's Theorem
All reducible reps of a finite group are fully reducible.

This is a corollary of the previous theorem. Since for a finite group it is always possible to choose a scalar product which makes the rep unitary, reducibility is equivalent to full reducibility.

A brief comment on where we are heading: we wish to determine all irreps of a group up to equivalence. Therefore, we need tools to determine whether one is dealing with an irrep, which can be done using one of Schur's lemmas, and whether the obtained irreps are inequivalent, which is done by means of characters to be defined later. The so-called character table specifies all inequivalent irreps of a group.

The following theorem, Schur's (second) lemma, provides an important practical tool to determine whether a rep is reducible or not. For a proof see Jones, section 4.1.

Theorem Schur's second lemma
Let D be a d-dim irrep of the group G, B a $d \times d$-matrix such that $\forall g \in G$: $D(g)B = BD(g)$, then the matrix B is proportional to the identity matrix $\mathbf{1} = \text{diag}(1, \ldots, 1)$: $B = \lambda \mathbf{1}$ with $\lambda \in \mathsf{C}$.

Schur's lemmas imply that if one finds a matrix $B \neq \lambda \mathbf{1}$ that commutes with all matrices of a matrix rep, then that rep is not an irrep. In this way it provides a tool to determine whether a rep is an irrep. This method is often easier to apply than to exclude that there exists a similarity transformation that brings the rep to reducible form or to exclude that there are no invariant subspaces. For finite groups one can find consequences of Schur's second lemma that are even easier to use to show that a rep is an irrep or not. This will be discussed in the next section on characters.

Remark
If $H < G$, i.e. H is a proper subgroup of G, then irreps of G restricted to H are not irreps of H necessarily. It is clear that if one restricts to a subset of elements and hence to a subset of matrices in the irrep, that there may be a matrix $B \neq \lambda \mathbf{1}$ that commutes with this subset, but not with the whole set. Consider for example the case where H is the center $Z(G)$ of G. If G is non-Abelian and has an irrep of dimension 2 or higher, then restricting this irrep to H cannot yield an irrep of H, since the center is always Abelian and Schur's second lemma implies that all irreps of an Abelian group must be 1-dimensional (note that 1-dimensional reps are by definition irreps).

2.3 Characters

We are interested in irreps *up to equivalence*, i.e., we do not count two irreps as different if they are equivalent. Therefore we look for a property that is invariant under similarity transformations.

Definition *character*
Let D be a d-dim rep of G. Then the mapping $\chi^D : G \to \mathsf{C}$ defined for all elements g of G by

$$\chi^D(g) = \mathrm{Tr} D(g) = \sum_{j=1}^{d} D(g)_{jj}$$

is said to be the character of the rep D.

Remark
(i) $\chi^D(e) = d$
(ii) Because $\mathrm{Tr}A$ is invariant under similarity transformations ($\mathrm{Tr}(ABC) = \mathrm{Tr}(CAB)$), $\chi^D = \chi^{D'}$ for any two equivalent reps. For the same reason a character is constant on each class of G: $\chi(hgh^{-1}) = \chi(g)$.

Characters can be used to differentiate between inequivalent irreps. This uses an orthogonality theorem, which we will state without proof, but can be proven solely by means of Schur's lemmas [see Jones, pages 62-65].

Theorem (First Orthogonality Theorem of Characters)
Let $D^{(\mu)}$ and $D^{(\nu)}$ be two irreps of the group G of finite order $[g]$ with dimensions n_μ and n_ν. If $\mu \neq \nu$ these irreps are supposed to be inequivalent. If $\chi^{(\mu)}$ and $\chi^{(\nu)}$ are characters of the irreps $D^{(\mu)}$ and $D^{(\nu)}$, then

$$\frac{1}{[g]} \sum_{g \in G} \chi^{(\mu)}(g) \chi^{(\nu)}(g)^* = \delta^{\mu\nu}.$$

Example D_3
We have encountered several reps of D_3. In the two-dimensional rep $D^{(3)}$ we find $\chi^{(3)}((E)) = 2$, $\chi^{(3)}((R)) = -1$ and $\chi^{(3)}((S)) = 0$. If we consider the characters as vectors in class space, then we have $\chi^{(3)} = (2, -1, 0)$.

For the one-dimensional rep $D^{(2)}$: $\chi^{(2)}((E)) = \chi^{(2)}((R)) = 1$, $\chi^{(2)}((S)) = -1$, so $\chi^{(2)} = (1, 1, -1)$.

For the three-dimensional rep D^V: $\chi^V((E)) = 3, \chi^V((R)) = 0$, $\chi^V((S)) = -1$, so $\chi^V = (3, 0, -1)$.

We see for instance that $\sum_g \chi^{(2)}(g)\chi^{(3)}(g) = 1(1\times 2)+2(1\times(-1))+3(-1\times 0) = 0$. However, $\sum_g \chi^{(3)}(g)\chi^V(g)$ does not vanish. Consequently, not all these reps can be irreps.

Corollary
A rep D of a group G of finite order $[g]$ is an irrep iff

$$\frac{1}{[g]} \sum_{g \in G} \left|\chi^{(\mu)}(g)\right|^2 = 1.$$

In practice, for finite groups this is the easiest way of finding out whether a rep is an irrep.

Returning to the reps of D_3: one can check easily that this identity is fulfilled by $\chi^{(2)}$ and $\chi^{(3)}$ of the group D_3, but not by χ^V. So $D^{(2)}$ and $D^{(3)}$ are irreps, D^V is not. Note that the trivial rep ($D^{(1)}$) is always an irrep.

Theorem

If G is a finite group, then the two irreps $D^{(\mu)}$ and $D^{(\nu)}$ are equivalent iff $\chi^{(\mu)} = \chi^{(\nu)}$.
Proof
If $D^{(\mu)}$ and $D^{(\nu)}$ are equivalent, then $\chi^{(\mu)} = \chi^{(\nu)}$. Suppose that $\chi^{(\mu)} = \chi^{(\nu)}$, but that $D^{(\mu)}$ and $D^{(\nu)}$ are not equivalent. From the first orthogonality theorem of characters it follows that

$$\frac{1}{[g]} \sum_{g \in G} \chi^{(\mu)}(g) \chi^{(\nu)}(g)^* = 0.$$

We may replace $\chi^{(\nu)}$ by $\chi^{(\mu)}$ in this expression, but then the sum is over positive numbers and must be different from zero. For instance, $\chi^{(\mu)}(e) = n_\mu$ always ($D^{(\mu)}(e)$ is always the $n_\mu \times n_\mu$ unit matrix). This is a contradiction, so the hypothesis that $D^{(\mu)}$ and $D^{(\nu)}$ are not equivalent must be false.
□

The first orthogonality theorem of characters can be phrased as a sum over classes K_i:

$$\frac{1}{[g]} \sum_{i} k_i \chi^{(\mu)}(K_i) \chi^{(\nu)}(K_i)^* = \delta^{\mu\nu},$$

where k_i is the number of elements in the class K_i. For a given irrep one can think of $\{\sqrt{k_1}\chi^{(\mu)}(K_1), \ldots, \sqrt{k_k}\chi^{(\mu)}(K_k)\}$ as a vector in k-dimensional space, where k is the number of classes. Then the orthogonality statement represents a complex scalar product of two vectors in this space, labelled by μ and ν respectively, which can take on r different values, the number of inequivalent irreps. But the number of linearly independent orthogonal vectors cannot exceed the dimensionality of the space: k. Therefore, the number of inequivalent irreps is less than or equal to the number of conjugacy classes: $r \leq k$.

The reverse can be concluded from a second orthogonality theorem on group characters, which we will state without proof.

Theorem Second Orthogonality Theorem
Let G be a finite group of order g, $\{K_i\}$ the set of its conjugacy classes, $\{D^{(\mu)}\}$ the set of its irreps up to equivalence, k_i is the number of elements in the class K_i, then

$$\frac{1}{[g]} \sum_{\mu} k_i \chi^{(\mu)}(K_i) \chi^{(\mu)}(K_j)^* = \delta_{ij}.$$

Viewing $\{\sqrt{k_i}\chi^{(1)}(K_i), \ldots, \sqrt{k_i}\chi^{(r)}(K_i)\}$ as a vector in r-dimensional space, where

r is the number of inequivalent irreps, leads to the conclusion that $k \leq r$. Hence, these numbers are in fact equal!

So the final, very useful result is

> For a finite group the number of irreps up to equivalence, is equal to the number of classes.

This shows the use of knowing the conjugacy classes. For example, C_3 is Abelian, which means each element forms a separate conjugacy class. Therefore, C_3 has three irreps, which are all 1-dimensional. D_3 also has three classes and hence, three inequivalent irreps.

We end this section by mentioning two additional results that are useful in the construction of the character table of a finite group (next section). Both results follow from analyzing the so-called regular representation (for which we refer to Jones). The first result is:

$$\sum_\mu n_\mu^2 = [g],$$

where the sum is over all inequivalent irreps $D^{(\mu)}$ with dimension n_μ. This result can be used for checking whether one has found all irreps. The second useful result applies to all elements $g \neq e$:

$$\sum_\mu n_\mu \chi^{(\mu)}(g) = 0.$$

This result can for instance be used to cross check a character table.

2.4 Character tables

Principal tools for the construction of a character table:

1. number of irreps r = number of conjugacy classes k
2. $\sum_\mu n_\mu^2 = [g]$
3. orthogonality:

$$\begin{aligned} \sum_i k_i \chi^{(\mu)}(K_i)\chi^{(\nu)}(K_i)^* &= [g]\delta^{\mu\nu} \\ \sum_\mu k_i \chi^{(\mu)}(K_i)\chi^{(\mu)}(K_j)^* &= [g]\delta_{ij} \end{aligned}$$

4. For Abelian groups all irreps are 1-dimensional (follows from tools 1 and 2 actually, or from Schur's lemma)

5. For 1-dimensional reps the character mapping is a homomorphism

Example: D_3
As we have seen D_3 has 3 conjugacy classes, hence also 3 irreps (using tool 1). There is always the trivial rep, which is 1-dimensional: $D^{(1)}$. Using tool 2, we find that there is another 1-dimensional and a 2-dimensional irrep: $D^{(2)}$ and $D^{(3)}$, that we already encountered. But even if we didn't find them already, their characters can be constructed easily using tools 3 and 5. To start with the latter: $\chi(RS_A) = \chi(R)\chi(S_A)$, but $\chi(RS_A) = \chi(S_C) = \chi(S_A)$, hence $\chi(R) = 1$. $\chi(E) = \chi(S_A^2) = \chi(S_A)^2 = 1$, hence $\chi(S_A) = \pm 1$. This gives the trivial ($\chi(S_A) = 1$) and the second 1-dimensional irrep ($\chi(S_A) = -1$). The third irrep is now obtained using tool 3 (and using that $\chi(E) = n_\mu$). The end-result is[1]:

	(E)	(R)	(S)
$D^{(1)}$	1	1	1
$D^{(2)}$	1	1	-1
$D^{(3)}$	2	-1	0

Note that all rows and columns satisfy orthogonality. For example, the second column: $2\times(1^2+1^2+(-1)^2)/6 = 1$, idem for the third one: $3\times(1^2+(-1)^2)/6 = 1$. Finally, note that the characters of third irrep for the elements $g \neq e$ could also have been obtained by using the result that:

$$\sum_\mu n_\mu \chi^{(\mu)}(g) = 0,$$

which can always be used as a way to check the correctness of the table.

Example: C_3
C_3 is a subgroup of D_3, but as already mentioned: irreps of a group are not necessarily also irreps of a subgroup. C_3 is an Abelian group of 3 elements, hence it has 3 classes, and therefore 3 1-dimensional irreps. There is always the trivial rep, hence the first row and column of the character table are already known. The rest follows from tool 5: $\chi(R^3) = 1$, hence $\chi(R)$ must be one of the three distinct roots of unity. Defining $\omega = \exp(i2\pi/3)$, one obtains:

[1]Jones uses in part crystallographic (Schönflies) notation for the groups (C_{3v}, etc) and classes ($2C_3$, C_6^3, etc) and Mulliken symbols for the irreps (A_i, B_i, E, etc), but since this lacks a full explanation, it is not used here.

	(E)	(R)	(R^2)
$D^{(1)}$	1	1	1
$D^{(2)}$	1	ω	ω^2
$D^{(3)}$	1	ω^2	ω

Note that $D^{(3)} = D^{(2)*}$, the complex conjugate rep of $D^{(2)}$. The complex conjugate of a rep is always also a rep, but it might be equivalent to the original rep. This is an example where it isn't.

Orthogonality can be checked, using that $1+\omega+\omega^2 = 0$, which follows for instance from $\omega^3 - 1 = (\omega - 1)(1 + \omega + \omega^2) = 0$.

Note of caution
A character table does not completely specify a group. The first example occurs at order 8: D_4 and the quaternion group Q have the same character table (see exercises 4.5 and 4.6 of Jones), even though the irreps themselves are not the same. Since the groups are not the same, it means that the irreps of the two groups with the same characters are simply not the same.

2.5 Decomposing reducible reps into irreps

It is useful to define a scalar product of two characters ϕ and χ as:

$$\langle \phi, \chi \rangle \equiv \frac{1}{[g]} \sum_{g \in G} \phi(g)\chi(g^{-1}).$$

Note that this scalar product is symmetric: $\langle \phi, \chi \rangle = \langle \chi, \phi \rangle$.

If D is unitary, i.e. $D(g^{-1}) = D(g)^{-1} = D(g)^\dagger$, then $\chi(g^{-1}) = \chi(g)^*$, such that orthogonality of characters can be written succinctly as $\langle \chi^{(\mu)}, \chi^{(\nu)} \rangle = \delta^{\mu\nu}$.

Theorem
Let G be a finite group of order $[g]$ and D any rep of G with character χ. If D is equivalent to the *direct sum* of the irreps $D^{(\mu)}$

$$D' = \bigoplus_\mu a_\mu D^{(\mu)}$$

then the numbers a_μ can be computed as

$$a_\mu = \langle \chi^{(\mu)}, \chi \rangle$$

Proof
If $SDS^{-1} = D' = \bigoplus_\mu a_\mu D^{(\mu)}$, then $\chi = \sum_\mu a_\mu \chi^{(\mu)}$. Using the orthogonality theorem for characters yields the result.
□

Notation of Jones: $\sum_\oplus$ instead of $\bigoplus$

Note that the numbers a_μ are in fact uniquely determined. Assume that $\sum_i a_i \chi^{(i)} = \sum_j b_j \chi^{(j)}$ with $a_i \neq b_i$, then equivalently $\sum_i (a_i - b_i)\chi^{(i)} = 0$. Since all $\chi^{(i)}$ are linearly independent, one would conclude: $a_i - b_i = 0 \; \forall i$, leading to a contradiction.

Let us next look at a reducible rep that we have encountered: D^V of D_3. Its characters are:

	(E)	(R)	(S)
D^V	3	0	-1

From $\langle \chi^V, \chi^V \rangle = 2$ we see that indeed this rep is reducible. One can find the decomposition of D^V in terms of irreps either by inspection of the character table (since the relation $\chi^V = \sum_\mu a_\mu \chi^{(\mu)}$ can only be satisfied for all g simultaneously by a unique set of numbers a_μ) or by calculating $a_\mu = \langle \chi^{(\mu)}, \chi^V \rangle$, to find:

$$D^V \sim D^{(2)} \oplus D^{(3)}.$$

In fact, this is also clear directly from the explicit D^V matrices given on page 23, which shows that

$$D^V(g) = \begin{pmatrix} D^{(3)}(g) & 0 \\ 0 & D^{(2)}(g) \end{pmatrix}.$$

There is no need for a basis transformation to bring D^V to block-diagonal form.

Let us now consider D^V of C_3:

	(E)	(R)	(R^2)
D^V	3	0	0

The decomposition of D^V into irreps is straightforward again:

$$D^V \sim D^{(1)} \oplus D^{(2)} \oplus D^{(3)}.$$

Clearly, D^V on page 23 is not yet written in this decomposed form, but one can by finding the appropriate basis transformation.

2.6 Application: invariant vectors

In Section 5.1(i) of Jones there is a nice application of the decomposition of D^V into irreps. It is explained how the existence of a permanent magnetic or electric dipole moment in a crystal (which has a certain point group as a symmetry group) is related to the fact of whether $D^{(1)}$ appears in this decomposition. Let us restrict first to crystals with a point group that only consists of rotations. The idea is that a dipole moment behaves as a vector under rotations and will thus transform according to D^V. A permanent dipole moment requires there to be an invariant direction into which it can point. Vectors pointing in that direction stay invariant under the transformation of the symmetry group of the crystal and thus "transform" according to the trivial irrep of the group. This can only happen if $\langle \chi^{(1)}, \chi^V \rangle \neq 0$.

As we have seen, the decomposition of D^V into irreps depends on the symmetry group. The rep D^V of the dihedral group D_3 (viewed as a subgroup of the rotation group $SO(3)$), does not contain the trivial irrep, it therefore does not allow for an invariant vector in the system. On the other hand, C_3 does allow for an invariant vector.

If one also considers point groups that include reflections, then it matters whether one deals with an invariant vector or axial vector. The latter behaves oppositely under reflections compared to a vector. An electric dipole moment is a vector, whereas a magnetic dipole moment is an axial vector, see the next chapter for discussion on this. Axial-vectors transform under the axial vector rep D^A, which coincides with D^V when restricted to rotations. For a permanent magnetic dipole moment to be allowed, the decomposition of D^A must include the trivial irrep, which again depends on the group.

Example: NH_3
Consider the ammonia molecule, consisting of three hydrogen atoms (A_1, A_2, A_3) and one nitrogen atom (A_4), shown in Fig. 2.2. The hydrogen atoms form an equilateral triangle. The symmetry group of the NH_3 molecule is usually called C_{3v}, which consists of the C_3 transformations of the equilateral triangle combined with reflections in the plane spanned by the origin, A_4 and one of the other A_i. It is not hard to see that this group is isomorphic, but not equal to D_3, where the latter is viewed as a group of *rotations* in three dimensions. Under the action of the reflections in C_{3v} vectors and axial vectors behave in an opposite manner. Whether a system with a C_{3v} symmetry allows (in principle) a permanent electric and/or magnetic dipole moment is subject of exercise 5.1 of Jones.

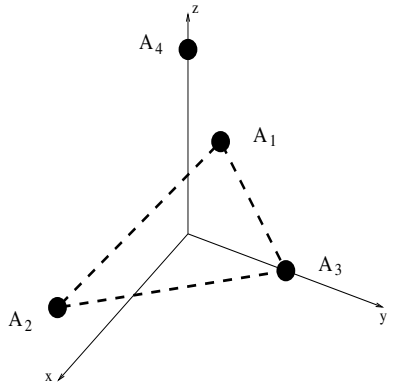


Figure 2.2: Geometrical representation of the ammonia molecule.

Example: Electron and neutron EDMs
The rep D^V of the group $SO(3)$ is an irrep (see next chapter), therefore, a spherically symmetric system does not allow for an invariant (axial) vector. There is no direction associated with the system. It is generally assumed that particles like the electron and the neutron are spherically symmetric and hence should not have an electric dipole moment (EDM). Measurements have shown that the electron and neutron EDM are indeed extremely small. Thus far, only upper bounds on their magnitude have been obtained, $|d_e| < 1.1 \cdot 10^{-29}\, e\,\mathrm{cm}$ and $|d_n| < 2.9 \cdot 10^{-26}\, e\,\mathrm{cm}$, which can be compared to the EDM of the water molecule, which in the same units is about $4 \cdot 10^{-9}\, e\,\mathrm{cm}$. The upper bounds indicate that the electron and the (charge distribution of the) neutron are incredibly round. Nevertheless, it is not expected that the EDMs are zero exactly. The spin in principle gives spin-1/2 particles a direction, but since spin $\vec{S}$ is an axial vector and the EDM $\vec{d}$ is a vector, it require parity violation to relate the two. In fact, it can be shown that it also requires time-reversal violation. The time-reversal violation in the weak interactions leads to only tiny EDMs for the electron and the neutron (and similar particles): $|d_e| \sim 10^{-38}\, e\,\mathrm{cm}$ and $|d_n| \sim 10^{-32}\, e\,\mathrm{cm}$. If larger EDM values are found in future experiments, then this would indicate new physics beyond the Standard Model of particle physics. Much progress regarding the search for such EDMs is expected in the coming years.

Note that we are considering (axial) vectors/directions that are invariant under *all* transformations in the group. Of course, each individual rotation does leave a specific direction invariant.

Lemma
If $R \in SO(3)$, then there exists a vector $\vec{f}$ with length $\|\vec{f}\| = 1$, such that $R\vec{f} = \vec{f}$.

Proof
$R\vec{f} = \vec{f}$ means: the matrix R has an eigenvalue equal to 1. This implies that $\det[R - I] = 0$, where $I = \mathrm{diag}(1, 1, 1)$ is the identity matrix in three dimensions. Now

$$\begin{aligned} \det[R - I] &= \det[R^{\mathsf{T}} - I^{\mathsf{T}}] = \det[R^{-1} - I] \\ &= \det R^{-1} \det(-I) \det[R - I] \\ &= -\det[R - I], \end{aligned}$$

where R^{T} is the transpose of the matrix R, being equal to R^{-1} and having a determinant equal to 1 as $R \in SO(3)$. So we can conclude that $\det[R - I] = 0$: there is indeed an eigenvalue equal to 1.
□

The eigenvector f may not be unique. This is easy to see: if we take for R the identity I, than any vector different from the null vector is an eigenvector with eigenvalue 1. For a given $\vec{f}$ of length 1, we may find two orthogonal vectors $\vec{g}$ and $\vec{h}$ such that $\{\vec{f}, \vec{g}, \vec{h}\}$ form an orthogonal basis for R^3. In this basis the matrix R has the form

$$R = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix}.$$

for some angle θ. All rotations about any axis over the same angle θ belong to the same class of $SO(3)$ and thus lead to the same value $\mathrm{Tr}\ R = 1 + 2\cos\theta$.

Remark [only for interested students]
Now that we have obtained the character of the rep D^V, $\chi^V(\theta) = 1 + 2\cos\theta$, we can establish the *crystallographic restriction theorem*: if a discrete group of displacements has more than one center of rotation, then there can only be 2, 3, 4, or 6-fold symmetry. Recall that an infinite three-dimensional lattice is defined by three basic lattice vectors $\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$ and by lattice coordinate vectors $\vec{n} = (n_1, n_2, n_3)$ with integer components. If one uses the lattice vectors a_i as a basis for the rep D^V, which differs just by a change of basis from the usual representation, the character is unaffected. Any two lattice points $\vec{r}$ and $\vec{r}'$ that are related by an $O(3)$ transformation R, in this basis must be represented by a matrix $D^V(R)$ that only contains integer entries. Therefore, $\chi^V(\theta) \in \mathsf{Z}$ and hence, nonzero θ can only take the angles $60°, 90°, 120°, 180°$, which correspond to 6, 4, 3, or 2-fold symmetry, respectively.

Chapter 3

Product representations in classical and quantum mechanics

[Topics in this chapter are covered in sections 3.2, 4.5, 5.1, 5.3, 6.3 of Jones.]

A product of two representations forms again a representation, the product representation, but it is often not irreducible even when the two original reps are irreducible. The decomposition of a product rep into irreps is called the Clebsch-Gordan series. The most familiar example from physics appears in Quantum Mechanics, in what is called "addition of angular momentum", where one considers Clebsch-Gordan decompositions and Clebsch-Gordan coefficients. The link with product representations and irreducibility will be discussed in this chapter. For a full understanding of this topic, the general transformations of quantum mechanical wave functions and operators, as well as the irreps of $SO(3)$ and $SU(2)$, will be discussed in some detail in this chapter. Examples from classical mechanics, such as the transformation properties of the electrical conductivity tensor of an inhomogeneous medium or material, will be given as well. We will start with a few simpler examples to keep in mind in the discussion of the general case.

3.1 Products of two vectors

Vectors in three dimensions, such as the position vector $\vec{r}$ and the momentum $\vec{p}$, transform under rotations and reflections according to the vector representation D^V of $O(3)$. The rep D^V is the *defining rep* of $O(3)$, which means its elements are defined by 3×3 matrices that act on the components of a three-vector $\vec{x} \in V = \mathsf{R}^3$.

On the other hand, the length of a vector, e.g. $|\vec{r}| = \sqrt{\vec{r}^2}$, is invariant under $O(3)$. It is a so-called scalar. A scalar "transforms" under the trivial rep, in order to be invariant under the action of the group. That is why the inner product $\vec{r}^2 = \vec{r}\cdot\vec{r}$ is also referred to as a *scalar* product. The often encountered Hamiltonian $H = \vec{p}^2/2m + V(|\vec{r}|)$ for example is an $O(3)$ scalar.

The two vectors in $\vec{r}_1 \cdot \vec{r}_2 = \sum_{i,j=1}^{3} \delta_{ij} r_1^i r_2^j$ each transform under the vector rep, but the scalar product as a whole transforms under the trivial rep. This means that in the product of two vector reps there is a component that transforms trivially, but there are also other parts. For instance, the outer product (also called vector product or cross product) of two vectors, written as $\vec{r}_1 \times \vec{r}_2$, transforms as a vector under rotations and oppositely to a vector under reflections, i.e. it transforms as an axial vector.

An electric field $\vec{E}$ transforms as a vector under $O(3)$, hence transforms under the vector representation D^V. A magnetic field $\vec{B}$, on the other hand, behaves oppositely to $\vec{E}$ under reflections, hence transforms as an axial vector under $O(3)$, i.e. under D^A. In the product of the vector rep and the axial vector rep there is no component that transforms trivially. The inner product of an axial vector and a vector is not invariant under reflections. Rather it transforms as a pseudo-scalar, which means it transforms trivially under rotations and picks up a minus sign under reflections. For example, the inner product $\vec{E} \cdot \vec{B}$ forms a pseudoscalar[1]. On the other hand, the outer product of a vector and an axial vector, such as $\vec{E} \times \vec{B}$, transforms as a vector (the name Poynting *vector* is thus appropriate). This means that in the decomposition of the product of D^V and D^A for $O(3)$ there must appear a D^V.

After these examples, we will now present a general discussion about products of representations and their decomposition into irreps, the so-called Clebsch-Gordan series. After that we will connect those results to addition of angular momentum in quantum mechanics, described in terms of the irreps of $SO(3)$ and $SU(2)$, that will also be discussed in some detail.

3.2 Tensor product representations

A vector is defined by its behavior under transformations $R : \vec{x} \mapsto \vec{x}'$ or in components $x'_n = R_{nm} x_m$. The matrices R_{nm} form a representation (D^V) of a

[1]Recall that for electromagnetic waves in vacuum, $\vec{E} \cdot \vec{B}$ actually vanishes. An example of a generally nonzero pseudoscalar is the (oriented) volume spanned by three vectors: $\vec{r}_1 \cdot (\vec{r}_2 \times \vec{r}_3)$.

group of transformations (it is useful to keep the example of rotations, $SO(3)$, in mind). Once a vector is defined this way, tensors are defined as objects that transform as products of vectors, e.g., $T_{n_1,\ldots,n_M}$ is a tensor element iff

$$T'_{n'_1,\ldots,n'_M} = R_{n'_1 n_1} \cdots R_{n'_M n_M} T_{n_1,\ldots,n_M}.$$

The object $R_{n'_1 n_1} \cdots R_{n'_M n_M}$ represents the transformation of the tensor. It is called the *tensor product* of its components $R_{n'_i n_i}$. We can use this idea for any rep of any group G. In the following theorem we state that the tensor product of two reps is again a rep, also referred to as a *direct product rep*. It suffices to consider products of irreps.

Theorem
If $D^{(\mu)}$ and $D^{(\nu)}$ are two irreps of a group G, with dimensions n_μ and n_ν resp., then the matrices with elements

$$D^{(\mu\times\nu)}_{mr,ns}(R) = D^{(\mu)}_{mn}(R) D^{(\nu)}_{rs}(R)$$

denoted by

$$D^{(\mu\times\nu)}(R) = D^{(\mu)}(R) \otimes D^{(\nu)}(R)$$

form a rep of G of dimension $n_\mu n_\nu$. The character $\chi^{(\mu\times\nu)}$ of $D^{(\mu\times\nu)}$ is given by $\chi^{(\mu\times\nu)}(R) = \chi^{(\mu)}(R)\chi^{(\nu)}(R)$.

Proof

(i) $\forall R_1, R_2 \in G$:

$$\begin{aligned} D^{(\mu\times\nu)}(R_1) D^{(\mu\times\nu)}(R_2) &= \Big(D^{(\mu)}(R_1) \otimes D^{(\nu)}(R_1)\Big)\Big(D^{(\mu)}(R_2) \otimes D^{(\nu)}(R_2)\Big) \\ &= D^{(\mu)}(R_1 R_2) \otimes D^{(\nu)}(R_1 R_2) \\ &= D^{(\mu\times\nu)}(R_1 R_2) \end{aligned}$$

so D is a rep.

(ii) Take traces to obtain the characters

$$\begin{aligned} \chi^{(\mu\times\nu)}(R) &= \sum_{j=1}^{n_\mu} \sum_{s=1}^{n_\nu} \Big(D^{(\mu)}(R) \otimes D^{(\nu)}(R)\Big)_{js,js} \\ &= \sum_j \sum_s D^{(\mu)}(R)_{jj} D^{(\nu)}(R)_{ss} \\ &= \chi^{(\mu)}(R)\chi^{(\nu)}(R). \end{aligned}$$

3.3 Clebsch-Gordan series

In general, the direct product rep $D^{(\mu)} \otimes D^{(\nu)}$ is reducible. If G is of finite order, then $D^{(\mu)} \otimes D^{(\nu)}$ is equivalent to a decomposable rep

$$D^{(\mu)} \otimes D^{(\nu)} = S^{-1} \left(\bigoplus_{\sigma} a^{\sigma}_{\mu\nu} D^{(\sigma)} \right) S, \tag{3.1}$$

with $D^{(\sigma)}$ irreps. The decomposition $\bigoplus_\sigma a^\sigma_{\mu\nu} D^{(\sigma)}$ is called the *Clebsch-Gordan series*. Its integer coefficients $a^\sigma_{\mu\nu}$ (which are not the Clebsch-Gordan coefficients!) indicate how many times a specific irrep appears, using the notation that $D^{(\mu)} \oplus D^{(\mu)} = 2D^{(\mu)}$. They can be computed straightforwardly:

$$\begin{aligned} a^\sigma_{\mu\nu} &= \frac{1}{[g]} \sum_{g\in G} \chi^{(\mu\times\nu)}(g) \chi^{(\sigma)}(g)^* \\ &= \frac{1}{[g]} \sum_{g\in G} \chi^{(\mu)}(g) \chi^{(\nu)}(g) \chi^{(\sigma)}(g)^* \end{aligned}$$

Let us look at what the decomposition of the direct product rep means in terms of the decomposition of its carrier space V. Let $\{\psi^{(\mu)}_m\}$ and $\{\psi^{(\nu)}_n\}$ be bases for the irreps $D^{(\mu)}$ and $D^{(\nu)}$ respectively. The second-rank tensors $\psi^{(\mu)}_m \psi^{(\nu)}_n$ form the basis for the representation $D^{(\mu\times\nu)}$, which in general is not an irrep. In other words, there are subspaces in the space spanned by the basis $\{\psi^{(\mu)}_m \psi^{(\nu)}_n\}$ that are invariant under the transformations of the group G. The decomposition of $D^{(\mu\times\nu)}$ into irreps $D^{(\sigma)}$ implies a basis decomposition:

$$\psi^{(\sigma)\alpha}_s = \sum_{m,n} \left(\begin{array}{cc|c} \mu & \nu & \sigma\alpha \\ m & n & s \end{array} \right) \psi^{(\mu)}_m \psi^{(\nu)}_n$$

where α runs from 1 to $a^\sigma_{\mu\nu}$ to label the bases of the irreps that appear repeatedly in the decomposition. The coefficients $\left(\begin{array}{cc|c} \mu & \nu & \sigma\alpha \\ m & n & s \end{array} \right)$ are called *Clebsch-Gordan* (CG) *coefficients*. These coefficients define the basis transformation matrix S in Equation (3.1).

Note that one cannot have two different linear combinations of irreps as CG decompositions. As for any decomposition of a reducible rep into irreps, it would imply $\sum_i a_i \chi^{(i)} = \sum_j b_j \chi^{(j)}$ with $a_i \neq b_i$, or equivalently $\sum_i (a_i - b_i)\chi^{(i)} = 0$.

Since all $\chi^{(i)}$ are linearly independent, one would conclude: $a_i - b_i = 0\ \forall i$, leading to a contradiction. As a result, often the CG decomposition (but not its CG coefficients) can be found by direct inspection of the character table, without the need to compute the $a^\sigma_{\mu\nu}$ factors.

Example D_3
Recall the character table of D_3:

D_3	(E)	(R)	(S)
$D^{(1)}$	1	1	1
$D^{(2)}$	1	1	-1
$D^{(3)}$	2	-1	0

We first consider tensor products of irreps and decompose them into irreps. Because the character determines the irrep uniquely, we find by direct inspection:

(i) $D^{(1)} \otimes D^{(\mu)} \sim D^{(\mu)} \quad \Rightarrow \quad a^\mu_{1\mu} = a^\mu_{\mu 1} = 1$
(ii) $D^{(2)} \otimes D^{(2)} \sim D^{(1)} \quad \Rightarrow \quad a^\mu_{22} = \delta_{1\mu}$
(iii) $D^{(2)} \otimes D^{(3)} \sim D^{(3)} \quad \Rightarrow \quad a^\mu_{23} = a^\mu_{32} = \delta_{3\mu}$

The case of $D^{(3)} \otimes D^{(3)}$ is less straightforward [Jones: page 75], although it too can be found by direct inspection of the characters. From $\chi^{(3\times 3)}(E) = 4$ we conclude that its dimension is 4, as it must be because $D^{(3)}$ is two-dimensional. The other characters are $\chi^{(3\times 3)}(R) = 1$ and $\chi^{(3\times 3)}(S) = 0$. The formula $D = \bigoplus_\mu a_\mu D^{(\mu)}$ plus orthogonality of characters of irreps implies

$$\frac{1}{[g]} \sum_{g\in G} \left|\chi^{(\mu\times\nu)}(g)\right|^2 = \sum_\mu a_\mu^2,$$

so we find for D_3

$$\frac{1}{6} \sum_{g\in D_3} \left|\chi^{(3\times 3)}(g)\right|^2 = 3.$$

The only solution is $\sum_\mu a_\mu^2 = 3 = 1 + 1 + 1$, so $a_1 = a_2 = a_3 = 1$. An elementary computation gives indeed

$$a^1_{33} = \frac{1}{6}(4 + 2 + 0) = 1, \quad a^2_{33} = \frac{1}{6}(4 + 2 + 0) = 1, \quad a^3_{33} = \frac{1}{6}(8 - 2 + 0) = 1.$$

This means:

$$D^{(3)} \otimes D^{(3)} \sim D^{(1)} \oplus D^{(2)} \oplus D^{(3)}.$$

The most interesting case is $D^V \otimes D^V$ [Jones: pages 80-82], which is frequently encountered in physics. It acts on tensors with elements T_{ij}. From the definition

$$D^{(V\times V)}_{kl,ij}(R) = D^V_{ki}(R) D^V_{lj}(R),$$

it is obvious that if the tensor T is (anti-)symmetric under the interchange of its two indices, i.e. $T_{ij} = \pm T_{ji}$, then also the transformed tensor T' is (anti-)symmetric: $T'_{kl} = \pm T'_{lk}$. Since any tensor T_{ij} can be split into symmetric and antisymmetric parts

$$T_{ij} = \frac{1}{2}(T_{ij} + T_{ji}) + \frac{1}{2}(T_{ij} - T_{ji}),$$

these two parts do not mix under the transformations and hence form invariant subspaces (although not necessarily the smallest ones). For example, the electrical conductivity tensor σ^{ij} ($j^i = \sigma^{ij} E^j$) is usually symmetric under the interchange of its two indices, which means it transforms according to the symmetric (+) part of $D^V \otimes D^V$:

$$D^{\pm}_{kl,ij}(R) = \frac{1}{2}\left[D^V_{ki}(R) D^V_{lj}(R) \pm D^V_{kj}(R) D^V_{li}(R)\right]$$

Jones writes these as $D^{(V\times V)_\pm}$. The corresponding characters are:

$$\chi^{\pm}(R) = \frac{1}{2}\left[(\chi^V(R))^2 \pm \chi^V(R^2)\right]$$

Since D^V is different for different groups, the decomposition into $D^\pm$ will be group dependent. For D_3 this leads to:

D_3	(E)	(R)	(S)
D^V	3	0	-1
D^+	6	0	2
D^-	3	0	-1

One sees that $D^+ \sim 2D^{(1)} \oplus 2D^{(3)}$ and $D^- \sim D^V \sim D^{(2)} \oplus D^{(3)}$. Since the trivial rep appears twice in the decomposition of D^+, it implies that a symmetric tensor σ_{ij} can adopt two forms that remain invariant under the action of D_3. These are $\sigma_{ij} = \delta_{ij}$ and $\sigma_{ij} = \delta_{i3}\delta_{j3}$, where 3 stands for the z-axis if the triangle is in the $x - y$ plane. As said, this is a group-dependent result. For further details see Jones pages 80-82, where also the rank-3 piezoelectric tensor p_{ijk} is mentioned, which requires consideration of $D^V \otimes D^V \otimes D^V$.

3.4 Transformations of wave functions

Transformations of coordinates, e.g. rotations in R^3, not only dictate how vectors and tensors transform, but also induce transformations in the space of functions of these coordinates, e.g. quantum mechanical wave functions. If one rotates "everything", nothing should change:

$$\psi'(\vec{r}\,') = \psi(\vec{r})$$

where $\vec{r}\,' = R\vec{r}$. Hence,

$$\psi'(\vec{r}) = \psi(R^{-1}\vec{r}) \equiv U(R)\psi(\vec{r})$$

U is an operator acting on the wave function, corresponding to the transformation $R \in G$. It follows the group multiplication of G when acting on $\psi(\vec{r})$, but may actually form a different group G'. So we define the mapping $U : G \to G'$, where G' is a group of operators, as follows

$$\forall R \in G,\ \forall \psi(\vec{r}) :\ (U(R)\psi)(R\vec{r}) = \psi(\vec{r}).$$

As said, it follows the group multiplication of G when acting on $\psi(\vec{r})$:

$$\forall \psi :\ (U(R_1)U(R_2))\psi = U(R_1 \circ R_2)\psi.$$

This is best seen by first defining $\phi(\vec{r}) \equiv U(R_2)\psi(\vec{r}) = \psi(R_2^{-1}\vec{r})$, to deduce $U(R_1)\phi(\vec{r}) = \phi(R_1^{-1}\vec{r}) = \psi(R_2^{-1}R_1^{-1}\vec{r}) = \psi((R_1R_2)^{-1}\vec{r}) = U(R_1R_2)\psi(\vec{r})$.

If one requires that the normalization of the wave function is preserved, $U(R)$ will be unitary. Therefore, $U(R)$ is a unitary operator rep of G when its action on functions ψ of $\vec{r} \in \mathsf{R}^3$ is considered. However, not all quantum mechanical wave functions are functions of $\vec{r}$, for example: spin states. In quantum mechanics it turns out that when $G = SO(3)$, then $G' = SU(2)$, which is the special unitary group of 2×2 complex, unitary matrices with determinant 1.

In the above the operators U act on the whole (Hilbert) space of wave functions, but that space may contain invariant subspaces. These subspaces lead to irreps of G'. Therefore, one can construct irreps of G' by just considering all transformations and identify invariant spaces. Starting with a specific wave function a certain set of wave functions can be obtained by considering all $R \in G$. So first construct the functions $\psi_R(\vec{r}) = U(R)\psi(\vec{r})$. Consider the set of all these functions $\{\psi_R | R \in G\}$. It is closed under the action of the group, since $U(R')\psi_R = \psi_{R'R}$ is again in the set. This subspace can have any dimension. For instance, it could be

1-dimensional for invariant wave functions, e.g. $\psi(r) = \int d\Omega\, \psi(\vec{r})$ is a rotationally invariant wave function. Now suppose the set $\{\psi_R | R \in G\}$ is d-dimensional. By Gram-Schmidt orthogonalization one can construct d orthonormal functions ψ_k, $k = 1, \ldots, d$, that form a basis for this subspace. So, any element of this set can be expanded in this basis:

$$U(R)\psi_k(\vec{r}) = \sum_{n=1}^{d} \psi_n(\vec{r})\, D(R)_{nk}, \quad k = 1, \ldots, d.$$

This means that D is a d-dim rep of G'. Hence, $\{\psi_1(\vec{r}), \ldots, \psi_d(\vec{r})\}$ form a *basis of the rep D of G'*. Using $\langle\psi_m|\psi_n\rangle = \delta_{mn}$ we find that the matrix D is formed by the "matrix elements" of the operator U:

$$D(R)_{mn} = \langle\psi_m|U(R)|\psi_n\rangle.$$

If this rep D is reducible, it can be decomposed into irreps.

3.5 Irreps of $SO(3)$ and $SU(2)$

The above described procedure allows us to identify irreps of $SO(3)$. Consider the wave functions $\psi_{nlm}(\vec{r}) = \langle\vec{r}|nlm\rangle = R_{nl}(r)Y_{lm}(\theta, \phi)$. Any rotation will transform this into $\sum_{m'} \psi_{nlm'} D^{(l)}_{m'm}(R)$, since under rotations the quantum numbers n and l do not change, only the quantum number m of the operator L_z does [see next chapter]. In other words, the invariant subspaces are labelled by the (integer) orbital quantum number l and are $2l+1$ dimensional. We observe that the Y_{lm}'s, or equivalently the states $|l, m\rangle$, form the basis for the irreps $D^{(l)}$ of $SO(3)$. For instance, the space formed by the three $l = 1$ angular momentum states $|1, m\rangle$ form a basis for a three-dimensional irrep of $SO(3)$. In fact, this $D^{(1)}$ irrep is equivalent to the defining or vector rep D^V of $SO(3)$ that is obtained by considering the action of $SO(3)$ on three-vectors $\vec{r}$. In quantum mechanics, it is common to consider a complex basis, in which the Cartesian vector $\vec{x} = (x, y, z)$ is transformed to the *spherical basis*: $(-(x+iy)/\sqrt{2}, z, (x-iy)/\sqrt{2})$ (cf. Jones: Eq. (3.14), exercise 3.1, and page 106). A unit vector $(x, y, z) = (\sin\theta\cos\varphi, \sin\theta\sin\varphi, \cos\theta)$ becomes in the spherical basis $\frac{1}{\sqrt{2}}(-\sin\theta e^{i\varphi}, \sqrt{2}\cos\theta, \sin\theta e^{-i\varphi}) = \sqrt{\frac{4\pi}{3}}(Y_{11}, Y_{10}, Y_{1,-1})$. This shows explicitly that $D^V \sim D^{(1)}$ for $SO(3)$. Note that since D^V is an irrep of $SO(3)$ that is not the trivial irrep, an $SO(3)$ invariant system does not allow any invariant vectors (cf. the discussion in the previous chapter).

If one includes spin, the effect of a rotation is different. The spin wave functions are not represented as functions of $\vec{r}$. Nevertheless, a rotation in coordinate space will modify the spin state too:

$$U(R)|s, m_s\rangle = \sum_{m'_s} |s, m'_s\rangle \, D^{(s)}_{m'_s m_s}(R),$$

in other words, we are after $D^{(s)}_{m'_s m_s}(R) = \langle s, m'_s|U(R)|s, m_s\rangle$, using that under a rotation a spin-s state will remain spin-s. This turns out to yield a $(2s+1)$-dimensional irrep of $SU(2)$ ($U \in SU(2)$). For integer s it also corresponds to an irrep of $SO(3)$, but for half-integer s only to a *projective rep* of $SO(3)$:

$$D(R_1)D(R_2) = e^{i\varphi(R_1,R_2)}D(R_1R_2).$$

Such projective reps appear naturally in quantum mechanics, where one allows for a change in the phase of wave functions under symmetry transformations. For instance, under a 2π-rotation $|s, m_s\rangle$ states for half-integer s values acquire a minus sign, as opposed to $|l, m\rangle$ states.

In quantum mechanics often one adds angular momenta, such as $\vec{J} = \vec{L} + \vec{S}$, to express states and observables in terms of the total angular momentum, which is often the only angular momentum that is conserved. The quantum number j can then take integer or half-integer values. In the case of integer j, $D^{(j)}_{m'_j m_j}(R) = \langle j, m'_j|U(R)|j, m_j\rangle$ forms an irrep of both $SU(2)$ and $SO(3)$, but in case of half-integer j only of $SU(2)$.

3.6 CG decompositions for $SO(3)$ and $SU(2)$

Let us now consider the CG decomposition of $D^V \otimes D^V$ into irreps for $SO(3)$. In general, a tensor T_{ij} can be decomposed as follows:

$$T_{ij} = \frac{1}{3}\delta_{ij}T_{kk} + \frac{1}{2}\epsilon_{ijk}\epsilon_{klm}T_{lm} + \frac{1}{2}\left(T_{ij} + T_{ji} - \frac{2}{3}\delta_{ij}T_{kk}\right),$$

where a summation over repeated indices is understood. The first term involving δ_{ij} is clearly invariant under rotations. Since the second term is antisymmetric and the third term is symmetric, they do not mix under $SO(3)$ transformations. The second (antisymmetric) term is simply $\frac{1}{2}(T_{ij} - T_{ji})$, which can be seen by using $\epsilon_{ijk}\,\epsilon_{klm} = \delta_{il}\,\delta_{jm} - \delta_{im}\,\delta_{jl}$. It has 3 linearly independent components. The

third (symmetric) term has 5 linearly independent components. The above decomposition of T_{ij} shows the CG decomposition $D^V \otimes D^V \sim D^{(0)} \oplus D^{(1)} \oplus D^{(2)}$ for $SO(3)$. This is often schematically written as

$$\mathbf{3} \otimes \mathbf{3} = \mathbf{1} \oplus \mathbf{3} \oplus \mathbf{5},$$

where the irreps are simply labelled by their dimension $\boldsymbol{d} = \mathbf{2}\boldsymbol{l} + \mathbf{1}$. More generally, the CG decompositions for $SO(3)$ are: $D^{(l_1)} \otimes D^{(l_2)} \sim \bigoplus_{l_3=|l_1-l_2|}^{l_1+l_2} D^{(l_3)}$, or

$$(\mathbf{2}\boldsymbol{l_1} + \mathbf{1}) \otimes (\mathbf{2}\boldsymbol{l_2} + \mathbf{1}) = \bigoplus_{l_3=|l_1-l_2|}^{l_1+l_2} (\mathbf{2}\boldsymbol{l_3} + \mathbf{1}).$$

This result is not only valid for $SO(3)$, i.e. integer l, but also for $SU(2)$ if one includes half-integer values j. All this should look familiar from the addition of angular momentum in quantum mechanics.

In quantum mechanics one encounters the CG decomposition when adding angular momenta. A tensor product of two states $|l, m\rangle$ is decomposed (without the need for an additional label α in this particular case) as follows:

$$|l_1, m_1\rangle \otimes |l_2, m_2\rangle = \sum_{l_3=|l_1-l_2|}^{l_1+l_2} \sum_{m_3=-l_3}^{l_3} \left(\begin{array}{cc|c} l_1 & l_2 & l_3 \\ m_1 & m_2 & m_3 \end{array} \right) |l_3, m_3\rangle,$$

This expresses the CG series in terms of the basis states of the irreps.

Another common way to write the CG coefficients is (replacing l_i by the more general angular momentum quantum number j_i to include spin): $\langle j_1 m_1 j_2 m_2 | j_3 m_3 \rangle$ or $\langle j_1 j_2; m_1 m_2 | j_3 m_3 \rangle$. Jones: $C(j_1 j_2 j_3; m_1 m_2 m_3)$. All are different ways to express that CG coefficients are functions of all quantum numbers involved.

3.7 Transformations of operators

Next we consider transformations of operators that act on wave functions. If one requires that $\mathcal{O}|\psi\rangle$ transforms as a wave function again, then $\mathcal{O}' = U(R)\mathcal{O}U^{-1}(R)$. If one demands that the normalization of the wave function is unchanged, then U must be unitary, such that $\mathcal{O}' = U(R)\mathcal{O}U^{\dagger}(R)$.

Also operators can transform according to irreps, which leads to the introduction of irreducible tensor operators:

Definition
The operator T^j_m is said to be an *irreducible tensor operator* if it transforms according to

$$U(R)T^j_m U(R)^{-1} = \sum_{m'=1}^{2j+1} T^j_{m'} D^j(R)_{m'm},$$

where D^j denotes an irrep of the group. This is written here in notation commonly used for $SO(3)$ and $SU(2)$, but it can be generalized to other groups.

A Hamiltonian H that is invariant under unitary transformations U, means that H transforms as a scalar operator: $H = U(R)HU^\dagger(R)$ or equivalently $[H, U] = 0$. It generally is a sum of scalar operators such as $\vec{p}^2$ and $\vec{L}\cdot\vec{S}$. Examples of vector operators are $\vec{J}$ and $\vec{r}$. Tensor operators arise for instance in multipole expansions.

Due to the very specific transformation behavior induced by the action of the group G, the matrix elements of irreducible tensor operators contain a part that is purely group theoretical and a "reduced" part that contains the dynamics. This insight simplifies the calculation of such matrix elements considerably. It is summarized in a theorem called the Wigner-Eckart theorem, which forms the basis of selection rules in Quantum Mechanics.

In the notation of Jones the Wigner-Eckart theorem is phrased as:

$$\langle j', m'|T^J_M|j, m\rangle = C(Jjj'; Mmm')\langle j'\|T^J\|j\rangle.$$

Here $\langle j'\|T^J\|j\rangle$ denotes the reduced matrix element. This result follows from the simple fact that $T^J_M|j, m\rangle$ transforms according to the tensor product rep $D^{(J)} \otimes D^{(j)}$, which can be CG decomposed and the above matrix element then selects the irrep $D^{(j')}$ from this decomposition. Since the end result must transform properly, i.e. exactly like $\langle j'm'|JMjm\rangle$, which is the CG coefficient, the proportionality constant can only depend on j, j', J, which do not change under the transformations of the group.

The Wigner-Eckart theorem allows one to calculate the matrix elements of vector operators, like the magnetic dipole moment $\vec{\mu}$. In quantum mechanics this is referred to as the projection theorem: for any vector operator $\vec{V}$ it holds that

$$\langle jm|\vec{V}|jm'\rangle = \langle jm|\vec{J}|jm'\rangle\langle j\|\vec{J}\cdot\vec{V}\|j\rangle/(\hbar^2 j(j+1)).$$

This follows from taking the Wigner-Eckart theorem expression for $\vec{V}$ and $\vec{J}$ and taking their ratio. The big advantage of this result is that it is usually much easier to calculate the matrix elements of a scalar operator $\vec{J}\cdot\vec{V}$ than of a vector operator V.

Chapter 4

Conserved quantities

[Topics in this chapter are covered in chapters 5.3, 6.1, 6.2, and some parts of chapter 10 of Jones.]

4.1 Consequences of symmetry

If a system is invariant under a set of transformations, then all its properties must be in agreement with that symmetry. In chapter 2 we discussed for example how to see whether a system allows for an invariant vector or not. The answers depends on the symmetry of the system. In this chapter we discuss in more detail the consequences of symmetries of a system in the form of conserved quantities, both for classical and quantum mechanical cases. Another consequence that will be discussed is that of degeneracy of energy levels, where different states of a system have the same energy. In the quantum mechanical case this is often a discrete set of energy levels, but in the classical case it is usually a continuous equipotential surface of one, two or three dimensions.

It is important to first emphasize the difference between the symmetries of the physical system and the symmetries of the potential or Hamiltonian of that system. Consider a classical potential $V(|\vec{r}|)$ experienced by a charged particle at position $\vec{r} = (x, y, z)$ in the field of an infinitely heavy charged particle situated at the origin. The potential is $O(3)$ invariant around $\vec{0}$, but the system itself and the force acting on the particle are not. The force $\vec{F} = -\vec{\nabla}V$ transforms as a vector. Since the potential V is central, the force $\vec{F}$ points in the direction of $\vec{r}$. As a consequence the torque $\vec{\tau} = \vec{r} \times \vec{F}$ must vanish[1]. This implies that the orbital

[1]Note that the torque does not vanish simply because the potential is invariant under reflections and the torque is an axial vector. The orbital angular momentum $\vec{L} = \vec{r} \times \vec{p}$ is an axial vector too and generally does not vanish.

angular momentum is conserved since $\vec{\tau} = d\vec{L}/dt$. Hence we see that rotational invariance of the potential implies conservation of angular momentum. This is an example of the general principle that invariances imply conservation laws. In this case we have three conserved quantities: L_x, L_y, L_z.

Next consider the case of a uniform electric field. A particle with charge q will then experience a Lorentz force $\vec{F} = q\vec{E}$. In this case the group of isometries (transformations that preserve distances) under which the corresponding potential is invariant, consist of rotations around and reflections in the electric field direction and translations transverse to it. Translation invariance in general implies momentum conservation ($V(\vec{r}) = V(\vec{r} + \vec{a}\,)$ implies $d\vec{p}/dt = \vec{F} = -\vec{\nabla}V(\vec{r}) = 0$), which in this example applies only to the momentum components transverse to the electric field.

We now turn to quantum mechanics. Recall that time evolution is generated by the Hamiltonian through the Schrödinger equation. If a Hamiltonian is invariant under rotations, then all its consequences, like the energy spectrum and the time evolution, must be compatible with rotational invariance. This does not mean that nothing is allowed to transform under rotations. The wave function solutions of the Schrödinger equation will transform according to certain representations of the rotation group $SO(3)$ (or $SU(2)$ rather, see chapter 3). Rotational invariance of the Hamiltonian implies that the wave functions that are related to each other by rotations must have the same energy, in other words, are degenerate. In quantum mechanics symmetry usually leads to degeneracy and degeneracy usually implies the presence of symmetry. The best-known example is that of the Coulomb potential. Its spectrum displays more symmetry than the rotational ($SO(3)$) symmetry that is apparent. This seeming 'accidental degeneracy' occurs because the Coulomb potential case actually is invariant under a larger symmetry group ($SO(4)$) than just rotational symmetry (see Chapter 7.2 of the book of Jones). This is true for both the classical and quantum mechanical cases.

In somewhat more detail, if a Hamiltonian H is invariant under a transformation U, then it means that H transforms as a scalar operator under U: $H = UHU^{-1}$, or equivalently $[H, U] = 0$. If ψ is a stationary state of the system satisfying $H\psi = E\psi$, then $[H, U] = 0$ implies that also $U\psi$ will be a stationary state with the same energy E:

$$[H, U(R)] = 0 \Rightarrow H(U(R)\psi) = E(U(R)\psi).$$

If $U\psi$ is not proportional to ψ itself, it means that there is degeneracy.

As we will discuss later in this chapter, invariance of a Hamiltonian under a set of

transformations also implies the existence of so-called constants of motion, which correspond to the conserved quantities in the quantum mechanical case. Recall that an operator $\mathcal{O}$ is a constant of motion if $[H, \mathcal{O}] = 0$ and $\partial\mathcal{O}/\partial t = 0$, such that its expectation value is conserved under time evolution:

$$\frac{d\langle\mathcal{O}\rangle}{dt} = \frac{1}{i\hbar}\langle[H, \mathcal{O}]\rangle + \langle\frac{\partial\mathcal{O}}{\partial t}\rangle = 0.$$

Symmetry of a Hamiltonian thus implies degeneracy and existence of constants of motion. To discuss this further we will first take a more detailed look at continuous symmetries and their "generators".

4.2 Continuous groups

The theory of continuous groups, i.e., continuous sets of elements with a composition law that fulfills the axioms of a group, is much more complicated than the theory of discrete groups. In the latter the elements can be enumerated, while in continuous groups the elements are given as functions of some variable or variables. Summation over the group elements needs to be replaced by integration and besides algebraic aspects also topological notions play a role, but these things are beyond the scope of this course.

The continuous groups encountered in physics are Lie groups, continuous groups whose elements depend analytically on a number of parameters (the number being the dimension of the Lie group). Lie groups are the subject of the Master course 'Lie groups in physics'. Here we will only briefly discuss some specific Lie groups.

Example $U(1)$
The Lie group $U(1)$ is defined as the unitary 1×1 matrices. It is the (Abelian) group of complex phases $e^{i\alpha}$, i.e. $\{z \in \mathsf{C} |\ |z| = 1\}$, viewed as a multiplicative subgroup of $\mathsf{C}\backslash\{0\}$. The set of elements can also be viewed as forming the unit circle S^1 in R^2. This group is very important in physics. It is for instance a symmetry in classical and quantum electrodynamics, and it is part of the symmetry group of the Standard Model of elementary particles.

Example $SO(3)$
Any element of $SO(3)$, i.e. any three-dimensional rotation, can be specified by three independent parameters: the angle of rotation, θ, and the direction about which the rotation takes place, given by a unit vector $\hat{n}$. This means that $SO(3)$ forms a three-dimensional Lie group. An element R of $SO(3)$, a rotation, is by

definition represented by a 3×3 matrix R_{ij} acting on three-dimensional vectors:

$$R(\theta\hat{n})_{ij} = \cos\theta\delta_{ij} + (1 - \cos\theta)n_i n_j + \sin\theta\epsilon_{ijk}n_k.$$

These matrices thus form the vector rep D^V of $SO(3)$. It can be shown that $R(\theta\hat{n})_{ij}$ can be written succinctly as an exponential:

$$R(\theta\hat{n}) = \exp(i\theta\sum_{i=1}^{3}\hat{n}_i L_i),$$

where the matrices L_i are given by:

$$L_1 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \quad L_2 = \begin{bmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{bmatrix}, \quad L_3 = \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

These L_i are called the "generators" of rotations in three dimensions. Or to be more precise, these L_i represent the generators of $SO(3)$ in the defining representation. Note that $L_i/\hbar$ satisfy angular momentum commutation relations, because:

$$[L_i, L_j] = i\epsilon_{ijk}L_k.$$

Example $SU(2)$
The group $SU(2)$ is defined as the set of complex 2×2 matrices that are unitary and have determinant equal to 1. A parametrization of all such matrices is given by

$$U = \begin{bmatrix} \alpha_1 + i\alpha_2 & \beta_1 + i\beta_2 \\ -\beta_1 + i\beta_2 & \alpha_1 - i\alpha_2 \end{bmatrix}, \quad \alpha_1^2 + \alpha_2^2 + \beta_1^2 + \beta_2^2 = 1.$$

The number of independent real parameters is three, hence $SU(2)$ is a three-dimensional Lie group. Reparameterizing U in terms of $x_1 = 2\beta_2, x_2 = 2\beta_1, x_3 = 2\alpha_2$, we can rewrite it as:

$$U(x_1, x_2, x_3) = \alpha_1\mathbf{1} + i\vec{x}\cdot\vec{\sigma}/2,$$

where $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ is formed by the well-known Pauli matrices:

$$\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

Upon a further reparametrization, $\alpha_1 = \cos(\theta/2)$ and $\vec{x} = 2\sin(\theta/2)\hat{n}$, with unit vector $\hat{n} = (n_1, n_2, n_3)$, one finds that every element $U \in SU(2)$ can be written in single exponential form:

$$U = \cos\frac{\theta}{2}\mathbf{1} + i\sin\frac{\theta}{2}\hat{n}\cdot\vec{\sigma} = \exp\left(i\sum_{i=1}^{3}\theta_i\frac{\sigma_i}{2}\right),$$

with $\theta_i = \theta n_i$. The Pauli matrices thus correspond to the generators of $SU(2)$ transformations. Again, to be more precise, the $\sigma_i/2$ represent the generators S_i of $SU(2)$ in its defining representation. The generators S_i of $SU(2)$ also satisfy angular momentum commutation relations (with $\hbar$ set equal to 1 or absorbed into the definition of S_i):

$$[S_i, S_j] = i\epsilon_{ijk}S_k.$$

The fact that the generators of spin transformations ($SU(2)$) and rotations ($SO(3)$) satisfy the same commutation relations, allows us to "add" spin and orbital angular momentum in Quantum Mechanics: $\mathbf{J} = \mathbf{L} + \mathbf{S}$.

Example *Lorentz group*
Extending the rotations to Lorentz transformations to form the Lorentz group, leads to a set of 6 generators: three generators J_i of rotations and three generators K_i of pure Lorentz transformations, which are also called boosts.

A general boosts is given by

$$\begin{aligned} x'^0 &= \gamma x^0 + \gamma\,\vec{\beta}\cdot\vec{x} \\ \vec{x}\,' &= \gamma\,\vec{\beta}x^0 + \frac{\gamma^2}{1+\gamma}\vec{\beta}\,(\vec{\beta}\cdot\vec{x}) + \vec{x} \end{aligned}$$

with $x^0 = ct$ and

$$\vec{\beta} = \frac{\vec{v}}{c},\ \gamma = \frac{1}{\sqrt{1-\vec{\beta}^2}}.$$

Because $\beta = |\vec{\beta}| \leq 1$, we can parametrize the pure Lorentz transformations alternatively in terms of a hyperbolic "angle" χ, also referred to as rapidity. Using the definitions $\gamma = \cosh\chi$, $\gamma\beta = \sinh\chi$ and $\hat{\beta} = \vec{\beta}/\beta$, a general boost takes the form:

$$\begin{aligned} x'^0 &= x^0\cosh\chi + \hat{\beta}\cdot\vec{x}\sinh\chi \\ \vec{x}\,' &= \hat{\beta}x^0\sinh\chi + \hat{\beta}\,(\hat{\beta}\cdot\vec{x})(\cosh\chi - 1) + \vec{x}. \end{aligned}$$

This expression can be used to obtain the generators K_i in the 4-dimensional defining rep of the Lorentz group.

A general Lorentz transformation can be uniquely written as a rotation followed by a boost. In terms of the generators a general element of the Lorentz group can be written as:

$$\Lambda = \exp\left(-i\,\vec{\chi}\cdot\vec{K}\right)\exp\left(-i\,\vec{\theta}\cdot\vec{J}\right).$$

The generators satisfy the following commutation relations (cf. chapter 10.3 of Jones):

$$\left[J^j, J^k\right] = i\epsilon_{jkl}J^l, \quad \left[J^j, K^k\right] = i\epsilon_{jkl}K^l, \quad \left[K^j, K^k\right] = -i\epsilon_{jkl}J^l.$$

Because the generators J_i and K_i do not commute, the Lorentz transformation Λ can in general not be written as one exponential (for matrices $e^A e^B \neq e^{A+B}$ in general).

Example *Poincaré group*
The Poincaré group (often also called the inhomogeneous Lorentz group) is the Lorentz group extended with translations in space and time. Any transformation belonging to the Poincaré group can be denoted by $(\Lambda|a)$, where a is a four-vector specifying a translation and Λ is a Lorentz transformation. Every element of the Poincaré group can be uniquely written as

$$(\Lambda|a) = (\mathbf{1}|a)(\Lambda|\mathbf{0}).$$

Translations are generated by the four-momentum operators P^μ (see next section). A translation along the four-vector a^μ is represented by:

$$(\mathbf{1}|a) = \exp(-ia_\mu P^\mu).$$

Hence, a general Poincaré transformation can be written as:

$$(\Lambda|a) = \exp(-ia_\mu P^\mu)\exp\left(-i\,\vec{\chi}\cdot\vec{K}\right)\exp\left(-i\,\vec{\theta}\cdot\vec{J}\right).$$

Again, as the various generators generally do not commute, this product of three exponentials can not be written as one exponential. P^μ and the generators of the Lorentz transformations satisfy (cf. chapter 10.4 of Jones):

$$\begin{aligned}
[K^j, P^0] &= -iP^j, \\
[K^j, P^k] &= iP^0 g^{jk} = -iP^0\delta_{jk}, \\
[J^l, P^0] &= 0, \\
[J^l, P^k] &= i\epsilon^{lkm}P_m.
\end{aligned}$$

Since the generator of time translations P^0 corresponds to the Hamiltonian, the first of these equations indicates that the generators of boosts K^i are not conserved quantities. On the other hand, the generators of the rotations J^i *are* conserved in a Poincaré invariant system.

Because translations in space and time commute, the corresponding generators should commute too:

$$\begin{aligned} [P^i, P^0] &= 0, \\ [P^i, P^j] &= 0. \end{aligned}$$

Here we see that the three-momentum is a conserved quantity in a Poincaré invariant system.

4.3 Conservation laws

Now we take a further look at the consequences of continuous symmetries of a Hamiltonian. As already mentioned in the beginning of this chapter, for a system that is invariant under a certain group of transformations U, the Hamiltonian commutes with all elements of the group: $H = UHU^{-1}$ or $[H, U] = 0$. For continuous groups this implies that the Hamiltonian commutes also with all generators and this in turn means that these generators are constants of motion, such that their expectation values are conserved under time evolution. For rotational symmetry this is the quantum mechanical analogue of conservation of angular momentum.

In the previous chapter we discussed the transformations of wave functions corresponding to rotations R in R^3:

$$\psi'(R\vec{r}) = \psi(\vec{r}) \Rightarrow \psi'(\vec{r}) = \psi(R^{-1}\vec{r}) \equiv U(R)\psi(\vec{r}).$$

Now consider an infinitesimal rotation $\vec{r} \to \vec{r}' = \vec{r} + \theta\ \hat{n} \times \vec{r}$. The wave function then transforms according to (up to order θ^2 terms):

$$\psi(R^{-1}\vec{r}) = \psi(\vec{r}) - \theta\ \hat{n} \cdot (\vec{r} \times \vec{\nabla})\psi(\vec{r}) = \left(1 - \frac{i}{\hbar}\theta\ \hat{n} \cdot \vec{L}\right)\psi(\vec{r}).$$

Here we see again that the L_i are the generators of rotations. One finds that

$$[H, U(R)] = 0\ \ \forall R\ \Rightarrow\ [H, L_i] = 0\ \ \forall i.$$

Hence, each generator L_i is a constant of motion. It also means that $[H, L_\pm] = 0$, which implies that for given l all states $|l, m\rangle$ of different m have the same energy.

To say it differently, the energy does not depend on the quantum number m. This could have been expected since for a rotationally invariant Hamiltonian all choices of quantization axis are equivalent, so projections on any quantization axis must have the same energy.

Despite the fact that $[H, L^2] = 0$, one cannot deduce that the energy must also be independent of the quantum number l. Since

$$[L^2, L_i] = 0 \quad \forall i \quad \Rightarrow \quad [L^2, U] = 0 \quad \forall U(R),$$

no transformation $U(R)$ can change the quantum number l. The fact that for the Coulomb potential the energy *is* independent of l is a special case. The Coulomb potential case has a larger symmetry ($SO(4)$) than just rotational symmetry. See Chapter 7.2 of Jones for more details.

Next we consider the space translations of R^3 as a set of continuous transformations. Recall the translation operator $T_{\vec{a}}$ that satisfies

$$T_{\vec{a}}\vec{r} = \vec{r}' = \vec{r} + \vec{a}, \quad (\vec{r}, \vec{a} \in \mathsf{R}^3).$$

Such translations also induce transformations in the space of functions of these coordinates, e.g. quantum mechanical wave functions. If one translates "everything", nothing should change:

$$\psi'(T_{\vec{a}}\, \vec{r}\,) = \psi(\vec{r}\,).$$

Hence,

$$\psi'(\vec{r}\,) = \psi(T_{\vec{a}}^{-1}\vec{r}\,) \equiv U_T(\vec{a})\psi(\vec{r}\,)$$

$U_T(\vec{a})$ is an operator acting on the wave function. Preservation of probability (or normalization) implies that it is a unitary operator. For an infinitesimal translation one finds:

$$\psi'(\vec{r}\,) = \psi(\vec{r} - \vec{a}) \approx \psi(\vec{r}\,) - \vec{a} \cdot \vec{\nabla}\psi(\vec{r}\,),$$

from which it follows that

$$U_T(\vec{a}) \approx \mathbf{1} - \frac{i}{\hbar}\vec{a} \cdot \vec{p}.$$

In other words, the momentum operators p^i are the generators of infinitesimal translations. For finite translations the translation operator is given by:

$$U_T(\vec{a}) = \exp\left(-\frac{i}{\hbar}\vec{a} \cdot \vec{p}\right).$$

If one considers a translationally invariant system, the corresponding Hamiltonian has to commute with all $U_T(\vec{a})$ and hence with the momentum operator. This means that each p^i is a constant of motion for a translationally invariant system, i.e. $d\langle\vec{p}\rangle/dt = 0$. In this way we see that translational invariance indeed implies momentum conservation.

These are examples of a general principle that invariance of a system under a set of transformation leads to conservation laws. For continuous symmetries, such as translations or rotations, the principle is known as Noether's theorem, which can be formulated as [F. Gieres, 1997]: "Covariance of the equations of motion with respect to a continuous transformation with n parameters implies the existence of n conserved quantities ("conserved charges" or "integrals of motion"), i.e. it implies conservation laws." Covariance means that the equations of motion retain their form under the transformations. In this case of continuous transformations the conserved charges are associated to conserved currents, also called Noether currents. Further information about this may be found in the course on Advanced Mechanics and/or Quantum Field Theory.

Invariances under a set of discrete transformations also lead to conservation laws, such as invariance under space reflections implies conservation of parity. Consider a Hamiltonian that is invariant under a space reflection P that acts on wave functions as $P\psi(x) = \psi(-x)$. The fact that $[H, P] = 0$, means that H and P can be diagonalized simultaneously, or in other words, they have simultaneous eigenfunctions. The eigenfunctions of P are the even and odd wave functions: $P\psi(x) = \pm\psi(x)$. Therefore, the stationary states are states of definite parity. Thus if the Hamiltonian is invariant under space reflections, then it implies that if a wave function is even (odd) under $x \to -x$, then it will remain even (odd) under time evolution. Since this concerns a discrete symmetry, there is in this case no associated conserved current.

4.4 Symmetry breaking & lifting of degeneracy

Consider (part of) the Hamiltonian describing an electron in an atom in a uniform external magnetic field $\vec{B}$:

$$H = -\frac{\hbar^2}{2m}\vec{\nabla}^{\,2} + V(|\vec{r}\,|) + \mu\vec{L}\cdot\vec{S} + \lambda(\vec{L} + 2\vec{S})\cdot\vec{B},$$

where μ, λ are some constants. Both the orbital angular momentum $\vec{L}$ and the intrinsic angular momentum or spin $\vec{S}$ transform as axial vectors. Therefore, the

spin-orbit coupling term $\propto \vec{L}\cdot\vec{S}$ is a scalar. Since the magnetic field $\vec{B}$ is an axial vector, one might be tempted to conclude that also the Zeeman term $\propto (\vec{L}+2\vec{S})\cdot\vec{B}$ is a scalar under rotations. However, from the perspective of the atom the external magnetic field $\vec{B}$ points in a fixed direction and therefore breaks the rotational invariance of the atomic system to which $\vec{L}$ and $\vec{S}$ belong. If one takes the magnetic field along the $\hat{z}$ direction, $\vec{B} = B\hat{z}$, then $(\vec{L} + 2\vec{S}) \cdot \vec{B} = B(L_z + 2S_z)$, which transforms like the z-component of an axial vector, rather than a scalar. The symmetry of the Hamiltonian is thus reduced to rotations around the magnetic field direction and reflections in the plane orthogonal to it (under which $\vec{B}$ is invariant). As a consequence of the reduced symmetry, the energy spectrum of the atom will show less degeneracy (barring accidental degeneracies).

The decomposition of reps into irreps can be used to discuss the lifting of degeneracy due to symmetry breaking. We will discuss this for the case that the symmetry is broken to a finite group of symmetry transformations.

Consider a Hamiltonian H describing an atom that is invariant under $SO(3)$ transformations. This implies that all states $|l, m\rangle$ with the same l have the same energy, i.e. there is a $(2l + 1)$-fold degeneracy. Now consider the atom as part of a crystal, with the rotational symmetry reduced to a finite point group G, that is a subgroup of $SO(3)$. The irreps of $SO(3)$ will in general not be irreps of its subgroups and one can simply calculate the decomposition of the irreps of $SO(3)$ into the irreps of G, by calculating $\langle\chi^{(\mu)}, \chi^{(l)}\rangle$ for the irreps $D^{(\mu)}$ of G and $D^{(l)}$ of $SO(3)$. Depending on the dimensionality of the irreps of G in this decomposition, one can see how the original $(2l + 1)$-fold degeneracy is lifted (barring accidental degeneracies). For example, consider a crystal with a C_3 symmetry. The irrep $D^{(1)}$ of $SO(3)$, which is equivalent to the vector rep D^V of $SO(3)$, is a reducible rep of C_3. In chapter 2 we obtained:

$$D^V \sim D^{(1)} \oplus D^{(2)} \oplus D^{(3)}.$$

Hence, the three-fold degeneracy of the $l = 1$ state of the free atom will in general be completely removed for the atom in a crystal with C_3 symmetry, yielding three $l = 1$ states with different energies. See chapter 5.3 of Jones for further discussion and examples.

In physics one encounters the breaking of symmetries very often. Symmetries are often not exact or not fully realized in nature. There are various kinds of symmetry breaking. There is so-called *explicit symmetry breaking*, as in the case of the fixed external magnetic field discussed above. The symmetry is then simply not present anymore, although often it is possible to consider the breaking to be

"small", which can then be taken into account as a correction or perturbation. Another form of symmetry breaking is called *spontaneous symmetry breaking*. In this case the ground state breaks a symmetry that is in principle present. The set of possible ground states is then itself symmetric, but each individual ground state is not. An example is a ferromagnet in which unpaired electron spins become aligned at low temperatures, leading to a nonzero magnetization in a certain direction. Any direction can appear in principle and all have the same energy, but by selecting a direction, the rotational invariance of the system is 'spontaneously' broken. Spontaneous symmetry breaking also occurs in particle physics, such as in the strong interaction (Nobel Prize in Physics 2008 for Y. Nambu) and in the Higgs mechanism (Nobel Prize in Physics 2013 for F. Englert & P. Higgs). Another form of symmetry breaking is *anomalous symmetry breaking*, in which a classical symmetry is broken at the quantum level.

Appendix A

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