Lecture Notes

Fall 2025

Group Theory

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Contents

Books on Group Theory useful for Physicists

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Part I

Finite Groups

Chapter 1

Definition and some examples of groups

Group theory provides the mathematical framework to describe and classify symmetries. Mankind has always been fascinated by symmetries[1]. One would thus expect that a theory of symmetries was constructed long ago, but, rather surprisingly, it was only recently constructed: in mathematics during the nineteenth century (the formal definition of a group was formulated in 1854 by Cayley), and in physics during the twentieth century (Poincaré completed Lorentz's transformations in 1904 by requiring that they form a group, Einstein found the symmetries of Special Relativity in 1905, and when Quantum Mechanics was constructed in 1925 and 1926, group theory was used to construct wavefunctions for many-electron systems).

The history of how the concept of group emerged is fascinating, but many readers, and most young readers, are not interested in the history of science, but prefer to cut to the chase. So we shall postpone describing the sources from which group theory flowed till the next chapter, and start right away in this chapter by giving the modern definition of a group (actually, more than one definition, but they are all equivalent).

1.1 Definition of a group

We shall now first give the standard abstract definition of a group, and afterwards present some examples of groups. There are other equivalent definitions of a group, and as an example we shall present the definition of a group based on "cancellations". As always with a definition of a mathematical concept, one should impose enough requirements so that one can prove nontrivial theorems, but not too many in order not to exclude interesting cases. In the case of group theory one is in the fortunate position that four seemingly weak and obvious requirements allow on the one hand many interesting theorems to be proven, and on the other hand many important physical systems to be described.

[1]Symmetries in decorations (for example, the 17 ways the Moors tiled planes or the 7 patterns of friezes of the Andeans), symmetries of geometrical objects (the 5 Platonic solids or the 14 Bravais lattices in three dimensional space or the 230 space crystallographic groups and the 17 plane crystallographic groups).

Definition of a group: A group G consists of a (finite or infinite) set of objects (called group elements), together with a law of composition $\otimes$ (called group multiplication, we shall soon drop the symbol $\otimes$) with the following four properties (also called group postulates):

(i) **closure**: if a and b are elements of G, then also $a \otimes b$ is an element of G. (Here b may be equal to a.)

(ii) **unit element**: there exists a group element e such that $e \otimes a = a \otimes e = a$ for all a in G.

(iii) **inverses**: for every element a in G there exists another element in G, denoted by a^{-1}, such that $a \otimes a^{-1} = a^{-1} \otimes a = e$. (Here a^{-1} may be equal to a.)

(iv) **associativity**: for any three elements a, b, c of G one has $a \otimes (b \otimes c) = (a \otimes b) \otimes c$. (Here some or all of a, b, c may be equal.)

The unit element is unique. Suppose there are two unit elements e and f. Then $ea = fa = a$, hence, by post multiplying with a^{-1}, $e = f$. Similarly one proves that the inverse elements are unique. Suppose $a^{-1}a = e$ and $b^{-1}a = e$. Then by right multiplication with a^{-1} one finds $a^{-1} = b^{-1}$. Group multiplication can take many forms: it may be equal to ordinary addition or multiplication, or multiplication of natural numbers modulo p (p a prime number), or it can be a particular operation, for example unions and intersections of sets. For physicists (and much of this course) it usually amounts to matrix multiplication, with matrices representing the abstract group elements. In what follows, we omit the symbol $\otimes$ in $a \otimes b$ and simply write ab.

If for all elements $ab = ba$, the group is called **abelian**[2]. Otherwise it is called **nonabelian**. There exist finite groups (groups with a finite number of elements), and infinite groups. There are many kinds of infinite groups: discrete infinite groups (such as translations on a lattice) and continuous infinite groups (such as rotations). A particular kind of continuous infinite groups which we shall discuss in detail, are the **Lie groups**.

In the building up of a group one encounters various systems with fewer postulates. We quote here a few but we will not study any of them in more detail, for a reference see [1].

Groupoïds: Only closure holds.

Semigroups: Closure plus associativity, but no unit or inverses.

Quasigroups: Closure and the equations $ax = b$ and $ya = b$ have for given a, b unique solutions x, y, but no associativity nor a unit element.

Loops: Quasigroups with an unit element.

Cancellation Semigroups: Semigroups with left- and right-cancellation properties.

Note: Different authors use different definitions.

[2] Named after the Norwegian mathematician Niels Henrik Abel, 1802–1829.

Comment 1. The four postulates were relatively late identified as postulates because in the particular models studied in the beginning, some properties were so obvious that they were not identified as postulates.

- the existence of an inverse was central in number theory (18th century)
- closure was a central issue for Galois (1830), who also introduced the term group
- the need for a postulate of an identity (in permutation groups) was noted by Cauchy in 1854
- the postulate of associativity was explicitly introduced by Cayley (1854). (In the particular models which were studied, associativity was automatically satisfied, so only when abstract groups were studied was the need for associativity noted.)

Comment 2: Associativity. The associative law $(ab)c = a(bc)$ was only imposed for three elements, and it states that in the expressions $a(bc)$ and $(ab)c$ one may omit the brackets. However, it implies that also in all more complicated expressions such as $[(ab)c][(de)(fg)]$ one may omit all brackets. For example this expression is equal to the expression $[(a(bc))d][e(fg)]$. To prove the assertion that one may omit all brackets in products of group elements, use induction w.r.t. the number of group elements. For three group elements the claim holds because it is a group postulate. For expressions with $n+1$ group elements, assume associativity holds for n elements. We shall show that one can always write two different expressions in the form of $B_1(B_2B_3)$ and $(B_1B_2)B_3$. Since B_1, B_2, B_3 are group elements, we can conclude that $(B_1B_2)B_3 = B_1(B_2B_3)$. Thus one may indeed omit all brackets in products of any number of group elements.

Let us now prove that two different expressions of $n+1$ group elements can always be written as $B_1(B_2B_3)$ and $(B_1B_2)B_3$. How does one multiply n elements? Since a binary operation allows multiplication of only two elements at a time, one first chooses a pair of adjacent a's and multiplies them; then, either one multiplies this new element by an a adjacent to it or one chooses two other adjacent a's and multiplies them. With each choice, the total number of factors decreases by one, so that eventually one is left with only two factors. Suppose now that

$$X = (a_1 \cdots a_i)(a_{i+1} \cdots a_n) \qquad \text{and} \qquad Y = (a_1 \cdots a_j)(a_{j+1} \cdots a_n) \tag{1.1}$$

are elements of G obtained by two people multiplying the a's together, each having made their own choices. The parentheses indicate the final multiplication each has just performed. For notational convenience, we assume that $i \leq j$. Since each of the final factors in X and in Y contains less than n of the a, the inductive hypothesis allows us to rearrange parentheses in them. Therefore, we may assume $i < j$ (or we are done) and write

$$X = (a_1 \cdots a_i)(a_{i+1} \cdots a_j)(a_{j+1} \cdots a_n) \quad \text{and} \quad Y = (a_1 \cdots a_i)(a_{i+1} \cdots a_j)(a_{j+1} \cdots a_n)\,. \tag{1.2}$$

If we denote $(a_1 \cdots a_i)$ by B_1, $(a_{i+1} \cdots a_j)$ by B_2 and $(a_{j+1} \cdots a_n)$ by B_3 we have $X = B_1(B_2B_3)$ and $Y = (B_1B_2)B_3$. Associativity then yields $X = Y$. (Rothman page 6.)

Comment 3: Left-units and left-inverses are enough. One can sharpen the definition of a group. Consider first finite groups. We claim that it is sufficient to require the existence of a left unit e_L and left inverses a_L^{-1}. Then, as we shall prove, e_L is also the right-unit e_R, and a_L^{-1} is also the right inverse a_R^{-1}. (Of course, the same is true if one interchanges left and right.)

Proof: We have $e_L a = a$ and $a_L^{-1} a = e_L$ for all a in G. We begin with proving that $e_L = e_R$ because we will need this in the proof that $a_L^{-1} = a_R^{-1}$. Consider now the set aG. We claim that all elements of aG are different. Indeed if $ag_1 = ag_2$, then by multiplying on the left with a_L^{-1} we obtain $g_1 = g_2$. Because the total number of elements of G, and thus also of aG, is finite, and all elements of aG are different, the set aG is a **permutation** of all elements of G. Given an element a in G, one must find this element a also in the set aG, so $ag = a$ for some g. But then multiplying on the left with a_L^{-1} yields $g = e_L$. So $ae_L = a$ for all a, and thus $e_L = e_R \equiv e$.

Similarly one must find the element e_L among the set aG, so $ag' = e_L$ for some g' in G. Multiplying again by a_L^{-1} on the left, and using $e_L = e_R$ we now obtain $g' = a_L^{-1} e_L = a_L^{-1} e_R = a_L^{-1}$. So $aa_L^{-1} = e$, and this proves that a_L^{-1} is also the right inverse: $a_L^{-1} = a_R^{-1} \equiv a^{-1}$.

In the proof we used the fact that for a finite group G the set aG is a permutation of all elements of G. It is interesting to ask whether the theorem is still true for infinite groups. One might wonder whether for infinite groups with only a left-unit and left-inverses the set aG is still equal to the set G. If for a given a one can always find any other element b among the set of elements aG, then one can solve the equation $ax = b$ with given a and b for suitable x, and then one can repeat the reasoning we presented above for finite groups. We shall prove that if a set G has a binary associative operation $\otimes$ (so closure and associativity hold), and if there exists a left-unit and a left-inverse for every group element, then the left-unit is also the right-unit, and the left-inverses are also right-inverses. Then we have a full group and then $gG = G$, because the equation $gg_1 = g_2$ has for any given g and g_2 a (unique) solution for g_1, namely $g_1 = g^{-1} g_2$.

Proof of $\boldsymbol{ae = ea}$. Given $ea = a$ and $a^{-1}a = e$ consider

$$a^{-1}(aa^{-1})a = (a^{-1}a)(a^{-1}a) = ee = e = a^{-1}a = a^{-1}(a^{-1}a)a\,. \tag{1.3}$$

Since $a^{-1} \in G$, it has a left inverse; acting with this left-inverse from the left yields

$$(aa^{-1})a = (a^{-1}a)a\,. \tag{1.4}$$

Then

$$ae = a(a^{-1}a) = (aa^{-1})a = (a^{-1}a)a = ea\,. \tag{1.5}$$

So $ae = ea$.

Proof of $\boldsymbol{aa^{-1} = a^{-1}a}$. Consider

$$(aa^{-1}) = a(a^{-1}a)a^{-1} = (aa^{-1})(aa^{-1})\,. \tag{1.6}$$

Since $aa^{-1} \in G$, it has a left-inverse; acting with it from the left yields

$$e = e(aa^{-1}) = aa^{-1}\,. \tag{1.7}$$

So $a^{-1}a = aa^{-1} = e$.

Comment 4: Right and left cancellations. In early studies of group theory (Cayley, Kronecker) an alternative definition of a **finite** group was used. This definition is no longer used, and for a first reading one may skip the following discussion. However, the whole of group theory is based on its postulates, so a deeper study of these postulates is warranted. Consider then the following group postulates:

(a) closure
(b) associativity
(c) right cancellation holds: if for any a, b and x, one has $ax = bx$, then this implies that $a = b$. (Equivalently, if $a \neq b$ then $ax \neq bx$ for all x.)
(d) left cancellation holds: if for any a, b, y one has $ya = yb$, then this implies that $a = b$. (Equivalently, if $a \neq b$ then $ya \neq yb$ for all y.)

The proof that for finite groups this set of four postulates is equivalent to the usual set of four postulates is based on the observation that for a finite group G the set of elements $G' = Gc$ is equal to the set of elements G. Indeed if G contains $G = \{a_1, a_2, \ldots, a_n\}$ then the elements of $G' = \{a_1c, a_2c, \ldots, a_nc\}$ are all different by postulate (c). Then, since the set of elements of G' is the same as the set of elements G, for any a_k in G there must be an element a_jc in G' such that $a_jc = a_k$. Similarly the set cG is equal to the set G by postulate (d).

We shall use these properties to first prove the existence of a unique unit element and then the existence of unique inverse elements a^{-1} for all a. The proof is surprisingly subtle. To prove the existence of a unit element we begin by noting that for given x and a there are always unique elements a_x^L and a_x^R satisfying

$$a_x^L a = x\,; \qquad a a_x^R = x \tag{1.8}$$

The subscript x in a_x^L and a_x^R indicates that these group elements in general depend on the choice of a and x. The uniqueness of a_x^L and a_x^R follows from right and left cancellations, respectively. Then we find for the particular case $x = a$ the following equations

$$a_e^L a = a\,; \qquad a a_e^R = a \tag{1.9}$$

where the subscript e indicates we hope to prove that a_e^L and a_e^R are equal to the unit element. To prove this, multiply x in (1.8) by a_e^L and a_e^R as follows

$$\begin{aligned} a_e^L x &= a_e^L(a a_x^R) = (a_e^L a) a_x^R = a a_x^R = x \\ x a_e^R &= (a_x^L a) a_e^R = a_x^L (a a_e^R) = a_x^L a = x\,. \end{aligned} \tag{1.10}$$

Thus, since x is an arbitrary group element, a_e^L is independent of a, and is the left unit, and similarly a_e^R is independent of a and is the right unit. To prove that they are equal, we take $x = a_e^L$ in $xa_e^R = x$ to obtain

$$a_e^L a_e^R = a_e^L \quad \text{but also} \quad a_e^L a_e^R = a_e^R \quad (\text{since } a_e^L x = x) \tag{1.11}$$

Thus $a_e^L = a_e^R = e$. The uniqueness of the unit element follows from the cancellation axioms: $ae = af$ implies $e = f$.

To prove the existence of a unique inverse we go back to $a_x^L a = x$ and $aa_x^R = x$ but now we take x equal to e, and denote for this case a_x^L by a_L^{-1} and a_x^R by a_R^{-1}. This notation suggests the next steps to be taken. We have

$$a_L^{-1} a = e\,; \qquad aa_R^{-1} = e \tag{1.12}$$

and post multiplying the first relation by a_R^{-1}, and premultiplying the second relation by a_L^{-1}, yields

$$\left.\begin{aligned} (a_L^{-1}a)a_R^{-1} = a_L^{-1}aa_R^{-1} = a_R^{-1} \\ a_L^{-1}(aa_R^{-1}) = a_L^{-1}aa_R^{-1} = a_L^{-1} \end{aligned}\right\} \text{hence } a_L^{-1} = a_R^{-1} = a^{-1}\,. \tag{1.13}$$

The uniqueness follows again from the cancellation axioms: if $aa^{-1} = ab^{-1}$, then $a^{-1} = b^{-1}$.

However, the equivalence of the axioms in comment 4 and the usual axioms can be violated for infinite groups. For example, the set of positive integers with group multiplication equal to ordinary multiplication satisfies closure, associativity, and the properties of left- and right- cancellation, but this set does not form a group since there are no inverses which are still integers. On the other hand, the set of positive rational numbers G is the same set as Gc for c a rational number, and in this case both criteria for forming a group are satisfied.

We shall not use the theorems in comment 3 and comment 4. Their practical value is small, but they illustrate in a beautiful way the necessity and the subtle interplay of the group postulates. For the interested reader we give two exercises.

Exercise. Does the existence of a left-unit and a right-inverse for a set G with a binary associative operation $\otimes$ always yield a group? *Answer:* No. Counterexample: define $x \otimes y = y$ for all x and y in G. Any x is left-unit, and $x^{-1} = e$ is right-inverse since $xe = e$, but this is of course not a group [2].

Exercise. Is left cancellation, instead of left cancellation and right cancellation, enough to define a group?

1.2 Examples of groups

We give now a few examples of finite groups and infinite groups. In future chapters we shall encounter many more groups, but the examples we have chosen give a preview of what is to come.

1.2.1 A finite group: discrete rotations in $\mathbb{R}^3$

Consider the rotations $R_x(\phi)$, $R_y(\phi)$, $R_z(\phi)$ around the x, y, z axis over an angle $\phi = \pi$. Drawing pictures or using the matrix representations

$$a = R_x(\pi) = \begin{pmatrix} 1 & & \\ & -1 & \\ & & -1 \end{pmatrix}; \quad b = R_y(\pi) = \begin{pmatrix} -1 & & \\ & 1 & \\ & & -1 \end{pmatrix}; \quad c = R_z(\pi) = \begin{pmatrix} -1 & & \\ & -1 & \\ & & 1 \end{pmatrix} \tag{1.14}$$

it is clear that $R_x(\pi)R_y(\pi) = R_y(\pi)R_z(\pi)$ and cyclic. Further $R_x(\pi)R_x(\pi) = I$ so we add the unit element (of course). Together with the unit element $e = I$ we get a finite abelian group of dimension 4

$$\begin{gathered} ea = a, \text{ etc}, \quad ab = ba = c, \quad bc = cb = a, \quad ca = ac = b \\ a^2 = b^2 = c^2 = e\,. \end{gathered} \tag{1.15}$$

This was one of the first groups to be studied. It is called the group of four, or Klein's group (due to the German mathematician Felix Klein), and denoted by V (four = vier in German, and Vierergruppe means group of four).

Now add rotations over $\phi = \frac{\pi}{2}$ and $\phi = \frac{3\pi}{2}$. The latter is the same as a rotation over $\phi = -\frac{\pi}{2}$ since a rotation over 2π yields the identity. Drawing pictures gets confusing, so we use matrices

$$\begin{gathered} R_x\left(\tfrac{\pi}{2}\right) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}; \quad R_y\left(\tfrac{\pi}{2}\right) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{pmatrix}; \quad R_z\left(\tfrac{\pi}{2}\right) = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \\ R_x\left(-\tfrac{\pi}{2}\right) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix}; \quad R_y\left(-\tfrac{\pi}{2}\right) = \begin{pmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}; \quad R_z\left(-\tfrac{\pi}{2}\right) = \begin{pmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{gathered} \tag{1.16}$$

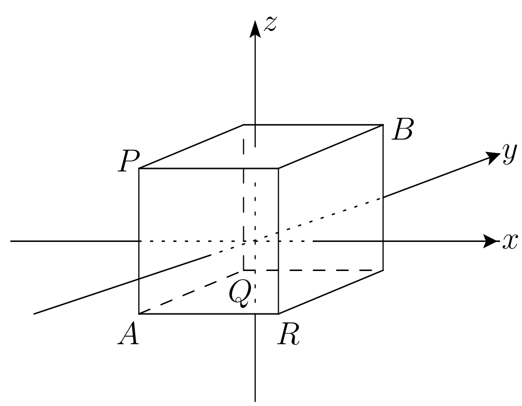
We take the active point of view: these matrices rotate vectors but the coordinate axes are left fixed. To check signs, act with $R_y\left(\frac{\pi}{2}\right)$ on a vector $\left(\begin{smallmatrix} 1 \\ 0 \\ 0 \end{smallmatrix}\right)$ along the x-axis; this yields the vector $\left(\begin{smallmatrix} 0 \\ 0 \\ -1 \end{smallmatrix}\right)$ along the minus z-axis, confirming that $R_y\left(\frac{\pi}{2}\right)$ is a clockwise rotation along the y-axis over an angle $\frac{\pi}{2}$. All 10 matrices (including the unit matrix) are orthogonal and have $\det R = 1$, so they are rotations.

Do they close? Let's check. We multiply a few pairs

$$
\begin{aligned}
R_z(\pi)R_x\left(\tfrac{\pi}{2}\right) &= \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} = R_{yz}(\pi)\,, \\
R_z\left(\tfrac{\pi}{2}\right)R_x\left(\tfrac{\pi}{2}\right) &= \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} = R_{xyz}\left(\tfrac{2\pi}{3}\right)\,.
\end{aligned}
\tag{1.17}
$$

In the first case we get a rotation along an axis $\left(\begin{smallmatrix}0\\1\\1\end{smallmatrix}\right)$ in the $+y,+z$ plane over an angle π; this rotation maps a vector along the x-axis to minus itself (consider the plane through the rotation axis $(0,1,1)$ and the x-axis), and it interchanges two vectors along the y and z axes. In the second case we get a rotation along an axis pointing in the $\left(\begin{smallmatrix}1\\1\\1\end{smallmatrix}\right)$ direction (between the $+x,+y$ and $+z$ direction) which maps $\vec{e}_x$ to $\vec{e}_y$, $\vec{e}_y$ to $\vec{e}_z$, and $\vec{e}_z$ to $\vec{e}_x$; looking at a picture we see that this is a clockwise rotation along the axes $\left(\begin{smallmatrix}1\\1\\1\end{smallmatrix}\right)$ over $\phi=\frac{2\pi}{3}$.

It gets complicated to work out all matrix products, but in this case we can use a geometric realization. Consider a cube. There are I) rotations about an axis through the middles of two opposite faces, or II) about diagonals such as AB, and III) about an axis connecting the middle of two opposite edges.



- There are 9 proper rotations about the axes through two faces, these are our previous R_x, R_y, R_z over $\phi=-\frac{\pi}{2},\pi,\frac{\pi}{2}$.

- There are 8 vertices, so 4 diagonals, (for example the diagonal from A to B) and for each diagonal two proper rotations (rotating P to Q, Q to R and R to P, or the other way round). In total 8 diagonal rotations. There are our previous rotations $R_{\pm x,\pm y,\pm z}\left(\frac{2\pi}{3} \text{ or } -\frac{2\pi}{3}\right)$. These are 8, not 16 rotations because for example $R_{x,y,z}\left(\frac{2\pi}{3}\right)=R_{-x,-y,-z}\left(-\frac{2\pi}{3}\right)$.

- Finally the rotations over π about axes through the middle of two opposite edges. There are 12 edges, so 6 "edge-diagonals", and thus 6 rotations of the cube. These are the matrices $R_{xy}(\pi)$, $R_{yz}(\pi)$, $R_{zx}(\pi)$ and $R_{-xy}(\pi)$, $R_{-yz}(\pi)$, $R_{-zx}(\pi)$.

These are all rotational symmetries of the cube. It follows that they form a group. The total number of group elements is $9 + 8 + 6 + 1$(for the unit)$= 24$. The group S_4 of the permutations of 4 objects has also 24 elements, so one is tempted to identify the group of rotations of the cube with S_4. This is correct: the group of rotations of the cube is isomorphic (has the same group multiplication table) to S_4.

$$R_{\text{rot}}(\text{cube}) = S_4 \,. \tag{1.18}$$

To see this, choose as carrier space (the space on which the rotations act) the 4 pairs of opposite vertices. The 24 rotations permute these 4 pairs in different pairs, so they form the group S_4.

There are also 24 ordinary and generalized reflections which map the cube into itself. They can be obtained by taking any rotation followed (or preceded) by a space inversion ($\vec{r} \to -\vec{r}$). Six of them can also be obtained by reflection about a place through two opposite edges, three more by reflection about the xy, yz, xz planes, but the remaining three are not reflections about any plane.

1.2.2 Lie groups defined by matrices

We shall study many matrix groups in this course, but here we pick a few to illustrate some general aspects. In all cases we shall consider **transformation groups** which act on **carrier spaces**. The carrier space will be the vectors in a linear vector space $\mathbb{R}^N$ (or $\mathbb{C}^N$ or $\mathbb{R}^{2N}$ or $\mathbb{C}^{2N}$), and we shall require that certain quadratic **forms** are invariant under group transformations. If one transformation leaves a form invariant, and the second does as well, then the product (first acting with one, then with the second) leaves the form invariant, thus **transformation groups guarantee closure** (when the product of two group elements is not yet a group element, add it to implement closure). Associativity, and the existence of unit and inverse group elements are also obvious, hence transformation groups are an excellent way to discover groups. One needs a bit more knowledge of matrix theory than is common, but we review it in the appendices.

Orthogonal groups. $\boldsymbol{SO(N)}$. Let $x' = Ox$ be a set of linear transformations, and require that the bilinear form $x \cdot x = \sum_{ij} x^i \delta_{ij} x^j$ is invariant.

$$x' \cdot x' = x \cdot x \tag{1.19}$$

Then $x^T O^T O x = x^T x$, but one cannot yet conclude that $O^T O = I$; for that we need $x^T O^T O y = x^T y$ with arbitrary x and y. But consider

$$\begin{aligned} (x' + y') \cdot (x' + y') &= x' \cdot x' + y' \cdot y' + x' \cdot y' + y' \cdot x' \\ (x + y) \cdot (x + y) &= x \cdot x + y \cdot y + x \cdot y + y \cdot x \end{aligned} \tag{1.20}$$

Since $x' \cdot x' = x \cdot x$ and $y' \cdot y' = y \cdot y$, and $x' \cdot y' = y' \cdot x'$ and $x \cdot y = y \cdot x$, we find

$$x' \cdot y' = x \cdot y \quad \Rightarrow \quad x^T O^T O y = x^T y \quad \Rightarrow \quad O^T O = I\,. \tag{1.21}$$

All matrices satisfying $O^T O = I$ are called orthogonal matrices, and they form a group because $O^{-1} = O^T$ is orthogonal ($(O^T)^T O^T = I$). We get the group

$$O(N, C) \text{ or } O(N, R) \tag{1.22}$$

depending on whether their entries are complex or real. Since $O^T O = I$, we deduce that $\det O = \pm 1$. All matrices with $\det O = +1$ form a subgroup denoted by $SO(N, C)$ or $SO(N, R)$ (because $\det(O_I O_{II}) = \det O_I \det O_{II} = +1$). The letter S stands for special and denotes that the determinant is one. Thus the space of group elements of $O(N, C$ or $R)$ is the union of two disjointed components

$$\boxed{O(N)} = \boxed{SO(N)} \cup \boxed{O(N) \text{ with } \det O = -1} \tag{1.23}$$

Comment. We used δ_{ij} in $x \cdot x$ to define $O(N)$, but one can begin more generally with a real or complex symmetric matrix H_{ij}. If it is real it can be diagonalized with an orthogonal matrix but if it is complex, it can first be transformed to a real diagonal matrix by $H \to U H U^T$ where U is a special unitary matrix. (Autonne-Takagi factorization. See appendix 1.II for a proof.) Requiring that the metric H_{ij} be nonsingular, the diagonal matrix D has the form $\begin{pmatrix} 1 & & & & & \\ & \ddots & & & & \\ & & 1 & & & \\ & & & -1 & & \\ & & & & \ddots & \\ & & & & & -1 \end{pmatrix} = \eta_{ij}$ (after scaling it as $S^T D S = D'$ with diagonal real matrices) with p plus signs and q minus signs ($p + q = N$). Then the quadratic form becomes $x^T \eta x$ and group elements must satisfy $O^T \eta O = \eta$. This yields the groups $O(p, q, C)$ or $O(p, q, R)$. We still find that $(\det O)^2 = 1$, and for $\det O = +1$ we get the groups $SO(p, q, C)$ and $SO(p, q, R)$.

Unitary groups. $\boldsymbol{SU(N)}$. Now consider a sesquilinear (half-linear) form $x \cdot x = \sum (x^i)^* x^i$. A more precise notation would be: $\bar{x} \cdot x = \bar{x}_i \delta^i{}_j x^j$ (summation over i, j understood), where $\bar{x}_i = (x^i)^*$, but we shall use instead the notation $x \cdot x$. We define again $x' = Ux$ with x complex vectors in $\mathbb{C}^N$ with inner product $x \cdot y$. We require that lengths are preserved.

$$x' \cdot x' = x \cdot x \quad \Rightarrow \quad x^\dagger U^\dagger U x = x^\dagger x\,. \tag{1.24}$$

Again we need $x^\dagger U^\dagger U y = x^\dagger y$ to conclude that $U^\dagger U = I$, but now $x \cdot y \neq y \cdot x$. But consider $x + \alpha y$ where α can be real or complex. Then

$$\begin{aligned} (x' + \alpha y') \cdot (x' + \alpha y') &= x' \cdot x' + \alpha^* \alpha (y' \cdot y') + \alpha (x' \cdot y') + \alpha^* (y' \cdot x') \\ (x + \alpha y) \cdot (x + \alpha y) &= x \cdot x + \alpha^* \alpha (y \cdot y) + \alpha (x \cdot y) + \alpha^* (y \cdot x) \end{aligned} \tag{1.25}$$

The diagonal terms are equal, see (1.24). For the off-diagonal term taking $\alpha = 1$ gives one set of relations, and taking $\alpha = i$ gives another set. Together they imply that $x' \cdot y' = x \cdot y$, so $U^\dagger U = I$. It follows from $U^\dagger U = I$ that $\det U \neq 0$, so inverses exist and $U^{-1} = U^\dagger$. It follows that the inverse group element U^{-1} is again unitary. We have a group $U(N, C)$ (but $U(N, R) = O(N, R)$). Again the requirement that $\det U = 1$ yields the subgroup $SU(N) = SU(N, C)$ (and $SU(N, R) = SO(N, R)$). Because $U(N, R) = O(N, R)$ and $SU(N, R) = SO(N, R)$ one usually denotes $U(N, C)$ by $U(N)$ and $SU(N, C)$ by $SU(N)$.

Comment. We could have started from $x \cdot x = (x^i)^* \eta_{ij} x^j$, and this yields the groups $U(p, q, C)$ and $SU(p, q, C)$ with $p + q = N$. They are usually denoted by $U(p, q)$ and $SU(p, q)$, respectively.

Symplectic groups. *Sp*(2*N*). Instead of $x^i \delta_{ij} y^j$, introduce an antisymmetric $2N \times 2N$ matrix $\Omega_{ij} = \left(\begin{smallmatrix} 0 & I \\ -I & 0 \end{smallmatrix}\right)$ and require that the bilinear $x\Omega y = x^i \Omega_{ij} y^j$ with real or complex x and y be invariant under $x \to x' = Mx$. (We cannot require that $x\Omega x$ is invariant because it vanishes due to antisymmetry of Ω.) We then find

$$x'\Omega y' = x\Omega y \quad \Rightarrow \quad x^T M^T \Omega M y = x^T \Omega y \quad \Rightarrow \quad \boxed{M^T \Omega M = \Omega}. \tag{1.26}$$

The matrices M satisfying this relation are called symplectic matrices. Since for any $N \times N$ antisymmetric matrix A one has $\det A = \det A^T = (-1)^N \det A$, we must consider $2N \times 2N$ matrices M. From (1.26) it follows that $\det M \neq 0$. For complex M these matrices form the group $Sp(2N, C)$. Closure holds because we have a transformation group, the unit element is I, and M^{-1} is again symplectic because multiplying $M^T \Omega M = \Omega$ by $M^{-1,T}$ and M^{-1} yields $\Omega = (M^T)^{-1} \Omega M^{-1}$ which proves that M^{-1} is symplectic. Requiring that M be real yields the group $Sp(2N, R)$. From (1.26) it follows that $(\det M)^2 = 1$. In fact, as we show in appendix 1.III, for $Sp(2N, C)$ (and thus a fortiori for $Sp(2N, R)$) one always has $\det M = 1$. So there is no subgroup $SSp(2N, C)$ or $SSp(2N, R)$.

Comment. One can begin with an arbitrary real or complex antisymmetric matrix A, but then there exists a unitary matrix U such that $UAU^T = \Omega$. So using Ω does not lose generality. For a proof see appendix 1.II.

Comment. Often one uses another form of the symplectic metric:

$$\Omega_2 = \begin{pmatrix} \begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix} & & \\ & \begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix} & \\ & & \ddots \end{pmatrix}_{2N \times 2N}. \tag{1.27}$$

The relation to $\Omega_1 = \left(\begin{smallmatrix} 0 & I \\ -I & 0 \end{smallmatrix}\right)_{2N\times 2N}$ is $\Omega_2 T = T\Omega_1$ where the similarity matrix T is real, symmetric and orthogonal: $T = T^T = T^{-1}$, and given by[3]

$$T(2N) = \left(\begin{array}{c|c} \begin{smallmatrix} 1 & 0 & \cdot & \cdot & \cdot \\ 0 & \cdot & \cdot & \cdot & \cdot \\ 0 & 1 & 0 & \cdot & \cdot \end{smallmatrix} & \begin{smallmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ 1 & 0 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{smallmatrix} \\ \vdots & \vdots \\ \hline \vdots & \vdots \\ \vdots & \vdots \\ 0 \; \cdot \; \cdot \; \cdot \; \cdot & \cdot \; \cdot \; \cdot \; \cdot \; 1 \end{array}\right)_{2N\times 2N} \quad ; \qquad T(4) = \left(\begin{array}{c|c} \begin{smallmatrix} 1 & 0 \\ 0 & 0 \end{smallmatrix} & \begin{smallmatrix} 0 & 0 \\ 1 & 0 \end{smallmatrix} \\ \hline \begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix} & \begin{smallmatrix} 0 & 0 \\ 0 & 1 \end{smallmatrix} \end{array}\right)_{4\times 4} . \tag{1.28}$$

USp(2N). The groups $SO(N,R)$ and $SU(N)$ are compact (meaning, for now at least, that their entries are bounded: $|\alpha_{ij}| \leq 1$). However, $Sp(2N,C)$ and $Sp(2N,R)$ are not compact. Compact groups play a preferred role in physics, and are also easier to deal with. To get a compact symplectic group, we can take the **intersection** of $Sp(2N,C)$ and $SU(2N)$ (or $U(2N)$ because $\det M = 1$ for $Sp(2N,C)$). This yields the compact group $USp(2N)$. These matrices are complex, so $USp(2N,C)$. The matrices $USp(2N,R)$ are the intersection of $Sp(2N,R)$ with $SU(2N,R) = SO(2N,R)$, so these are the real $2N\times 2N$ matrices that are both symplectic and orthogonal. Matrices near the unit element can always be written as exponentials

$$M = e^m \, . \tag{1.29}$$

Then one can consider the special case that m is small, expand the exponent, and keep only terms linear in m. For symplectic matrices (real or complex) this yields $M = I + m + \mathcal{O}(m^2)$ and

$$m^T\Omega + \Omega m = 0\, ; \quad m = \begin{pmatrix} A & B \\ C & D \end{pmatrix} \quad \Rightarrow \quad \begin{array}{l} B - B^T = 0 \\ C - C^T = 0 \\ A + D^T = 0 \end{array} \tag{1.30}$$

where A, B, C and D are $N\times N$ matrices. If the matrices m are also orthogonal we also get

$$m^T + m = 0 \quad \Rightarrow \quad A^T + A = 0\, ; \quad D^T + D = 0\, ; \quad B + C^T = 0\, . \tag{1.31}$$

The resulting set of matrices has the following form

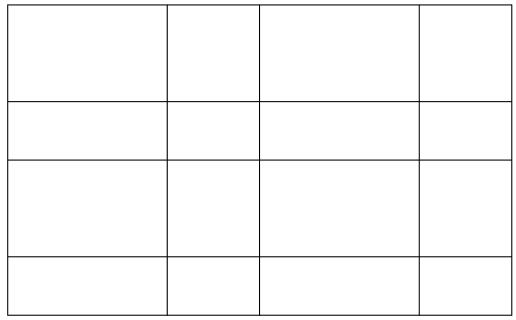
$$m = \begin{pmatrix} A & S \\ -S & A \end{pmatrix} \tag{1.32}$$

with A antisymmetric and real and S symmetric and real for $OSp(2N,R)$. For $USp(2N,C)$ both A and S are complex. Exponentiating these matrices gives the group elements of $USp(2N)$ or $OSp(2N)$.

---

[3] Relabeling rows and columns as $123456\cdots \to 135\cdots|246\cdots$ amounts to $e_1 \to e_1$, $e_2 \to e_{N+1}$, $e_3 \to e_2$, $e_4 \to e_{N+2}$, etc. This yields T.

Comment 1. If one takes the intersection of $SU(p,q)$ and $Sp(2N,C)$ one gets the group $USp(p,q,C)$. Its matrices have the form of 16 blocks of size $p\times p$, $p\times q$, $q\times p$ and $q\times q$.



(1.33)

Comment2 . The word symplectic means "composed" in Greek. Since $\Omega^2=-I$, Ω looks like $i=\sqrt{-1}$ (where the letter i stands for imaginary, introduced by Descartes), but since the word complex (meaning composed in Latin, complex numbers $a+bi$ are composed numbers in an Argand diagram) was already used, Weyl translated the word complex from Latin to Greek, obtaining symplectic.

Comment 3. Canonical transformations $\hat{x}=X(x,p,t)$ and $\hat{p}=P(x,p,t)$ preserve by definition the canonical commutation relations. Symplectic transformations preserve by definition the Poisson brackets. It follows that a transformation is canonical iff it is symplectic, see appendix to chapter 6 in [3]

$$J^T\Omega J=\Omega \qquad \text{where } J=\begin{pmatrix} \frac{\partial X}{\partial x} & \frac{\partial X}{\partial p} \\ \frac{\partial P}{\partial x} & \frac{\partial P}{\partial p} \end{pmatrix} \tag{1.34}$$

Comment 4. There exist also superalgebras which are denoted by $OSp(M|2N)$, but they have nothing to do with the matrices of $OSp(2N)$. They have orthogonal matrices $SO(M,R)$ and symplectic matrices $Sp(2N,R)$ along the diagonal, and leave the bilinear form $x^i\delta_{ij}x^j+\theta^\alpha C_{\alpha\beta}\theta^\beta$ invariant, where $C_{\alpha\beta}$ is the charge conjugation matrix and θ^α are anticommuting coordinates.

1.2.3 A group of sets

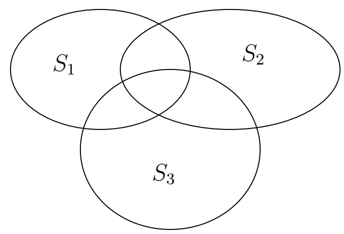
Only to show that group multiplication need not be ordinary multiplication or matrix multiplication, we construct an example with sets. Consider a set Σ and all its subsets S_J including the whole set Σ and the empty set $\varnothing$. Multiplication of two sets S_1 and S_2 can be defined as the union of sets $S_1\cup S_2$, or one can take the intersection $S_1\cap S_2$, or, as a third case, one can define group multiplication of two sets S_1 and S_2 as the union from which the intersection is removed

$$S_1\otimes S_2=(S_1\cup S_2)/(S_1\cap S_2)\,. \tag{1.35}$$

The operator $*$ defined by $S_1\otimes S_2=S_1\cup S_2$ does not yield a group because although there is a unit element ($\varnothing$, the empty set, which satisfies $S\cup\varnothing=\varnothing\cup S=S$), there is not always an inverse ($S^{-1} \otimes S = S^{-1} \cup S = \varnothing$ has no solution if S is not empty). Associativity holds.

The definition of $S_1 \otimes S_2 = S_1 \cap S_2$ does not yield a group either because again a unit element exists ($e = \Sigma$ because $S_1 \cap \Sigma = \Sigma \cap S_1 = S_1$), but no inverses exist ($S^{-1} \otimes S = S^{-1} \cap S = \Sigma$ has no solution because $S \cap S^{-1}$ is not larger than S, so for no S^{-1} does one get $S \cap S^{-1}$ equal to Σ). Associativity holds also in this case.

The definition of $S_1 \otimes S_2 = (S_1 \cup S_2)/(S_1 \cap S_2)$ does lead to a group. Closure holds, and there is a unit element ($e = \varnothing$), and inverses do exist ($S^{-1} = S$, because then $S \otimes S^{-1} = (S \cup S)/(S \cap S) = S/S = \varnothing$). To check associativity is an amusing exercise: draw blobs which intersect in the most general way and take it from there.



Comment: We give a few more examples of operations that are not associative.

1) Define $p * q = \frac{p}{q}$ for real p and q.

2) Define $p * q = p^q$. Clearly $(2^3)^5 \neq 2^{3^5}$.

1.2.4 Quaternions and octonions

One can define complex numbers by $a + bi$ where a, b are real numbers, and $i^2 = -1$. Hamilton tried to generalize the complex numbers. Complex numbers $z = a + bi$, with $z^* = a - bi$ have the following properties

Closure: One can add and multiply complex numbers, and the result is again a complex number. For example, $(a + bi)(c + di) = (ac - bd) + (ad + bc)i$.

Norm: The norm of the product is the product of the norms: $|z_1 z_2| = |z_1||z_2|$ with $|z|^2 = a^2 + b^2$. Indeed, $|z_1 z_2|^2 = (ac - bd)^2 + (ad + bc)^2$ which is equal to $(a^2 + b^2)(c^2 + d^2)$ as one easily checks (the cross terms cancel).

Division algebra:[4] If $z_1 z_2 = 0$ either $z_1 = 0$ or $z_2 = 0$. For complex numbers this is true: if $z_1 z_2 = 0$, then $z_1 z_2 z_2^* = z_1 |z_2|^2 = 0$, hence either $z_1 = 0$, or $z_2 = 0$.

Any system with these three properties is called a **normed division algebra**. So complex numbers form a normed division algebra. Hamilton tried to generalize the complex numbers to $q = a + bI + cJ$ with two imaginary units I and J but could not find a solution. However, with

[4] In an algebra one can add and multiply.

three imaginary units I, J, K he found a solution in 1843, which he called quaternions because they contained 4 real numbers a, b, c and d

$$\begin{aligned} q &= aE + bI + cJ + dK\,, \quad I^2 = J^2 = K^2 = -E\,, \quad IJ = K = -JI \text{ and cyclic.} \\ q^* &= aE - bI - cJ - dK \end{aligned} \tag{1.36}$$

One can prove abstractly that this is a normed division algebra, but one can also use a simple faithful[5] representation in terms of 2×2 matrices (the Pauli matrices, which were known to the mathematicians long before Pauli)

$$I = -i\sigma_1\,; \quad J = -i\sigma_2\,; \quad K = -i\sigma_3\,; \quad E = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right). \tag{1.37}$$

Then

$$q = \begin{pmatrix} a - id & -ib - c \\ -ib + c & a + id \end{pmatrix} \tag{1.38}$$

and $|q|^2 = qq^* = (a^2 + b^2 + c^2 + d^2)E = (\det q)E$. Hence we define the norm of q by $|q|^2 = \det q$. We can now easily prove that the q's form a normed division algebra

Closure: Obvious from $(-i\sigma_i)(-i\sigma_j) = \epsilon_{ijk}(-i\sigma_k) - \delta_{ij}$.

Norm: $|q_1 q_2| = |q_1||q_2|$ because $\det(q_1 q_2) = \det q_1 \det q_2$.

Division algebra: If $q_1 q_2 = 0$ then $q_1(q_2 q_2^*) = q_1(a_2^2 + b_2^2 + c_2^2 + d_2^2) = 0$ if $q_1 = 0$ or $q_2 = 0$.

After this success, the race was on for further normed division algebras. Cayley found another normed division algebra in 1845, two years after Hamilton found the quaternions. These "Cayley numbers" are also called octonions, because they contain 8 real numbers $a_0, \cdots a_7$

$$O = a_0 + a_1 e_1 + \cdots + a_7 e_7 \text{ with } e_i e_j = f_{ij}{}^k e_k - \delta_{ij} \text{ and } \{e_i, e_j\} = -2\delta_{ij}\,. \tag{1.39}$$

The "structure constants" $f_{ij}{}^k$ are totally antisymmetric (the $f_{ijk} = f_{ij}{}^k$ satisfy $f_{ijk} = -f_{jik} = -f_{ikj}$), and the only nonvanishing ones are given by

$$f_{12}{}^4 = f_{13}{}^7 = f_{15}{}^6 = f_{23}{}^5 = f_{26}{}^7 = f_{34}{}^6 = f_{45}{}^7 = 1\,. \tag{1.40}$$

The closure of octonions follows from $e_i e_j = -\delta_{ij} + f_{ij}{}^k e_k$. There is a norm $|O|$ defined by $|O|^2 = O^* O$ where $O^* = a_0 - a_1 e_1 \cdots - a_7 e_7$. One finds easily that $|O|^2 = a_0^2 + a_1^2 + \cdots + a_7^2$. It is a normed algebra, $|O_1 O_2| = |O_1||O_2|$. This is not obvious, but Cayley found the values for $f_{ij}{}^k$

[5] A matrix representation is faithful if no two different group elements correspond to the same matrix.

such that this is true. For example, consider

$$
\begin{gathered}
O_1O_2 = (a_1e_1 + a_2e_2)(a_3e_3 + a_4e_4) = a_1a_3e_7 + a_1a_4(-e_2) + a_2a_3e_5 + a_2a_4e_1 \\
\left.\begin{array}{c}
|O_1|^2 = a_1^2 + a_2^2\,; \qquad |O_2|^2 = a_3^2 + a_4^2 \\
|O_1O_2|^2 = (a_1a_3)^2 + (a_1a_4)^2 + (a_2a_3)^2 + (a_2a_4)^2
\end{array}\right\} \quad |O_1|^2|O_2|^2 = |O_1O_2|^2\,.
\end{gathered}
\tag{1.41}
$$

Finally, this is also a division algebra, because with $e_i^* = -e_i$ one gets $O^* = a_0 - a_1e_1 \cdots - a_7e_7$, and $OO^* = |O|^2$. Then if $O_1O_2 = 0$, also $O_1O_2O_2^* = O_1(|O_2|^2){=}0$, hence either $O_1 = 0$ or $O_2 = 0$. Cayley also proved that there are no further solutions with more than 7 imaginary units, hence we have the following

Theorem: The only normed division algebras are the real numbers, the complex numbers, the quaternions and the octonions.

What has all this to do with group theory? The $\pm 1, \pm i$ of complex numbers form a group of order 4, called Z_4, and the $\pm 1, \pm I, \pm J, \pm K$ of quaternions also form a group of order 8, called the quaternion group and denoted by Q. (Recall that the order of a group is the number of its elements.) However the octonions do not form a group because they are not associative! It is easy to check the nonassociativity in an example

$$
\begin{aligned}
(e_1e_2)e_5 &= e_4e_5 = e_7 \\
e_1(e_2e_5) &= e_1(-e_3) = -e_7
\end{aligned}
\tag{1.42}
$$

For fun we write down the octonion multiplication table.

(1.43)

	I	e_1	e_2	e_3	e_4	e_5	e_6	e_7
I	I	e_1	e_2	e_3	e_4	e_5	e_6	e_7
e_1	e_1	$-I$	e_4	e_7	$-e_2$	e_6	$-e_5$	$-e_3$
e_2	e_2	$-e_4$	$-I$	e_5	e_1	$-e_3$	e_7	$-e_6$
e_3	e_3	$-e_7$	$-e_5$	$-I$	e_6	e_2	$-e_4$	e_1
e_4	e_4	e_2	$-e_1$	$-e_6$	$-I$	e_7	e_3	$-e_5$
e_5	e_5	$-e_6$	e_3	$-e_2$	$-e_7$	$-I$	e_1	e_4
e_6	e_6	e_5	$-e_7$	e_4	$-e_3$	$-e_1$	$-I$	e_2
e_7	e_7	e_3	e_6	$-e_1$	e_5	$-e_4$	$-e_2$	I

One may note certain regularities. For example, if $i \neq j$ then $e_ie_j = -e_je_i$ which agrees with the total antisymmetry of $f_{ijk} = f_{ij}{}^k$. Also, if $e_ie_j = e_k$ then $e_{i+1}e_{j+1} = e_{k+1} \mod 7$, and $e_{2i}e_{2j} = e_{2k} \mod 7$. The 16×16 multiplication table for the 16 group elements $\pm I$, $\pm e_1$, $\cdots, \pm e_7$ can be constructed. It is a Latin square, see section 2.1 for a definition of a Latin square, but as we show there, not every Latin square corresponds to a group, and also here we are not dealing with a group. Despite these shortcomings, octonions play a role in supergravity theories.

1.3 Exercise

The Lorentz group. Maxwell did not know that his equations had symmetries, and Lorentz came close to finding them in 1904, but Poincaré found an error[6] and still generously called the corrected transformation laws the Lorentz group transformations, and he showed that they form a group. Poincaré noted that to prove that the Maxwell equations have the same form in the moving frame as in the frame at rest, one must transform both the coordinates x, y, z, t and the electromagnetic fields $\vec{E}$ and $\vec{B}$. Here we only consider the transformation rules of the coordinates, and we consider only boosts along the x-axis. They form a one-parameter Lie group, whose parameter is the velocity v of a moving observer with respect to an observer at rest. Consider then the following "Lorentz transformations"

$$x' = \frac{x + vt}{\sqrt{1 - \frac{v^2}{c^2}}}\,; \quad t' = \frac{t + \frac{v}{c^2}x}{\sqrt{1 - \frac{v^2}{c^2}}}\,; \quad y' = y\,; \quad z' = z\,, \tag{1.44}$$

where v is bounded by $-c < v < c$. Let $L(v)$ be the set of transformations from x, t to x', t'. Show that the set of all $L(v)$ form a group, namely, show that the four group postulates are satisfied.

1.I Diagonalization of a real antisymmetric matrix

The diagonalization of a real symmetric $N \times N$ matrix S by a real orthogonal matrix O is well-known from quantum mechanics

$$O^T S O = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_N \end{pmatrix} \tag{1.45}$$

with real λ_j. We prove here that a real antisymmetric $2N \times 2N$ matrix A can be cast into symplectic form by a real orthogonal $2N \times 2N$ matrix O

$$O^T A O = \begin{pmatrix} \begin{smallmatrix} 0 & \mu_1 \\ -\mu_1 & 0 \end{smallmatrix} & & \\ & \ddots & \\ & & \begin{smallmatrix} 0 & \mu_N \\ -\mu_N & 0 \end{smallmatrix} \end{pmatrix}, \tag{1.46}$$

with real positive μ_j.

[6] Lorentz obtained $x' = \gamma x + \beta\gamma x^0$ and $(x^0)' = \gamma x^0 + \frac{\beta}{\gamma}x$. Poincaré added $(x^0)' = \beta^2\gamma x$ and obtained $(x^0)' = \gamma x^0 + \beta\gamma x$.

The eigenvalues of A are purely imaginary: $Az = \lambda z$ and $Az^* = \lambda^* z^*$ imply that $\lambda = i\mu$ with real μ. (Define $(z,z) = \sum z_i^* z_i$ and use $(z, Az) = \lambda(z,z) = (-Az, z) = -\lambda^*(z,z)$ with $(z,z) > 0$.) Hence $A\,\mathrm{Re}z = -\mu\,\mathrm{Im}z$ and $A\,\mathrm{Im}z = \mu\,\mathrm{Re}z$. The eigenvalues and eigenvectors come in pairs λ_J, λ_J^* and (z_J, z_J^*) with $J = 1, \cdots, N$. We choose from each pair (z_J, z_J^*) the eigenvector with eigenvalue $i\mu_J$ with positive μ_J, and denote these eigenvectors by w_J with $J = 1, \cdots, N$. We decompose them in real and imaginary parts, and define the $2N \times 2N$ matrix O as follows

$$O = (\mathrm{Re}w_1, \mathrm{Im}w_1, \cdots, \mathrm{Re}w_N, \mathrm{Im}w_N) \tag{1.47}$$

It is clear that O is real, and satisfies

$$AO = O \begin{pmatrix} \begin{smallmatrix} 0 & \mu_1 \\ -\mu_1 & 0 \end{smallmatrix} & & \\ & \ddots & \\ & & \begin{smallmatrix} 0 & \mu_N \\ -\mu_N & 0 \end{smallmatrix} \end{pmatrix} \tag{1.48}$$

with $\mu_j \geq 0$. To prove that O is orthogonal, we note that

$$\begin{aligned} (w_J, Aw_K) &= i\mu_K(w_J, w_K) = -(Aw_J, w_K) = i\mu_J(w_J, w_K) \\ (w_J^*, Aw_K) &= i\mu_K(w_J^*, w_K) = -(Aw_J^*, w_K) = -i\mu_J(w_J^*, w_K)\,. \end{aligned} \tag{1.49}$$

Hence for $J \neq K$, both $(w_J, w_K) = 0$ and $(w_J^*, w_K) = 0$. Then also $(w_J^*, w_K^*) = 0$ and $(w_J, w_K^*) = 0$. Hence $(w_J \pm w_J^*, w_K \pm w_K^*) = 0$ which proves that the columns for $J \neq K$ are orthogonal. For $J = K$ we only have $(w_J^*, w_J) = 0$, but its imaginary part is proportional to $(\mathrm{Re}w_J, \mathrm{Im}w_J)$ and vanishes. (Its real part states that $(\mathrm{Re}w_J, \mathrm{Re}w_J)$ is equal to $(\mathrm{Im}w_J, \mathrm{Im}w_J)$.) If some of the μ_J vanishes, we are free to choose the corresponding $\mathrm{Re}w_J$ and $\mathrm{Im}w_J$ to be orthogonal.

1.II Diagonalization of a complex symmetric or antisymmetric matrix

It is well-known that a real symmetric matrix can be diagonalized by a real orthogonal matrix, and a real antisymmetric nonsingular matrix in $2N$ dimensions can be cast into the symplectic form $\Omega = \left(\begin{smallmatrix} 0 & I \\ -I & 0 \end{smallmatrix}\right)$. But this is also possible for complex symmetric or antisymmetric matrices. For complex symmetric matrices this is the Autonne-Takagi theorem from the 1900's, and for complex antisymmetric matrices a proof can be found in [4] (where it is used to write the central charges of supersymmetry algebras in canonical form). We give here the proof for antiysmmetric matrices, but the proof for symmetric matrices goes the same way.

We prove the matrix theorem that a general antisymmetric complex $2N \times 2N$ matrix Z^{ij} can be brought to symplectic form by a unitary matrix W as follows

$$WZW^T = \begin{pmatrix} 0 & +\mu_1 & & & & \\ -\mu_1 & 0 & & & 0 & \\ & & \ddots & & & \\ & & & & 0 & +\mu_n \\ & 0 & & & -\mu_n & 0 \end{pmatrix} ; \quad \mu_1, \cdots, \mu_n \geq 0 \tag{1.50}$$

By a further rescaling with diagonal matrices $S = \left(\frac{1}{\sqrt{\mu_1}}, \frac{1}{\sqrt{\mu_1}}, \cdots, \frac{1}{\sqrt{\mu_n}}, \frac{1}{\sqrt{\mu_n}}\right)$ we obtain $SWZ(SW)^T$ with all μ_j equal to one. (Note the W^T instead of W^{-1}. If the matrix is odd-dimensional, there is an additional zero in the last diagonal entry.) The proof is based on two observations:

(i) $Z(Z^*Z) = (ZZ^*)Z$ where $-Z^*Z = +Z^\dagger Z$ is positive semi-definite and hermitian, and so can be diagonalized by a unitary matrix.

(ii) For an antisymmetric unitary matrix A^{ij}, the complex conjugate A^* commutes with A, since $A^* = (A^T)^{-1} = -A^{-1}$. Hence $A + A^*$ and $i(A - A^*)$ are real antisymmetric matrices which commute with each other. Such matrices can be brought simultaneously into symplectic form

$$\begin{pmatrix} 0 & +\mu_1 & & & & \\ -\mu_1 & 0 & & & 0 & \\ & & \ddots & & & \\ & & & & 0 & +\mu_n \\ & 0 & & & -\mu_n & 0 \end{pmatrix} ; \quad \mu_1, \cdots, \mu_n \geq 0 \tag{1.51}$$

by a real orthogonal matrix O.

Let us now give the proof.

The matrix $H = Z^\dagger Z = -Z^*Z$ can be diagonalized by unitary V and has eigenvalues $h_\mu \geq 0$ according to (i). Hence $VHV^{-1} = H_D$. Consider now the identity $ZH - H^*Z = 0$. After multiplication by V^* on the left and V^{-1} on the right, one obtains

$$V^*(ZH - H^*Z)V^{-1} = (V^*ZV^{-1})H_D - H_D(V^*ZV^{-1}) = 0 \tag{1.52}$$

Hence $(V^*ZV^{-1})_{\mu\nu}(h_\mu - h_\nu) = 0$, so that V^*ZV^{-1} consists of blocks along the diagonal, different blocks corresponding to different h_ν. Call $V^*ZV^{-1} = \psi$ in such a block. Clearly ψ is antisymmetric (since $V^* = V^{-1,T}$). Since the matrix $\psi\psi^\dagger = (V^*ZV^{-1})(V^*ZV^{-1})^\dagger$ is equal to $V^*(ZZ^\dagger)(V^*)^{-1}$, which is equal to $(V(-Z^*Z)V^{-1})^* = H_D$, we see that $\psi\psi^\dagger = H_D$. If $h_\mu = 0, \psi = 0$ while if $h_\mu \neq 0$, then $h_\mu^{-\frac{1}{2}}\psi \equiv A$ is unitary and antisymmetric. Because A is antisymmetric, and ReA and ImA

ommute (because A is unitary, see (ii)), we can apply (ii) to obtain

$$O\,\mathrm{Re}A\,O^T = \begin{pmatrix} 0 & +\mu_1 & & & \\ -\mu_1 & 0 & & & 0 \\ & & \ddots & & \\ & 0 & & 0 & +\mu_n \\ & & & -\mu_n & 0 \end{pmatrix}; \quad O\,\mathrm{Im}A\,O^T = \begin{pmatrix} 0 & +\nu_1 & & & \\ -\nu_1 & 0 & & & 0 \\ & & \ddots & & \\ & 0 & & 0 & +\nu_n \\ & & & -\nu_n & 0 \end{pmatrix};$$

$$OAO^T = \begin{pmatrix} 0 & +z_1 & & & \\ -z_1 & 0 & & & 0 \\ & & \ddots & & \\ & 0 & & 0 & +z_n \\ & & & -z_n & 0 \end{pmatrix} \tag{1.53}$$

where O is real orthogonal and $z_j = \mu_j + i\nu_j$. But since A, and hence OAO^T, is unitary, the z_j's are phases $e^{i\phi_j}$. Hence

$$\widehat{A} \equiv OAO^{-1} = \begin{pmatrix} 0 & +e^{i\alpha} & & & \\ -e^{i\alpha} & 0 & & & 0 \\ & & \ddots & & \\ & 0 & & 0 & +e^{i\beta} \\ & & & -e^{i\beta} & 0 \end{pmatrix} \tag{1.54}$$

Consider now the unitary matrix $U = \mathrm{diag}(e^{-i\frac{\alpha}{2}}, e^{-i\frac{\alpha}{2}}, e^{-i\frac{\beta}{2}}, \cdots)$. Then $U\widehat{A}U^T = (UO)\big(\psi h^{-\frac{1}{2}}\big)(UO)^T$ $= (UO)V^* Z h^{-\frac{1}{2}} V^{-1}(UO)^T$ is a matrix which consists of 2×2 blocks $i\sigma^2$. (By $\psi h^{-\frac{1}{2}}$ we mean a block diagonal matrix with $\psi_\mu h_\mu^{-\frac{1}{2}}$ in each block.) Hence $WZW^T = \prod_\mu h_\mu^{\frac{1}{2}}(i\sigma^2)$ where the matrix $W = UOV^*$ is unitary, and thus the theorem in (1.50) is proved.

1.III Complex antisymmetric matrices, Pfaffians, and symplectic matrices

In this appendix we shall first prove that the determinant of an $2N\times 2N$ complex (or real) symplectic matrix is $+1$, and then show that the determinant of a complex (or real) antisymmetric $2N\times 2N$ matrix A factorizes into the square of its Pfaffian [5]

$$\det M = +1\,, \qquad \det A = (\mathrm{Pf}\,A)^2\,. \tag{1.55}$$

We shall use the result of the previous appendix that a complex (or real) antisymmetric matrix A can be brought to the form $\Omega = \left(\begin{smallmatrix} 0 & I \\ -I & 0 \end{smallmatrix}\right)$ by a complex nonsingular matrix B

$$B^T A B = \begin{pmatrix} \begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix} & & \\ & \ddots & \\ & & \begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix} \end{pmatrix} . \tag{1.56}$$

The Pfaffian is defined as follows

$$\mathrm{Pf}\, A = \frac{1}{2^n n!} \epsilon_{i_1 j_1 \cdots i_n j_n} A_{i_1 j_1} \cdots A_{i_n j_n} \tag{1.57}$$

We shall prove that for an arbitrary complex matrix B

$$\mathrm{Pf}(B^T A B) = (\mathrm{Pf}\, A)(\det B) \tag{1.58}$$

To prove this, we rearrange the terms in $\mathrm{Pf}(B^T A B)$

$$\begin{aligned} \mathrm{Pf}(B^T A B) &= \frac{1}{2^n n!} \epsilon_{i_1 j_1 \cdots i_n j_n} (B^T_{i_1 k_1} A_{k_1 l_1} B_{l_1 j_1}) \cdots (B^T_{i_n k_n} A_{k_n l_n} B_{l_n j_n}) \\ &= \frac{1}{2^n n!} \left(\epsilon_{i_1 j_1 \cdots i_n j_n} B_{k_1 i_1} B_{l_1 j_1} \cdots B_{k_n i_n} B_{l_n j_n} \right) \left(A_{k_1 l_1} \cdots A_{k_n l_n} \right) \end{aligned} \tag{1.59}$$

The first expression inside parentheses is the definition of a determinant

$$\epsilon_{i_1 j_1 \cdots i_n j_n} B_{k_1 i_1} B_{l_1 j_1} \cdots B_{k_n i_n} B_{l_n j_n} = \epsilon_{k_1 l_1 \cdots k_n l_n} \det B \tag{1.60}$$

Substituting this into (1.59) yields

$$\mathrm{Pf}(B^T A B) = \left(\frac{1}{2^n n!} \epsilon_{k_1 l_1 \cdots k_n l_n} A_{k_1 l_1} \cdots A_{k_n l_n} \right) \det B = (\mathrm{Pf}\, A)(\det B) . \tag{1.61}$$

We now apply this relation to symplectic matrices M which satisfy $M^T \Omega M = \Omega$. So we set in (1.61) the matrix B equal to M, and A equal to Ω, and then we use $M^T \Omega M = \Omega$. This yields

$$\mathrm{Pf}(M^T \Omega M) = \mathrm{Pf}\, \Omega = (\mathrm{Pf}\, \Omega)(\det M) . \tag{1.62}$$

Since $\mathrm{Pf}\, \Omega \neq 0$ we have proven that symplectic matrices have unit determinant

$$\det M = +1 . \tag{1.63}$$

To prove the relation $\det A = (\mathrm{Pf}\, A)^2$, we begin with (1.61) which we square

$$(\mathrm{Pf}(B^T A B))^2 = (\mathrm{Pf}\, A)^2 (\det B)^2 \tag{1.64}$$

There is another expression containing $(\det B)^2$,

$$\det(B^T AB) = \det A(\det B)^2 \tag{1.65}$$

Taking the ratio of (1.64) and (1.65), the factors $(\det B)^2$ cancel, and one obtains

$$\frac{(\mathrm{Pf}(B^T AB))^2}{\det(B^T AB)} = \frac{(\mathrm{Pf}\, A)^2}{\det A} \tag{1.66}$$

This relation holds for all nonsingular complex (or real) B, and we shall choose a particular B which will allow us to evaluate the left-hand side. We choose for B the matrix W of the previous appendix which casts A into the 2×2 block diagonal form

$$W^T AW = \begin{pmatrix} \begin{smallmatrix} 0 & \mu_1 \\ -\mu_1 & 0 \end{smallmatrix} & & \\ & \ddots & \\ & & \begin{smallmatrix} 0 & \mu_n \\ -\mu_n & 0 \end{smallmatrix} \end{pmatrix} \tag{1.67}$$

Then $\mathrm{Pf}(W^T AW) = \mu_1 \cdots \mu_n$ and $\det(W^T AW) = \mu_1^2 \cdots \mu_n^2$, so the left-hand side of (1.66) is unity, and this proves

$$\det A = (\mathrm{Pf}\, A)^2\,. \tag{1.68}$$

For example

$$N = 1: \quad A = \left(\begin{smallmatrix} 0 & a \\ -a & 0 \end{smallmatrix}\right), \quad \mathrm{Pf}\, A = 0\,, \quad \det A = (\mathrm{Pf}\, A)^2 \tag{1.69}$$

$$N = 2: \quad A = \begin{pmatrix} 0 & a & b & c \\ -a & 0 & d & e \\ -b & -d & 0 & f \\ -c & -e & -f & 0 \end{pmatrix}, \quad \mathrm{Pf} = af - be + cd\,, \quad \det A = (\mathrm{Pf}\, A)^2\,. \tag{1.70}$$

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Chapter 2

A brief history of group theory

Applications of group theory to physics started in the twentieth century. Consider as an example Albert Einstein and Special Relativity (1905) [1]. Until that time physicists had studied particular dynamical models but the symmetries of these models were not noticed or they played a minor role. (In Maxwell's 1865 theory of Electromagnetism, its relativistic symmetry was discovered by Poincaré 40 years later, and its gauge invariance was even later discovered by Weyl in 1919.) Einstein put symmetry first and dynamics later. He required the relativistic invariance of any physical theory, and in doing so, it turned out that this determined dynamics to some extent. The most spectacular example was his theory of gravitation (General Relativity) where symmetry (general coordinate invariance) determines the dynamics (the Einstein field equations) completely. As Yang has succinctly said: "Symmetry dictates interactions".

However, for most physicists this approach of putting symmetry ahead of interactions was a bridge too far. Lorentz must have felt that Einstein cheated [1]. He wrote that Einstein proposed relativistic symmetry but did not prove it. With the advent of Quantum Mechanics in the 1920's, matters got worse. A small but growing set of physicists started using group theory instead of detailed calculations to solve problems concerning symmetries of wave functions. Most physicists initially disliked the use of group theory in physics. To get a feeling for a typical reaction we quote [2] from the autobiography of John Slater (of the Slater determinant):

> It was at this point that Wigner, Hund, Heitler, and Weyl entered the picture with their "Gruppenpest": the pest of the group theory... The authors of the "Gruppenpest" wrote papers which were incomprehensible to those like me who had not studied group theory, in which they applied these theoretical results to the study of the many electron problem. The practical consequences appeared to be negligible, but everyone felt that to be in the mainstream one had to learn about it. Yet there were no good texts from which one could learn group theory. It was a frustrating experience, worthy of the name of a pest. I had what I can only describe as a feeling of outrage at the turn which the subject had taken....

Slater then wrote his paper on the Slater determinant which could be used instead of group theory to antisymmetrize wave functions of electrons. We continue with Slater's autobiography.

> As soon as this paper became known, it was obvious that a great many other physicists were as disgusted as I had been with the group-theoretical approach to the problem. As I heard later, there were remarks made such as "Slater has slain the 'Gruppenpest' ". I believe that no other piece of work I have done was so universally popular.

The term "Gruppenpest" was coined by Pauli (according to Wigner). Probably physicists in the 1920's and 1930's felt that there was something fishy about getting results by only using symmetries and not performing painful explicit calculations using particular dynamical interactions.

When the $SU(3)$ symmetry of hadrons made from up, down and strange quarks was introduced into particle physics in the 1960s, similar feelings of outrage occurred. We quote from the introduction to Harry Lipkin's book "Lie Groups for Pedestrians" [3]

> As a graduate student in experimental physics, I found the study of group theory considered to be a useless 'high-brow' luxury. Furthermore all attempts to follow a lecture course resulted in a losing battle with characters, cosets, classes, invariant subgroups, normal divisors and assorted lemmas. It was impossible to learn all the definitions of new terms defined in one lecture and remember them until the next lecture. The result was complete chaos.
>
> It was a great surprise to find later on that (1) techniques based on group theory can be useful; (2) they can be learned and used without memorizing the large number of definitions and lemmas which frighten the uninitiated. Angular momentum is presented in elementary quantum mechanics courses without a detailed analysis of the Lie group of continuous rotations in three dimensions. The student learns about angular momentum multiplets and coupling of angular momenta without realizing that these are the irreducible representations of the rotation group. He also does not realize that the algebraic properties of other Lie groups can be applied to physical problems in the same way as he has used angular momentum algebra, with no need for characters, classes, cosets, etc.

Nowadays, group theory has become an indispensable tool in physics, but it has become so popular that there are physicists who only use group theory and not, for example, quantum field theory, to solve physical problems. This is the other extreme. Howard Georgi writes in his textbook [4]

> Symmetry is a tool that should be used to determine the underlying dynamics, which must in turn explain the success (or failure) of the symmetry arguments. Group theory is a useful technique, but it is no substitute for physics.

We shall discuss group theory, first its mathematical properties and then its applications to physics. We shall not use any quantum field theory, but we hope that our presentation is not so enchanting that newcomers decide to surrender to the beauty of group theory and forsake the messiness of quantum field theory. Let us now explain how group theory came into being. This is a historical account; we give dates to illustrate the developments of ideas in time. In what follows many group-theoretical concepts are mentioned; these will be explained in subsequent chapters and thus the text below may also serve as a (partial) list of topics to be discussed.

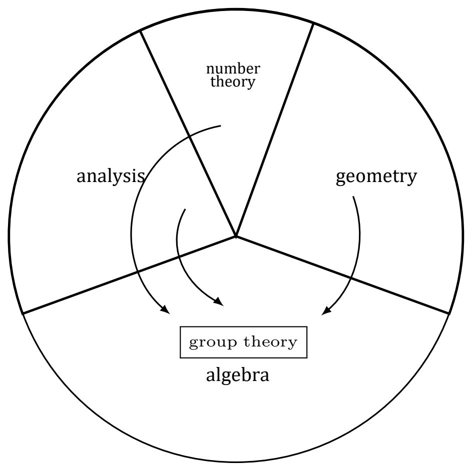


Figure 2.1: The four main areas of mathematics are number theory, analysis, algebra and geometry. (Some mathematicians add algebraic geometry to this list.) Group theory is part of algebra, but its roots lie in early studies in all four main areas.

The origins of group theory go back to the four main areas in mathematics: number theory (the older term is arithmetics), algebraic properties of the roots of polynomial equations, symmetries of geometrical objects, and symmetries of differential equations (leading to Lie groups). We shall later give examples. All these examples have some algebraic properties in common, and abstracting these properties from the particular models, one arrived at the abstract concept of a group.

A very rough history of group theory in mathematics is as follows:

- before 1800: studies in number theory (Pythagoras (550 B.C.), Euclid (300 B.C.), Diophantus (3rd century), and, more recently, Fermat (1640), Euler (1741), Lagrange (1771), Gauss (1801) and many others). The number systems studied by these mathematicians formed finite groups, although this was not realized in these early studies.

- before 1830: symmetries in geometry (symmetries of polyhedra and polygons, and maximally symmetric spaces and non-Euclidean geometries for which Euclid's fifth postulate no longer holds, leading to the hyperbolic geometry of Gausz (1824), Lobachevski (1826) and Bolyai (1832). These symmetries formed finite and infinite groups.

- 1800-1830: studies of the roots of quintic polynomial equations. The solution of the quadratic equation was already known to Babylonians (1600 BC), and the cubic equation and quartic equation were solved by Cardano, del Ferro, Ferrari, Tartaglia and others around 1545. (Earlier (1079), Omar Khayyam had solved particular cases of the cubic equation.) For these three cases all solutions are radical solutions. (A radical solution is a solution only involving n^{th} roots; radix = root in Latin). However, for more than two centuries, no proof could be found that all solutions of any quintic equation were radical. Lagrange (1771) noted that certain polynomials[1] depending on the roots of an n^{th} order polynomial took on only m values if one permuted these roots in $n!$ ways, and found that for $n = 4$ one got $m < n$ (namely $m = 3$), but for $n = 5$ he got $m > n$ (namely $m = 6$). His work introduced permutations as a tool for solving the quintic. Abel (1824) proved that there exist particular quintic equations whose roots are not all radical and Galois (1830) derived necessary and sufficient conditions to decide which quintic equations have only radical roots and which do not. All these studies used permutations of roots, so **group theory started out as the theory of permutations** (the older term is substitutions).

Lagrange

Abel

Galois

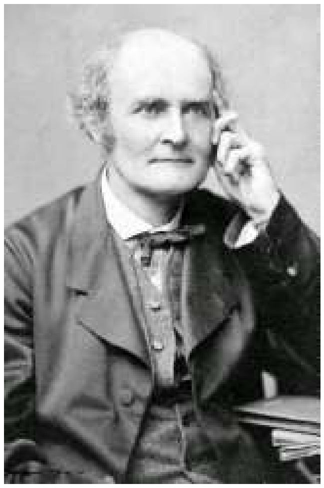
- 1830-1860: studies of permutations in general, leading to a formal definition of abstract groups by Cayley (1854). Cayley also showed that every finite group is a (sub)group of a permutation group[2] S_n for suitable n, thus all the work done in the period 1800-1830 on permutation groups was not in vain.[3]

- 1860-present: properties of abstract groups, and the theory of matrix representations of finite groups and characters by Frobenius (1890's) and others. Sophus Lie and Felix Klein were students together in 1869 in Berlin. Felix Klein (1874) championed studying geometries

[1] See [5]. For example, for polynomial equations with $n = 4$, Lagrange constructed a corresponding cubic equation whose roots were $x_1x_2 + x_3x_4$, $x_1x_3 + x_2x_4$ and $x_1x_4 + x_2x_3$ where x_1, x_2, x_3 and x_4 are the roots of the 4^{th} order polynomial equation. We discuss this in more detail in appendix 2.I.

[2] A finite group is a group with a finite number of elements, and the permutation group S_n is the group whose elements are the permutations of n objects.

[3] Cayley gave a definition of abstract **finite** groups because he viewed them as subgroups of S_n. In 1882 Dijck (later ennobled to von Dijck) gave a definition of any abstract group in terms of group generators.



Cayley

Frobenius

Klein

by concentrating on their symmetries. He studied transformations of points of particular geometries which were permutations of these points, and his work led to a development of group theory which is an alternative to the approach based on permutation groups, namely the **transformation groups**. By studying polyhedra or automorphic functions and other objects, he found the corresponding finite groups. He saw disadvantages in the focus on abstract group theory; as he wrote [6]

> ...the abstract formulation is excellent for the working out of proofs but it does not help one find new ideas and methods... in general, the disadvantage of the [abstract] method is that it fails to encourage thought.

Lie

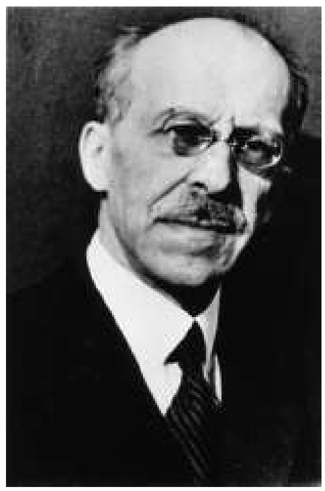
Killing

Cartan

Sophius Lie (1884) introduced the study of continuous groups. He studied transformation groups acting on differential equations. Killing (1880-1900) studied simple Lie algebras and discovered the four series of compact classical groups $SU(N)$, $SO(2N+1)$, $USp(2N)$ and

$SO(2N)$ and the five exceptional Lie groups.[4] Cartan subsequently classified all real forms of the simple Lie algebras. Killing introduced Cartan generators and Cartan introduced the Killing metric. Maschke (1898) proved that all reducible matrix representations of finite groups are completely reducible. Schur (1905) obtained his lemmas and proved that all irreducible matrix representations (irreps) of finite groups can be made unitary. Cartan and Weyl determined all unitary (and hence finite-dimensional) matrix representations of all simple compact Lie algebras. The Peter-Weyl theorem (1927) (Peter was a student of Weyl) proved the L_2-completeness of characters, and the orthonormality of the matrix elements of the unitary irreducible representations (irreps) of simple compact groups. (An example well-known to physicists are the Y^l_m of quantum mechanics, which form a complete set of irreps for scalars of $SU(2)$.) Differential geometry was combined with group theory yielding

Maschke



Issai Schur

Weyl

the Maurer-Cartan equations. Group manifolds and coset manifolds were introduced with vielbeins and connections, and integration on them became possible with the Haar measure (1933). New formulations of Lie algebras led to the Chevalley basis (1955) instead of the Cartan-Weyl basis (1925) and the Serre relations (1987). Young tableaux (1900) and Dynkin diagrams (1947) replaced Killing's root diagrams (1889). In the 1970s, a new type of Lie algebras was discovered by physicists: the superalgebras, and this led to explosive developments in physics and mathematics. Lie algebras and superalgebras were extended to loop groups, affine Lie algebras, and Kac-Moody algebras. Finally, between 1955 and 2004, based on the work of hundreds of mathematicians, the complete classification of all finite simple groups was achieved.

[4] Actually, Killing only explicitly constructed G_2 and claimed that there existed six exceptional Lie groups. Cartan proved that there were only five, and constructed them in his Ph.D. of 1894. In 1914 he constructed all real forms of the simple Lie algebras.


Chevalley


Dynkin

Serre

In physics groups were introduced in the 20th century. Poincaré identified (1905) the Lorentz group in the transformations Lorentz had used (1904) to analyze the Maxwell equations, and which led to Special Relativity (1905). After General Relativity had been constructed in 1915, spaces with a cosmological constant were introduced, and this led to the group theory of anti-de Sitter spaces and de Sitter spaces. The local scale (Weyl) invariance of Maxwell theory (1865) led to the conformal group (1908) which plays a central role in string theory. In the 1930s, Weyl, Wigner, van der Waerden (the 3 W's) and others applied group theory to quantum mechanics, for example, the Wigner-Eckart theorem (1930). Wigner constructed the infinite-dimensional unitary irreps


Poincaré


Wigner


van der Waerden

of the noncompact non-semisimple Poincaré algebra and the noncompact simple Lorentz group (1939). In solid state physics, the theory of matrix representations was applied to the symmetry groups of molecules, and this gave detailed information about their (Raman and infrared) spectra. In the 1940s and 1950s, applications to nuclear physics followed (for example Wigner's $SU(4)$ combining spin and isospin applied to nuclei with N nucleons), and in the 1960s, group theory became central in particle physics (the eightfold way of Gell-Mann and Zweig (1963) and later the $SU(3) \times SU(2) \times U(1)$ gauge symmetry of the Standard Model, and the Grand Unified Theories based on the groups $SU(5)$ or $SO(10)$ or other groups). In superstring theory, the modular group and the Virasoro algebra led to applications of discrete infinite groups.

Summary. One can summarize our short history as follows: up to the 1880s group theory was the theory of "specialized" groups: the permutation groups (due to polynomial equations), the abelian groups (due to number theory), and the finite and infinite transformation groups (due to geometry and analysis). From the 1880s to the 1910s, a theory of abstract groups was developed. After the 1920s, the field became so large that it split into different directions: classification of finite groups, topological groups, loop groups, and other extensions.

We now give examples of mathematical structures which were studied before 1800, in which we can recognize a group structure. The first example is in number theory (section 2.1), the second in geometry (section 2.2), the third in algebra (appendix 2.I), and the fourth in analysis (differential equations, appendix 2.II).

2.1 Number Theory: finite abelian groups

Number theory is an area in mathematics with few practitioners and high standards. With hindsight we can see that early number theorists were dealing with systems with the structure of a group. As an example, following Fermat (1640), we consider all positive integers smaller than p, where p is a prime number. For example, if $p = 5$, the set of elements G is given by $G = \{1, 2, 3, 4\}$. We define group multiplication $\otimes$ as ordinary multiplication modulo p, so for example $2 \otimes 3 = 1$ if $p = 5$. This yields an abelian group as we now show.

- Closure holds because if $a \otimes b = c \bmod p = c + kp$ then $0 \leq c < p$, but $c = 0$ is not possible because otherwise a and/or b would be divisible by p. Hence c lies in G.
- The unit element is clearly the number 1.
- Inverses exist because $aG = Ga = G$ (aG is a permutation of G, see before).
- Associativity holds because in the relation $((a \otimes b \bmod p) \otimes c) \bmod p = a \otimes (b \otimes c \bmod p) \bmod p$ all terms due to mod p are of the form kp and can be dropped.

One can, following Cayley, construct the group multiplication table for such groups. It is a $p \times p$ matrix with in the kl entry the product of the group elements a_k and a_l. This yields a so-called **Latin square** (the name is due to Euler who used Latin characters for the entries). An $n \times n$ Latin square contains n numbers such that the numbers in each row and each column are different. For our example with $p = 5$ the table reads as follows

G	1	2	3	4
1	1	2	3	4
2	2	4	1	3
3	3	1	4	2
4	4	3	2	1

Clearly each row and each column contains a permutation of the elements of G. This guarantees closure and the existence of a unit element and inverses. Each group with n elements yields an $n \times n$ Latin square, but the converse is not true: there exist Latin squares which do not correspond to groups. They can only violate associativity.[5] The simplest example has 5 elements.

	e	a	b	c	d
e	e	a	b	c	d
a	a	e	d	b	c
b	b	c	e	d	a
c	c	d	a	e	b
d	d	b	c	a	e

This Latin square violates associativity so it does not correspond to a group; for example

$$(ab)c = dc = a$$
$$a(bc) = ad = c$$

This is the only Latin square with $n = 5$ that violates associativity (up to permuting rows and columns, and other equivalence operations, see Google).

Exercise. The Euler function. Consider an integer $m > 0$ which is not necessarily a prime. The set of all positive integers $0 < k < m$ which are prime with respect to m is denoted by $S(m)$. For example, for $m = 6$ we get $S(6) = \{1, 5\}$. The number of integers contained in $S(m)$ is called the Euler function $\phi(m)$. By definition $\phi(1) = 1$, and it follows that $\phi(2) = 1$, $\phi(3) = 2$, $\phi(4) = 2$, $\phi(5) = 4$, $\phi(6) = 2$, $\phi(7) = 6$, $\phi(8) = 4$, $\phi(9) = 6$, $\phi(10) = 4$. Show that $S(m)$ forms a group if group multiplication is defined as ordinary multiplication modulo m. $S(m)$ groups with the same number of elements need not be isomorphic (for now, we mean by isomorphic that they have the same group multiplication table; the notion of isomorphism is introduced later). For example, $S(5)$ and $S(8)$ have each 4 elements, but the corresponding groups are "different" (not isomorphic), namely Z_4 and V (see later). Construct the Latin squares for $S(5)$, $S(8)$ and $S(10)$.

We shall not study number theory in this book, but for fun we include two more exercises on group theory.

Exercise. Fermat's "little theorem" from 1640: prove that

Theorem: $n^p = n \mod p$, where n is a natural number and p a prime number. (p has to be a prime number, for example $2^3 = 2 \mod 3$ but $2^4 \neq 2 \mod 4$. *Hint:* Use induction with respect to n. Use, and try to prove, that $\binom{p}{k}$ for $k < p$ is an integer proportional to p.)

[5] If only closure, identity and inverses exist, one calls such structures quasi-groups. If only closure holds one has a groupoid, and if closure and associativity holds, one has a semigroup. None of these structures will be of interest to us.

Exercise. **Wilson's theorem** from 1771: prove that

Theorem: n is prime iff $(n-1)! = -1 \mod n$. (The acronym iff means "if and only if". For example $n = 3 \Leftrightarrow 2 = -1 \mod 3$, but $n = 4 \not\Leftrightarrow 6 = -1 \mod 4$. So any prime p divides $(p-1)!+1$, for example 5 divides $(5-1)!+1$.) Lagrange found a proof in 1771. (*Hint:* The numbers $k \leq p-2$ come in pairs a, a^{-1}, or, equivalently, the equation $k^2 = 1 \mod p$ has as solutions only $k = 1$ and $k = p-1$, because $(p-1)^2 = 1 \mod p$.)

2.2 Geometry: transformation groups

Our next example of the origins of group theory concerns the symmetries of a regular tetrahedron. Instead of the generic term symmetry we shall use the more precise term isometry. **An isometry** is a transformation ϕ which maps one-to-one the points x of a manifold into the points of the manifold (it permutes the points of the manifold) and which preserves distances

$$d(\phi(x), \phi(y)) = d(x, y) . \tag{2.1}$$

The manifolds we consider are real linear vector spaces and we assume that there exists a real inner product (x, y),

$$|x-y|^2 = (x-y, x-y) , \tag{2.2}$$

in terms of which distances are defined $d(\phi(x), \phi(y)) = |\phi(x) - \phi(y)|$. Isometries need not keep the origin fixed, for example translations are isometries. Isometries which keep the origin fixed are linear transformations.[6] They form "transformation groups" which act on "carrier spaces". For example, one may choose as carrier spaces the vertices of a regular tetrahedron. Denote the vertices by $1, 2, 3, 4$ as indicated in figure 2.2. Clearly, any permutation of the vertices is

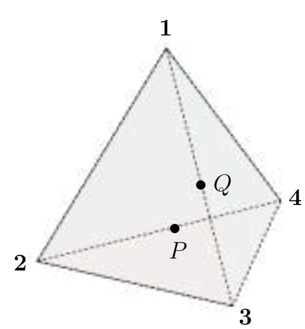


Figure 2.2: A regular tetrahedron. Rotations over angles $\pm\frac{2\pi}{3}$ about an axis going throught a vertex yield $4 \times 2 = 8$ proper rotations. Rotations about a "midline" (here PQ in the figure) over an angle π yield 3 rotations. Six of the isometries with $\det O = -1$ are due to a reflection about a plane through one of the edges. The six remaining isometries with $\det O = -1$ can be obtained by rotating about a midline over $\frac{\pi}{2}$, followed by space inversion.

[6] $(\phi(x) - \phi(y), \phi(x) - \phi(y)) = (x-y, x-y)$ implies $(\phi(x), \phi(y)) = (x, y)$.

an isometry.[7] Hence there are 24 isometries. They consist of 12 rotations, and 12 generalized reflections, isometries whose 3×3 matrix representations satisfies $\det \mathcal{O} = -1$. The rotations satisfy $\det \mathcal{O} = 1$ and are easily identified:

- 8 rotations over $\pm 120°$ keeping a vertex fixed
- 3 rotations over $180°$ about an axis through the midpoint of two opposite edges

Together with the unit element this gives 12 rotations. They form by themselves a group (check!). One can introduce a notation for permutations in terms of cycles. The k-cycle $(a_1, \ldots, a_k)$ means: move (vertex) a_1 to the place of a_2, a_2 to a_3, …, a_k to a_1. Note that cycles are cyclic: $(a_1, \ldots, a_l) = (a_2, \ldots, a_l, a_1) = (a_3, \ldots, a_l, a_1, a_2)$ etc. The inverse of $(a_1, \ldots, a_l)$ is $(a_l, \ldots, a_1)$ and the unit element will be denoted by (1). Then the two rotations about the top vertex in figure 2.2 correspond to (234) and (432). The rotation about the axis through the middle of the edges 12 and 34 corresponds to $(12)(34)$.

To evaluate products of cycles we read the instructions from left to right: so $(24)(34)$ states that 2 goes to 4, which goes to 3; 3 goes to 4; and 4 goes to 2. Thus $(24)(34) = (234)$. So the 3-cycles are a product of two 2-cycles. On the other hand $(1234) = (14)(24)(34)$. We call a product of cycles even (odd) if it can be written with an even (odd) number of 2-cycles. The unit element (1) contains zero 2-cycles, so it is by definition even. So, **the rotations correspond $1-1$ to the even permutations**.

It follows that the isometries with $\det \mathcal{O} = -1$ correspond to the odd permutations. Let's identify them. The reflection about a plane containing the edge (13) interchanges the vertices 2 and 4, so it corresponds to the permutation (24) which is indeed odd. In this way we recover 6 reflections about a plane. There must be 6 further isometries with $\det \mathcal{O} = -1$, and they can be obtained as the product of the twelve rotations with any of these six reflections[8], for example $(12)(234) = (1342)$ (or $(234)(12) = (2341) = (1234)$). There are indeed 12 isometries with $\det \mathcal{O} = -1$; they correspond to the 6 permutations (ab) and the 6 permutations $(abcd)$.

The product of two permutations is a permutation, and the product of two even permutations is again an even permutation. Then the isometries and the rotations each form a group. What is the group of isometries of a regular tetrahedron? It is the group of permutations of the 4 vertices, hence it is S_4. What is the group of rotations of a regular tetrahedron? It is the group of even

[7]Some mathematicians (for example Coxeter in his "Introduction to Geometry", page 29) define a transformation as "a one-to-one" map of points in the plane (or in space)...", so for them the carrier space is the plane or a (3-dimensional) space. For us it can be any set of geometrical objects, for example the set of the 4 vertices, or the set of all the 6 edges, or the set of all the 4 faces, or the pairs of opposite edges, etc. With this definition, a polyhedron is mapped into itself. For example, space inversion is a transformation which permutes all points of the cube and which preserves distances. So space inversion is one of the isometries of the cube.

[8]One can also make a rotation along the axis through the midpoint of two opposite edges over an angle $\frac{\pi}{2}$, followed by space inversion. In figure 2.2 a rotation over $\frac{\pi}{2}$ around PQ yields the following figure $\begin{smallmatrix} 1' & - & 3' \\ & \times & \\ 2 & - & 4 \end{smallmatrix}$ where $1', 3'$ are the vertices 1 and 3 after the rotation, and $2, 4$ are the vertices before the rotation, and $\times$ denotes the center of the tetrahedron. Space inversion maps $1'$ to 4 and $3'$ to 2, and also $4'$ to 3 and $2'$ to 1. So this isometry corresponds to (1432). There are 6 such isometries (3 midlines, angles $\pm\frac{\pi}{2}$).

permutations. For a given n, the subset of even permutations forms a group which is called the **alternating group** and is denoted by A_n. Hence the group of rotations of the tetrahedron is A_4.

Exercise. Determine the isometry group of the cube. (Hint: the 8 vertices of the cube form two tetrahedra with opposite orientation. Space inversion interchanges them.)

Answer: $G(\text{cube}) = S_4 \cup \sigma S_4$ where σ denotes space inversion. The rotations of the cube form also a group S_4, but it is not the S_4 in $S_4 \cup \sigma S_4$ because half of the isometries of this latter S_4 have $\det O = -1$. Rather the 12 rotations of the first S_4 and σ times the 12 generalized reflections of the S_4 in σS_4 form the S_4 whose 24 elements are the rotations of the cube and these have all determinant $+1$.

*2.I Algebra: the quintic polynomial equation

We now show how group theory emerged from algebra. In 1770 and 1771, Lagrange developed an approach to solving polynomial equations. It was heavily based on symmetry, namely on the invariance of certain functions depending on the coefficients of the polynomial equation and its roots, under permutations of those roots. This work evolved into the theory of permutation groups and led some mathematicians to suspect that not every quintic polynomial is solvable by radicals. More practically, it gave a method to solve cubic and quartic equations, which simplify various methods that had been known since the Renaissance. We shall consider in some detail the case of the quartic polynomial equation, but the discussion is involved, and for a first reading we recommend skipping it.

Consider the following equation for complex b, c, d and e

$$\begin{aligned} f(x) &= x^4 + bx^3 + cx^2 + dx + e = 0 \\ &= (x-\alpha_1)(x-\alpha_2)(x-\alpha_3)(x-\alpha_4) \end{aligned} \tag{2.3}$$

$$b = -\sum_j \alpha_j; \quad c = \sum_{i<j} \alpha_i\alpha_j; \quad d = -\sum_{i<j<k} \alpha_i\alpha_j\alpha_k; \quad e = \alpha_1\alpha_2\alpha_3\alpha_4 \tag{2.4}$$

The problem is to find the roots α_j if the coefficients b, c, d and e are given. To find the roots α_i, Lagrange begins by considering a polynomial $h(\alpha_1, \alpha_2, \alpha_3, \alpha_4)$ and constructing its orbit by acting with S_4 on h. The polynomial which will give the solution[9] is $h = (\alpha_1 + \alpha_2)(\alpha_3 + \alpha_4)$, and its orbit

[9] There is no construction which yields h for the quintic polynomial equation, and, in fact, Lagrange spent the last years of his life trying to find a suitable h for the quintic problem. He failed, of course, because we now know that the quintic has in general nonradical solutions and his method breaks down for the quintic.

is given by

$$
\begin{aligned}
\gamma_{12} &= (\alpha_1+\alpha_2)(\alpha_3+\alpha_4) \\
\gamma_{13} &= (\alpha_1+\alpha_3)(\alpha_2+\alpha_4) \\
\gamma_{14} &= (\alpha_1+\alpha_4)(\alpha_2+\alpha_3)
\end{aligned} \tag{2.5}
$$

So there are 4 roots, but only 3 combinations γ_{1j}. Next he constructs a monic polynomial having (2.5) as roots. It is called the *resolvent cubic* of $f(x)$ and given by $g(x) = (x-\gamma_{12})(x-\gamma_{13})(x-\gamma_{14})$. Two properties are true by construction. Permuting the α_i permutes the γ_{1j}, and permuting the γ_{1j} leaves $g(x)$ invariant. We may therefore conclude that the coefficients of $g(x)$ are symmetric polynomials in $\alpha_1, \alpha_2, \alpha_3, \alpha_4$. This means that they are algebraic functions of the *elementary* symmetric polynomials $e_n(\alpha_1, \alpha_2, \alpha_3, \alpha_4)$, which are just equal to $\pm$ the coefficients of $f(x)$, see (2.3). The explicit expression for $g(x)$ in terms of symmetric polynomials follows from brute force

$$
\begin{aligned}
g(x) &= (x-\gamma_{12})(x-\gamma_{13})(x-\gamma_{14}) \\
&= x^3 - 2cx^2 + (c^2 + bd - 4e)x + (d^2 + b^2e - bcd)
\end{aligned} \tag{2.6}
$$

Given the cubic equation $g(x) = 0$ in terms of b, c, d and e, we assume that a method for solving cubic equations is known. So we have now a simpler problem: given b, c, d, e we must find the γ_{1j}. We could discuss how one fixes the γ_{1j} using Lagrange's method for cubic equations, but Lagrange's method for the cubic equation is much more complicated than for the quartic, so we shall use Cardano's method for the cubic equation in (2.6). Thus we may assume that the γ_{1j} as functions of b, c, d, e are known.

It is still not obvious that the original problem of solving a quartic equation has been reduced to the simpler problem of solving a cubic equation. However, the next step will hopefully convince us of this. Define the quantities $\beta_{ij} = \alpha_i + \alpha_j$ with $i \neq j$. Of the six β_{ij}, only three of them (β_{1j}) are needed to recover the roots of $f(x)$:

$$
\begin{aligned}
2\alpha_1 &= +b + \beta_{12} + \beta_{13} + \beta_{14} \\
2\alpha_2 &= -b + \beta_{12} - \beta_{13} - \beta_{14} \\
2\alpha_3 &= -b - \beta_{12} + \beta_{13} - \beta_{14} \\
2\alpha_4 &= -b - \beta_{12} - \beta_{13} + \beta_{14}
\end{aligned} \tag{2.7}
$$

Here we have used the fact that $-b = \alpha_1 + \alpha_2 + \alpha_3 + \alpha_4$ — it is the first elementary symmetric polynomial in α_i, just as e is the last one. If we could determine the β_{1j} in terms of γ_{1j}, we would have a solution for the α_j. The key is that each of the three β_{1j} satisfies a quadratic equation depending on γ_{1j} and b. Indeed,

$$\begin{aligned} \beta_{12}+\beta_{34} &= -b \ , \ \beta_{12}\beta_{34}=\gamma_{12} \ \Rightarrow \ h_2(x)=x^2+bx+\gamma_{12}=(x-\beta_{12})(x-\beta_{34}) \\ \beta_{13}+\beta_{24} &= -b \ , \ \beta_{13}\beta_{24}=\gamma_{13} \ \Rightarrow \ h_3(x)=x^2+bx+\gamma_{13}=(x-\beta_{13})(x-\beta_{24}) \\ \beta_{14}+\beta_{23} &= -b \ , \ \beta_{14}\beta_{23}=\gamma_{14} \ \Rightarrow \ h_4(x)=x^2+bx+\gamma_{14}=(x-\beta_{14})(x-\beta_{23}) \end{aligned} \tag{2.8}$$

where $\beta_{34}=-b-\beta_{12}$, $\beta_{24}=-b-\beta_{13}$ and $\beta_{23}=-b-\beta_{14}$. We can solve the quadratic equations $h_j(x)=0$ since b and γ_{1j} are known. So this gives the β_{12}, β_{13}, β_{14} in terms of b,c,d,e, and thus α_1, α_2, α_3, α_4 in terms of b,c,d,e. However, when we solve $h_2(x)$ and find $x=\frac{-b\pm\sqrt{b^2-4\gamma_{12}}}{2}$, there is still the minor problem of determining which solution is β_{12} and which is β_{34}. Considering $h_3(x)$ and $h_4(x)$ as well, there are 8 ways to choose the signs. In principle, we could try all combinations one-by-one and stop when all $f(\alpha_i)=0$, but there is a more elegant approach. The key observation is that going between the two solutions, *e.g.* mapping β_{12} to β_{34}, can be achieved by sending

$$\beta_{1j}\mapsto\beta'_{1j}=-b-\beta_{1j} \tag{2.9}$$

Now by inspection, if we replace any *two* of the β_{1j} by β'_{1j}, each α_i in (2.7) will be replaced by another α_i. For example, replacing β_{12} by β'_{12} and β_{13} by β'_{13} has as effect that α_1 is interchanged with α_4, and α_2 with α_3. In other words, out of 8 sign choices, there are 4 choices that give the same correct answer and 4 choices that gives the same incorrect answer. We move within a group of 4 by applying (2.9) an even number of times, and we move between the groups by applying (2.9) an odd number of times. To choose the right one, we exploit the fact that a certain product of the square roots is again a symmetric function of the α_i.

$$\begin{aligned} \delta &= (2\beta_{12}+b)(2\beta_{13}+b)(2\beta_{14}+b) \\ &= 4bc-8d-b^3 \end{aligned} \tag{2.10}$$

Since $2\beta_{12}+b=\pm\sqrt{b^2-4\gamma_{12}}$, it is clear that δ agrees with $\sqrt{b^2-4\gamma_{12}}\sqrt{b^2-4\gamma_{13}}\sqrt{b^2-4\gamma_{14}}$ up to a sign. Therefore the last step of the algorithm is as follows. We compute candidates for the β_{1j} by choosing positive square roots and multiply these square roots together. If we get $4bc-8d-b^3$ we stop. If we get minus this number, we send one of the β_{1j} to β'_{1j}, or equivalently, change the sign for one of the square roots. We then go back through (2.7) and solve the original problem.

These steps can be illustrated with the following example

$$f(x)=x^4+2x^3+2x^2+4x+4 \tag{2.11}$$

From these coefficients, we write down the resolvent cubic. Unlike (2.11), it can be factored with the rational root test.[10] (For that reason we began with (2.11).)

$$\begin{aligned} g(x) &= x^3 - 4x^2 - 4x + 16 \\ &= (x-2)(x+2)(x-4) \end{aligned} \tag{2.12}$$

Choosing $\gamma_{12} = 4$, $\gamma_{13} = 2$ and $\gamma_{14} = -2$, we have from (2.8) sign ambiguities

$$\begin{aligned} \pm\sqrt{b^2 - 4\gamma_{12}} &= \pm 2i\sqrt{3} \\ \pm\sqrt{b^2 - 4\gamma_{13}} &= \pm 2i \\ \pm\sqrt{b^2 - 4\gamma_{14}} &= \pm 2\sqrt{3} \end{aligned} \tag{2.13}$$

The product of these must be δ which from (2.10) is -24. This means that all positive signs in (2.13) is a valid choice. Hence, $\frac{-b+\sqrt{b^2-4\gamma_{1j}}}{2}$ is β_{1j} rather than β'_{1j}. Writing the expressions for $\beta_{ij} = (-b + \sqrt{b^2 - 4\gamma_{ij}})/2$ down yields

$$\begin{aligned} \beta_{12} &= -1 + i\sqrt{3} \\ \beta_{13} &= -1 + i \\ \beta_{14} &= -1 + \sqrt{3} \end{aligned} \tag{2.14}$$

Going through (2.7) with these numbers finally yields

$$\begin{aligned} \alpha_1 &= \frac{-1+\sqrt{3}}{2} + \frac{1+\sqrt{3}}{2}i \\ \alpha_2 &= \frac{-1-\sqrt{3}}{2} + \frac{-1+\sqrt{3}}{2}i \\ \alpha_3 &= \frac{-1-\sqrt{3}}{2} + \frac{1-\sqrt{3}}{2}i \\ \alpha_4 &= \frac{-1+\sqrt{3}}{2} + \frac{-1-\sqrt{3}}{2}i \end{aligned} \tag{2.15}$$

This is the way Lagrange solved quartic polynomial equations.

Cardano's method for cubic equations. For completeness we review Cardano's method. The cubic equation $Ax^3 + Bx^2 + Cx + D = 0$ is first "depressed", meaning that the x^2 term is eliminated by shifting $x = x' + x_0$ and choosing x_0 suitably. Dividing by A we obtain $x'^3 + ax' + b = 0$. Next set $x' = \alpha\left(z + \frac{1}{z}\right)$ where α is a new parameter which will be chosen such that it simplifies the

[10] If a polynomial $P(x) = a_n x^n + \cdots + a_0$ with integer a_j has a rational root $x = p/q$ (with of course p and q relative primes), then multiplying $P(p/q)$ by q^n and moving the term with a_0 to the right-hand side and factoring out p on the left-hand side, shows that p divides a_0. Similarly, moving the term with a_n to the right-hand side shows that q divides a_n. So one may try as roots the ratios p/q where p is a divisor of a_0, and q is a divisor of a_n.

cubic equation. We obtain

$$\alpha^3 z^3 + (3\alpha^3 + \alpha a)z + (3\alpha^3 + \alpha a)\tfrac{1}{z} + \alpha^3 \tfrac{1}{z^3} + b = 0 \tag{2.16}$$

Setting $3\alpha^2 + a = 0$, both(!) terms with z and $\frac{1}{z}$ cancel, and defining $z^3 = t$, we get a quadratic equation for t, namely

$$\alpha^3 t^2 + bt + \alpha^3 = 0 \tag{2.17}$$

Solving for t and substituting $t = z^3$ we find the solutions for z in terms of quadratic and cubic roots, and from them the solutions for x'.

If we apply this method to (2.12), one finds easily $x_0 = \frac{4}{3}$ and

$$g(x') = x'^3 + ax' + b = (x')^3 - \tfrac{28}{3}x' + \tfrac{160}{27} = 0 \tag{2.18}$$

Then, setting $x' = \alpha\left(z + \frac{1}{z}\right)$, we find straightforwardly $\alpha^2 = \frac{28}{9}$ and $z^3 = t = (-10 \pm 9i\sqrt{3})/7\sqrt{7}$ which is a phase. The three solutions for z contain cubic roots of terms with quadratic roots. However, casting these expressions into simpler form seems quite difficult. Working backwards, the root $x = 2$ corresponds to $x' = \frac{2}{3}$, and this yields the phase $z = (1 \pm 3i\sqrt{3})/\sqrt{28}$. The cube of this expression yields the two values of t, but it is not easy to see without working backwards which of the six values of $z = t^{1/3} = \left[(-10 \pm 9i\sqrt{3})/7\sqrt{7}\right]^{1/3}$ can be simplified to $(1 \pm 3i\sqrt{3})/\sqrt{28}$. Thus, in this example at least, if one wants to obtain explicit expressions for the roots, Lagrange's method is simpler than Cardano's method.

Ferrari's method for the quartic equation. Also for completeness we review how the quartic equation was solved in terms of radicals by Ferrari in 1540, and published by his mentor Cardano in 1545 in the same book where he also published the solution of the cubic equation. Given the equation $Ax^4 + Bx^3 + Cx^2 + Dx + E = 0$, we divide by A and remove the term with x^3 by shifting x. To solve the equation $x^4 + ax^2 + bx + c = 0$ complete the squares as follows

$$\left(x^2 + \tfrac{a}{2}\right)^2 = \tfrac{a^2}{4} - bx - c \tag{2.19}$$

The right-hand side is not a pure square, but Ferrari's trick was to introduce a new parameter m and to choose it such that also the right-hand side becomes a square

$$\left(x^2 + \tfrac{a}{2} + m\right)^2 = 2mx^2 + am + m^2 + \tfrac{a^2}{4} - bx - c \tag{2.20}$$

The right-hand side will be a pure square in x if the discriminant of the quadratic equation in x vanishes

$$D = b^2 - 8m\left(am + m^2 + \tfrac{a^2}{4} - c\right) = 0 \tag{2.21}$$

This is a cubic equation in m, which can be solved in terms of radicals. Then also all solutions for x will be in terms of radicals. There seem to be 12 solutions for x (three for m, two for the pure squares, and two for the final quadratic equation for x), but only four are different.

Of course, some roots may involve roots of negative numbers, which was a problem in the 1540's, but the Italian physicist Bombelli discussed in his book L'Algebra of 1572 how to use the imaginary unit i to solve algebraic equations.

To obtain an example with nice roots we first choose values for m, a, b, c such that the discriminant D vanishes. Then we reconstruct the corresponding quartic equation, and apply the procedure of Ferrari. In this way we are guaranteed to obtain nice solutions.

In order that the leading term $2mx^2$ in D in (2.20) is a simple nice square we choose $m = 2$, and then the right-hand side should factorize, yielding two equal roots $x = \frac{b}{4m}$. For that reason we take $b = 4m = 8$. Then D becomes $D = 64 - 16\big(2a + 4 + \frac{a^2}{4} - c\big) = -16\big(2a + \frac{a^2}{4} - c\big)$. Setting $a = 2$ we find from $D = 0$ for c the value $c = 5$.

Thus we forget how we obtained the quartic equation and start from

$$x^4 + 2x^2 + 8x + 5 = 0\,. \tag{2.22}$$

Then we add a new parameter m as in (2.20). Anticipating that D vanishes, this can be written as

$$(x^2 + 1 + m)^2 = 2m\big(x - \tfrac{b}{4m}\big)^2 = 2m\big(x - \tfrac{2}{m}\big)^2\,. \tag{2.23}$$

The discriminant in (2.21) equals $D = 64 - 8m(2m + m^2 - 4)$. In principle we should solve this equation with Cardano's method (laborious!) but we already constructed one solution for m, namely $m = 2$. The other two solutions are twice $m = -2$. The corresponding equations for x and their solutions are as follows

$$\left.\begin{array}{rl} m = 2: & (x^2 + 3) = \pm 2(x - 1) \\ m = -2: & (x^2 - 1) = \pm 2i(x + 1) \end{array}\right\} \; x = 1 \pm 2i, -1, -1\,. \tag{2.24}$$

There are clearly 4 solutions, not 12.

*2.II Differential equations: Lie groups

Finally we discuss how group theory emerged from analysis. Abel and Galois, continuing the work of Lagrange, used permutation groups in their endeavours to construct solutions of polynomial equations, and this is one of the ways group theory originated. Klein and Lie continued these studies, and started investigating how groups act on objects (transformation groups). Klein studied their action on geometrical objects such as polyhedra, and this led to finite groups. Lie decided to investigate whether group theory can be used to construct solutions of differential equations (both ordinary and partial), and this led to continuous infinite groups which are nowadays called

Lie groups. The basic idea is to consider the set of symmetries of a differential equation, where by definition a symmetry is a transformation that maps (in a way to be discussed) solutions of the differential equation into solutions. Anyone who is already familiar with Lie groups as they occur in physics is perhaps surprised to learn that they first occurred in the theory of differential equations. However, that groups will be found is clear from the following observation: if one symmetry maps solutions to solutions, and a second symmetry does the same, then the product of two symmetries also does the same. Hence closure is guaranteed and it is clear that one will get groups. There is a large literature on the subject, but we shall be content with a few examples which illustrate the procedure to obtain Lie groups, rather than giving existence proofs.

Typical examples of symmetries of differential equations are translations, rotations and scale transformations, but there are usually more, less intuitive, symmetries. Different differential equations produce different groups. The Lie groups that are found this way are often not very nice groups, being neither semi-simple, nor any of the classical groups, and often solvable. Moreover, these groups may act nonlinearly on the coordinates and the functions, taking one outside the domain of (matrix) representation theory. Because the space of smooth functions is infinite dimensional, we shall get infinite dimensional realizations of the Lie groups. As a result, global properties are difficult to analyze, and a simpler approach is to study the group elements near the unit element, yielding "Lie algebra generators", differential operators X_k, which, after having been found, can (in principle at least) be exponentiated to yield the group elements of the symmetries of the system.[11] Lie considered continuous symmetry groups, although in some cases there are also discrete symmetries (like parity). The great advantage of continuous symmetry groups, as we shall see, is that one can use computer programs to determine systematically all generators X_k of the symmetries of a given differential equation.

What is the use of these symmetries of differential equations? First of all, one can use them to construct new solutions, and decompose the space of all solutions into "orbits" of the symmetry group. This leads to a classification of solutions, and in turn, a classification of differential equations. We shall not discuss these issues. Next, one can use the symmetries to reduce the degree of an ordinary differential equation from a nth order equation to an $(n-1)$th order equation. For $n = 1$, one gets even explicit formulas for the general solution. For partial differential equations, one cannot reduce their degree in this manner, but one can construct particular solutions, which are often of great use in physics. There are very many more aspects of the role of group theory in the area of differential equations (Hamiltonian systems, relation between symmetries and conservation laws, generalized Lie-Poisson structures), but we refer to the literature, for example the introduction of [7]. A readable account on an introductory level is in [8].

Example 1. Consider the heat equation $\partial_x\partial_x u = \partial_t u$. Let us be more explicit by what is meant by a map from one solution to another solution. Given a differential equation, for example

[11] We use the notation X_k for the differential operators which form a realization of the abstract Lie algebra with generators L_k.

$\partial_x \partial_x u(x,t) = \partial_t u(x,t)$, consider the transformation

$$x \to x^*(\lambda, x, t, u)\,; \quad t \to t^*(\lambda, x, t, u)\,; \quad u \to u^*(\lambda, x, t, u)\,, \tag{2.25}$$

where x^*, t^*, u^* can be any (linear or nonlinear) functions of x, t, u, λ, where λ is a real continuous parameter (as we shall see, a group parameter of the Lie group). For example if $x^* = e^\lambda x$, $t^* = e^{2\lambda} t$, $u^* = u$, and if u is a solution of the heat equation $\partial_x \partial_x u = \partial_t u$, then also $\tilde{u}(x,t) = u^*(x^*, t^*)$ is a solution

$$\begin{aligned} \partial_x \partial_x \tilde{u}(x,t) &= e^\lambda \partial_y e^\lambda \partial_y u(y,\tau) = e^{2\lambda} \partial_y \partial_y u(y,\tau) \quad \text{with } y = e^\lambda x,\ \tau = e^{2\lambda} t \\ \partial_t \tilde{u}(x,t) &= \partial_t u(e^\lambda x, e^{2\lambda} t) = e^{2\lambda} \partial_\tau u(y,\tau)\,. \end{aligned} \tag{2.26}$$

Clearly $\tilde{u}(x,t)$ is also a solution, $\partial_x \partial_x \tilde{u}(x,t) = \partial_t \tilde{u}(x,t)$.

Expanding in terms of λ, the terms of order λ^k separately satisfy the differential equation for any k. In the example

$$\begin{aligned} x^* = x + x^{(1)} + x^{(2)} + \cdots\,, &\qquad x^{(1)} = \lambda x \\ t^{(1)} = 2\lambda t\,; &\qquad u^{(1)} = 0\,. \end{aligned} \tag{2.27}$$

The transformations near $\lambda = 0$ can be written as a differential operator X acting on x, t, u. In the example $X = x\partial_x + 2t\partial_t$ and $Xu = x\partial_x u + 2t\partial_t u$ will satisfy the heat equation. As a second symmetry consider space translations $x \to x^* = x + \lambda$, $t = t^*$, $u = u^*$. The function $\tilde{u}(x,t) = u(x+\lambda, t)$ obviously still satisfies the heat equation, and the differential operator for this symmetry is $X = \partial_x$. As a third example, consider the transformation $u(x,) \to \tilde{u}(x,t) = e^\lambda u(x,t)$. Now $X = u\partial_u$. The X's are to be considered the generators of a group, in the sense that $e^{\lambda X}$ generates a corresponding one-parameter group element, and if there are k symmetries, we get k generators $X_1, \cdots, X_k$, and a general group element can be written as

$$g = e^{\lambda^1 X_1} e^{\lambda^2 X_2} \cdots e^{\lambda^k X_k}\,. \tag{2.28}$$

These group generators satisfy an algebra: they form a linear vector space A with elements $V = \sum_k \lambda^k X_k$, and the commutators of two X_k operators close. Indeed, each $X_k u$ satisfies the differential equation, hence also $X_k X_l u$ satisfies it, and a fortiori $[X_k, X_l]u$ is again a solution. If $[X_k, X_l]$ lies in A we found nothing new, but if $[X_k, X_l]$ is not a linear combination of the X_k we already got, we add it to the list of X_k. In the way we obtain **closure** of the commutators of the differential operators X_k. We have now a closed **algebra**. (In an algebra one has two operations: addition in a linear vector space, and "multiplication" where here the "product" of X_k and X_l is their commutator.)

The complete set of Lie algebra generators for the heat equation is as follows[12]

$$\begin{aligned} &X_1 = \partial_x\,; \quad X_2 = \partial_t\,; \quad X_3 = u\partial_u\,; \quad X_4 = x\partial_x + 2t\partial_t\,; \\ &X_5 = 2t\partial_x + xu\partial_u\,; \quad X_6 = 4tx\partial_x + 4t^2\partial_t + (x^2+2t)u\partial_u \end{aligned} \tag{2.29}$$

The first four operators generate space and time translations, scaling of u, and separate scaling of x and t, but it is not obvious that X_5 and X_6 generate symmetries. They do, however, as one can prove by checking that

$$\tilde{u}_5(x,t) = 2t\partial_x u + xu \quad \text{satisfies } \partial_x\partial_x\tilde{u}_5 = \partial_t\tilde{u}_5\,, \tag{2.30}$$

and similarly (with obviously more work) for X_6. (In the expressions for $\partial_x\partial_x\tilde{u}_5$ and $\partial_t\tilde{u}_5$ one should substitute $\partial_t u = \partial_x\partial_x u$.)

The commutators can be collected in the analogue of a Latin square, as an 6×6 matrix A with the entries A_{jk} equal to $[X_j, X_k]$

$$\begin{array}{c|cccccc} & X_1 & X_2 & X_3 & X_4 & X_5 & X_6 \\ \hline X_1 & 0 & 0 & 0 & X_1 & X_3 & 2X_5 \\ X_2 & 0 & 0 & 0 & 2X_2 & 2X_1 & 4X_4+2X_3 \\ X_3 & 0 & 0 & 0 & 0 & 0 & 0 \\ X_4 & -X_1 & -2X_2 & 0 & 0 & X_5 & 2X_6 \\ X_5 & -X_3 & -2X_1 & 0 & -X_5 & 0 & 0 \\ X_6 & -2X_5 & -4X_4-2X_3 & 0 & -2X_6 & 0 & 0 \end{array} \tag{2.31}$$

To identify the corresponding abstract Lie algebra A we note that (X_1, X_3, X_5) form a subalgebra M, and $(X_2, X_4 + \frac{1}{2}X_3, X_6)$ another subalgebra N of the following form:

$$A = M \cup N\,; \quad [M,M] \subset M\,; \quad [N,N] \subset N\,; \quad [M,N] \subset M\,. \tag{2.32}$$

Thus N is an ideal of M (an ideal is like an invariant subgroup, but now an invariant subalgebra). Reordering the generators this structure becomes manifest

$$\begin{array}{c|ccc:ccc} & X_1 & X_3 & X_5 & X_2 & X_4+\frac{1}{2}X_3 & X_6 \\ \hline X_1 & 0 & 0 & X_3 & 0 & X_1 & 2X_5 \\ X_3 & 0 & 0 & 0 & 0 & 0 & 0 \\ X_5 & -X_3 & 0 & 0 & -2X_1 & -X_5 & 0 \\ \hdashline X_2 & 0 & 0 & 2X_1 & 0 & 2X_2 & 4X_4+2X_3 \\ X_4+\frac{1}{2}X_3 & -X_1 & 0 & X_5 & -2X_2 & 0 & 2X_6 \\ X_6 & -2X_5 & 0 & 0 & -4X_4-2X_3 & -2X_6 & 0 \end{array} \tag{2.33}$$

[12] This example is taken from section 2.6 of the excellent textbook [9]. There are some misprints in their formulas which we have corrected.

The Lie algebra spanned by (X_1, X_3, X_5) is non-semisimple because X_3 is an abelian ideal (X_3 commutes with X_1 and X_5). To identify it, we write it as

$$\begin{aligned} [L_0, L_+] &= 0 \quad \text{with } L_0 = \tfrac{1}{2}X_3 \text{ and } L_+ = X_5 \\ [L_0, L_-] &= 0 \quad \text{with } L_- = X_1 \\ [L_+, L_-] &= -2L_0 \end{aligned} \tag{2.34}$$

This is a Wigner-Inönü group contraction of the algebra of the group $SL(2,\mathbb{R}) = SO(2,1)$, known from angular momentum theory

$$[L_0, L_\pm] = \pm L_\pm\,; \quad [L_+, L_-] = -2L_0 \tag{2.35}$$

(As usual $L_\pm = L_1 \pm iL_2$ and $L_0 = L_3$, but our L_1, L_2, L_3 are antihermitian.) Setting $L_\pm = \sqrt{a}\tilde{L}_\pm$ and $L_0 = a\tilde{L}_0$, and taking the limit $a \to \infty$, yields (2.34).

The Lie algebra spanned by $(X_2, X_4 + \frac{1}{2}X_3, X_6)$ is easier to identify. Defining arbitrarily $X_2 = T_1$, $4X_4 + 2X_3 = T_2$, $X_6 = T_3$ we get

$$\left.\begin{aligned} [T_1, T_2] &= 2T_1 \\ [T_2, T_3] &= 2T_3 \\ [T_3, T_1] &= -T_2 \end{aligned}\right\} \Rightarrow \quad \begin{aligned} [L_0, L_\pm] &= \pm L_\pm \\ [L_+, L_-] &= -2L_0 \end{aligned} \tag{2.36}$$

with $L_0 = \frac{1}{2}T_2$, $L_+ = T_3$ and $L_- = T_1$. This is the group algebra $so(2,1)$. Hence, the symmetry algebra of the heat kernel is the semidirect sum (we use lowercase letters for the algebra)

$$so(2,1)_{\text{contracted}} \otimes so(2,1) \tag{2.37}$$

Exponentiation of the algebra yields the corresponding group. The exponentiation of X_1, X_3 and X_4 yields symmetries we identified before, but the exponentiation of X_5 and X_6 is tedious, see [10]. The results are as follows

$$\begin{aligned} \tilde{u}_5(x,t) &= e^{\lambda x + \lambda^2 t} u(x + 2\lambda t, t) \\ \tilde{u}_6(x,t) &= \frac{1}{\sqrt{|1+\gamma t|}} e^{-\frac{\gamma x^2}{4(1+\gamma t)}} u\left(\frac{x}{1+\gamma t}, \frac{t}{1+\gamma t}\right) \end{aligned} \tag{2.38}$$

The function $u(x,t) = 1$ is, of course, a solution of the heat equation, and substituting this into $\tilde{u}_6$ we obtain the Green function for the heat equation. As to $\tilde{u}_5$, it is easy to check that it is a solution, but we are not aware of a physical interpretation.

Example 2. The Laplace equation $\Box u = 0$ with $\Box = \sum_{i=1}^n \partial_{x^i}\partial_{x^i}$. Following the same steps as before, we find the following infinitesimal symmetries

$P = \frac{\partial}{\partial x^i}$ (translations).

$L_{ij} = x_i \partial_{x^j} - x_j \partial_{x^i}$ ($\frac{1}{2}n(n-1)$ rotations).

$D = \sum_l x^l \frac{\partial}{\partial x^l}$ (dilatations)

$K = x_k (x^j \frac{\partial}{\partial x^j}) - \frac{1}{2} x^2 \frac{\partial}{\partial x^k} + (\frac{n-2}{2}) x^k u \frac{\partial}{\partial u}$ (n conformal boosts)

$A = u \frac{\partial}{\partial u}$ (rescaling $u \to \lambda u$)

$B = B(x) \frac{\partial}{\partial u}$ with $\Box B = 0$.

The transformations generated by P, L, D and K form the conformal algebra $so(n-1,1)$ in Euclidean space which leaves the line element $dx^i dx^i = 0$ invariant, but the operators A and B are present because we can also transform the scalar function u (see the comments later).

Example 3. Symmetries of $(\nabla u)^2 dx^1 \cdots dx^n$. The generators are

$$P_i = \frac{\partial}{\partial x^i}\,; \quad L_{ij} = x_i \frac{\partial}{\partial x^j} - x_j \frac{\partial}{\partial x^i}\,; \quad T = \frac{\partial}{\partial u}\,; \quad D = -x^i \frac{\partial}{\partial x^i} + \left(\frac{n}{2} - 1\right) u \frac{\partial}{\partial u} \tag{2.39}$$

The finite symmetry transformation for D is

$$(x^i)^* = -\lambda x^i\,; \quad u^* = e^{\lambda \frac{n}{2} - 1} u\,. \tag{2.40}$$

The symmetry group is the Euclidean Poincaré group, augmented with dilatations and a shift of u.

Example 4. Burgers' modified heat equation $u_{xx} + (u_x)^2 = u_t$. This is the simplest extension of the heat equation with both dissipation and nonlinear effects. The Lie algebra of the symmetry generators resembles strongly the result for the heat equation

$$\begin{gathered} L_1 = \partial_x\,; \quad L_2 = \partial_t\,; \quad L_3 = \partial_u\,; \quad L_4 = x\partial_x + 2t\partial_t\,; \\ L_5 = 2t\partial_x + x\partial_u\,; \quad L_6 = 4tx\partial_x + 4t^2\partial_t + (x^2 + 2t)\partial_u \end{gathered} \tag{2.41}$$

Only in L_3, L_5 and L_6 has a factor u been deleted as compared to the generators for the heat equation.

Example 5. The Korteweg-de Vries equation

$$u_t + u_{xxx} + u u_x = 0\,. \tag{2.42}$$

This is a higher order nonlinear partial differential equation, and describes long waves in shallow water. The symmetry generators are ∂_x, ∂_t, $t\partial_x + \partial_u$, $x\partial_x + 3t\partial_t - 2u\partial_u$ (space translations, time translations, Galilean boosts, and scale transformations).

Exponentiation shows that if $u = f(x,t)$ is a solution of KdV equation, so are

$$u_1 = f(x-\lambda_1, t)\,; \quad u_2 = f(x, t-\lambda_2)\,; \quad u_3 = f(x-\lambda t, t)+\lambda\,; \quad u_4 = e^{-2\lambda} f(e^{-\lambda}x, e^{-3\lambda}t) \tag{2.43}$$

The commutation relations are

	L_1	L_2	L_3	L_4
L_1	0	0	0	L_1
L_2	0	0	L_1	$3L_2$
L_3	0	$-L_1$	0	$-2L_3$
L_4	$-L_1$	$-3L_2$	$2L_3$	0

The algebra is the semi-direct sum $(L_1, L_2) \otimes (L_3, L_4)$ where (L_1, L_2) form an abelian ideal, and (L_3, L_4) form a two-dimensional subalgebra of the form $[L_3, L_4] = -2L_3$.

Comment 1. We expanded the finite transformation rules of x and u in the heat equation in terms of a Taylor expansion in λ, and studied the terms linear in λ. They separately mapped solutions into solutions, and formed a Lie algebra. One can also keep the terms of any other order in λ; they, too, yield functions which satisfy the differential equation. This is generally true, and is fun to check for the heat equation.

Comment 2. Our aim was to show how groups arise from the symmetries of (linear or nonlinear, ordinary or partial) differential equations. But this approach can be used to actually construct solutions (see Example 1), or to simplify the differential equations.

Comment 3. Most of the algebras we have encountered were pretty ugly: nonsemisimple and abelian. Klein's approach to symmetries of polyhedra yielded interesting but finite groups. Nice (simple) Lie algebras are encountered in particle physics if one puts particles in multiplets. We shall concentrate on these algebras, but we mention here Levi's theorem:

Levi's Theorem. Every Lie algebra is a semidirect sum of its radical and a semisimple Lie algebra.
(A semisimple Lie algebra is a direct sum of simple Lie algebras, a simple Lie algebra has no ideals, the radical is the maximal solvable ideal, and for a solvable algebra L the series $[L, L] \subset L_1$, $[L_1, L_1] \subset L_2$, $\cdots$ stops.) One can identify the radical in the examples discussed above. For example, for the Poincaré group, the translations form the radical.

Comment 4. How does one know whether one has found all symmetries? One can write down the most general expressions for the Lie algebra generators X_k, and require closure. Obviously, this is hopelessly complicated to do by hand, but computer programs have been written which do this task, and this has become an active research field. In our example of the heat equation $\partial_x\partial_x u = \partial_t u$ there are further symmetries, for example $u \to u + \lambda$, yielding $X_7 = \partial_u$. Taking the commutators of X_7 with the $X_1, \cdots, X_6$ given above, yields $X_8 = x\partial_u$ and $X_9 = (x^2+2t)\partial_u$. These X_8 and X_9 generate the translation $u \to u + x$ and $u \to u + x^2 + 2t$. It becomes now clear that any shift $u \to u + B(x,t)$ is a symmetry as long as B satisfies the heat equation $\partial_x\partial_x B = \partial_t B$. The space of such $B(x,t)$ is infinite dimensional, and if one restricts the definition of Lie groups by requiring that they have only a finite number of generators, one usually omits writing B's (as we did. However, in the Laplace equation we included B's).

Comment 5. Not all operators for the heat kernel in (2.29) are antihermitian, but by adding polynomials in x and t they can be made antihermitian. The following operators are antihermitian

$$\begin{gathered}\hat{X}_1 = \partial_x\,; \quad \hat{X}_2 = \partial_t\,; \quad \hat{X}_3 = X_3 + \tfrac{1}{2}\,; \\ \hat{X}_4 = X_4 + \tfrac{3}{2}\,; \quad \hat{X}_5 = X_5 + \tfrac{1}{2}x\,; \quad \hat{X}_6 = X_6 + 7t + \tfrac{1}{2}x^2\,. \end{gathered} \tag{2.44}$$

The commutation relations for the $\hat{X}$ are the same as for the X in (2.31) and (2.33). This closure follows of course from the fact that the commutator of two antihermitian operators is antihermitian, but decomposing $\hat{X}_k = X_k + P_k$ where P_k are polynomials in x, t, u, then P_k satisfy $[X_k, P_l] - [X_l, P_k] = f_{kl}{}^m P_m$ where $f_{kl}{}^m$ are given by $[X_k, X_l] = f_{kl}{}^m X_m$. This is a good check on the expressions for X_k and P_k. Perhaps imposing antihermiticity may be useful as an algorithm for other complicated cases. (We have not found a discussion of this observation in the literature.)

Comment 6. We also have not found an application of these ideas of Lie to superalgebras in the literature either. This might be an interesting topic.

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Chapter 3

Basic concepts in Group Theory - I

3.1 Order of a group. Subgroups.

The **order of a group G**, denoted by $|G|$, is the number of elements of G. So the order of the group of isometries of a regular tetrahedron is 24. A **subgroup** H is a subset of group elements of G which by themselves form a group. One must check closure, and the presence of a unity[1] and inverses, but associativity need not be checked because G is already associative. We already encountered an example: A_n is a subgroup of S_n.

3.2 Left (right) cosets

Left Cosets. Let H be a subgroup of order $k+1$ with elements

$$H = eH = (e, h_1, \cdots, h_k) \tag{3.1}$$

$$\text{Pick } a \text{ not in } H \text{ and form } aH = (a, ah_1, \cdots, ah_k) \tag{3.2}$$

$$\text{Pick } b \text{ not in } H \text{ and not in } aH\text{: } bH = (b, bh_1, \cdots, bh_k) \tag{3.3}$$

$$\vdots \tag{3.4}$$

$$\text{Pick } c \text{ not in } H,\ aH,\ bH, \cdots\text{: } cH = (c, ch_1, \cdots, ch_k). \tag{3.5}$$

The sets $H, aH, bH, \cdots, cH$ are called left-coset elements (so each coset element contains $k+1$ group elements). The collection of all coset elements is called the coset.

Theorem: All group elements of a given coset element are different.

Proof: Assume $ah_k = ah_l$, but $h_k \neq h_l$, then by multiplication with a^{-1} we obtain $h_k = h_l$,

[1]The unit element and inverses in G are the same as the unit element and inverses in H. For example, the unit element e_H for H must satisfy $e_H h = h e_H = h$ for all group elements h in H. Taking $h = e_H$ implies that $e_H e_H = e_H$. So the unit element for H must be the same as the unit element for G. Similarly for the inverse of group element h in H.

which is a contradiction.

Theorem: Group elements in different coset elements are different.

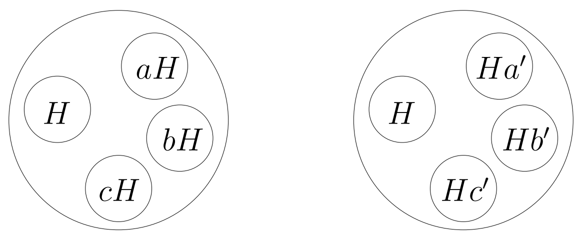
Proof: If $ah_k = bh_l$ then $b = ah_k h_l^{-1} = ah'$, contradiction.

Thus all group elements in all left-coset elements are different, and the total set of group elements is just the group G. Then the following is clear: The total number of group elements of G is equal to the number of group elements in H times the number n_{cosets} of left-coset elements.

3.3 Lagrange's theorem

Lagrange's[2] Theorem: The order of a subgroup H is a divisor of the order of the group G.

$$|G| = |H| \times n_{cosets}. \tag{3.6}$$



Pictorially, we see that G decomposes into non-overlapping coset elements, all of which are equally large (contain the same number of group elements).

Comment. We constructed a left-coset element aH by picking a group element a and multiplying it with all elements of the subgroup H. But we can also pick any other group element $a' = ah$ in this coset aH and construct the set $a'H$, because $a'H = (ah)H = a(hH) = aH$. So all group elements in a given coset element appear on equal footing.

One can also consider right-coset elements H, Ha', Hb', $\cdots$, Hc' where a' is not in H, b' is not in H or Ha', etc. Again $|G| = |H| \times n_{cosets}$, which shows that the number of left-coset elements is equal to the number of right-coset elements. However, in general the left-coset elements aH are not equal to the right-coset elements Ha.[3]

[2] Lagrange (1771) did not prove Lagrange's theorem in its general form but only for polynomials of the kind we discussed before. Gausz (1801) proved it for the positive integers modulo a prime number p, which form a group as we also discussed before. Cauchy (1844) proved it for S_n. Finally, the French mathematicians Camille Jordan (not to be confused with the German physicist Pascual Jordan of quantum mechanics) proved it for general groups in 1861.

[3] One can still establish a 1–1 correspondence between left-coset elements and right-coset elements as follows $f(aH) = Ha^{-1}$. If one picks any other group element a' in aH, it is still true that $f(a'H) = Ha'^{-1}$, so this is really a map from coset elements to coset elements. Other maps, for example $f(aH) = Ha$, do not have this property.

3.4 Normal (invariant) subgroups

It is natural to ask: when are the left-coset elements equal to the right-coset elements? When is $gH = Hg$ for all g in G? (When is **the set** $g, gh_1, \cdots, gh_k$ equal to **the set** $g, h_1g, \cdots, h_kg$? Note that we do not require that $gh_i = h_ig$ for a fixed h_i.) Those subgroups for which this is true are called **normal (or invariant) subgroups**. They are denoted by N. (They are a special case of subgroups H. They are in some sense the equivalent of prime numbers, because any finite group can be built from normal subgroups in a way we will discuss later, just as any natural number can be decomposed into a product of prime numbers.) An equivalent definition of a normal subgroup N is the set of all group elements n for which

$$gng^{-1} \text{ lies in } N \text{ for all } g \text{ in } G.$$

(Prove the equivalence yourself.) Here comes a surprise:

Theorem: The set of coset elements of a normal subgroup form themselves another group, called the **quotient group** and denoted by G/N.

Proof: The group elements of G/N are $N, aN, bN, \cdots$ and group multiplication is defined as follows

$$(aN)(bN) = (ab)N \qquad \text{because } Nb = bN \text{ and } NN = N. \tag{3.7}$$

The unit element is $eN = N$. Inverses of coset elements are again coset elements $(aN)^{-1} = a^{-1}N$ (this defines $(aN)^{-1}$). Associativity holds for the quotient group because it holds for G.

3.5 Order of a group element

The **order of a group element g**, denoted by $|g|$, is defined as follows: construct the sequence

$$e, g, g^2, g^3, \cdots, g^k = e, \tag{3.8}$$

where $g^2 = gg$, etc. For a finite group one must at some point repeat an element. Suppose the first time this happens is when we reach g^r. So $g^r = g^s$ for $r > s$. Then $g^{r-s} = g^k = e$ is the first time e appears in the sequence. So all group elements $e, g, g^2, \cdots, g^{k-1}$ in (3.8) are different. Then the order of g is k.

For any group element g with $g^k = e$ the sequence $e, g, g^2, \cdots g^{k-1}$ forms a subgroup, called the **cyclic group Z_k** of order k. It follows from Lagrange's theorem that the order of a group element is a divisor of the order of G.

Theorem: For $p =$ prime number Z_p has no nontrivial subgroups.

Proof: Use Lagrange's theorem. So if one picks any element g of Z_p, the set $e, g, \cdots, g^{p-1}$ reproduces the whole group Z_p.

Another set of groups we will often encounter are the **permutation groups $\boldsymbol{S_n}$**. The group S_n is the group of permutations of n objects, and $|S_n| = n!$.

3.6 Direct product groups

The **direct product** of two groups, denoted by $G_1 \otimes G_2$, is the set of elements (g_i, g'_j) where g_i lies in G_1, and g'_j in G_2. Group multiplication is derived as follows

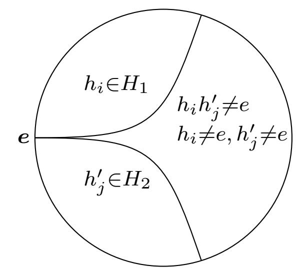
$$(g_1, g'_1)(g_2, g'_2) = (g_1 g_2, g'_1 g'_2). \tag{3.9}$$

Closure clearly holds and we leave as an exercise to check that $G_1 \otimes G_2$ is again a group.

Often the following situation occurs. A given group G has two subgroups H_1 and H_2 satisfying the following properties:

(i) They have only the unit element e in common, $H_1 \cap H_2 = e$.

(ii) All group elements of G can be written as $h_i h'_j$ where h_i are the group elements of H_1 and h'_j those of H_2 (see the figure).



(iii) All h_i commute with h'_j.

So we can obtain all group elements of G by multiplying H_1 and H_2

$$G = H_1 H_2 \,. \tag{3.10}$$

There is then an isomorphism between $H_1 H_2$ and $H_1 \otimes H_2$: namely a $1-1$ map ϕ from the elements of $H_1 H_2$ onto all elements of $H_1 \otimes H_2$ such that group multiplication is the same. This map is

$$\phi(h_i h'_j) = (h_i, h'_j) \ . \tag{3.11}$$

So then we may also write $G = H_1 \times H_2$.

We considered here two subgroups whose elements commute: $h_{1i} h_{2j} = h_{2j} h_{1i}$ for $h_{1i} \in H_1$ and $h_{2j} \in H_2$. One can also consider the case that **both** H_1 and H_2 are normal subgroups and $H_1 \cap H_2 = e$; then it is still true[4] that $H_1 \times H_2$ is isomorphic to $H_1 H_2$. If only H_1 is normal and H_2 is a subgroup, then one can define a semi-direct product.

[4] Calling the normal subgroups N_1 and N_2, the group elements of $N_1 \times N_2$ are again (n_{1i}, n_{2j}) but the group elements of $N_1 N_2$ can be written as $n_{1i} n_{2j}$. Group multiplication for the $N_1 \times N_2$ is defined as $(n_{1i}, n_{2j})(n_{1k}, n_{2l}) = (n_{1i} n_{1k}, n_{2j} n_{2l})$ but for $N_1 N_2$ we get $(n_{1i} n_{2j})(n_{1k} n_{2l})$ whereas we need $n_{1i} n_{1k} n_{2j} n_{2l}$ for isomorphy. Actually, n_{1i} and n_{2j} commute: consider $n_{1i} n_{2j} n_{1i}^{-1} n_{2j}^{-1}$. It can be written as $(n_{1i} n_{2j} n_{1i}^{-1}) n_{2j}^{-1}$ which lies in N_2 or as $n_{1i}(n_{2j} n_{1i}^{-1} n_{2j}^{-1})$ which lies in N_1. Since $N_1 \cap N_2 = e$ by assumption, we get $n_{1i} n_{2j} = n_{2j} n_{1i}$.

3.7 Semi-direct product groups

We defined the direct product of two subgroups H_1 and H_2 of a group G before. If G is the direct product of H_1 and H_2 they should satisfy $H_1 \cap H_2 = e$, $[H_1, H_2] = 0$ and $G = H_1 H_2$. We now consider the product structure of a group in terms of one normal subgroup N and one subgroup H. If G is the semi-direct product of N and H, one uses the notation $G = N \rtimes H$. The requirements are[5]

1) N is normal subgroup of G.

2) H is subgroup of G.

3) $N \cap H = e$.

4) $G = NH$.

Since N is normal, all group elements of G can be written as $g = nh$ with n in N and h in H. This is a group: closure holds since if $g_1 = n_1 h_1$ and $g_2 = n_2 h_2$, then $g_1 g_2 = n_1 h_1 n_2 h_2 = n_1 (h_1 n_2 h_1^{-1}) h_1 h_2 = \tilde{n}\tilde{h}$. The unit is of course e, and if $g = nh$ then $g^{-1} = h^{-1} n^{-1} = (h^{-1} n^{-1} h) h^{-1} = \tilde{n}\tilde{h}$. Some examples are ($D_n$ will be defined in the next chapter)

$$\begin{gathered} D_n = Z_n \rtimes Z_2\,; \qquad S_n = A_n \rtimes Z_2\,; \\ \text{Poincaré group} = \text{translations} \rtimes \text{Lorentz transformations}. \end{gathered} \tag{3.12}$$

Theorem: If $n = pq$ where p, q are coprime (relatively prime, denoted by $(p, q) = 1$, they have no integer in common except the number one), then $Z_p \otimes Z_q = Z_{pq}$.

For example: $Z_3 \otimes Z_2 = Z_6$. If the elements of Z_6 are $e, a, a^2, \cdots, a^5$, we define $Z_2 = (e, a^3)$ and $Z_3 = (e, a^2, a^4)$. Then the set of 6 elements $(e, a^3) \otimes (e, a^2, a^4)$ reproduces the set of elements of Z_6, and $a^3 \times a^2 = a^5$ and $a^3 \times a^4 = a$ generate Z_6 (they have order 6). Conversely, if $Z_2 = (e, a)$ and $Z_3 = (e, b, b^2)$ and a and b commute, then $Z_2 \otimes Z_3$ forms the cyclic group Z_6 because it is generated by the group element ab (or ab^2).

The proof of this theorem uses the algorithm of Euclid (if $(p, q) = 1$ there exist integers r and s such that $rp + sq = 1$. For example, if $(p, q) = (2, 3)$ then (r, s) can be $(2, -1)$, $(5, -3)$, $(8, -5)$ or $(-1, 1)$, $(-4, 3)$, $\cdots$, in general $(r, s) = (2 + 3l, -1 - 2l)$ with $l = \cdots, -1, 0, +1, +2)$.

Note that if $(p, q) \neq 1$ (if p and q are not coprime, for example if $p = 2$ and $q = 2$) then it is not true that $Z_p \otimes Z_q = Z_{pq}$. For example Z_4 has an element of order 4, but all elements of $Z_2 \otimes Z_2$ (except e) have order 2. Thus the theorem can be sharpened to: $Z_p \otimes Z_q$ is equal (isomorphic) to Z_{pq} if and only if $(p, q) = 1$.

Exercise. Check that $Z_3 \otimes Z_4 = Z_{12}$ if $Z_3 = (e, a, a^2)$ and $Z_4 = (e, b, b^2, b^3)$ and $ab = ba$. Then show that $Z_{12} = (e, c, c^2, \cdots, c^{11})$ can be written as $Z_3 \otimes Z_4$.

[5] One can define a more general semi-direct product structure, see Ramond, but we shall not need it.

Exercise. Show that the intersections $G_1 \cap G_2$, $H_1 \cap H_2$, $N_1 \cap N_2$ of the groups G_j, subgroups H_j and normal subgroups N_j are again groups, subgroups and normal subgroups, respectively.

Exercise. Show that if H is a subgroup of G, and H' is a subgroup of H, then H' is a subgroup of G. If N is a normal subgroup of G, and N' is a normal subgroup of N, is N' then a normal subgroup of G? (The answer is no, see next chapter.)

Chapter 4

Examples of finite groups

We now present several examples of finite groups for two reasons: to illustrate the general theorems, we have encountered so far, but also because these examples play an important role in applications to problems in physics.

4.1 Permutations and cycles

4.2 The symmetric groups S_n and the alternating groups A_n

4.3 The Klein group V

The rotations $a = R_x(\pi)$, $b = R_y(\pi)$, $c = R_z(\pi)$ around the x, y and z-axis over an angle π, together with the unit element e (no rotation) form a group denoted by V. One may check that $a^2 = b^2 = c^2 = e$ and $ab = ba = c$, $ac = ca = b$ and $bc = cb = a$. So $|V| = 4$. This group is called the Klein group (after Felix Klein), or the four-group (Vierer Gruppe in German (vier=four), which explains the notation V). The group multiplication table is:

V	e	a	b	c
e	e	a	b	c
a	a	e	c	b
b	b	c	e	a
c	c	b	a	e

A finite group is abelian if and only if its group multiplication table is symmetric about the diagonal. Hence V is abelian and $V = (e, a) \otimes (e, b) = Z_2 \otimes Z_2$. Further, order a = order b = order $c = 2$. Any nontrivial subgroup H of V must have $|H| = 2$, so $H = (e, a)$ (or $H = (e, b)$ or $H = (e, c)$). For an abelian group all subgroups are normal, and $V/H = (H, bH) = Z_2$ if $H = (e, a)$.

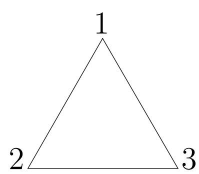
4.4 The dihedral groups D_n

The isometries of a regular n-polygon in a plane form the dihedral group D_n. They consist of n rotations around an axis perpendicular to the plane forming the group Z_n, and n reflections in the plane[1]. So the order of D_n is $2n$. One can define D_n by giving its group multiplication tables but that becomes cumbersome for larger n. Instead one uses the concept of **a presentation**: a subset of group elements which satisfy some relations, and whose products generate the whole group. For D_n a presentation is

$$D_n = \{a, b | a^n = e, b^2 = e, bab^{-1} = a^{-1}\} \tag{4.1}$$

Here a is a rotation over $\frac{2\pi}{n}$, and b is a reflection. Since $ba = a^{-1}b$, the set of group elements is $e, a, a^2, \cdots, a^{n-1}$ and $b, ab, \cdots, a^{n-1}b$. Sometimes there is more than one presentation to define a group.

***D_3*.** We consider first the regular triangle, and use cycles to denote the group elements.



$$\left.\begin{array}{c} \text{3 rotations: } e, (123), (132) \\ \text{3 reflections: } (23), (13), (12) \end{array}\right\} \text{closure holds.}$$

The rotations form a subgroup by themselves (the product of two rotations is again a rotation). Like the tetrahedron, every permutation of the vertices $1, 2, 3$ corresponds to a different isometry, and every isometry corresponds to a different permutation, so: the group of isometries of the triangle is $D_3 = S_3$, and the representation of D_3 in terms of 2×2 matrices is **faithful**[2]. Clearly, $|D_3| = 6$. The group $D_3 = S_3$ is nonabelian:

$$\left.\begin{array}{l} (12)(123) = (13) \\ (123)(12) = (23) \end{array}\right\} \text{ and } (13) \neq (23). \tag{4.2}$$

The subgroup A_3 of even permutations consists of $e, (123)$ and (132). (Recall that $(abc) = (ac)(bc)$ so all (abc) are even permutations.) So the subgroup of rotations of the triangle is $Z_3 = A_3$.

We claim that A_3 is a normal subgroup of S_3. The left-coset elements of S_3 are A_3 and gA_3 where g is any of $(23), (13)$ or (12). The right coset elements are A_3 and A_3g. It follows that the sets gA_3 and A_3g are equal (because they are the set of all odd permutations), so A_3 is a normal

[1] Any reflection can be obtained as the product of a rotation and a particular reflection. Note that a reflection in the plane is equivalent to a rotation in 3-dimensional space. For example, the reflection about the x-axis in the plane gives the same result as a rotation around the x-axis over an angle π.

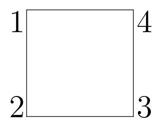
[2] A representation of a group is faithful if different group elements correspond to different matrices of the representation. Then the representation uniquely characterizes the abstract group. The 2×2 matrices representing D_3 are easily constructed: the 4 rotations have $\det M = +1$ and the 4 reflections have $\det M = -1$. Then it is clear that this representation is faithful.

subgroup of S_3. Then the quotient group S_3/A_3 has order 2, so it must be Z_2

$$S_3/A_3 = Z_2. \tag{4.3}$$

For example G/A_3 consists of $E = A_3$ and $B = (12)A_3$, and the set E, B has the same group multiplication table as e and (12).

***D*₄.** The regular square has isometry group D_4.



4 rotations: $e, (1234), (13)(24), (1432)$
4 reflections: $(12)(34), (14)(23), (24), (13)$

(The reflections are about the x-axis, y-axis, or about the two diagonals.) Closure holds ("obviously" because there are no further symmetries, but you can check it by evaluating all products ab). Note that D_4 is a subgroup of S_4 (D_4 has 8 elements, S_4 has 24 elements). This agrees with Lagrange's theorem: 8 is a divisor of 24. The rotations form a subgroup of D_4 of order 4 (and again Lagrange's theorem is satisfied: 4 is a divisor of 8). D_4 is not a normal subgroup of S_4; one can check this by tedious computation, but in the next section where we introduce the concept of classes, and then it becomes at once clear that D_4 is not normal in S_4 because D_4 is not composed of entire classes of S_4.

It is clear that the rotations form the subgroup Z_4 (they are generated by the rotation over 90°). But we can find other subgroups, for example

$$\begin{aligned} H_I &= \big(e, (13)\big) & H_{III} &= \big(e, (13)(24), (13), (24)\big) \\ H_{II} &= \big(e, (13)(24)\big) & H_{IV} &= Z_4 = \big(e, (1234), (13)(24), (1432)\big) \end{aligned} \tag{4.4}$$

Clearly, $H_I = Z_2$ and $H_{II} = Z_2$. But also H_{III} is known:

$$H_{III} = \big(e, (13)\big) \otimes \big(e, (24)\big) = Z_2 \otimes Z_2 = V. \tag{4.5}$$

(We used that (13) and (24) commute. They commute because they act on different vertices. The group element $g = (13)(24)$ corresponds to a rotation over π around the z-axis in R^3, but it corresponds also to space inversion in the plane.)

Which ones of these subgroups are normal in D_4? Both $H_{III} = V$ and $H_{IV} = Z_4$ are normal in D_4 because in each case there are only two coset elements of the quotient group, and H is a coset element which is common to the left cosets and the right cosets. So the other two coset elements (gH and Hg) must also be equal. Clearly the quotient groups D_4/Z_4 and D_4/V are Z_2 (the group with two elements is unique).

Are $H_{III} = V$ and $H_{IV} = Z_4$ also normal subgroups of S_4? A subgroup H' of a subgroup H of a group G is a subgroup H' of G. Take $H' = H_{IV}$, $H = D_4$ and $G = S_4$. Then $|S_4|/|H_{IV}| = 6$ and

Lagrange's theorem is satisfied: 6 is a divisor of 24. Also $|S_4|/|H_{III}| = 6$ agrees with Lagrange's theorem. If H_{III} and H_{IV} were normal subgroups of S_4, the cosets S_4/H_{III} and S_4/H_{IV} would be groups of order 6, and since the only groups of order 6 are[3] D_3 and Z_6, the quotient groups S_4/H_{III} and S_4/H_{IV} would be isomorphic to D_3 or Z_6. But are they normal subgroups? The answer is no as one can explicitly check[4]. (It can be more easily proven using the notion of classes, see next chapter.)

But what about H_I and H_{II}: are they also normal in D_4? Let's begin with $H_I = \big(e, (13)\big)$. The 4 left-coset elements are

$$\begin{aligned} H_I &= \big(e,(13)\big)\,; & (24)H_I &= \big((24),(24)(13)\big)\,; \\ (12)(34)H_I &= \big((12)(34),(12)(34)(13) = (1234)\big)\,; & (14)(23)H_I &= \big((14)(23),(1423)\big)\,. \end{aligned} \tag{4.6}$$

The 4 right-coset elements are

$$\begin{aligned} H_I &= \big(e,(13)\big)\,; & H_I(24) &= \big((24),(24)(13)\big)\,; \\ H_I(12)(34) &= \big((12)(34),(1432)\big)\,; & H_I(14)(23) &= \big((14)(23),(1234)\big)\,. \end{aligned} \tag{4.7}$$

Not all coset elements satisfy $aH_I = H_I a$, so H_I is not normal in D_4.

Now consider $H_{II} = \big(e, (13)(24)\big)$. Again we work out the left-coset elements and the right-coset elements. The 4 left-coset elements are

$$\begin{aligned} H_{II} &= \big(e,(13)(24)\big)\,; & (24)H_{II} &= \big((24),(13)\big)\,; \\ (14)(23)H_{II} &= \big((14)(23),(12)(34)\big)\,; & (1234)H_{II} &= \big((1234),(1432)\big)\,. \end{aligned} \tag{4.8}$$

The 4 right-coset elements are

$$\begin{aligned} H_{II} &= \big(e,(13)(24)\big)\,; & H_{II}(24) &= \big((24),(13)\big)\,; \\ H_{II}(14)(23) &= \big((14)(23),(12)(34)\big)\,; & H_{II}(1234) &= \big((1234),(1432)\big)\,. \end{aligned} \tag{4.9}$$

Now all left-coset elements and right-coset elements are equal, so H_{II} is normal in D_4.

Abstractly, both H_I and H_{II} are the same as Z_2 (they are isomorphic: they have the same group multiplication table). But the group multiplication rules of H_I and H_{II} with the rest of $G = D_4$ are different, and this explains why H_{II} can be a normal subgroup of G while H_I is not. (Again, this follows more easily from the class structure, see next chapter.)

[3]This claim can be proven by studying all possibilities. For $|G| = 4$, one can prove with some effort that the only groups of order 4 are V and Z_4, but for $|G| \geq 6$ the proofs become quite tedious. Other methods can then be used.

[4]For example the sets $(12)H_{III}$ and $H_{III}(12)$ are different, and also the sets $(12)H_{IV}$ and $H_{IV}(12)$ are different.

4.5 The quaternion group $\mathbb{Q}$

The quaternions I, J and K can be represented by a set of 2×2 matrices which were invented by Hamilton[5] and satisfy $I^2 = J^2 = K^2 = -E$ where E is the unit 2×2 matrix, and further $IJ = -JI = K$ and cyclic. They form a group whose 8 elements are $\pm I$, $\pm J$, $\pm K$, $\pm E$. (Note that $-I$, $-J$ and $-K$ are different group elements from I, J and K. In a group one can multiply elements (using group multiplication), but not also add or subtract elements.) This group is nonabelian (for example IJ is not equal to JI). For future use we note that $I^{-1} = -I$, $J^{-1} = -J$ and $K^{-1} = -K$ and $KJK^{-1} = J^{-1}$ $(-KJK = -J)$. For the quaternion group a presentation is

$$\mathbb{Q} : \left\{ I, J \,|\, I^4 = E, J^2 = I^2, JIJ^{-1} = I^{-1} \right\}. \tag{4.10}$$

This is actually the case $n = 2$ of an infinite class of groups Q_{2n} called the dicyclic groups, which we discuss next.

4.6 The dicyclic (binary dihedral) groups Q_{2n}

The dicyclic groups are defined by the following presentation with two generating group elements a and b

$$Q_{2n} : \left\langle a, b \,|\, a^{2n} = e, b^2 = a^n, bab^{-1} = a^{-1} \right\rangle \tag{4.11}$$

(This looks like the dihedral groups, but dihedral groups have $b^2 = e$.) Their order is $4n$. For $n = 2$ we get $a^4 = e$ and $b^2 = a^2$. Then a is I and $b = J$ where I and J are quaternions. The group elements are the set of 8 elements e, a, a^2, a^3 and b, ab, a^2b, a^3b. Other group elements such as ba^k can be reduced to the set of 8 by using $ba = a^{-1}b$. So Q_4 is the group of quaternions, often denoted by $\mathbb{Q}$. Generalizing to $n > 2$, it is clear that there are $4n$ group elements: those of the form a^k and those of the form a^kb. (The a^k form the cyclic group Z_{2n} and the ba^k double the number of group elements, and this may explain the name dicyclic groups.)

[5] In terms of the usual Pauli matrices $\sigma_1 = \left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right)$, $\sigma_2 = \left(\begin{smallmatrix} 0 & -i \\ i & 0 \end{smallmatrix}\right)$ and $\sigma_3 = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ one has $I = -i\sigma_1$, $J = -i\sigma_2$ and $K = -i\sigma_3$.

Chapter 5

Basic concepts in Group Theory - II

5.1 Homomorphism

A **homomorphism** ϕ is a map of a group G into[1] a group $\widetilde{G}$ which satisfies $\phi(a)\phi(b) = \phi(ab)$ for all a and b in G. (It preserves the group structure: the map of the product is the product of the maps.) The unit e in G is mapped to the unit e' in $\widetilde{G}$ because $\phi(e)\phi(b) = \phi(b)$, so $\phi(e) = e'$. But there may be more group elements which are mapped to e', and the total set is called the **kernel** of the map ϕ. Note that $\phi(a^{-1})\phi(a) = e'$, so $\phi(a^{-1})$ is the group element in $\widetilde{G}$ that is the inverse of the group element $\phi(a)$ in $\widetilde{G}$

$$\phi(a^{-1}) = \big(\phi(a)\big)^{-1} . \tag{5.1}$$

The image of G lies inside $\widetilde{G}$ and forms a group G' (check).

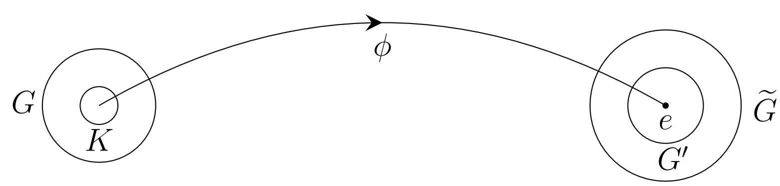


Figure 5.1: The image of G lies inside $\widetilde{G}$ and forms the group G'. The set K of group elements of G that are mapped into the unit element e of $\widetilde{G}$ (and of G') is called the kernel of G and is a normal subgroup of G. The quotient G/K is isomorphic to G'.

[1] If the map from G to $\widetilde{G}$ is **onto** $\widetilde{G}$, such a homomorphism is called an epimorphism (epi means onto in Greek.) However, there is no special name for a homomorphism from G **into** $\widetilde{G}$. (The term endomorphism (endo means into in Greek) refers to a homomorphism from G into G itself (not into $\widetilde{G}$). For finite groups, an endomorphism that is also an isomorphism is an automorphism. So an automorphism is a 1–1 map ϕ from G onto itself which preserves the group structure, $\phi(a)\phi(b) = \phi(ab)$. For infinite groups, an isomorphic homomorphism need not be an automorphism, it can be "into" instead of "onto". For example if $G = \mathbb{Z}$ (the set of integers with addition) the homomorphism $\phi(n) = 2n$ is an isomorphism (it is 1–1) but not an automorphism (the odd integers lie outside the image).

Theorem: The kernel K of a homomorphism is a normal subgroup.

Proof: If $\phi(a) = e'$ and $\phi(b) = e'$, then also $\phi(ab) = e'$ so closure holds. As we already showed, e lies in the kernel K. If a lies in K, then also a^{-1} lies in K because $\phi(a)\phi(a^{-1}) = e'$ and if $\phi(a) = e'$, then $e'\phi(a^{-1}) = e'$ which implies that $\phi(a^{-1}) = e'$, hence a^{-1} lies in K. And because G is associative, also K is associative. So K forms a group. To show that it is a normal subgroup we must show that for all g in G, gkg^{-1} lies in K if k lies in K. That is clear: $\phi(gkg^{-1}) = \phi(g)e'\phi(g^{-1}) = \phi(g)\phi(g^{-1}) = e'$. So K is a normal subgroup. This will be useful for the construction of matrix representations of G. ■

5.2 Isomorphism

An **isomorphism** is a 1–1 map of a group G **onto** a group G' which satisfies $\phi(a)\phi(b) = \phi(ab)$. In other words, the group multiplication tables for G and G' are the same: one can not tell G and G' apart. Because K is normal, for a homomorphism of G into $\widetilde{G}$, the quotient G/K is a group, and we leave as an exercise to show that G/K is isomorphic to G'. (G' is the image of G in $\widetilde{G}$.)

We now prove Cayley's theorem which gives a relation between abstract groups and permutation groups. It is with Sylow's theorems (to be discussed) and after Lagrange's theorem the most important theorem of finite group theory. Early work by Lagrange, Abel, Galois, Cauchy, C. Jordan and others dealt exclusively with permutation groups, but slowly the notion of abstract groups emerged: groups which were only defined by their group multiplication rules (the Cayley tables), but not by a particular realization as for example rotations of particular geometrized objects such as polyhedra. Cayley, who invented the group multiplication table (and thus the concept of abstract groups) must have asked himself at some time what the relation is between abstract groups, and permutation groups. He solved this problem completely and simply.

5.3 Cayley's theorem

Cayley's Theorem (1845): A group G with n elements is isomorphic to a (sub)group of the permutation group S_n. (The group S_n is the group of permutations of n objects and isomorphic means having the same group multiplication table.)

Proof: To prove this theorem, note that if one acts with a given group element a on the group elements $g_0 = e, g_1, \cdots, g_{n-1}$ by right-multiplication this yields a permutation of the elements of G. (We discussed this before: all elements $a, g_1a, \cdots, g_{n-1}a$ are different, and the number of these elements is the same as the number of elements in G, so the action of a on G by right-multiplication is a particular permutation of the n group elements of G.) In this way one associates to any particular group element a particular permutation Π_a of S_n. If g_k is mapped to g_ka for all

$k = 0, \cdots, n-1$ we can denote this permutation as follows

$$G\phi(a) = Ga\,; \quad \phi(a) = \Pi_a = \begin{pmatrix} g_0 \cdots g_{n-1} \\ g_0 a \cdots g_{n-1} a \end{pmatrix} \tag{5.2}$$

This map ϕ from G into S_n is a homomorphism because if a effects a permutation Π_a, and b a permutation of Π_b, then Π_a followed[2] by Π_b is the permutation Π_{ab}

$$\begin{gathered} (G\Pi_a)\Pi_b = \begin{pmatrix} g_0 \cdots g_{n-1} \\ g_0 a \cdots g_{n-1} a \end{pmatrix} \Pi_b = \begin{pmatrix} g_0 \cdots g_{n-1} \\ g_0 ab \cdots g_{n-1} ab \end{pmatrix} = G\Pi_{ab} \\ \phi(a)\phi(b) = \phi(ab)\,. \end{gathered} \tag{5.3}$$

Since $\Pi_a\Pi_b$ acting on g is equal to Π_{ab} acting on g **for all g**, we have $\Pi_a\Pi_b = \Pi_{ab}$. The map Π is actually an isomorphism because its kernel is only the unit element

$$\text{If } \Pi_a = \Pi_b \text{ then } a = b.$$

(Two different group elements ($a \neq b$) give different permutation ($\Pi_a \neq \Pi_b$).) So any group G of order n is isomorphic to a particular subgroup of S_n (or even to S_n itself). One calls this representation of G in terms of this subgroup of permutations the **regular representation**. Note that the regular representation views the group as a transformation group G which acts on itself: the carrier space is G itself. ■

5.4 Classes. Order of a class.

The concept of classes also plays an important role in the construction of matrix representations of groups.[3] A class is constructed as follows; pick a group element a and construct the set of elements gag^{-1} for all g in G. Call this class C_a. Having constructed C_a, pick a group element b that does not lie in C_a and construct the set gbg^{-1} for all g in G. This is the class C_b. Go on in this way until no elements are left. The class containing the unit element consists of only the unit element because $geg^{-1} = e$. If one picks an element a' in the class C_a, and one forms the set of a group elements $ga'g^{-1}$, one obtains the same class C_a. The proof is easy: $a' = \hat{g}a\hat{g}^{-1}$ for some $\hat{g}$ in G because a' lies in C_a. Then the set $C_{a'}$ of elements $ga'g^{-1}$ for all g in G is equal to the set of all elements $g\hat{g}a\hat{g}g^{-1}$ which is the set of all gag^{-1} which is C_a. So, all group elements of a given class are on equal footing. The total number of group elements in a given class C_a is called the order of

[2] Because we defined that the product of cycles should read from left to right, we need right multiplication for the Cayley theorem. If one still reads products of cycles from left to right, but one uses left-multiplication, one finds an "anti-isomorphism", $\phi(a)\phi(b) = \phi(ba)$ (or an isomorphism for the inverses of group elements: $\phi(a^{-1})\phi(b^{-1}) = \phi(a^{-1}b^{-1})$). Of course, if one reads the product of cycles from right to left and one uses left multiplication by a, one finds again an isomorphism.

[3] One usually means by the term representation a realization of a group in terms of matrices, so "matrix representations" is a pleonasm, but to stress that we are using matrices we sometimes will use the term matrix representations.

that class and denoted by $|C_a|$. The classes of S_n consist of e, all (ab), all (abc), all $(ab)(cd)$, $\cdots$, all $(a_1 \cdots a_n)$. For example, there are 5 classes in S_4.

Comment. In applications to physics the map $a \to gag^{-1}$ corresponds to choosing a different basis, and it follows that all elements in a given class describe the same physics.

Theorem: Two different classes have no group element in common.

Proof: If $gag^{-1} = g'bg'^{-1}$, where a lies in C_a and b lies in C_b, then $b = (g'^{-1}g)a(g'^{-1}g)^{-1} = (g'')^{-1}ag''$ would lie in C_a, which is a contradiction. ■

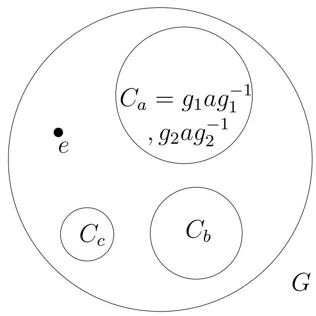


Figure 5.2:

Thus just as a group G decomposes into left-(or right-)cosets, the group G also splits up into nonoverlapping classes. However, different coset elements have always the same number of group elements, while different classes have in general different numbers of group elements. Before we discuss classes further, we introduce two related concepts.

5.5 Centralizer. Center.

The **centralizer Z_a of a group element a** is the set of all group elements that commute with a. This set clearly forms a subgroup (check).

The **center Z_G of a group G** is the set of group elements that commute with all group elements. They form an abelian invariant subgroup (check). Clearly Z_G always contains e, but sometimes it contains more elements. For an abelian group the center is the whole group itself (check). The intersection of the centralizers of all group elements is the center of the group.

There is a relation between classes and normal subgroups which makes it often easy to determine all normal subgroups N of a given group G

Theorem: A normal subgroup N consists of entire classes.

Proof: Let N be a normal subgroup, and pick a group element n_1 in N. Then the set gn_1g^{-1} for all g forms a class C_{n_1}, but at the same time all gn_1g^{-1} lie in N. So the whole class C_{n_1} lies in N. Next pick another element n_2 in N that does not lie in the class C_{n_1}. Again gn_2g^{-1} for all g

gives an entire class which lies in N. Hence N consists of entire classes. (Of course, one of these classes is the unit element e, which forms a class by itself as we have discussed earlier.) ■

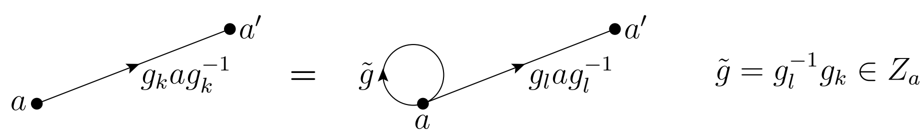
As an example, consider the dihedral group D_4 of chapter 4. The 8 group elements form the following 5 classes: (e), (12)(34) and (14)(23), (13) and (24), (1234) and (4321), and finally (13)(24). Hence the subgroup $H_I = \big(e, (13)\big)$ is not normal, the subgroup $H_{II} = \big(e, (13), (24)\big)$ is a normal subgroup since it is a subgroup composed of entire classes, the subgroup $H_{III} = \big(e, (13), (24), (13)(24)\big)$ is also a normal subgroup, and the subgroup $H_{IV} = \big(e, (1234), (13)(24), (4321)\big)$ is normal. The geometrical meaning of the group elements of H_{III} is a rotation over π and two reflections about the diagonals of a square. Also the subgroup H_V of a rotation over π of a square and two reflections about the x-axis and the y-axis forms a normal group; its elements are (13)(24), (12)(34) and (14)(23).

Comment. We see here very clearly that all elements of a class describe the same "physics" (geometry in this case). For example, (13) and (24) both describe reflection about a diagonal of a square, and all (both) such reflections are geometrically the same. Similarly the rotations (1234) and (4321) are geometrically the same as they rotate over angle $\frac{\pi}{2}$ and $-\frac{\pi}{2}$, respectively. But the rotation over π, corresponding to (13)(24) forms a class by itself.

Just as the order of the coset elements $H, aH, bH, \cdots$ is a divisor of the order $|G|$ of the group, the same holds for the order of a class, as we now prove.

Theorem: The order of a class is a divisor of the order of the group.

Proof: Consider the set of elements gag^{-1} for fixed a and all g in G. They form the class C_a. Let there be m elements $g_1, g_2, \cdots g_k, \cdots g_m$ such that $g_k a g_k^{-1} = a'$ for all m elements with a' an element of C_a. Then two such elements satisfy $g_k a g_k^{-1} = g_l a g_l^{-1}$, hence $g_l^{-1} g_k$ commutes with a: it lies in the centralizer of a. So the set of all g_k which map a in C_a into a' in C_a is given by $g_l Z_a$ where Z_a keeps a fixed and g_l is one particular group element which maps a to a' (since $g_k = g_l g_l^{-1} g_k = g_l \tilde{g}$ with $\tilde{g}$ in Z_a). Pictorially



Likewise the set of group elements that map a in C_a into another group element a'' in C_a is given by $g_j Z_a$ where g_j is any particular group element of G that maps a to a''. Thus it follows that the total number of group elements is equal to the number of group elements in Z_a times the number of group elements in C_a: $|G| = |Z_a||C_a|$. One could have started with a group element a' instead of a to construct the class $C_{a'}$. We already showed that $C_a = C_{a'}$. It follows that $|Z_a| = |Z_{a'}| = |Z_{a''}| \cdots$ for all group elements a, a', a'' in the class C_a which contains a. Hence $|Z_a|$ and $|C_a|$ are "class functions": they do depend on the class, but not on individual group elements in a given class: $|Z_a| = |Z_{a'}|$ and $|C_a| = |C_{a'}|$. ■

Next we define a particular normal subgroup which will tell us later how many one-dimensional representations a given group G has.

5.6 Commutator subgroup

Definition: The **commutator subgroup $C(G)$** is the group generated by all group elements of the form $aba^{-1}b^{-1}$ for all a and b in G ("generated" means: start with this set, and add products of these elements if needed and products of these products, $\cdots$ etc, to achieve closure).

It is clear that $C(G)$ forms a group:

1) Closure: by construction.
2) The unit element is contained in $C(G)$ because $aa^{-1}a^{-1}a = e$.
3) The inverse of $aba^{-1}b^{-1}$ is $bab^{-1}a^{-1}$ which lies in $C(G)$.
4) Associativity holds because it holds in G.

We claim that $C(G)$ is a normal subgroup.

Theorem: $C(G)$ is a normal subgroup.

Proof: We must show that $g(aba^{-1}b^{-1})g^{-1}$ lies in $C(G)$ for all g in G. This is true

$$g(aba^{-1}b^{-1})g^{-1} = (gag^{-1})(gbg^{-1})(gag^{-1})^{-1}(gbg^{-1})^{-1} = a'b'(a')^{-1}(b')^{-1}\,. \tag{5.4}$$

Similarly products of the generators $aba^{-1}b^{-1}$ lie in $C(G)$:

$$g(aba^{-1}b^{-1}cdc^{-1}d^{-1})g^{-1} = (gag^{-1})\cdots(gd^{-1}g^{-1}) = \left(a'b'a'^{-1}b'^{-1}\right)\left(c'd'c'^{-1}d'^{-1}\right) \tag{5.5}$$

which lies in $C(G)$ (because we included them to obtain closure). ■

Because $C(G)$ is a normal subgroup, the quotient $G/C(G)$ is also a group. But it is a special group as the next two theorems show.

Theorem: $G/C(G)$ is abelian.

Proof: Since $C(G)b = bC(G)$ for a normal subgroup we have

$$aC(G)bC(G) = abC(G). \tag{5.6}$$

Now $aC(G)$ or $bC(G)$ or $abC(G)$ need not be equal to $C(G)$, but $abC(G) = baC(G)$ since $b^{-1}a^{-1}baC(G) = C(G)$. (For any group or subgroup H, the set of elements hH is the same as the set of elements of H because hH is only a permutation of the elements of H. For $H = C(G)$ the elements are $h = b^{-1}a^{-1}ba$ and products thereof.) ■

The final property of $C(G)$ which we shall need is

Theorem: $C(G)$ is the smallest normal subgroup N of G such that G/N is abelian (it is a commutative quotient group). Of course e is always a normal subgroup of any group G, but G/e is not abelian in general. On the other hand, G is also a subgroup of G, and $G/G = e$ is always abelian. For a nonabelian group G we need a larger subgroup than e in order that $G/C(G)$ be abelian. The claim is that the smallest normal subgroup of G such that G/N is still abelian, is $C(G)$. For matrix representations we need the largest abelian quotient G/N, because this will enable us to get rid of all one-dimensional representations.

Proof: We already saw that $C(G)$ is a normal subgroup and that $G/C(G)$ is abelian. We now must show that any other normal subgroup N with abelian G/N contains $C(G)$. Suppose we have found such an N, then $aNbN = abN$ is equal to $bNaN = baN$. But the relation $abN = baN$ can be rewritten as $a^{-1}b^{-1}abN = N$, so the elements $a^{-1}b^{-1}ab$ lie in N. This proves that N contains $C(G)$. ■

Comment. $C(G)$ "measures" how nonabelian G is: if G is abelian $C(G)$ is very small ($C(G) = e$). A group for which $C(G)$ is equal to the whole group G is called a **perfect group**. Thus a perfect group is as nonabelian as possible. For a perfect group G, the elements $aba^{-1}b^{-1}$ generate the whole group G. What is so perfect about a perfect group? In number theory a perfect number is a number that is equal to the sum of its divisors except itself. For example $6 = 1 + 2 + 3$ and $28 = 1+2+4+7+14$. A perfect group is a group that is equal to the union of its abelian quotients. (An abelian quotient of a group G is a group G/N which is abelian. All normal subgroups N of G such that G/N is abelian, contain $C(G)$. Hence all abelian quotients are contained in the quotient $G/C(G)$ as we have shown. Thus for a perfect group G is equal to $C(G)$.)

Figure 5.3: If N is a normal subgroup of G, and G/N is abelian, then N contains $C(G)$. Hence $G/C(G)$ contains all G/N.

5.7 Simple and perfect groups

As an amusing aside we mention that there is a relation between **simple groups** and **perfect groups**. We shall discuss simple groups later, but here we only need their definitions: a simple group is a group which has no nontrivial normal subgroups (e and G are always trivial subgroups) and a perfect group is a group G which has no nontrivial abelian quotients. All nonabelian simple groups are perfect, but not all perfect groups are simple. An obvious counterexample is the direct product of two simple groups, which is perfect, but not simple (if $G = G_1 \times G_2$ and G_1 and G_2 are simple, then $I \times G_2$ and $G_1 \times I$ are normal subgroups of G).

5.8 Class multiplication

Now we return to classes, and discuss **class multiplication**, the multiplication of two classes. Given classes C_a and C_b we define by C_aC_b the set of elements obtained by multiplying any element in C_a with any element in C_b, in that order. We claim that the set of group elements C_aC_b is a sum (we really should call it a union) of entire classes

$$C_aC_b = \sum_c f_{ab}{}^c C_c \qquad (a, b, c \text{ label classes}) \tag{5.7}$$

where $f_{ab}{}^c$ are nonnegative integers. Note that if one produces a group element g_c in C_aC_b more than once, say twice, then we count it twice on the right-hand side. This explains why $f_{ab}{}^c$ can be larger than one. The total number of elements is the same on both sides; in fact one can write

$$|C_a||C_b| = \sum_c f_{ab}{}^c |C_c| \tag{5.8}$$

where we now have really a sum of numbers, and not a union of sets. Let us begin by proving that C_aC_b is equal to C_bC_a, so $f_{ab}{}^c$ is symmetric, $f_{ab}{}^c = f_{ba}{}^c$. The proof is as follows: for any group element g_a in C_a and g_b in C_b we obtain

$$g_a g_b = (g_b g_b^{-1}) g_a g_b = g_b (g_b^{-1} g_a g_b) \in C_b C_a. \tag{5.9}$$

So any group element in C_aC_b lies also in C_bC_a, and thus also any group element in C_bC_a lies in C_aC_b. This proves that the two sets of group elements C_aC_b and C_bC_a are equal. Hence $f_{ab}{}^c$ is symmetric in ab.

We want now to prove that the set of group elements C_aC_b is a sum (union) of entire classes. First note that $gC_ag^{-1} = C_a$ (because gC_ag^{-1} lies in C_a, and any group element a in C_a is contained in gC_ag^{-1} because $g^{-1}ag$ lies in C_a and $a = g(g^{-1}ag)g^{-1}$). Hence $C_aC_b = (gC_ag^{-1})(gC_bg^{-1}) = g(C_aC_b)g^{-1}$. Thus the set $\mathcal{C} = C_aC_b$ of group elements is invariant under conjugation: $g\mathcal{C}g^{-1} = \mathcal{C}$.

Consider now a group element $\hat{g}$ that lies in the set of group elements C_aC_b. Since $g(C_aC_b)g^{-1} = C_aC_b$, it follows that $g\hat{g}g^{-1}$ lies in C_aC_b, for all g in G. Hence the whole class to which $\hat{g}$ belongs, is part of C_aC_b. This proves the following theorem.

Theorem: The set C_aC_b is a union of entire classes: $C_aC_b = \sum_c f_{ab}{}^c C_c$, where $f_{ab}{}^c$ are nonnegative integers.

If an element $\hat{g}$ is produced k times if one multiplies the group elements in C_a and those in C_b, then the corresponding $f_{ab}{}^c$ has the value k.

Example: Let the 3 classes of S_3 be denoted by C_1, C_2, C_3, where C_k contains the k-cycles. Then

$$\begin{aligned} C_2C_2 &= 3C_1 + 3C_3 \\ C_2C_3 &= 2C_2 \\ C_3C_3 &= 2C_1 + C_3 \,. \end{aligned} \tag{5.10}$$

We end this chapter with an application which uses classes. Whereas Lagrange's theorem states that the order of a subgroup H of a group G is a divisor of the order of G, Cauchy's theorem is in a sense the inverse of Lagrange's theorem:

*5.9 Cauchy's theorem on subgroups

Cauchy's Theorem (1844). If the order of a group G is divisible by a **prime number** $\boldsymbol{p}$, then G contains a subgroup of order p. (Equivalently, then G contains a group element of order p.) (Warning: When p divides $|G|$, there need not exist a subgroup H of **index** p, namely there need not exist a subgroup H for which $\frac{|G|}{|H|}$ (the order of the quotient G/H, i.e., the number of coset elements) is equal to p. Example: A_4 has order 12 and subgroups of order $p = 2$, but no subgroup of order $\frac{12}{p} = 6$.[4])

As a warming-up exercise we consider the case $p = 2$. Consider a group G and the pairs g_i, g_i^{-1} with $g_i^{-1} \neq g_i$, and further the elements g_k with $g_k^{-1} = g_k$. If the order of G is even, the number of g_k must be odd in order that the total number of group elements (pairs g_i, g_i^{-1}, e and the g_k) be even. So then there is indeed a subgroup of order 2 (e, g_k for any k).

We now give the general proof and consider first abelian G, and then use the result for nonabelian G.

If G is abelian, pick an element a in G. If the order r of a is divisible by p, then $a^{r/p}$ generates a group $H = Z_p$. If $|a|$ is not divisible by p, the order of the quotient G/H is divisible by p (because $|G/H| = \frac{|G|}{|H|}$ and $|G|$ but not $|H|$ is divisible by p). For abelian groups the quotient G/H is a group, and this group has order less than G, so the proof is given.

If G is nonabelian, we can divide its elements into two classes: in one class we have the g for which $g^{-1} \neq g$, while in the other class $g^{-1} = g$ (so $g^2 = e$). If one constructs the classes of G, the order of given class C_i is equal to the order of G divided by the order of the normalizer of any

[4]The only subgroups of order 6 are Z_6 and S_3, but A_4 has no group element of order 6, and S_3 has 3 group elements of order 2 $\{(12), (13), (23)\}$ that do not commute with each other while A_4 has no such elements. Interesting factoid: A_4 is the smallest group G which does **not** have a subgroup whose (non-prime) order is a divisor of $|G|$.

element g_i in C_i: $|C_i| = \frac{|G|}{|N(g_i)|}$. Then the order of G is given by the following expression

$$|G| = |Z| + \sum_i \frac{|G|}{|N(g_i)|} \tag{5.11}$$

where Z denotes the center (the classes with one element). If one of the $|N(g_i)|$ is divisible by p, we are done. If not, each of the $\frac{|G|}{|N(g_i)|}$ is divisible by p. Also $|G|$ is by assumption divisible by p. So $|Z|$ is divisible by p. Then, as we have seen for abelian groups, there is a subgroup of order p.

Cauchy's theorem on p-groups was extended by the Norwegian mathematician Ludvig Sylow in his three theorems of 1872. We shall not prove these theorems, but apply them in several examples. If a group G has order $|G| = p^k r$ where p does not divide r, one calls a subgroup of order p^k a Sylow p-subgroup. Any subgroup of order p to some power is called a p-subgroup. So Cauchy's theorem says that for any p in $|G| = p^k r$ there exists a p-subgroup. The Sylow theorems made statements about the number n_p of Sylow p-subgroups, and their properties.

*5.10 Sylow theorems on subgroups

Theorem Sylow I: A finite group G has a Sylow p-subgroup for every prime p in its order, and every p-subgroup lies in some Sylow p-subgroup of G.

Theorem Sylow II: For every prime p, the Sylow p-subgroups of G are conjugate. (If H and K are Sylow p-groups of G, then there exists an element g in G with $gHg^{-1} = K$.) If there is only one Sylow p-subgroup, it is self-conjugate, hence a normal subgroup.

Theorem Sylow III: Let n_p be the number of Sylow p-subgroups of a finite group G of order $|G| = p^k m$ where p does not divide m. Then n_p divides m, $n_p = 1 \mod p$, and $n_p = |G/N(P)|$ where P is a Sylow p-subgroup, and $N(P)$ its normalizer.

We now given some examples [1, 2].

Example 1. Consider a group G of order $|G| = pq$ where both p and q are prime. Sylow III tells us that n_p divides q, so $n_p = 1, q$. Similarly, $n_q = 1, p$. We also have $n_p = 1, p+1, \cdots$, so if $p \geq q$ we get $n_p = 1$. Since $n_q = 1, 1+q, 1+2q$, we get a group either if $n_q = 1$, in which case $G_{pq} = Z_p \times Z_q$, or if $n_q = p$ but then p should be equal to one of the $1+q$, $1+2q$, $\cdots$. For example there is only one group G_{15} namely $Z_5 \times Z_3$, but for G_{21} we get two groups: $Z_7 \times Z_3$ and $Z_7 \rtimes Z_3$. The latter case is the Frobenius group with $n_7 = 1$ and $n_q = 7 (= 1+2q$ with $q = 3)$. Since $n_7 = 1$, there is only one subgroup of order 7, and Sylow II tells us that it is conjugate to itself, hence it is a normal subgroup, and the Frobenius group is not simple.

Example 2. Consider all groups whose order is given by $|G| = 84 = 2^2 \cdot 3 \cdot 7$. In this case $n_7 = 1, 2, 3, 4, 6, 12$ and $n_7 = 1, 8, 15, \cdots$, so $n_7 = 1$. Thus there is a subgroup of order 7, and it is a normal subgroup. So there are no simple groups of order 84. This illustrates how useful the Sylow theorems are for the classification of all simple groups.

Example 3. Consider the integers $0, 1, \cdots, 11 \mod 12$, and define group multiplication as addition modulo 12. This yields the group $\mathbb{Z}/12$ of order $2^2 \cdot 3$. It has $n_3 = 1, 4$ and $n_2 = 1, 3$. For $\mathbb{Z}/12$ the only Sylow 2-subgroup is $\{0, 3, 6, 9\} = \langle 3 \rangle$ and the only Sylow 3-subgroup is $\{0, 4, 8\} = \langle 4 \rangle$. Hence $\mathbb{Z}/12$ corresponds to $n_2 = 1$ and $n_3 = 1$ and $\mathbb{Z}/12 = Z_{12} = Z_4 \times Z_3$. There are 5 groups of order 12: $Z_4 \times Z_3$, $Q_6 = Z_3 \rtimes Z_4$, $Z_6 \times Z_2$, $D_6 = Z_6 \rtimes Z_2$ and A_4. In the next example we study A_4.

Example 4. In A_4 there is one subgroup of order 4, so the only Sylow 2-subgroup is[5]

$$\{(1), (12)(34), (13)(24), (14)(23)\} = \big\langle (12)(34), (14)(23) \big\rangle \ . \tag{5.12}$$

There are four Sylow 3-subgroups:

$$\begin{aligned} &\{(1), (123), (132)\} = \big\langle (123) \big\rangle \ , \quad \{(1), (124), (142)\} = \big\langle (124) \big\rangle \ , \\ &\{(1), (134), (143)\} = \big\langle (134) \big\rangle \ , \quad \{(1), (234), (243)\} = \big\langle (234) \big\rangle \ . \end{aligned} \tag{5.13}$$

Clearly, A_4 corresponds to the case $n_2 = 1$, $n_3 = 4$.

Example 5. In D_6 there are three Sylow 2-subgroups:

$$\{1, r^3, s, r^3 s\} = \big\langle r^3, s \big\rangle \ ; \quad \{1, r^3, rs, r^4 s\} = \big\langle r^3, rs \big\rangle \ ; \quad \{1, r^3, r^2 s, r^5 s\} = \big\langle r^3, r^2 s \big\rangle \ . \tag{5.14}$$

(Note that $(rs)^2 = (r^2 s)^2 = (r^3 s)^2 = (r^4 s)^2 = (r^5 s)^2 = e$.) The only Sylow 3-subgroup of D_6 is $\{1, r^2, r^4\} = \langle r^2 \rangle$. Hence D_6 corresponds to the case $n_2 = 3$, $n_3 = 1$. Each of the Sylow 2-subgroups is isomorphic to V, and they are conjugate:

$$r \big\langle r^3, s \big\rangle r^5 = \big\langle r^3, r^2 s \big\rangle \text{ and } r^2 \big\langle r^3, s \big\rangle r^4 = \big\langle r^3, rs \big\rangle \ . \tag{5.15}$$

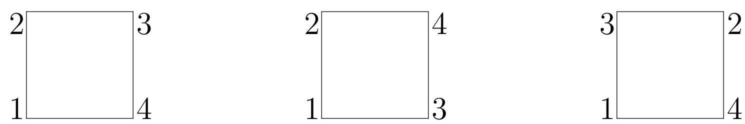
The Sylow 3-subgroup is self-conjugate, a normal subgroup.

Example 6. For $Z_6 \times Z_2 = Z_3 \times Z_2 \times Z_2$ it is clear that $n_2 = 1$ and $n_3 = 1$. This solves a question that arose in problem 3: there were 5 inequivalent groups of order 12 but only 4 combinations of n_2 and n_3. Clearly, at least one pair of groups should have the same n_2 and n_3. We found such a pair: Z_{12} and $Z_6 \times Z_2$. Actually also Q_6 has $n_2 = n_3 = 1$.

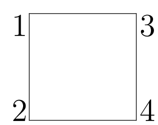
[5] Any subgroup of A_4 that contains a 3-cycle, contains all 3-cycles, which would yield a subgroup of order larger than 4. That leaves (5.12).

Example 7. In S_4, the Sylow 3-subgroups are the Sylow 3-subgroups of A_4 (an element of order 3 in S_4 must be a 3-cycle, and they all lie in A_4). We determined the Sylow 3-subgroups of A_4 in (5.13); there are four of them.

There are three Sylow 2-subgroups of S_4 (subgroups of order 8), and they are interesting to work out since they can be understood as copies of D_4 inside S_4. The number of ways to label the four vertices of a square as 1, 2, 3, and 4 is $4! = 24$, but up to rotations and reflections of the square there are really just three different ways of carrying out the labeling, as follows.



Every other labeling of the square is a rotated or reflected version of one of these three squares. For example, the square below is obtained from the middle square above by reflecting across a horizontal line through the middle of the square.



When D_4 acts on a square with labeled vertices, each motion of D_4 creates a permutation of the four vertices, and this permutation is an element of S_4. For example, a 90-degree rotation of the square is a 4-cycle on the vertices. In this way we obtain a copy of D_4 inside S_4. The three essentially different labelings of the vertices of the square above embed D_4 into S_4 as three different subgroups of order 8:

$$\begin{aligned}
&\{1, (1234), (1432), (12)(34), (13)(24), (14)(23), (13), (24)\} = \big\langle (1234), (13) \big\rangle\,, \\
&\{1, (1243), (1342), (12)(34), (13)(24), (14)(23), (14), (23)\} = \big\langle (1243), (14) \big\rangle\,, \\
&\{1, (1324), (1423), (12)(34), (13)(24), (14)(23), (12), (34)\} = \big\langle (1324), (12) \big\rangle\,.
\end{aligned} \tag{5.16}$$

These are the Sylow 2-subgroups of S_4.

Example 8. The Chevalley group $SL(2, 3)$ (nonsingular 2×2 matrices with entries $-1, 0, +1$ mod 3) has order 24.[6] It is not isomorphic to S_4 since its center $\{\pm I_2\}$ is nontrivial. The Sylow theorems tell us that $n_2 = 1$ and $n_3 = 1, 4$. By explicit calculation, $SL(2, 3)$ has only 8 elements of order 2:

$$\begin{gathered}
\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix}, \\
\begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \begin{pmatrix} -1 & -1 \\ -1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & -1 \\ -1 & -1 \end{pmatrix}.
\end{gathered} \tag{5.17}$$

[6]If $m = \left(\begin{smallmatrix} a & b \\ c & d \end{smallmatrix}\right)$, one can pick a, b in $3 \times 3 - 1 = 8$ ways and c, d in $3 \times 3 - 3 = 6$ ways. Requiring the determinant to be $+1$ halves the number of matrices.

These form the only Sylow 2-subgroup. It is isomorphic to Q_8 by labeling the matrices in the first row as $1, i, j, k$ and the matrices in the second row as $-1, -i, -j, -k$.

There are four Sylow 3-subgroups of $SL(2,3)$:

$$\left\langle \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \right\rangle, \quad \left\langle \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \right\rangle, \quad \left\langle \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix} \right\rangle, \text{ and } \left\langle \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix} \right\rangle. \tag{5.18}$$

Hence $n_2 = 1$ amd $n_3 = 4$ for $SL(2,3)$.

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Chapter 6

All groups of order $|G| \leq 24$. Simple groups.

As an application of what we have learned so far, but even more because mostly groups of low order play an important role in physics, we give a list of all finite groups of order $|G| \leq 24$. Any group whose order is a prime number is a cyclic group, as we showed, and we also recall that $Z_{pq} = Z_p \times Z_q$ if and only if p and q are coprime $\big((p,q) = 1\big)$, but if $(p,q) > 1$ then Z_{pq} and $Z_p \times Z_q$ are different groups (they are not isomorphic). We also recall that we introduced two infinite families of finite groups: the dihedral group D_n of order $2n$, and the dicyclic (binary dihedral) group Q_n also of order $2n$. We shall encounter below a new kind of finite groups, the Chevalley groups (also called groups of Lie type). Their entries are elements of a finite field as we shall discuss.

Before we give the list, we derive by direct means all possible groups for the cases $|G| = 3$ and $|G| = 4$. For $|G| > 4$ it becomes increasingly difficult to use this kind of approach, and other methods must be used.

$|G| = 3$: The group elements are e, a, b. Then ab cannot be equal to a or b ($ab = a$ implies $b = e$), so $ab = e$. Similarly $ba = e$, so the group is abelian. Next we note that a^2 cannot be equal to a or e ($a^2 = e$ and $ab = e$ imply that $a = b$). Hence $a^2 = b$. Similarly $b^2 = a$. Thus the group elements are e, a, a^2 which is the cyclic group Z_3. There are no other groups with $|G| = 3$.

$|G| = 4$: The group elements are e, a, b, c. From Lagrange's theorem we know that the order of any $g \neq e$ in G can only be 2 or 4. Let there be an element of order 4, say a. Then $a^4 = e$, and the set e, a, a^2, a^3 gives Z_4. If on the other hand there is no element of order 4, we have $a^2 = b^2 = c^2 = e$. Then ab can only be equal to c ($ab = e$ and $a^2 = e$ imply $b = a$). Similarly, $bc = a$ and $ac = b$. This is V, "the group of four". There are no other groups with $|G| = 4$.

Here is the list (stars denote nonabelian groups). Isomorphisms are given in parentheses in the third column, and we identify the groups in the last column. We begin with the first 15 groups, they are easy to write down and require no new concepts. Then we discuss the case $|G| = 16$ where we find 14 groups, 3 of which involve slight generalizations of semidirect products. The cases $|G| = 17, 18, 19$ are not remarkable, but at $|G| = 20$ we find for the first time Chevalley groups. Chevalley groups are further discussed in chapter 10.

Order $\|G\|$	Group	Isomorphisms	Name
2	Z_2	$= D_1$	cyclic (dihedral)
3	Z_3	$= A_3$	cyclic (alternating)
4	Z_4		cyclic (dicyclic)
4	V	$= D_2 = Q_2 = Z_2 \times Z_2$	Klein's four-group (dihedral)
5	Z_5		cyclic
6	Z_6	$= Z_2 \times Z_3$	cyclic
6*	D_3	$= S_3 = Z_3 \rtimes Z_2$	dihedral (permutation)
7	Z_7		cyclic
8	Z_8		cyclic
8	$Z_4 \times Z_2$		direct product of cyclic
8	$Z_2 \times Z_2 \times Z_2$	$= D_2 \times Z_2 = V \times Z_2$	direct product of cyclic
8*	D_4		dihedral
8*	$\mathbb{Q}$	$= Q_4$	quaternion (dicyclic)
9	Z_9		cyclic
9	$Z_3 \times Z_3$		direct product of cyclic
10	Z_{10}	$= Z_2 \times Z_5$	cyclic
10*	D_5	$= Z_5 \rtimes Z_2$	dihedral
11	Z_{11}		cyclic
12	Z_{12}	$Z_4 \times Z_3$	cyclic
12	$Z_6 \times Z_2$	$= Z_3 \times Z_2 \times Z_2 = Z_3 \times D_2$	direct product of cyclic
12*	D_6	$Z_6 \rtimes Z_2' = D_3 \times Z_2 = D_3' \rtimes Z_2'$	dihedral
12*	Q_6	$= Z_3 \rtimes Z_4$	dicyclic (binary dihedral)
12*	A_4		tetrahedral rotations (alternating)
13	Z_{13}		cyclic
14	Z_{14}	$= Z_2 \times Z_7$	cyclic
14*	D_7	$= Z_7 \rtimes Z_2$	dihedral
15	Z_{15}	$= Z_3 \times Z_5$	cyclic

Some discussion is needed. Consider the group D_6 with the 12 group elements $(e, a, a^2, a^3, a^4, a^5)$ and $(b, ab, a^2b, a^3b, a^4b, a^5b)$ with $bab^{-1} = a^{-1}$ and $a^6 = e = b^2$. It follows that $ba = a^5b$, hence $ba^2 = a^4b$ and $ba^3 = a^3b$. So a^3 and b commute. It can be written both as a direct product and as a semi-direct product (in fact, in two ways as a semi-direct product)

$$D_6 = D_3 \times Z_2 = (e, a^2, a^4, b, a^2b, a^4b) \times (e, a^3)$$
$$D_6 = D_3' \rtimes Z_2 = (e, a^2, a^4, ab, a^3b, a^5b) \rtimes (e, b)$$
$$D_6 = Z_6 \rtimes Z_2 = (e, a, a^2, a^3, a^4, a^5) \rtimes (e, b)$$

If we define $Z_2 = (e, a^3)$ and $Z_2' = (e, b)$ then

$$D_6 = D_3 \times Z_2 = D_3' \rtimes Z_2' = Z_6 \rtimes Z_2' . \tag{6.1}$$

The groups D_3 and D_3' are isomorphic ($\phi(a) = a$, $\phi(b) = ab$. Note that $(ab)^2 = e$.).

For Q_6 with the presentation $a^6 = e$, $b^2 = a^3$ and $bab^{-1} = a^{-1}$ (hence $ba = a^5b$ and $(ab)^2 = b^2 = a^3$) one has the same set of group elements as D_6 (but of course different multiplication rules). Then

$$Q_6 = Z_3 \rtimes Z_4 = (e, a^2, a^4) \rtimes (e, ab, a^3, a^4b) \tag{6.2}$$

Note that there is no group $Z_2 \rtimes Z_3$ at order 6 or $Z_5 \rtimes Z_3$ at order 15. To explain this, we now derive a criterion to decide when $Z_m(a) \rtimes Z_n(b)$ is a group if $bab^{-1} = a^k$. Obviously for $k = 1$ we get an abelian group.

Theorem: The presentation $G = \{a, b \,|\, a^m = b^n = e,\ bab^{-1} = a^k\}$ yields only a group if $1 = k^n \mod m$ for $1 \leq k < m$. For $k = 1$ one gets an abelian group.

Proof: Multiply $ba = a^kb$ by b^{n-1} on the left. This yields $a = b^{n-1}a^kb$. Next use $ba^k = a^{k^2}b$, so $b^{n-1}a^kb = a^{k^n}$. Hence, for consistency, k should be given by $1 = k^n \mod m$.

Example 1. For the case $Z_2 \rtimes Z_3$ we get $1 = k^3 \mod 2$, whose only solution is $k = 1$, but that leads back to $Z_2 \times Z_3$. For the case $Z_5 \rtimes Z_3$ we find the condition $1 = k^3 \mod 5$ for $1 \leq k < 5$. The only solution is $k = 1$. Similarly $Z_3 \rtimes Z_5$ yields the condition $1 = k^5 \mod 3$ whose only solution is $k = 1$. So we get only an abelian group. Since $n_5 = 1$ and $n_3 = 1$, the only group of order 15 is $Z_{15} = Z_5 \times Z_3$.

Example 2. For $Z_{21} = Z_7 \rtimes Z_3$ we get $1 = k^3 \mod 7$ for $1 \leq k < 7$. Now the solutions for k are $k = 1, 2, 4$. Sylow yields $n_7 = 1$, and $n_3 = 1, 7$ and $n_3 = 1, 4, 7, \cdots$. So $n_3 = 1, 7$. For $n_3 = 1$ we get $Z_7 \times Z_3$ (with $k = 1$) while for $n_3 = 7$ we get the Frobenius group (with $k = 2$ or $k = 4$) which has seven Sylow 3-groups. Cayley's theorem states that the Frobenius group is a subgroup of a permutation group S_n. It is natural to try S_7, and to realize a by the permutation $a = (1234567)$. Consider the case $k = 2$. Since $ba = a^2b$ so $bab^{-1} = a^2$, the permutation b must replace $a = (1234567)$ by $a^2 = (1357246)$. So $b = (235)(476)$. The seven Sylow 3-groups of the Frobenius group are then generated by $b, ab, \cdots, a^6b$. That yields the following Sylow 3-groups:

(e, b, b^2), (e, ab, a^3b^2), (e, a^2b, a^6b^2), (e, a^3b, a^2b^2), (e, a^4b, a^5b^2), (e, a^5b, ab^2) and (e, a^6b, a^3b^2). Sylow II tells us that they are conjugate, and indeed $g(e, b, b^2)g^{-1} = (e, a^kb, a^{3k \mod 7}b^2)$ for $g = a, ab, \cdots$. We leave the case $k = 4$ as an exercise.

We continue the above table to see whether new groups enter the stage. At $|G| = 16$ there are 14 groups, namely 5 abelian groups and 9 nonabelian groups. The 5 abelian groups are easily found:
$\boldsymbol{|G| = 16}$**:** 5 abelian: Z_{16}, $Z_8 \times Z_2$, $Z_4 \times Z_4$, $Z_4 \times Z_2 \times Z_2$, $Z_2 \times Z_2 \times Z_2 \times Z_2$.
They are all different, for example, Z_{16} is the only group with an element of order 16. But with the knowledge we have developed so far, we get only 6 nonabelian groups:
$\boldsymbol{|G| = 16^*}$**:** 6 nonabelian: $D_8 = Z_8 \otimes Z_2$, $Z_4 \otimes Z_4$, $(Z_4 \times Z_2) \otimes Z_2 = (Z_2 \times Z_2) \otimes Z_4$, Q_8, $Q_4 \times Z_2$, $(Z_4 \otimes Z_2) \times Z_2 = D_4 \times Z_2$.
Of the three remaining groups one is defined in terms of a "semi-dihedral" group in which one replaces the usual xax^{-1} of a dihedral group by xax^{-n}, the second involves a modified semidirect product in which one replaces again $xax^{-1} = a^{-1}$ by $xax^{-1} = a^n$, and third (the "Pauli group") involves a "central direct product" where one identifies the two central subgroups of the two defining groups.
$\boldsymbol{|G| = 16^*}$**:** 3 further nonabelian:

- $SD(16)$ (semidihedral group): $\{a, b | a^8 = b^2 = e, bab^{-1} = a^3\}$.
- $M(16)$: modular group of order 16: $\{a, x | a^8 = x^2 = e, xax^{-1} = a^5\}$.
- "Pauli group": Generated by $\sigma_x, \sigma_y, \sigma_z$ (the Dirac group in $3 + 0$ dimensions). It has 16 elements $\pm I, \pm iI, \pm\sigma_x, \pm i\sigma_x, \pm\sigma_y, \pm i\sigma_y, \pm\sigma_z, \pm i\sigma_z$. It is also "the central product" of D_4 and Z_4, namely $\{a, x, y | a^4 = x^2 = e, xax^{-1} = a^{-1}, ay = ya, xy = yx, \boxed{a^2 = y^2}\}$. Note that a^2 is a central element of D_4 and y^2 of Z_4.

Summary: Up to and including order 16, one only finds "the usual" groups: direct products of abelian groups, various abelian groups with semidirect product, groups involving D_n and Q_n, and groups with modified semidirect products (replacing $xax^{-1} = a^{-1}$ by $xax^{-1} = a^n$).

We go on with the list of groups, increasing the order in order to find out whether at some point new groups enter the stage.

$\boldsymbol{|G| = 17}$**:** Z_{17}.

$\boldsymbol{|G| = 18}$**:** 5 groups: $D_9, Z_{18}, S_3 \times Z_3, Dih(H)$ and $Z_6 \times Z_3$. $Dih(H)$ is the generalized dihedral group, a semidirect product of an abelian group with a Z_2 which is defined by taking the inverse of the abelian group. $Dih(H) = H \rtimes Z_2$ where $Z_2 = (e, \sigma)$ and $h\sigma = h^{-1}$.

$|G| = 19$: Z_{19}.

$|G| = 20$: Five groups of order 20:

$$Q_{10}\,; \quad Z_{20}\,; \quad GA(1,5)\,; \quad D_{10}\,; \quad Z_{10} \times Z_2\,. \tag{6.3}$$

Here for the first time a new kind of group appears: **Chevalley groups**. These are groups over finite fields. $GA(m,n)$ are the affine groups defined by $\left(\begin{smallmatrix} a & b \\ 0 & 1 \end{smallmatrix}\right)$ with a an $m \times m$ matrix over a field $F(n)$ with entries $0, 1, 2, 3, \cdots, n-1 \mod n$ and b a column vector with entries $0, 1, \cdots, n-1$. Of course, the determinant should be nonvanishing. The group $GA(1,5)$ has order $4 \times 5 = 20$ ($a = 1, 2, 3, 4$ and $b = 0, 1, 2, 3, 4$). Chevalley discovered these groups in 1956, after the subject of finite groups had not moved much since the late 1890's. Chevalley groups are also called groups of Lie type because one can construct finite groups by taking Lie group elements with group parameters from a finite field.

$|G| = 21$: $Z_{21} = Z_7 \times Z_3$ and $Z_7 \rtimes Z_3$ (Frobenius group).

$|G| = 22$: D_{11} and $Z_{22} = Z_{11} \times Z_2$.

$|G| = 23$: Z_{23}.

$|G| = 24$: 15 groups, 3 abelian, 12 nonabelian of which one is a Chevalley group, none are simple.

- 3 abelian: $Z_{24} = Z_8 \times Z_3$, $Z_{12} \times Z_2 = Z_6 \times Z_4 = Z_4 \times Z_3 \times Z_2$, $Z_3 \times Z_2 \times Z_2 \times Z_2$.
- 9 nonabelian direct products: D_{12}, Q_{12}, $D_6 \times Z_2$, $Q_6 \times Z_2$, $D_4 \times Z_3$, $Q_4 \times Z_3$, S_4, $A_4 \times Z_2$, $S_3 \times Z_4$.
- 3 semi-direct products and Chevalley groups: $Z_3 \rtimes Z_8$, $SL(2,3)$, $Z_3 \rtimes D_4 = (Z_3 \times Z_2) \rtimes Z_2 = D_6 \rtimes Z_2 = (Z_3 \rtimes Z_2) \times Z_2$.

6.1 Simple groups

An important class of groups are the simple groups. A simple group is by definition a group without any nontrivial normal subgroups. (The unit e and the group G itself are trivial normal subgroups.) One can construct all finite groups from simple groups by a (complicated) construction which we do not discuss. One class of simple groups are the cyclic groups of order p (where p is prime). Beyond that the first nontrivial simple group is A_5, the alternating group of order 60, so all groups in our list except the Z_p are not simple: they contain normal subgroups. In particular A_4 contains a normal subgroup V, so it is not simple. In fact, V is abelian, and one can sharpen the concept of simple to simple and semisimple. In particular, when we discuss Lie groups, we shall need the notion of a semisimple group, so let us define it here already for finite groups. A **semisimple group** is a group without any abelian normal subgroups (but it may have nonabelian normal subgroups). The cyclic groups Z_{pq} with $(p,q)=1$ are not semisimple because they have abelian subgroups (namely Z_p and Z_q). The dihedral groups are also non-semisimple because the rotation subgroup of them is normal and abelian.

Any finite group can be decomposed in a "composition series", a series of nested groups

$$G \triangleright H_1 \triangleright H_2 \cdots \triangleright H_k \triangleright e \tag{6.4}$$

where H_1 is **a** maximal normal subgroup of G, H_2 is **a** maximal normal subgroup of H_1, $\cdots$, H_k has no normal subgroups (H_k is simple), and e is of course the unit element.

The choice of maximal subgroups inside a given group is not unique (there can be different normal subgroups each of which cannot be extended to an even bigger normal subgroup), but the Jordan-Hölder-Schreier theorem states that two composition series of the same group are isomorphic (by isomorphic it is meant: any quotient group H_k/H_{k+1} of one composition series is isomorphic to a quotient group H'_l/H'_{l+1} of the other composition series). Thus two composition series have the same length, and there is a 1–1 map between the factor groups. The decomposition of a finite group into a composition series is similar to the decomposition of a positive integer into prime numbers, hence the classification problem of all simple groups is like the classification of all prime numbers (which is of course much harder in the first case than in the second case).

However a given composition series may correspond to different groups, hence the classification of finite groups requires more work than only classifying all composition series. The classification of all simple finite groups was completed in 1983 and 2004[1] with the following results. There are four types of simple groups

1) Cyclic groups Z_p with p prime. We showed they do not contain any nontrivial subgroups, hence they certainly do no contain any nontrivial normal subgroups, so they are simple.

2) Alternating groups A_n for $n \geq 5$. Of course $A_3 \cong Z_3$ is contained in 1), and A_4 has a nontrivial normal subgroup, namely Klein's group V (which is abelian, so A_4 is not even semisimple). The proof that A_5 is simple can easily be given by using that any normal subgroup contains entire classes. (The order of A_5 is 60, and its 5 classes have orders 1, 15, 20, 12, 12. There is no combination of these 5 numbers which includes 1 and sums up to one of the nontrivial divisors of 60 which are 30, 20, 15, 12, 10, 6, 5, 4, 3, 2.) However, the proof that A_n is simple for $n \geq 6$ is more involved. We reproduce it below for the interested reader, but we shall not need the simplicity of A_n for $n \geq 6$, so in a first reading we recommend skipping this proof.

3) Groups of Lie type. The group elements of these groups are represented by $m \times m$ matrices

[1] Gorenstein gave a complete classification in 1983 but an error was found, and corrected by Ashbacher and Smith in 2004.

of Lie **algebras** whose entries are not real or complex numbers, but elements of a finite field. A class of these groups called $PSL_m(p^n)$ are $m \times m$ matrices, whose entries are nonnegative integers modulo p^n with p a prime number. For $m = 2$ (2×2 matrices) the $PSL_2(p^n)$ are simple if $p > 3$, while for $m \geq 3$ all of them are simple [1, chapter 8].

4) 26 isolated groups (not part of infinite families) which are called the sporadic groups. The largest of them is called the Monster group, and it contains the following 20 smaller sporadic groups as subgroups or quotients of subgroups. They consists of:

   (a) the 5 Matthieu groups, found in the 1860's; the largest is the Monster group.

   (b) 7 more groups that show up in the studies of the automorphism group of the Leech lattice;

   (c) finally 8 further groups.

   The remaining 6 sporadic groups are not contained in the Monster group. The Leech lattice and the Monster group play a role in string theory. For a readable introduction to the groups of Lie type and the sporadic groups see [2].

6.1.1 Simplicity of A_n for $n \neq 4$

Let us now prove that the A_n for $n \geq 5$ are simple. The proof is based on the following three observations:

1) all even permutations can be written as products of 3-cycles (or as a single 3-cycle).

2) any given 3-cycle (abc) is related to any other 3-cycle (pqr) (where some or all of abc can be equal to some or all of pqr) by a similarity transformation: $(abc) = S^{-1}(pqr)S$. So a normal subgroup with one 3-cycle contains all 3-cycles.

3) any permutation which is part of a normal subgroup N produces a 3-cycle by taking products with suitable other cycles in N. Thus N contains all 3-cycles (step 2), and hence all even permutations (step 1), so $N = A_n$. This proves that N is trivial.

We present now the proofs of these three steps.

1) Every n-cycle is a product of 2-cycles (transpositions)

$$(a_1 \cdots a_n) = (a_n a_{n-1})(a_{n-1} a_{n-2}) \cdots (a_3 a_2)(a_2 a_1)\,. \tag{6.5}$$

   Even permutations have an even number of transpositions, and any product of two transpositions is equal to a 3-cycle or a product of 3-cycles

$$\begin{aligned} (12)(34) &= (234)(123) \\ (12)(23) &= (132) \end{aligned} \tag{6.6}$$

2) two different 3-cycles can have 2,1 or no permutands (objects to be permuted) in common. In each case they are conjugated in A_n

$$
\begin{aligned}
(123) &= (l3k)(12k)(k3l) \\
(123) &= (24)(k3)(14k)(24)(k3) \\
(123) &= (14)(521)(36)(456)(36)(125)(14)
\end{aligned}
\tag{6.7}
$$

3) any element π of a normal subgroup N can be written in terms of disjoint cycles. We shall now analyze separately the following cases:

(i) π contains at least one 5-or-more cycle;

(ii) π contains at least one 4-cycle and no 5-or-more cycles;

(iii) π contains products of 2-cycles and 3-cycles. Then π^2 contains only 3-cycles and π^3 contains only 2-cycles. We shall consider these two special cases separately.

In each of these cases we shall show that there is a 3-cycle in N.

(i) If $\pi \in N$ contains at least one 5-or-more cycle $\pi = (1234 \cdots k)(\cdots)(\cdots)$ with $k > 4$, then also $(123)^{-1}\pi(123)$ lies in N, and also $\pi^{-1}(123)^{-1}\pi(123)$ lies in N. We find

$$
\begin{aligned}
(123)^{-1}\pi(123) &= (3124 \cdots k)(\cdots)(\cdots) \\
\pi^{-1}(123)^{-1}\pi(123) &= (k \cdots 4321)(3124 \cdots k) = (3k2)
\end{aligned}
\tag{6.8}
$$

so there is a 3-cycle in N.

(ii) if $\pi \in N$ contains at least one 4-cycle $\pi = (1234)(\cdots)(\cdots)$ where the cycles $(\cdots)$ contain only 2, 3, 4 cycles, then $\pi^2 = (13)(24)(\cdots)(\cdots)(\cdots)$ contains only 2-cycles and 3-cycles. So we study these cases next.

(iii) if $\pi \in N$ contains only 2-cycles and 3-cycles, then π^2 contains only 3-cycles (case (iv)) and π^3 contains only 2-cycles (case (v)). We study these two cases separately.

(iv) if $\pi \in N$ contains only 3-cycles $\pi = (123)(456)(\cdots)$, then also $\pi_1 = (14)(25)\pi(14)(25)$ lies in N, and also $\pi^{-1}\pi_1$ lies in N. We show that $\pi^{-1}\pi_1$ contains only 2-cycles (case (v))

$$
\begin{aligned}
\pi_1 &= (14)(25)(123)(456)(\cdots)(14)(25) = (126)(453)(\cdots) \\
\pi^{-1}\pi_1 &= (321)(654)(126)(453) = (52)(36)
\end{aligned}
\tag{6.9}
$$

So there is an element in N that only contains 2-cycles. Go now to case (v).

(v) if $\pi \in N$ contains only 2-cycles then the following cycles lie also in N:

$$\begin{aligned}
\pi &= (12)(34)(56)(78)(\cdots) \quad \text{(the case of two transpositions is covered by (6.6))}\\
\pi_1 &= (23)(56)\pi(23)(56) = (23)(56)[(12)(34)(56)(78)(\cdots)](23)(56)\\
&= (13)(24)(56)(78)(\cdots)\\
\pi_2 &= \pi^{-1}\pi_1 = (87)(65)(43)(21)(13)(24)(56)(78) = (14)(23)
\end{aligned} \tag{6.10}$$

Now use (6.6) to show that also in this case N contains a 3-cycle.

This concludes the proof that a normal subgroup N of A_n for $n \geq 6$ contains a 3-cycle, hence $N = A_n$.

6.2 The icosahedron and A_5

The icosahedron (eikosi is 20 and hedron means face or plane in Greek) is a regular surface in 3 dimensions with 20 faces. It consists of a cap on top of 5 equilateral triangles, another cap at the bottom also with 5 equilateral triangles, and a belt in between with 10 equilateral triangles. We put the icosahedron on a table with one vertex touching the table (the bottom vertex), and precisely above it the opposite vertex (the top vertex). We cut the icosahedron with an upper horizontal plane between the upper cap and the belt, and a lower horizontal plane between the belt and the lower cap. The intersection of the upper horizontal plane with the icosahedron yields a pentagon, and the intersection of the lower horizontal plane with the icosahedron yields another but oppositely oriented pentagon. We can now easily identify the vertices, edges and faces.

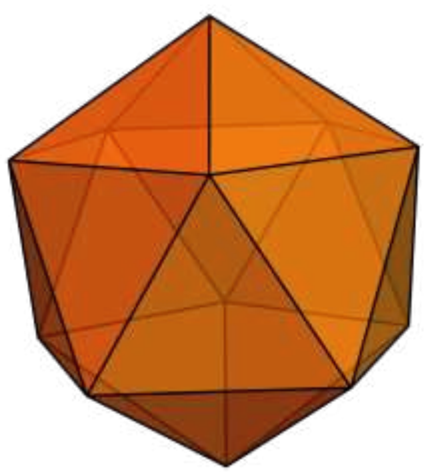

Figure 6.1: The icosahedron.

The top and bottom vertex, together with the two horizontal pentagons, yield 12 vertices. The 5 edges from the top vertex to the upper pentagon, and the 5 edges of the upper pentagon yield 10 edges. Similarly the bottom cap and the lower pentagon yield 10 edges. Next the belt contains 10 edges which connect the upper pentagon to the lower pentagon. Thus there are 30 edges. Finally, the faces are also easily counted: 5 faces in the upper cap, 5 faces in the lower cap, and 10 faces in the belt yield 20 faces. The Euler formula $V - E + F = 2$ is satisfied: $12 - 30 + 20 = 2$.

The symmetries of this polyhedron consists of rotations and (generalized) reflections. Let us first consider the rotations. Rotations in 3 dimensions are around an axis, and for symmetry reason an axis must either join two opposite vertices, or the middle of two opposite faces, or the middle of two opposite edges. We denote these rotations by R_{vv}, R_{ff} and R_{ee}, respectively.

For a given axis between two vertices, there are four genuine rotations over angles $\pm 72^\circ$ and $\pm 2 \times 72^\circ$ ($5 \times 72 = 360$). There are 6 axes for these rotations, so the total number of these rotations is $4 \times 6 = 24$

$$R_{vv} = 24\,. \tag{6.11}$$

If one puts the icosahedron on a table such that it rests on one triangle one finds another horizontal but oppositely oriented triangle on top. There are two genuine rotations about the vertical axis through the middle of these two faces, and since there are 20 faces, there are 10 such axes, yielding $2 \times 10 = 20$ rotations

$$R_{ff} = 20\,. \tag{6.12}$$

Finally, we can put the icosahedron on the table such that it rests on one of its edges at the bottom. There is then another diametrically opposite edge on top; this edge is horizontal and parallel to the edge at the bottom, and there is an axis connecting the middles of these two edges. We call the axes connecting two opposite edges **crosslines**, they will play a crucial role in what follows. Since there are 15 crosslines, there are 15 rotations over 180° about these crosslines, hence

$$R_{ee} = 15\,. \tag{6.13}$$

Together with the unit element (no rotation at all) we find 60 group elements

$$R_{vv} + R_{ff} + R_{ee} + 1 = 24 + 20 + 15 + 1 = 60\,. \tag{6.14}$$

Thus the group of rotations has order 60.

Which group is this? We know by now several groups of order 60[2]: D_{30}, A_5, Q_{30}, Z_{60}. We can rule out the cyclic group Z_{60} as the group of rotations is clearly nonabelian. We also rule out the dihedral group D_{30} as it involves symmetries of a polygon in a plane, not a polyhedron in 3 dimensions. The dicyclic group Q_{30} has no a priori pros or cons, but the alternating group A_5 has a big pro: the abelian group of rotations about an axis connecting two opposite vertices is Z_5 of order 5. So our strategy now is to view the rotations as a transformation group which acts on a carrier space containing 5 objects of the icosahedron. Which 5 objects? Not the vertices (12), or edges (30), or faces (20). Pairs of faces yield 10 objects, not 5. But let us look at the 15 crosslines.

[2]The total number of groups of order 60 is 13, of which only 2 are abelian ($Z_{60} = Z_3 \times Z_5 \times Z_4$ and $Z_{30} \times Z_2 = Z_3 \times Z_5 \times Z_2 \times Z_2$).

They can be divided into **five pairs of triplets of orthogonal crosslines** as we now discuss.

It is not too difficult to find three crosslines that are mutually orthogonal. Having found one such triplet, the other four triplets can be obtained by the four rotations about an axis connecting two opposite vertices. (Of course, the crosslines in one triplet cannot be orthogonal to the crosslines in another triplet.) If one has good stereographic insight, one can readily identify a triplet: let the icosahedron rest on a table on one of its edges. The opposite edge on top is parallel and above it, so one crossline of the triplet is the vertical line connecting the middles of these two horizontal edges. If the bottom edge is parallel to the direction of sight, there are two horizontal parallel edges perpendicular to the line of sight; they yield the second crossline. Finally, there are also two vertical parallel edges perpendicular to the line of sight which yield the third crossline. For readers with less stereographic insight, we shall project the icosahedron (resting on one vertex) onto a plane at the bottom. Then one finds in the projective plane the following complicated figure: the center corresponding to the top and bottom vertex, one (say red) pentagon connected to the center by 5 red radii, and another (say blue) pentagon, oppositely oriented, and connected to the center by 5 blue radii. Finally, the 10 edges in the belt are projected to the 10 (say green) edges of the decagon (10-gon) formed by the two pentagons.

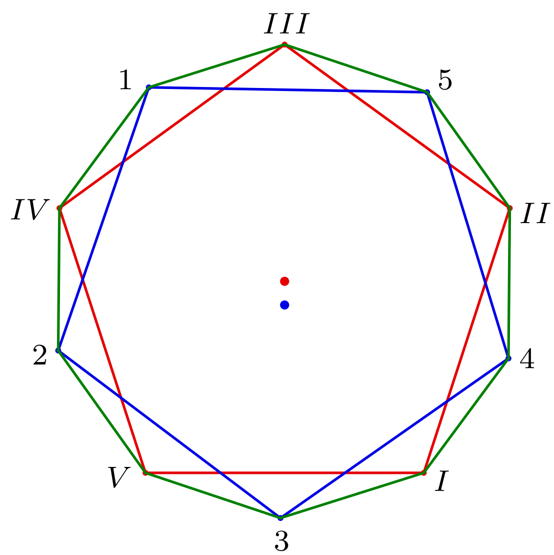

Figure 6.2: The projected icosahedron. The center is due to the top vertex (red dot) and the bottom vertex (blue dot). If one pulls the red and blue dots apart, the icosahedron reappears, the same way as a folded lantern appears if one opens it.

To identify a triplet, we begin with the crossline from the middle of the red edge (15) on top in the figure to the middle of the blue edge (VI) at the bottom. The second crossline connects the middle of the edge (II4) with the middle of the edge (2IV). And the third crossline connects the middle of the edge (03) to the middle of the edge (0III). The corresponding crosslines in 3-dimensions are orthogonal. So the five pairs of crosslines form a 5-dimensional representation of A_5.

So far we discussed the rotations of an icosahedron. What about the (generalized) reflections?

One can obtain 60 generalized reflections by taking the product of one particular reflection with 60 rotations. Together one obtains then 120 isometries, and one might expect that the full symmetry group of an icosahedron is S_5. However, that is incorrect as becomes clear if we consider the isometry σ of space inversion. It commutes with A_5, and hence also with the generalized reflections σA_5. Hence the symmetry group of an icosahedron contains a central element. On the other hand, S_5 does not contain a central element[3]. Hence the symmetry group of an icosahedron is $A_5 \cup \sigma A_5$, and not S_5.

Exercise. Identify all 13 groups of order 60, of which 2 are abelian.

Solution: All abelian groups are cyclic groups, or direct products of cyclic groups. Since 60 has many divisors: $1, 2, 3, 4, 5, 6, 10, 12, 15, 20, 30$, one might expect that the number of abelian groups of order 60 is large. However, there are also many isometries

$$\begin{aligned} &Z_2 \times Z_3 = Z_6,\ Z_2 \times Z_5 = Z_{10},\ Z_2 \times Z_{15} = Z_{30},\ Z_3 \times Z_5 = Z_{15}, \\ &\qquad Z_3 \times Z_4 = Z_{12},\ Z_3 \times Z_{10} = Z_{30},\ Z_3 \times Z_{20} = Z_{60} \text{ and more} \end{aligned} \tag{6.15}$$

and the number of inequivalent abelian groups is only 2

$$\begin{gathered} Z_{60} = Z_5 \times Z_{12} = Z_5 \times Z_4 \times Z_3 = Z_{20} \times Z_3 = Z_{15} \times Z_4\,; \\ Z_{30} \times Z_2 = Z_5 \times Z_3 \times Z_2 \times Z_2 = Z_{15} \times Z_2 \times Z_2\,. \end{gathered} \tag{6.16}$$

Most of the remaining 11 nonabelian groups can be constructed using D_n and Q_{2n} groups, namely

$$\begin{gathered} D_3,\ D_5,\ D_6,\ D_{10},\ D_{15},\ D_{30}\,; \\ Q_2,\ Q_6,\ Q_{10},\ Q_{30}\,. \end{gathered} \tag{6.17}$$

The groups D_4, D_8, D_{12} and Q_4, Q_8, Q_{12} cannot be used (Lagrange's theorem). However, just as $Q_6 = Z_3 \rtimes Z_4$, also $Q_{10} = Z_5 \rtimes Z_5$, $Q_{30} = Z_{15} \rtimes Z_4$ and $Q_2 = V$. Some of the isomorphisms for the D_n groups were given before. Then one finds the following 7 groups

$$\begin{gathered} (Z_5 \rtimes Z_4) \times Z_3 = Q_{10} \times Z_3\,; \qquad D_3 \times D_5\,; \\ (Z_3 \rtimes Z_4) \times Z_5 = Q_6 \times Z_5\,; \qquad D_3 \times Z_{10}\,; \\ Z_{15} \rtimes Z_4 = Q_{30}\,; \qquad D_5 \times Z_6\,; \qquad D_{30}\,. \end{gathered} \tag{6.18}$$

Then there are two groups with A_n groups

$$A_5\,; \qquad A_4 \times Z_5\,. \tag{6.19}$$

[3]Realizing S_5 in terms of cycles, no group element is kept fixed by all similarity transformations gag^{-1}.

The final two nonabelian groups of order 60 are

$$\mathrm{Hol}(A_5) \times Z_3\,; \qquad \left\{a, b | a^5 = b^4 = e; bab^{-1} = a^2\right\}. \tag{6.20}$$

The group $\mathrm{Hol}(A_5)$ is a discrete group with matrices of affine type $M = \begin{pmatrix} \boxed{5\times 5} & \boxed{} \\ \varnothing & 1 \end{pmatrix}$.

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Chapter 7

Reducibility and unitarity of matrix representations of finite groups

Groups usually appear in physics as matrices, for example, matrices inside covariant derivatives of field theories, or matrices acting on the atoms in molecules. It is thus crucial to know which matrices can represent a given group. This is the subject of this chapter. It is at this point that mathematics and physics part ways. In mathematics one is primarily interested in properties of abstract groups, whereas in physics the emphasis is on matrices associated with physical systems.

We define a matrix representation of a group as a set of matrices $M(g)$, one matrix M for each group element g, satisfying

$$M(g_1)M(g_2) = M(g_1g_2). \tag{7.1}$$

The set of matrices $M(g)$ forms a group since all four group axioms are satisfied. Thus a matrix representation[1] is a homomorphism from the group G into the set of $n \times n$ (real or complex) matrices (in general not an isomorphism). Only particular values of n can occur for a given group, and we shall determine these values. In some cases the matrices are real, in other cases complex, and there is a third possibility (pseudoreal) which we shall define and discuss later.

Before we begin, we make some general statements. Taking $g_2 = e$ yields $M(g_1)M(e) = M(g_1)$, hence $M(e)$ is the unit element for the set of matrices $M(g)$. Taking $g_2 = g^{-1}$ yields $M(g_1)M(g_1^{-1}) = M(e)$. Without loss of generality[2] we choose $M(e)$ to be the $n \times n$ unit matrix I, and then $M(g^{-1})$ is the inverse of the matrix $M(g)$. Hence, **all matrices $\boldsymbol{M(g)}$ are nonsingular**.

There is always the **trivial representation** where all $M(g)$ are equal to the number 1. Clearly $M(g_1)M(g_2) = M(g_1g_2)$ if $M(g) = 1$ for all g. Another representation that always exists is the

[1] In mathematics one defines a representation of a group G as a homomorphism from G into the group of permutations of a set X. In the case of matrix representations, X is R^n and the permutations are the linear transformations of R^n into itself.

[2] If $M(e)$ has a kernel $M(e)x = 0$, these vectors x are also in the kernel of the $M(g)$ because $M(g)M(e)x = M(g)x = 0$. Thus the kernel forms an invariant subspace. Maschke's theorem (see later) then states that one can choose a basis such that all matrices are in the block form $M(g) = \begin{pmatrix} \overline{M}(g) & 0 \\ 0 & 0 \end{pmatrix}$ where $\overline{M}(g)$ are nonsingular. Without loss of generality we can drop the null space. If we define $\overline{M}(g^{-1}) = \overline{M}(g)^{-1}$, it follows that $\overline{M}(e)$ is the unit matrix.

regular representation: for fixed a the map $G \to G$ given by $g \to ag$ is a permutation Π_a of the group elements of G, and to each Π_a corresponds a matrix with only entries equal to 1 or 0. However, there is usually an easy way to find further representations by using quotient groups: if N is a normal subgroup of G, we have seen that G/N is a group. Suppose one has a particular matrix representation $\bar{M}$ for G/N whose matrices are $\bar{M}(aN)$, $\bar{M}(bN), \cdots$ where aN, $bN, \cdots$ are the coset elements. Then it can at once be extended to a matrix representation M of G by defining that $M(n) = e$ for all n in N. Indeed, in that case $\bar{M}(an) = M(a)$, so M is the same for all group elements in a coset element. If for the coset elements one has $\bar{M}(aN)\bar{M}(bN) = \bar{M}(aNbN) = \bar{M}(abN)$, then, since any group element g can be written as an for some a in a coset element aN, one has $M(g_1)M(g_2) = M(an_1)M(bn_2) = \bar{M}(aN)\bar{M}(bN) = \bar{M}(abN) = M((an_1)(bn_2)) = M(g_1g_2)$ since $an_1bn_2 = abn_3 \in abN$. So, **any matrix representation of a quotient group yields a matrix representation of the group**.

7.1 Faithful matrix representation. Reducibility.

A **faithful** matrix representation $M(g)$ of a group G satisfies: if $g_1 \neq g_2$ then $M(g_1) \neq M(g_2)$. Then knowing the matrices uniquely identifies the corresponding group elements. On the other hand, if the matrix representation M is not faithful, there are several elements of G which form the kernel K of the homomorphism, and in that case the matrices M form a faithful representation of the quotient group G/K. It is then a good strategy first to determine the matrix representations of G/K, and then to extend them to G as discussed above. (Recall that K is an invariant subgroup.)

There are two properties which all matrix representations of finite groups possess, but which only hold for a special class of Lie groups (namely the compact Lie groups, to be defined later): they are **completely reducible** and can be made **unitary**. If a representation (the set of all $n \times n$ matrices $M(g)$ acting in an n-dimensional space V) has a nontrivial invariant subspace W (so W is not empty and not the whole space), it is called a **reducible representation**. Complete reducibility means that one can write all matrices in block form, and each block is irreducible.

The proof of complete reducibility is sometimes given by first making the matrices $M(g)$ unitary by another basis change $M'(g) = VM(g)V^{-1}$, but it is a property of linear vector spaces, and has nothing to do with unitarity. It is called **Maschke's theorem** (1898 and 1899) and the proof is as follows.

Suppose the matrices $M(g)$ act in a linear vector space $\mathbb{V}$, and suppose there is a subspace W which is mapped into itself by all $M(g)$. We call such a subspace an invariant subspace (invariant under the action of all $M(g)$). If we choose a basis in W, and complete the basis by choosing some further basis vectors in some arbitrary but definite way, then a vector v in $\mathbb{V}$ can be decomposed as $\boldsymbol{v} = \boldsymbol{w} + \boldsymbol{z}$ where $\boldsymbol{w}$ lies in W and $\boldsymbol{z}$ is a linear combination of the further basis vectors. Then the action of $M(g)$ on $\boldsymbol{v}$ has the following structure

$$M(g)\boldsymbol{w} = \boldsymbol{w}' \qquad (W \text{ is an invariant subspace}) \tag{7.2}$$

$$M(g)\boldsymbol{z} = \boldsymbol{w}'' + \boldsymbol{z}'' \qquad (M(g)\boldsymbol{z} \text{ can be anything}) \tag{7.3}$$

The vectors $\boldsymbol{w}'' + \boldsymbol{z}''$ contain in general a nonvanishing part $\boldsymbol{w}''$ in W, and $M(g)$ acting on $\left(\begin{smallmatrix} z \\ w \end{smallmatrix}\right)$ has the form

$$M(g) = \begin{pmatrix} M_1(g) & A(g) \\ 0 & M_2(g) \end{pmatrix} \tag{7.4}$$

where the matrices $M_1(g)$ and $M_2(g)$ form two separate matrix representations.[3] The claim of Maschke's theorem is that one can remove A by a clever basis choice. A basis change is implemented by a similarity transformation. So we want to find a matrix S such that for all g

$$M(g)S = SD(g) \quad \text{with} \quad D(g) = \begin{pmatrix} M_1(g) & 0 \\ 0 & M_2(g) \end{pmatrix} \tag{7.5}$$

If one has found such a matrix S but the blocks $M_1(g)$ and $M_2(g)$ themselves are reducible, one can apply the theorem again. Then the final set of blocks $M_1(g)$, $M_2(g)$, $M_3(g), \cdots$ are not reducible (cannot be cast into triangular form) and each block is called **irreducible**. Matrices with a triangular form are called reducible and matrices in block form are called completely reduced. Hence the theorem states that for finite groups a reducible representation is completely reducible. Irreducible matrix representations will from now on be called **irreps**.

7.2 Maschke's theorem on complete reducibility

Theorem (Maschke, 1898): A reducible representation of a finite group is completely reducible.

Proof: We claim that S is given by the following matrix

$$S = \frac{1}{|G|} \sum_g M(g^{-1})D(g) \quad \text{with } |G| = \text{order}\, G \tag{7.6}$$

One sometimes finds proofs in which one analyzes each of the blocks of this matrix equation separately, but it is simpler not to decompose this matrix equation at all. Substituting (7.4) and

[3]From $M(g)M(g') = M(gg')$ we learn that $M_1(gg') = M_1(g)M_1(g')$ and $M_2(gg') = M_2(g)M_2(g')$ (matrix representations). So $M_1(g)$ and $M_2(g)$ are representations of G and $D(g) = \left(\begin{smallmatrix} M_1(g) & 0 \\ 0 & M_2(g) \end{smallmatrix}\right)$ forms also a representation of G. Further $A(gg') = A(g)M_2(g') + M_1(g)A(g')$, so if the matrices $M(g)$ form a representation, then $M(g^{-1})$ contains $A(g^{-1})$ given by $A(g^{-1}) = -M_1(g^{-1})A(g)M_2(g^{-1})$. One can check that $M(g)M(g^{-1})$ is equal to the unit matrix.

(7.5) one finds that S has the form[4]

$$S = \sum_g \frac{1}{|G|} \begin{pmatrix} M_1(g^{-1}) & A(g^{-1}) \\ 0 & M_2(g^{-1}) \end{pmatrix} \begin{pmatrix} M_1(g) & 0 \\ 0 & M_2(g) \end{pmatrix} = \begin{pmatrix} I & * \\ 0 & I \end{pmatrix} \tag{7.7}$$

hence S is invertible and the claim is that

$$D(g) = S^{-1} M(g) S \,. \tag{7.8}$$

For the proof, we just write out the products of matrices

$$\begin{aligned} M(g)S &= \frac{1}{|G|} \sum_{g'} M(g) M(g'^{-1}) D(g') \\ &= \frac{1}{|G|} \sum_{g'} M(gg'^{-1}) D(g') \quad \text{(group property for } M) \\ &= \frac{1}{|G|} \sum_{g'} M(gg'^{-1}) D(g' g^{-1}) D(g) \quad \text{(group property for } D) \\ &= \frac{1}{|G|} \sum_{g''} M(g'') D(g''^{-1}) D(g) \quad \text{with } g'' = gg'^{-1}. \end{aligned} \tag{7.9}$$

This is indeed equal to $SD(g)$

$$SD(g) = \frac{1}{|G|} \sum_{g'} M(g'^{-1}) D(g') D(g) = \frac{1}{|G|} \sum_{g''} M(g'') D(g''^{-1}) D(g) \,. \tag{7.10}$$

because summing over all g' is the same as summing over all $(g'')^{-1}$. Hence we can bring all $M(g)$ simultaneously to block form by a similarity transformation. (Note that in general S does not lie in the group of matrices $M(g)$.)

Next we prove the other property of any irrep of finite groups, their unitarity. For unitarity we need an inner product, so we consider $n \times n$ matrices $M(g)^i{}_j$ with $i, j = 1, \cdots, n$, which act in an n-dimensional space, and define an inner product in this space by

$$(x, y) = \sum_{i=1}^{n} (x^i)^* y^i \,. \tag{7.11}$$

7.3 Schur's theorem on unitary representations

Theorem (Schur, 1905): Any irrep of a finite group can be made unitary by a similarity transformation.

[4]The normalization factor $\frac{1}{|G|}$ in (7.6) was chosen in order to obtain the unit matrix on the diagonal in (7.7), but this normalization is not essential.

Proof: We want to prove that there exists a matrix S such that

$$SM(g)S^{-1} = \tilde{M}(g) \quad \text{where} \;\; \tilde{M}(g)\tilde{M}^{\dagger}(g) = I \;\; \text{for all } g \in G. \tag{7.12}$$

So we must find a matrix S such that $SM(g)(S^{-1}S^{-1,\dagger})M(g)^{\dagger}S^{\dagger} = I$ for all g. If $S^{-1}S^{-1,\dagger}$ were to be given by $\sum_{g'} M(g')M(g')^{\dagger}$, then we could repeat the observation used in (7.9) that $M(g)$ times $\sum_{g'} M(g')M(g')^{\dagger}$ is equal to $\sum_{g''} M(g'')M(g'')^{\dagger}M(g)^{\dagger,-1}$. So how do we find the relation between $S^{-1}S^{-1,\dagger}$ and $\sum_{g'} M(g')M(g')^{\dagger}$?

Consider the matrix

$$H = \sum_g M(g)M(g)^{\dagger} \tag{7.13}$$

The sum (we cannot add group elements but we can add matrices) is over all group elements, and is well-defined since we are considering finite groups. It is clear that $H^{\dagger} = H$ and H is positive definite:

$$(x, Hx) = (x^i)^* H^i{}_j x^j = \sum_g \left| M(g)^{\dagger} x \right|^2 > 0 \quad (i, j = 1, \cdots, n) \tag{7.14}$$

(For no x is any of the $M(g)^{\dagger}x = 0$ because the matrices $M(g)$ are nonsingular.) A hermitian matrix can be diagonalized by unitary matrix, and since H is positive definite, this diagonal matrix also has positive entries on the diagonal

$$UHU^{-1} = D = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} \quad \text{with all } \lambda_j > 0\,. \tag{7.15}$$

Then we can take the square root $D^{\frac{1}{2}}$ which is also diagonal and positive definite. The same holds for $D^{-\frac{1}{2}}$. Define next

$$S = D^{-\frac{1}{2}}U \text{ and } \tilde{M}(g) = SM(g)S^{-1}. \tag{7.16}$$

Then $S^{-1}S^{-1,\dagger} = U^{-1}D^{-1}U = H = \sum_{g'} M(g')M(g')^{\dagger}$, so we have found the relation between the matrix S and the matrix $M(g)$. Now it is straightforward to verify that the matrices $\tilde{M}$ are unitary

$$\begin{aligned}
\tilde{M}(g)\tilde{M}(g)^{\dagger} &= \left(SM(g)S^{-1}\right)\left(SM(g)S^{-1}\right)^{\dagger} \\
&= \left(D^{-\frac{1}{2}}UM(g)U^{-1}D^{\frac{1}{2}}\right)\left(D^{\frac{1}{2}}UM(g)^{\dagger}U^{-1}D^{-\frac{1}{2}}\right) \;\; \text{since } U^{\dagger} = U^{-1} \\
&= D^{-\frac{1}{2}}UM(g)HM(g)^{\dagger}U^{-1}D^{-\frac{1}{2}} \\
&= \sum_{g'} D^{-\frac{1}{2}}U\big(M(g)M(g')\big)\big(M(g')^{\dagger}M(g)^{\dagger}\big)U^{-1}D^{-\frac{1}{2}} \quad \text{using (7.13)} \\
&= \sum_{g''} D^{-\frac{1}{2}}UM(g'')M(g'')^{\dagger}U^{-1}D^{-\frac{1}{2}} \quad \text{with } g'' = gg' \\
&= D^{-\frac{1}{2}}UHU^{-1}D^{-\frac{1}{2}} \quad \text{using again (7.13)} \\
&= D^{-\frac{1}{2}}DD^{-\frac{1}{2}} = I\,.
\end{aligned} \tag{7.17}$$

This proves that without loss of generality one can always assume, as we shall do from now on, that all matrices of an irrep of a finite group are unitary. ■

Finally we prove the celebrated **Schur lemmas**. They are properties of linear vector spaces, like Maschke's theorem, and hold whether or not the irrep is unitary.[5] The first lemma states that the set of matrices $M(g)$ of an irrep is sufficiently "'dense" that no matrix except I can commute with all of the $M(g)$.

7.4 Schur's two lemmas

Lemma I (Schur, 1907): Any matrix $\boldsymbol{A}$ that commutes with all matrices $\boldsymbol{M(g)}$ of an irrep, is proportional to the unit matrix: $\boldsymbol{A = \alpha I}$.

Proof: Assume $[A, M(g)] = 0$ for all g. Consider all eigenvectors of A with eigenvalue λ, $Ax = \lambda x$. (There is always one **eigenvalue** λ.) They span a linear vector space V_λ, so x lies in V_λ. Then $M(g)Ax = M(g)\lambda x = \lambda M(g)x = A(M(g)x)$. So, also $M(g)x$ lies in V_λ. Thus the space V_λ is transformed into itself by all matrices $M(g)$: it is an invariant subspace. But since the $M(g)$ form an irreducible representation, the only invariant space is the whole space. (The space is not empty: we started with at least one eigenvector x.) So $Ax = \lambda x$ for all x in the whole n-dimensional space. This implies $A = \lambda I$. ■

The first Schur lemma makes a statement about the commutator of a matrix A and the matrices $M(g)$ of one given irrep. The second Schur lemma deals with two irreps.

Lemma II (Schur, 1907): If for two irreps of a finite group with matrices $\boldsymbol{M_I(g)}$ and $\boldsymbol{M_{II}(g)}$ there is a matrix $\boldsymbol{B}$ which intertwines these irreps,

$$\boldsymbol{M_I(g)B = BM_{II}(g)}\,, \tag{7.18}$$

then $\boldsymbol{B = 0}$ if $\boldsymbol{M_I}$ and $\boldsymbol{M_{II}}$ are inequivalent, but if $\boldsymbol{M_I}$ and $\boldsymbol{M_{II}}$ are equivalent[6], then $\det \boldsymbol{B \neq 0}$. (Of course, $B = 0$ is another, trivial, solution.)

Proof: Let the matrices $M_I(g)$ be larger (or equal) in size than the matrices $M_{II}(g)$. Then the matrix B is an $m \times n$ matrix with $m \geq n$. The matrix B maps then any vector x in the smaller space R^n into a vector in the large space R^m. Act now with the matrix equation in (7.18) on a

[5]There exist proofs where one first decomposes A into a real and an imaginary part. Such a decomposition requires that the irrep has been made unitary, but that is unnecessary. (If $[M(g), A] = 0$ also $[M(g), A^\dagger] = 0$ since $[M(g), A]^\dagger = [A^\dagger, M(g)^\dagger] = [A^\dagger, M(g)^{-1}] = [A^\dagger, M(g^{-1})] = 0$. We used the unitarity of the matrices $M(g)$. One can then take linear combination of A and $A^\dagger$ which are real.)

[6]Two irreps with matrices $M_I(g)$ and $M_{II}(g)$ are called equivalent if $M_I(g) = SM_{II}(g)S^{-1}$ for all g. Note that S must be the same matrix for all g. If this relation does not hold, the two irreps are called inequivalent.

vector x in R^n

$$\begin{pmatrix} & & \\ & M_I(g) & \\ & & \end{pmatrix} \underbrace{\begin{pmatrix} \\ B \\ \\ \end{pmatrix}^{(x)}}_{y} = \underbrace{\begin{pmatrix} \\ B \\ \\ \end{pmatrix}^{\big(M_{II}(g)\big)(x)}}_{y'} . \tag{7.19}$$

Denote the subspace $y = Bx$ for all x by S. So the vector $y = Bx$ for all x form a linear vector subspace of dimension n in the bigger space R^m. Then

$$M_I(g)y = y' \tag{7.20}$$

and y and y' both lie in S. So S is an invariant subspace of $\mathbb{R}^m$ of dimension $d \leq n$ (because the rank of B is $d \leq n$). Since $M_I(g)$ was supposed to be irreducible, and if $m > n$, S must be empty, hence $B = 0$ if $m > n$. This proves the first part of the theorem.

If $m = n$, the equation $M_I(g)y = y'$ can only be satisfied either if all y' span the whole space $\mathbb{R}^m$, or if all y' vanish. If all $y' = BM_{II}(g)x$ for a given g and all x span the whole space, $\det M_{II}(g) \neq 0$ and $\det B \neq 0$. Then M_I and M_{II} are equivalent: $M_I(g) = BM_{II}(g)B^{-1}$. But if all y' vanish, namely if all $BM_{II}(g)x$ vanish for all x and all g, then all Bz (with $z = M_{II}(g)x$) vanish for all z in $\mathbb{R}^n$ (recall that $M_{II}(g)$ are invertible). But then the whole space S is the null space, and $B = 0$. ■

Alternative proof (see Tinkham's book): If one assumes that all matrices have been made unitary, a simpler proof can be given. Suppose again that

$$M_I(g)B = BM_{II}(g) \quad \text{for all } g \tag{7.21}$$

Hermitian conjugation and assuming unitarity yields

$$B^\dagger M_I(g) = M_{II}(g)B^\dagger \quad \text{for all } g \tag{7.22}$$

since $M_I(g)^\dagger = M_I(g)^{-1} = M_I(g^{-1})$ and similarly for $M_{II}(g)$. Then the $m \times m$ matrix $BB^\dagger$ commutes with all $M_I(g)$. But the lemma I tells us that $BB^\dagger$ is proportional to the unit matrix. So either $BB^\dagger = 0$ or if $BB^\dagger = \alpha I$ with $\alpha \neq 0$, $\det B \neq 0$. In the latter case M_I and M_{II} are equivalent, while in the former case we have $|B^\dagger y|^2 = 0$ for all y, which implies $B = 0$.

7.5 The orthogonality relations for irreps

Schur's lemmas have a very important application: they allow us to prove that the matrix elements of unitary irreps are orthogonal. Suppose one is given two irreps, $R^{(i)}$ and $R^{(j)}$, the first being given by matrices $M^{(i)}(g)^\mu{}_\nu$ where $\mu, \nu = 1, \cdots, n$, and the second being given by $M^{(j)}(g)^\alpha{}_\beta$ where $\alpha, \beta = 1, \cdots, m$. Each matrix element of a given irrep $M^{(i)}(g)^\mu{}_\nu$ is a function of g, and we view this function as a vector in a $|G|$-dimensional space. So the claim is that all these vectors (all matrix elements of all inequivalent irreps) are orthonormal.

Theorem (Schur): $$\sum_g \left((M^{(i)}(g)^*)_\mu{}^\nu (M^{(j)}(g)^\alpha{}_\beta)\right) = \delta^\alpha_\mu \delta^\nu_\beta \delta^j_i \frac{|G|}{\dim R^i} \tag{7.23}$$

where[7] $(M^{(i)}(g)^*)_\mu{}^\nu \equiv (M^{(i)}(g)^\mu{}_\nu)^*$. By $\dim R^i$ we mean the dimension of the matrices $M^{(i)}(g)$.

Proof: The normalization can be checked for the unit representation (set $i = j$ and $\dim R^i = 1$). To apply Schur's lemma we need a matrix A that intertwines $M^{(i)}$ and $M^{(j)}$. Since the irreps can be assumed to be unitary, we have

$$\left(M^{(i)}(g)^\mu{}_\nu\right)^* = M^{(i)}\left(g^{-1}\right)^\nu{}_\mu\,. \tag{7.24}$$

Consider then the following matrix

$$A = \sum_g M^{(i)}(g) X M^{(j)}\left(g^{-1}\right) \tag{7.25}$$

where X is any rectangular matrix. It interpolates between the irreps R^i and R^j

$$\begin{aligned} M^{(i)}(g)A &= \sum_{g'} M^{(i)}(g)\Big(M^{(i)}(g')XM^{(j)}\left(g'^{-1}\right)\Big) = \sum_{g'} M^{(i)}(gg')XM^{(j)}\left(g'^{-1}\right) \\ &= \sum_{g''}\Big(M^{(i)}(g'')XM^{(j)}\left(g''^{-1}\right)\Big) M^{(j)}(g) \qquad \text{with } g''=gg' \\ &= AM^{(j)}(g)\,. \end{aligned} \tag{7.26}$$

Hence, if $R^{(i)}$ and $R^{(j)}$ are inequivalent, Schur's lemma states that $A = 0$,

$$\sum_g M^{(i)}(g)^\mu{}_\nu X^\nu{}_\alpha M^{(j)}\left(g^{-1}\right)^\alpha{}_\beta = 0 \;\text{ if } i \neq j\;. \tag{7.27}$$

Taking $X^\nu{}_\alpha = 1$ for a particular value of ν and α, and vanishing for all other values, we obtain

$$\sum_g M^{(i)}(g)^\mu{}_\nu M^{(j)}\left(g^{-1}\right)^\alpha{}_\beta = 0\,. \tag{7.28}$$

which proves the theorem for the case that $i \neq j$.

[7] We use here a notation which is not necessary but very useful for unitary matrices: complex conjugation maps an upper index to a lower index, and vice-versa. With this notation equation (7.23) becomes manifestly covariant: it fixes all Kronecker delta functions on the right-hand side with one index up and the other index down. Let us derive (7.24) in excruciating detail. We begin with the definition of hermitian conjugation $(x, My) = (M^\dagger x, y)$ where $(x, y) = (x^*)_\mu y^\mu$ (summed over μ). Then $(M^\dagger x, y) = (M^\dagger x)^*_\nu y^\nu = ((M^\dagger)^\nu{}_\mu x^\mu)^* y^\nu = ((M^\dagger)^\nu{}_\mu)^*(x^*)_\mu y^\nu$. Thus $M^\mu{}_\nu = ((M^\dagger)^\nu{}_\mu)^*$. Now we use the unitarity of the matrices $M(g)$: $M^\dagger(g) = M^{-1}(g) = M(g^{-1})$. So $M^\mu{}_\nu(g) = (M^\nu{}_\mu(g^{-1}))^*$ which is (7.24).

When $i = j$ (i.e., when the irreps are equivalent), Schur's lemma states that $A = \alpha I$ for some α. Then

$$\sum_g M^{(i)}(g)^\mu{}_\nu X^\nu{}_\rho M^{(i)}\left(g^{-1}\right)^\rho{}_\sigma = \alpha\delta^\mu{}_\sigma \,, \tag{7.29}$$

where α depends on ν, ρ and i. Choosing again $X^\nu{}_\rho = 1$ for a particular value of ν and ρ now yields

$$\sum_g M^{(i)}(g)^\mu{}_\nu M^{(i)}\left(g^{-1}\right)^\rho{}_\sigma = \alpha_\nu^{(i)\rho}\delta^\mu{}_\sigma \,. \tag{7.30}$$

Summing over $\mu = \sigma$ fixes α

$$\sum_{g,\mu} M^{(i)}(g)^\mu{}_\nu M^{(i)}\left(g^{-1}\right)^\rho{}_\mu = \sum_g I_\nu{}^\rho = |G|\delta_\nu{}^\rho = \dim R^i \alpha_\nu^{(i)\rho} \tag{7.31}$$

hence $\alpha_\nu^{(i)\rho} = \frac{|G|}{\dim R^i}\delta_\nu{}^\rho$. Substitution of this result and (7.24) into (7.29) yields (7.23). This concludes the proof of the orthogonality relations. ■

Comment. Many of the results for finite groups also hold for **compact** Lie groups. For example, all finite-dimensional reps can be made unitary by a suitable similarity transformation (but there exist in addition infinite-dimensional reps which are not unitarizable). The orthogonality relations of matrix elements of irreps hold again. For example, for $SU(2)$ with group elements $e^{-i\alpha J_3}e^{-i\beta J_2}e^{-i\gamma J_3} \equiv e^{\alpha T_3}e^{\beta T_2}e^{\gamma T_3}$ there exist matrices $\left(D^j(\alpha,\beta,\gamma)\right)^m{}_n$ for any $j = 0, \frac{1}{2}, 1, \cdots$. So j labels the irrep. The matrix elements are parametrized by $m, n = j, j-1, \cdots, -j$, and α, β, γ label the group elements. One can decompose these irreps as follows

$$\left(D^j(\alpha,\beta,\gamma)\right)^m{}_n = e^{-i\alpha m}\left(d^j(\beta)\right)^m{}_n e^{-i\gamma m} \tag{7.32}$$

where $\left(d^j(\beta)\right)^m{}_n$ are real orthogonal $(2j+1)\times(2j+1)$ matrices.[8] Just as for finite groups, the irreps satisfy the following orthogonality relations

$$\int d\tau_A \left(D^j(A)^m{}_n\right)^* \left(D^{j'}(A)\right)^{m'}{}_{n'} = \delta_j^{j'}\delta_m^{m'}\delta_n^{n'}\frac{\mathrm{vol}(G)}{\dim R^j} \tag{7.33}$$

where $\dim R^j = 2j+1$, $\mathrm{vol}(G) = 16\pi^2$, A denotes the triplet α, β, γ, and

$$\int \tau_A = \int_0^{2\pi} d\alpha \int_{-1}^{+1} d\cos\theta \int_{-2\pi}^{2\pi} d\gamma \tag{7.34}$$

is the Haar measure for $SU(2)$. (For $SO(2)$ one has $\int_0^{2\pi} d\gamma$.) These D-functions provide the connections between quantum mechanics with Y_m^l's and group theory for the group $SU(2)$, but we shall use general groups, not only $SU(2)$, and for that reason we shall not study these D-functions

[8]The spherical harmonics $Y^l{}_m(\theta,\phi)$ are related to the "D functions" as $Y^l{}_m(\theta,\phi) = \left(\frac{2l+1}{4\pi}\right)^{\frac{1}{2}}\left(D^l(\phi,\theta,0)^m{}_0\right)^*$ and the Legendre polynomials $P_l(\cos\theta)$ are related by $P_l(\cos\theta) = \left(d^l(\theta)\right)^0{}_0$.

any further. However, for the interested reader we recommend the quite detailed textbook by Wu-Ki Tung.

Chapter 8

Three theorems on matrix representations. Character Tables.

There are three main theorems which give information about which matrix irreps (irreducible representations) are possible for finite groups. We shall first state them, then apply them in a simple example, next introduce and discuss characters, then work through a less simple example, and finally prove the three theorems[1].

Theorem 1: The number of one-dimensional irreps is equal to the order of G divided by the order of the commutator subgroup

$$\boldsymbol{n_{1-\mathrm{dim}} = \frac{|G|}{|C(G)|}} \tag{8.1}$$

Theorem 2: The number of inequivalent irreps is equal to the number of classes

$$\boldsymbol{n_{irreps} = n_C} \tag{8.2}$$

Theorem 3: The order of a group is equal to the sum of the squares of the dimensions d_i of all the inequivalent irreps R^i

$$\boldsymbol{|G| = \sum_i (d_i)^2} \tag{8.3}$$

Comment 1. Usually one is not interested in one-dimensional irreps, so theorem 1 is only useful in so far as it gives some information on irreps one would like to get rid of. Theorem 2 states that one should first determine the number of classes, and then this number is equal to the number

[1] There exists a fourth theorem which restricts which irreps are possible: the dimension of any irrep of a group G is a divisor of the index of each of the maximal normal abelian subgroups of G. So the theorem is only useful for nonsemisimple Lie groups. For example, the quaternion group $\mathbb{Q} = Q_4$ has 4 nontrivial normal abelian subgroups of which 3 are maximal (the normal subgroup $\{\pm e, \pm I\}$, and the same with J and K). These three groups have order 4, hence index 2. Thus the irreps of $\mathbb{Q}$ can only have dimensions 1 or 2. The proof of this theorem (that I know of) is complicated and not that useful for our purposes, so for that reason we shall not discuss it any more.

of the one-dimensional irreps of theorems, plus the number of higher-dimensional irreps. Finally theorem 3 gives another relation between the number of one-dimensional and higher-dimensional irreps. Often there is only one solution to the Diophantine equation $|G| = \sum_i d_i^2$, given $n_{1-\text{dim}}$ from theorem 1.

Let us now give a simple example.

8.1 $G = S_3$

The group elements of S_3 are the elements of the permutation group of 3 objects: $S_3 = \{e, (12), (13), (23), (123), (132)\}$. We already encountered this group as the isometry group D_3 of an equilateral triangle (3 rotations, 3 reflections). The permutands $1, 2, 3$ correspond to the vertices of the triangle. So S_3 is isomorphic to D_3. The isometries of an equilateral triangle when viewed as linear transformations in the plane give a 2-dimensional irrep. However, we can also identify the permutands 1, 2 and 3 with the x, y and z-axis of a 3-dimensional space, and then (12) is a transformation which interchanges the x- and y-coordinates of a 3-dimensional vector, while (123) maps for example the vector $(0, 0, 1)$ to $(1, 0, 0)$. This yields a 3-dimensional irrep. So we have already two representations: the first in a 2-dimensional space (the plane), and the second in a 3-dimensional space (x, y, z space).

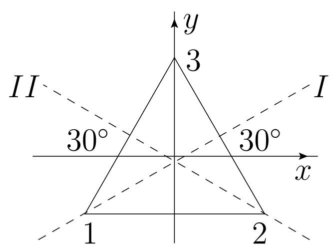


Figure 8.1: The vertices $1, 2, 3$ correspond to the unit vectors $\begin{pmatrix} -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2} \end{pmatrix}$, $\begin{pmatrix} \frac{1}{2}\sqrt{3} \\ -\frac{1}{2} \end{pmatrix}$ and $\binom{0}{1}$, respectively. The diagonals I and II lie along the unit vectors $\left(\frac{1}{2}\sqrt{3}, \frac{1}{2}\right)$ and $\left(-\frac{1}{2}\sqrt{3}, \frac{1}{2}\right)$.

Let us begin with the former. The set of matrices of this rep is as follows

$$e = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$(123) = \begin{array}{c}\text{rotation of vectors in} \\ \text{the } x\text{-}y \text{ plane over } 120^\circ\end{array} = \begin{pmatrix} \cos 120^\circ & -\sin 120^\circ \\ \sin 120^\circ & \cos 120^\circ \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix}$$

$$(132) = \begin{array}{c}\text{rotation of vectors in} \\ \text{the } x\text{-}y \text{ plane over } -120^\circ\end{array} = \begin{pmatrix} \cos(-120^\circ) & -\sin(-120^\circ) \\ \sin(-120^\circ) & \cos(-120^\circ) \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix}$$

$$(12) = \text{reflection about } y\text{-axis} = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$(23) = \text{reflection about diagonal I} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix} \quad \left(\text{maps } \begin{pmatrix} 1 \\ 0 \end{pmatrix} \text{ to } \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2}\sqrt{3} \end{pmatrix} \text{ etc.}\right)$$

$$(13) = \text{reflection about diagonal II} = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix} \quad \left(\text{maps } \begin{pmatrix} -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2} \end{pmatrix} \text{ to } \begin{pmatrix} 0 \\ 1 \end{pmatrix}\right) \tag{8.4}$$

The rotations have $\det M = +1$, and the reflections have $\det M = -1$. One may check the relation $M(g_1)M(g_2) = M(g_1g_2)$ in a few cases, for example[2]

$$M(12)M(13) = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix} = M(132) \tag{8.5}$$

This representation is faithful: all 6 matrices are different. It is also unitary (it is orthogonal and real, hence unitary). And finally, it is irreducible: there is no simultaneous eigenvector of all six matrices $M(g)$. Hence we have found a two-dimensional irrep.

The other representation is even easier to write down, but we shall see that it is reducible, and decomposing it into a 1×1 "block" and a 2×2 block, the 2×2 block will be "similar" to the irrep we constructed above. "Similar" means that $M^{(1)}(g) = SM^{(2)}(g)S^{-1}$ for all g with S independent of g. This matrix representation is in terms of the following 3×3 matrices

$$M(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad M(123) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}; \quad M(132) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix};$$

$$M(12) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad M(13) = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}; \quad M(23) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{8.6}$$

For example, the matrix for (123) maps $e_1 = (1,0,0)$ to $e_2 = (0,1,0)$, $e_2 = (0,1,0)$ to $e_3 = (0,0,1)$ and $e_3 = (0,0,1)$ to $e_1 = (1,0,0)$. Again we may check

$$M(12)M(13) = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} = M(132). \tag{8.7}$$

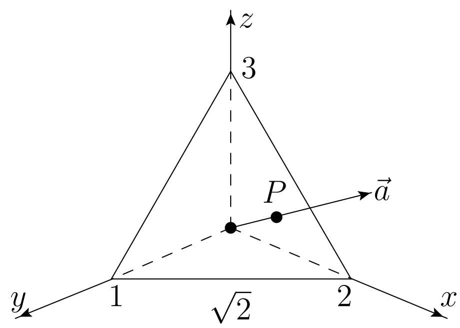
We have obtained a homomorphism from $G = S_3$ into the group $\widetilde{G}$ of six 3×3 real nonsingular matrices, and since the kernel is e, this is an isomorphism between S^3 and the six 3×3 matrices.

[2] We follow here the active point of view: vectors in the x-y plane are transformed, but the coordinate axes are kept fixed. Then we should read products of cycles from right to left, so $(12)(13) = (132)$. If one transforms instead the coordinates, then the inverses of these matrices (the transposed matrices in this case) form a representation of the group S_3 defined by reading products of cycles from left to right.

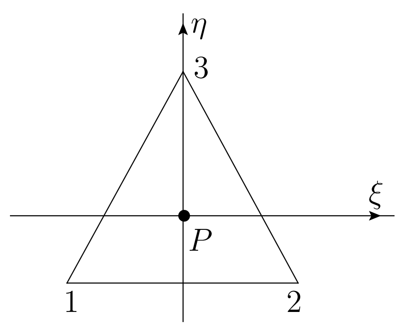
However, this representation has a one-dimensional invariant subspace: the vector $\left(\begin{smallmatrix}1\\1\\1\end{smallmatrix}\right)$ is kept fixed by all six 3-dimensional matrices. So this representation is faithful but reducible. Maschke's theorem says that we should be able to choose a different basis where all matrices get the following block form

$$SM(g)S^{-1} = \bar{M}(g) \text{ where } \bar{M}(g) = \left(\begin{array}{c|cc} 1 & 0 & 0 \\ \hline 0 & \multicolumn{2}{c}{\multirow{2}{*}{$M(g)_{2\times 2}$}} \\ 0 & & \end{array}\right) \tag{8.8}$$

We could construct the matrix S and then obtain explicit expressions for the matrices in the 2×2 block, but we can find the 2×2 matrices $M(g)_{2\times 2}$ more easily by elementary geometry. Consider a simplex whose base is a triangle with vertices on the x-axis, y-axis and z-axis a distance 1 from the origin.



The vector $\vec{a} = (1, 1, 1)$ intersects the simplex at a point P at right angles to the simplex. Looking down on the simplex along the line from $(1, 1, 1)$ to the origin $(0, 0, 0)$, we see the following triangle



We choose new axes ξ and η through the intersection point P. Then we have exactly the same situation as when we considered the triangle, hence

$$SM(g)_{3\times 3}S^{-1} = \begin{pmatrix} 1 & 0 \quad 0 \\ 0 & \multirow{2}{*}{$M(g)_{2\times 2}$} \\ 0 & \end{pmatrix} \tag{8.9}$$

where $M(g)_{2\times 2}$ is the same set of matrices as found in (8.4). So, we have so far found two irreps: a 2-dimensional irrep and the unit irrep ($M(g) = 1$ for all g). We now use the three theorems to see whether there are still irreps missing.

Theorem 1: For theorem 1 we need the commutator subgroup $C(G)$. It is given by $\big(e, (123), (132)\big)$. Hence $\frac{|G|}{|C(G)|} = \frac{6}{3} = 2$: there are 2 one-dimensional irreps. The quotient group $G/C(G)$ is isomorphic to Z_2 (it has only 2 elements), so it has two one-dimensional irreps:

$$\begin{array}{c|cc} & C(G) & (12)C(G) \\ \hline \bar{M}^I(g) & 1 & 1 \\ \bar{M}^{II}(g) & 1 & -1 \end{array} \tag{8.10}$$

Then the two one-dimensional irreps for the group $G = S_3$ itself are at once obtained by "lifting" (see below) the irrep of G/H to an irrep for G.

$$\begin{array}{c|cccccc} & e & (123) & (132) & (12) & (13) & (23) \\ \hline M^I(g) & 1 & 1 & 1 & 1 & 1 & 1 \\ M^{II}(g) & 1 & 1 & 1 & -1 & -1 & -1 \end{array} \tag{8.11}$$

Theorem 2: Since there are 3 classes of S_3:

$$\boxed{e} \quad \boxed{(123), (132)} \quad \boxed{(12), (13), (23)} \tag{8.12}$$

the number of irreps is 3. But we have already got 3 irreps: the 2 one-dimensional irreps and the 2-dimensional irrep! So there are no further irreps.

Theorem 3: Theorem 3 gives confirmation of the results already obtained: $|G| = 6 = \sum_{i=1}^{3} d_i^2 = 1^2 + 1^2 + 2^2$.

8.2 Characters

In this example, we found the higher-dimensional irrep from geometrical arguments. Often one lacks such arguments, and then the 3 theorems and the requirement $M(g_1)M(g_2) = M(g_1 g_2)$ are the only information available. We already saw that we needed a basis change (from x, y, z axes to new axes a, ξ, η), but finding such basis changes becomes complicated. Some properties of matrices are basis-independent: the trace, the determinant, and in fact all coefficients of λ^k of the characteristic equation $\det(M - \lambda I)$ for $k = 0, \cdots, n-1$. (The term without λ yields $\det M$, the term with $(-\lambda)^{n-1}$ yields $\operatorname{tr} M$, and the terms with λ^1, $\lambda^3, \cdots, \lambda^{n-2}$ give other basis-independent objects.) The simplest basis-independent object one can construct from $M(g)$ is its trace $\operatorname{tr} M(g) \equiv \chi(g)$. (The notation $\chi(g)$ is arbitrary but standard.) These traces are called **characters** (so the trace of $M(g)$ is the character $\chi(g)$): they characterize the essential part of the matrices $M(g)$ (not the part that depends on the choice of basis).

The characters of all group elements in a given class are the same (since the trace satisfies $\operatorname{tr} M(g)M(a)M(g^{-1}) = \operatorname{tr} M(a)$). Hence **characters are class functions**. So we may write $\chi(C_a)$ instead of $\chi(a)$, where C_a denotes the class to which a belongs. We can then construct a character table: an array where we plot the characters $\chi(C_a)$ of different irreps against the classes C_a. Theorem 2 states that this is a square array. Here is the character table for S_3:

S_3	e [1]	(123) [2]	(12) [3]
$\chi^{(1)}$	1	1	1
$\chi^{(1')}$	1	1	-1
$\chi^{(2)}$	2	-1	0

(8.13)

The numbers in square brackets [ ] are the orders of the classes, and we only wrote down one group element for each class (called a class representative). We obtained the first two rows from (8.11). To obtain the last row, we just took the traces of the 2×2 matrices in (8.4).

There is a wonderful check on character tables provided by the orthogonality relations of the matrix elements of (in)equivalent irreps. Tracing (7.23) over (μ, ν) and (α, β) yields

$$\sum_g \left(\chi^{(i)}(g)\right)^* \chi^{(j)}(g) = \sum_{a=1}^{n_C} \chi^{(i)}(C_a)^* \chi^{(j)}(C_a)|C_a| = |G|\delta_i^j \,. \tag{8.14}$$

Clearly, $\sqrt{\frac{|C_a|}{|G|}}\chi^{(i)}(C_a)$ are orthonormal vectors in a n_C-dimensional complex space. Let's check this equation for S_3. There are 9 cases ($i, j = 1, 1', 2$) but we only record 4 of them (omitting parentheses around i and j for notational simplicity)

$$\begin{aligned}
\chi^1(e)^*\chi^1(e) \times 1 + \chi^1(123)^*\chi^1(123) \times 2 + \chi^1(12)^*\chi^1(12) \times 3 &= 1 + 2 + 3 = 6 \\
\chi^1(e)^*\chi^{1'}(e) \times 1 + \chi^1(123)^*\chi^{1'}(123) \times 2 + \chi^1(12)^*\chi^{1'}(12) \times 3 &= 1 + 2 - 3 = 0 \\
\chi^{1'}(e)^*\chi^2(e) \times 1 + \chi^{1'}(123)^*\chi^2(123) \times 2 + \chi^{1'}(12)^*\chi^2(12) \times 3 &= 2 - 2 + 0 = 0 \\
\chi^2(e)^*\chi^2(e) \times 1 + \chi^2(123)^*\chi^2(123) \times 2 + \chi^2(12)^*\chi^2(12) \times 3 &= 4 + 2 + 0 = 6.
\end{aligned} \tag{8.15}$$

Summarizing: We have seen that characters of irreps satisfy orthogonality relations. This, together with the 3 theorems, often allows us in a rather simple way to obtain much information we need for physical applications. Further information is obtained from the theory of characters, to which we now turn.

Consider an arbitrary, in general reducible, representation R with matrices $M(g)$. According to Maschke's theorem, it can be brought to block form, with irreps in the blocks, hence upon taking its trace, we find

$$\chi(g) = \sum_i n_i \chi^{(i)}(g) \tag{8.16}$$

where the n_i are nonnegative integers. Using the orthogonality relations for the characters of irreps we shall now obtain two theorems which are very useful for applications.

The inner product of χ with χ^i yields

Theorem I. $(\chi^{(i)}, \chi) = \sum_g \chi^{(i)}(g)^* \chi(g) = n_i \, \text{order}\, G$.

This tells us how often an irrep $R^{(i)}$ is contained in R. The inner product of χ with itself yields

Theorem II. $(\chi, \chi) = \sum_{i,j} n_i n_j \sum_g \chi^{(i)}(g)^* \chi^{(j)}(g) = \text{order}\, G \sum_i n_i^2$.

If $(\chi, \chi) = \text{order}\, G$, then χ is irreducible, but if (χ, χ) is larger than order G, the rep $R(g)$ is reducible. One can then compute the number of times n_i that the irrep $R^{(i)}$ is contained in R from theorem I, and theorem II is then a check.

For any finite group there exists a particular reducible representation, **the regular representation**, which will play a central role in our analysis of irreps, because it contains all of them. It is constructed as follows. Let $\{g_1, \cdots, g_n\}$ be the group elements of a group G, and fix one element a (so a is one of the g_i). Multiplying the group elements by a **on the left**, we get the set $\{ag_1, \cdots ag_n\}$. If we write the group elements $(g_1, \cdots g_n)$ as a column vector, then there is a $|G|$-dimensional matrix $M^{reg}(a)$ which permutes the elements the same way as $g_i \to ag_i$ does. The map $a \to M^{reg}(a)$ yields the regular representation. It is faithful but (except for $G = \{e\}$) reducible. An explicit form for the matrices $M^{reg}(g_i)$ can be obtained as follows. Define

$$M^{reg}(a)^k{}_l = \begin{cases} 1 & \text{if } ag_l = g_k \\ 0 & \text{if } ag_l \neq g_k \end{cases} . \tag{8.17}$$

Then we can write the product ag_l as follows

$$ag_l = \sum_{k'=1}^{|G|} g_{k'} M^{reg}(a)^{k'}{}_l \quad \text{for } l = 1, \cdots, |G| \tag{8.18}$$

To show that the matrices $M^{reg}(g)$ form indeed a representation, consider the product $(ab)g_l = a(bg_l)$ and apply (8.18)

$$\begin{aligned}(ab)g_l &= \sum_{k'} g_{k'} M^{reg}(ab)^{k'}{}_l = a(bg_l) = a \sum_{l'} g_{l'} M^{reg}(b)^{l'}{}_l \\ &= \sum_{l'} (ag_{l'}) M^{reg}(b)^{l'}{}_l = \sum_{k'l'} g_{k'} M^{reg}(a)^{k'}{}_{l'} M^{reg}(b)^{l'}{}_l \end{aligned} \tag{8.19}$$

Equating the coefficients of $g_{k'}$ shows that $M^{reg}(a)M^{reg}(b) = M^{reg}(ab)$.

Given two irreps $R^{(i)}$ and $R^{(j)}$ with matrices $M^{(i)}(g)^\mu{}_\nu$ and $M^{(j)}(g)^\alpha{}_\beta$, one can form the **tensor product** $R^{(i)} \times R^{(j)}$, and the matrix representation corresponding to the tensor product is given by

$$M^{(ij)}(g)^{\mu\alpha}{}_{\nu\beta} = M^{(i)}(g)^\mu{}_\nu M^{(j)}(g)^\alpha{}_\beta \, . \tag{8.20}$$

The character of the tensor product representation is obtained by tracing the matrix of the tensor product, i.e., summing over $\mu\alpha = \nu\beta$. This amounts to summing over $\mu = \nu$ and $\alpha = \beta$

$$\begin{aligned} M^{(ij)}(g)^{\mu\alpha}{}_{\mu\alpha} &= M^{(i)}(g)^{\mu}{}_{\mu} M^{(j)}(g)^{\alpha}{}_{\alpha} \\ \chi^{(ij)}(g) &= \chi^{(i)}(g)\chi^{(j)}(g) \end{aligned} \tag{8.21}$$

The matrices $M^{(ij)}$ form a matrix representation of G, $M^{(ij)}(g_1)M^{(ij)}(g_2) = M^{(ij)}(g_1 g_2)$ as one easily can verify, hence **the product of characters is a character**. The (usually reducible) character $\chi^{(ij)}(g)$ can be expanded into the characters of the irreps

$$\chi^{(ij)}(g) = \sum_k n_k^{(ij)} \chi^{(k)}(g) \tag{8.22}$$

where $n_k^{(ij)}$ is given by

$$n_k^{(ij)} \,\mathrm{order}\, G = \sum_g \left(\chi^k(g)\right)^* \chi^{(ij)}(g) = \sum_g \left(\chi^k(g)\right)^* \chi^i(g)\chi^j(g)\,. \tag{8.23}$$

The $n_k^{(ij)}$ are nonnegative integers which depend of course on k but also on the irreps $R^{(i)}$ and $R^{(j)}$ which combined to yield $R^{(ij)}$.

One can now construct **the Clebsch-Gordan series** for the expansion of the product of two irreps $R^{(i)}$ and $R^{(j)}$ into irreps $R^{(k)}$. This generalizes the addition of angular momenta j_1 and j_2 in quantum mechanics, where the well-known formula $j_1 \times j_2 = j_1 + j_2, j_1 + j_2 - 1, \cdots, j_1 - j_2$ for $j_1 \geq j_2$ is shorthand for

$$M^{(j_1)}(g)^{\mu}{}_{\nu} M^{(j_2)}(g)^{\alpha}{}_{\beta} = S \begin{pmatrix} M^{j_1+j_2} & & & \\ & M^{j_1+j_2-1} & & \\ & & \ddots & \\ & & & M^{j_1-j_2} \end{pmatrix} S^{-1} \tag{8.24}$$

Taking traces yields

$$\chi^{j_1}\chi^{j_2} = \chi^{j_1+j_2} + \chi^{j_1+j_2-1} + \cdots + \chi^{j_1-j_2}\,. \tag{8.25}$$

Similarly, for an arbitrary finite group

$$\chi^i(g)\chi^j(g) = \sum_k n_k^{(ij)} \chi^k(g) \tag{8.26}$$

which can be written symbolically as

$$\boldsymbol{i} \times \boldsymbol{j} = \boldsymbol{k_1} + \boldsymbol{k_2} + \cdots + \boldsymbol{k_p} \tag{8.27}$$

where each $\boldsymbol{k_j}$ denotes an irrep $R^{(j)}$. Some of the $\boldsymbol{k_j}$ may be equal; in that case the corresponding matrix representation $R^{(j)}(g)$ occurs more than once. Often one writes instead of $\boldsymbol{k_j}$ the dimensions of the irreps. If two (or more) irreps have the same dimensions, one adds superscripts to the dimensions which distinguish the irreps. For example, one may find a formula such as $\mathbf{3} \times \mathbf{3} = \mathbf{1} + \mathbf{1'} + \mathbf{1''} + \mathbf{3} + \mathbf{3}$.

Given a normal subgroup N of a group G, a representation of the quotient group G/N can be **lifted** to a representation of G itself as follows

$$M^{(G)}(g) = M^{(G/N)}(gN) \tag{8.28}$$

To each element g of G, we assign the matrix $M^{(G/N)}(gN)$ of the coset to which it belongs. One can check that this yields a representation of G, namely

$$M^{(G)}(g_1)M^{(G)}(g_2) = M^{(G)}(g_1 g_2) \tag{8.29}$$

if $M^{(G/N)}$ is a representation of the quotient group

$$M^{(G/N)}(aN)M^{(G/N)}(bN) = M^{(G/N)}(abN)\,. \tag{8.30}$$

Taking the trace of (8.28) we find

$$\chi^{(G)}(g) = \chi^{(G/N)}(gN) \tag{8.31}$$

Given a character $\chi^{(G/N)}$ of a quotient group, we can construct a character of the group G as indicated. This is often a useful way to construct characters of G.

This lifting of an rep of the quotient group to a rep of the group itself is particularly useful when one considers the commutator subgroup. The quotient group $G/C(G)$ is abelian, and as we now show, for an abelian group all irreps are one-dimensional. These one-dimensional irreps are easy to construct, and **there are no other one-dimensional irreps of G** in addition to those of $G/C(G)$, so the problem of constructing all one-dimensional irreps of a group G is solved.

To prove that all irreps of an abelian group are one-dimensional, consider the equation for an irrep

$$M^{(i)}(g_1)M^{(i)}(g_2) = M^{(i)}(g_1 g_2)\,. \tag{8.32}$$

For an abelian group $g_1 g_2 = g_2 g_1$, hence we find

$$M^{(i)}(g_1)M^{(i)}(g_2) = M^{(i)}(g_2)M^{(i)}(g_1)\,. \tag{8.33}$$

For fixed g_1, the matrix $A = M^{(i)}(g_1)$ commutes with all matrices $M^{(i)}(g_2)$ of the irrep. Schur's lemma states then that $A = \lambda I$. Hence the matrix $M^{(i)}(g_1)$, and hence all matrices $M^{(i)}(g)$ for all g of an irrep, are proportional to the unit matrix. Then each entry on the diagonal is an irrep of G, so the irreps are one-dimensional.

8.3 $G = S_5$

As a less easy exercise, to become familiar with the methods used to determine characters, we construct the character table of the symmetric group S_5. For this case we have no recourse to geometrical methods, we have only the algebraic methods discussed before. There are 7 classes; we write them down together with their order

$$e\,[1],\ (ij)\,[10],\ (ijk)\,[20],\ (ij)(kl)\,[15],\ (ijkl)\,[30],\ (ij)(klm)\,[20],\ (ijklm)\,[24] \tag{8.34}$$

where $i, j, \cdots$ run from 1 to $n = 5$. As a check we add the order of the classes, and indeed obtain the order of S_5 which is $5! = 120$

$$1 + 10 + 20 + 15 + 30 + 20 + 24 = 120\,. \tag{8.35}$$

As another check, we note that the order of each class is a divisor of the order (120) of the group S_5.

The commutator subgroup[3] $C(G)$ is generated by the group elements $aba^{-1}b^{-1}$ which are most easily evaluated by noting that $ba^{-1}b^{-1}$ is obtained by replacing in a^{-1} the permutands $ij\cdots$ according to the prescription given by b^{-1}. (We evaluate products of cycles from left to right changing the permutations in a according to the prescription in b^{-1}.) So **all group elements $\boldsymbol{ba^{-1}b^{-1}}$ have the same cycle structure as the group element $\boldsymbol{a^{-1}}$**, and by choosing for a and b a particular element in each of the 7 classes (a so-called class representative), we find the elements of $C(G)$. In particular for $a = (ij)$ the set $aba^{-1}b^{-1}$ for $b = (ik)$ contains[4] (ikj), while for $a = (ijklm)$ and $b = (ij)$ the set $aba^{-1}b^{-1}$ contains $(ijklm)(ijmlk) = (imj)$. Furthermore, $(523)(124) = (54123)$. Recalling that $C(G)$ is a normal subgroup, and that normal subgroups consist of entire classes, we conclude that $C(G)$ is the set of all even permutations

$$C(G) = A_5\,. \tag{8.36}$$

Then the number of one-dimensional irreps is $|S_5|/|A_5| = 2$ and it is easy to write them down, using that A_5 is a normal subgroup and $G/A_5 \simeq Z_2$.

(8.37)

S_5	$e\,[1]$	$(ij)\,[10]$	$(ijk)\,[20]$	$(ij)(kl)\,[15]$	$(ijkl)\,[30]$	$(ij)(klm)\,[20]$	$(ijklm)\,[24]$
χ_1	1	1	1	1	1	1	1
χ_1'	1	-1	1	1	-1	-1	1

[3]A simple argument that proves that $C(S_5) = A_5$ uses advanced knowledge, namely that all A_n for $n \neq 4$ are simple. We proved this in chapter 7. Any normal subgroup of G with only even elements is also a normal subgroup of A_5, but A_5 has no normal subgroups. Thus the commutator subgroup of S_5 (which is a normal subgroup of S_5) can only be A_5 or S_5. But $C(A_5)$ contains only even permutations, hence $C(S_5) = A_5$. In the text we use direct pedestrian methods to obtain this result.

[4]First evaluate $ba^{-1}b^{-1}$. For $a^{-1} = (ij)$ and $b^{-1} = (ki)$ we get for example, $ba^{-1}b^{-1} = (kj)$ and then $a(ba^{-1}b^{-1})$ yields $(ij)(kj) = (ikj)$ so (ikj) lies in $C(G)$.

There is always the trivial (unit) character χ_1, and the character χ_1' corresponds to $\chi_1' = +1$ on A_5 and $\chi_1' = -1$ on the classes with uneven permutations.

The permutations of 5 objects yield a reducible representation in terms of 5×5 matrices with $+1$ or 0 as entries. The 5-dimensional vector $v = (1, 1, \cdots, 1)$ is invariant under these matrices, and yields the unit character, hence there is a 4×4 matrix representation of S_5 whose trace gives a character χ_4. It is given by $\chi_4 = \chi_5 - \chi_1$. Then the product $\chi_4 \chi_1'$ (which differs from χ_4) is another 4-dimensional character. (Recall that the product of characters is a character.) We shall check that they are irreducible, but first we write them down.

S_5	$e\,[1]$	$(ij)\,[10]$	$(ijk)\,[20]$	$(ij)(kl)\,[15]$	$(ijkl)\,[30]$	$(ij)(klm)\,[20]$	$(ijklm)\,[24]$
χ_5	5	3	2	1	1	0	0
χ_4	4	2	1	0	0	-1	-1
χ_4'	4	-2	1	0	0	1	-1

(8.38)

Since $\sum_{a=1}^{n_C} \chi_4^2(C_a)|C_a| = 4^2 \times 1 + 2^2 \times 10 + 1^2 \times 20 + (-1)^2 \times 20 + (-1)^2 \times 24 = 120 = |S_5|$, the representations yielding χ_4 and χ_4' are irreducible. They are orthogonal to χ_1 and χ_1' (since $4 \pm 2 \times 10 + 1 \times 20 \mp 1 \times 20 - 1 \times 24 = 0$).

We have obtained 4 characters $(\chi_1, \chi_1', \chi_4, \chi_4')$ so we need 3 more characters. We get these by using **tensor methods**. We discussed them in more generality before, but here we only need a particular case. Taking the direct product of two **4** representations, we get a reducible representation **16** spanned by tensors $v^I w^J$, with $(I, J = 1, \cdots, 4)$, which we decompose into a symmetric representation S of dimension **10** and an antisymmetric representation A of dimension **6**. A basis is given by $s^{IJ} = v^I w^J + v^J w^I$ and $a^{IJ} = v^I w^J - v^J w^I$, and they transform as follows

$$
\begin{aligned}
s'^{IJ} &= \tfrac{1}{2}\left(M^I{}_K M^J{}_L + M^J{}_K M^I{}_L\right) s^{KL} \equiv M^{IJ}_{sym\,KL} s^{KL} \\
a'^{IJ} &= \tfrac{1}{2}\left(M^I{}_K M^J{}_L - M^J{}_K M^I{}_L\right) a^{KL} \equiv M^{IJ}_{anti\,KL} a^{KL} .
\end{aligned}
\tag{8.39}
$$

The trace of the matrices $M^I{}_J$ yields the character χ_4. The trace of M_{sym} and M_{anti} is obtained by summing over $IJ = KL$, hence $I = K$ and $J = L$, and using $M(g)M(g) = M(g^2)$, we find that the characters of the S and A representations are given by

$$
\begin{aligned}
\chi_S(g) &= \tfrac{1}{2}\left(\chi_4^2(g) + \chi_4(g^2)\right) \\
\chi_A(g) &= \tfrac{1}{2}\left(\chi_4^2(g) - \chi_4(g^2)\right) .
\end{aligned}
\tag{8.40}
$$

We shall see that χ_A is irreducible, but χ_S is reducible. To evaluate $\chi_4(g^2)$, note that $(ij)^2 = (ij)(ij) = 1$, $(ijk)^2 = (ijk)(ijk) = (ikj)$, $\big((ij)(kl)\big)^2 = (1)$, $(ijkl)^2 = (ik)(jl)$, $\big((ij)(klm)\big)^2 = (kml)$, $(ijklm)^2 = (ikmjl)$. These relations are of the form $g^2 = g'$ where g' lies in some cases in another class than g, and they allow us to express $\chi_4(g^2) = \chi_4(g')$ in terms of $\chi_4(g)$. The results for the characters $\chi_4(g)$, $\chi_4^2(g)$, $\chi_4(g^2)$, χ_A and χ_S are as follows

S_5	$e\,[1]$	$(ij)\,[10]$	$(ijk)\,[20]$	$(ij)(kl)\,[15]$	$(ijkl)\,[30]$	$(ij)(klm)\,[20]$	$(ijklm)\,[24]$
χ_4	4	2	1	0	0	-1	-1
χ_4^2	16	4	1	0	0	1	1
$\chi_4(g^2)$	4	4	1	4	0	1	-1
χ_A	6	0	0	-2	0	0	1
χ_S	10	4	1	2	0	1	0

(8.41)

Of course, $\chi_A(e) = 6$ because it is the character of a 6-dimensional representation, but now we show that χ_A is irreducible

$$\sum_{a=1}^{n_C} \chi_A^2(C_a)|C_a| = 6^2 \times 1 + (-2)^2 \times 15 + 1^2 \times 24 = 120 = |S_5|. \tag{8.42}$$

As checks one may verify that χ_A is orthogonal to $\chi_1, \chi_1', \chi_4, \chi_4'$. Note that $\chi_A\chi_1'$ is the same character as χ_A, so there is no inequivalent χ_A' character.

At this point we have obtained 5 of the 7 characters. The remaining two characters can be obtained from χ_S. Recall that for any character χ one has $\chi = \sum m_j \chi^j$ (where j labels the 7 irreducible characters), and $(\chi, \chi) = (\sum m_j^2) \times |S_5|$. Applied to χ_S we find

$$(\chi_S, \chi_S) = 10^2 \times 1 + 4^2 \times 10 + 1^2 \times 20 + 2^2 \times 15 + 1^2 \times 20 = 360. \tag{8.43}$$

Hence $\sum m_j^2 = 3$, which implies that χ_S contains 3 of the 7 irreducible characters, each only once. It is easy to check that χ_S contains χ_1 and χ_4 once $\big((\chi_S, \chi_1) = 120$ and $(\chi_S, \chi_4) = 120\big)$, but χ_1', χ_4' and χ_A are not present in χ_S $\big((\chi_S, \chi_1') = 0, (\chi_S, \chi_4') = 0$ and $(\chi_S, \chi_A) = 0\big)$. So we have found another character: it is $\chi_5 = \chi_S - \chi_1 - \chi_4$. Then the last of the 7 characters is given by $\chi_5\chi_1'$. The complete character table is as follows (denoting χ_A by χ_6 for uniformity of notation)

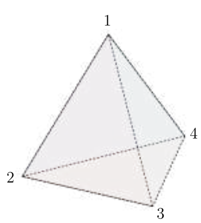
S_5	$e\,[1]$	$(ij)\,[10]$	$(ijk)\,[20]$	$(ij)(kl)\,[15]$	$(ijkl)\,[30]$	$(ij)(klm)\,[20]$	$(ijklm)\,[24]$
χ_1	1	1	1	1	1	1	1
χ_1'	1	-1	1	1	-1	-1	1
χ_4	4	2	1	0	0	-1	-1
χ_4'	4	-2	1	0	0	1	-1
χ_5	5	1	-1	1	-1	1	0
χ_5'	5	-1	-1	1	1	-1	0
χ_6	6	0	0	-2	0	0	1

(8.44)

Comment. In this example we never needed to construct the explicit form of the matrices $M(g)$ for any of the irreps, and fortunately, all we need for physical applications are their traces (the characters). This is a huge simplification, but it raises the question whether one looses information if one only uses the traces of the matrices $M(g)$. Specifically: could it be that more than one group produces the same traces (the same character table)? In physical applications we usually know the symmetry group G, and then this problem does not arise. But in the inverse case, where one only knows the characters, in a few cases there are indeed more than one group with the same characters. An example is the quaternion group $\mathbb{Q} = Q_4$ and the dihedral group D_4 which have the same character table.

8.4 $G = A_4$

For the group S_n, group elements with a given cycle structure sometimes form one class, but for the group A_n it sometimes happens that a class of S_n with even permutations splits into two classes. We show this for the case of A_4. The group of rotation of a tetrahedron is the order 12 group A_4. Since A_4 is not in the list of simple finite groups, it has a nontrivial normal subgroup: the order 4 subgroup containing the 3 rotations about the axes through the middle of pairs of opposing edges. This is the commutator subgroup. Hence there are 3 one-dimensional irreps, and hence there is one 3-dimensional irrep ($12 = 1^2 + 1^2 + 1^2 + 3^2$). It follows that there should be 3 classes. One class contains the unit element, another class the 3 rotations mentioned above. Thus the remaining 8 rotations about axes through a vertex and the middle of the opposing face should form **two** separate classes. To work this out, we write the 12 group elements in cycle notation where $1, 2, 3, 4$ refer to the 4 vertices of the tetrahedron.



$$\begin{array}{cc} (234) & (243) \\ (341) & (314) \\ (412) & (421) \\ (123) & (132) \end{array} \qquad \boxed{\begin{array}{c} (13)(24) \\ (14)(23) \\ (12)(34) \end{array}} \qquad \boxed{e} \tag{8.45}$$

All group elements are represented by even cycles, so group elements differing by one permutation **must** lie in different classes. By using that SgS^{-1} just means changing the permutations in g according to the prescription S, we can take one of the 8 3-cycles, and evaluate SgS^{-1} with S the 3 twins. That yields the following two classes

$$\boxed{\begin{array}{cc} (123), & (341) \\ (214), & (432) \end{array}} \quad \text{and} \quad \boxed{\begin{array}{cc} (132), & (431) \\ (124), & (342) \end{array}} \tag{8.46}$$

Since $G/C(G) = Z_3$, the 3 one-dimensional irreps are obvious. The 3-dimensional irrep consists of the 3-dimensional rotations of the tetrahedron. The character table becomes then

$$\begin{array}{c|cccc} A_4 & e\,[1] & (123)\,[4] & (132)\,[4] & (ij)(kl)\,[3] \\ \hline \chi_1 & 1 & 1 & 1 & 1 \\ \chi_1' & 1 & e^{\frac{2\pi i}{3}} & e^{-\frac{2\pi i}{3}} & 1 \\ \chi_1'' & 1 & e^{-\frac{2\pi i}{3}} & e^{\frac{2\pi i}{3}} & 1 \\ \chi_3 & 3 & 0 & 0 & -1 \end{array} \tag{8.47}$$

Exercise 1. Show that the character tables for $\mathbb{Q}$ and D_4 are equal.

Exercise 2. Consider the character table for S_5 in (8.44). The sum of the squares of the entries in a given row, each square multiplied by the order of the corresponding class, equals 120. Similarly, the sum of the squares of the entries of a given column, multiplied by the order of the corresponding class, equals 120. Explain this observation. This yields an excellent check on any character table.

8.5 Proofs of the three theorems

We now prove the three theorems in (8.1), (8.2) and (8.3). It turns out that to prove theorem 2 we need theorem 3, so we shall consider first the proof of theorem 1, then of theorem 3, and finally of theorem 2.

Proof of Theorem 1: $\boldsymbol{n_{1-dim} = \frac{|G|}{|C(G)|}}$. We recall that the commutator subgroup $C(G)$ is an invariant subgroup of G, and $G/C(G)$ is abelian. **Every irrep of an abelian group is one-dimensional**, because from $M(g_1)M(g_2) = M(g_1g_2) = M(g_2g_1) = M(g_2)M(g_1)$ it follows that for fixed g_1 the matrix $M(g_1)$ commutes with all matrices $M(g_2)$. Then Schur's lemma tells us that $M(g_1)$ is proportional to the unit matrix, and thus all irreps of an abelian group are one-dimensional.

Since for an abelian group the number of classes is equal to the number of group elements, it follows that an abelian group has as many one-dimensional irreps as it has group elements. Thus $G/C(G)$ has precisely $\frac{|G|}{|C(G)|}$ one-dimensional irreps.

Every irrep of a quotient group G/N can be extended ("lifted") to an irrep of G by stipulating that $M(g)$ for all group elements in a given class is the same as $M(\bar{g})$ for a group element $\bar{g}$ in the coset group. Then all group elements of $C(G)$ have $M(e) = I$, all group elements $g' = gag^{-1}$ for all g in the class C_a have $M(g') = M(C_a)$ etc.

Thus there are at least as many one-dimensional irreps of G as $\frac{|G|}{|C(G)|}$. To show that there are no more, assume the contrary: assume there exists a one-dimensional irrep of G which is not one of the $\frac{|G|}{|C(G)|}$ irreps. The kernel of this irrep forms a normal subgroup N of G, and the quotient group G/N contains the group elements $N, aN, bN, \cdots$. Let ϕ be the homomorphism from G/N onto the one-dimensional irrep G'. Since G/N is isomorphic to G', and G' is abelian, the quotient group is abelian. The normal subgroup contains $C(G)$ and any (one-dimensional) irrep of $G/C(G)$ can be extended to G. Thus the set of one-dimensional irreps of G/N is contained in the set of one-dimensional irreps of $G/C(G)$, and thus there are no more one-dimensional irreps of G than $\frac{|G|}{|C(G)|}$. This proves Theorem 1.

Proof of Theorem 3: $|G| = \sum_i (d_i)^2$. In the regular representation $M^{reg}(e)$ is of course the unit matrix, but $M^{reg}(a)$ for $a \neq e$ contains only zeros along the diagonal

$$M^{reg}(e) = \begin{pmatrix} 1 & & & & \varnothing \\ & 1 & & & \\ & & 1 & & \\ & & & \ddots & \\ & \varnothing & & & 1 \end{pmatrix}; \qquad M^{reg}(a) = \begin{pmatrix} 0 & & & & \\ & 0 & & * & \\ & & 0 & & \\ & * & & \ddots & \\ & & & & 0 \end{pmatrix} \tag{8.48}$$

because $g_i e = g_j$ with $g_j = g_i$ and $g_i a = g_j$ with $g_j \neq g_i$ if $a \neq e$. The regular representation satisfies the definition of a representation

$$M^{reg}(g_1)M^{reg}(g_2) = M^{reg}(g_1 g_2) \tag{8.49}$$

We know from Maschke's theorem that M^{reg} can be brought to block form by a similarity transformation, such that each block forms an irreducible representation. Since the trace is basis independent, it follows that

$$\chi^{reg}(g) = \sum_i n_i \chi^i(g) \tag{8.50}$$

where the sum runs over all irreps (all blocks) in R^{reg}. Now use the orthogonality relations to obtain

$$\frac{1}{|G|} \sum_g \left(\chi^{(i)}(g)\right)^* \chi^{reg}(g) = n_i \tag{8.51}$$

However, $\chi^{reg}(g)$ is only nonzero if $g = e$, and then $\chi^{reg}(e) = |G|$. Hence

$$\frac{1}{|G|} \chi^{reg}(e) \chi^{(i)}(e)^* = \left(\chi^i(e)\right)^* \tag{8.52}$$

But in any irrep $M^{(i)}(g)$ the matrix $M^{(i)}(e)$ is the unit matrix, hence $\chi^{(i)}(e) = \dim R^i = d_i$. So we finally get

$$n_i = d_i\,. \tag{8.53}$$

We conclude: the regular representation contains the irrep $R^{(i)}$ as many as d_i times. So in block form we find

$$SM^{reg}S^{-1} = \begin{pmatrix} \ddots & & & & \\ & \underbrace{R^{(i)} & \ddots & R^{(i)}}_{d_i \text{ times}} & \\ & & & & \ddots \end{pmatrix}, \quad d_i = \dim R_i \tag{8.54}$$

Hence $\operatorname{tr} M^{reg}(e) = |G| = \sum_i (d_i) d_i$. This proves the relation

$$|G| = \textstyle\sum_i (d_i)^2 \,. \tag{8.55}$$

Proof of Theorem 2: $\boldsymbol{n_{irreps} = n_C}$. We have shown that the characters of the irreps of a finite group are orthonormal vectors $v^{(i)}(C_a) = \chi^{(i)}(C_a)\sqrt{\frac{|C_a|}{|G|}}$. The index i labels the vectors, and the index a labels the components of the vectors. Because there cannot be more orthonormal vectors in an n-dimensional space than n, the number of characters is at most equal to the number of cosets: $n_{irreps} \leq n_C$. Our aim is to show that $n_{irreps} = n_C$.

We shall need some properties of class multiplication. As shown in chapter 5

$$C_i C_j = \sum_k c_{ij}{}^k C_k \tag{8.56}$$

The nonnegative numbers $c_{ij}{}^k$ satisfy the following 4 properties

1) $c_{ij}{}^k = c_{ji}{}^k$ because if g_i lies in C_i and g_j lies in C_j then $g_i g_j$ lies in $C_i C_j$ but $g_i g_j = (g_i g_j g_i^{-1}) g_i$ lies in $C_j C_i$. Thus every group element in $C_i C_j$ lies also in $C_j C_i$ and vice-versa, which proves that $C_i C_j = C_j C_i$.

2) $c_{1j}{}^k = \delta_j{}^k$ where $C_1 = e$. This follows from $eC_j = c_{1j}{}^k C_k = C_j$.

3) $c_{jk}{}^1 = |C_j| \delta_{jk^{-1}}$. For a given class C_j we denote by $C_{j^{-1}}$ the class which contains the inverses of the group elements in C_j. Then $C_j C_{j^{-1}} = |C_j| e +$ other classes because for each element in C_j the inverse of this element appears in $C_{j^{-1}}$. The set of $C_j C_{l^{-1}}$ with $l \neq j$ does not contain any unit element, hence $C_{jl^{-1}}{}^m = 0$ for any m if $l \neq j$. Together these results yield $c_{jl^{-1}}{}^1 = |C_j| \delta_{jl}$. Setting l^{-1} equal to k yields the result above.

4) $\gamma_i^{(p)} \gamma_j^{(p)} = \sum_k c_{ij}{}^k \gamma_k^{(p)}$ where $\gamma_i^{(p)}$ will be defined. Consider the sum of all matrices $M^{(p)}(g)$ of an irrep p for all group elements g in a class C_i

$$\sum_{g \in C_i} M^{(p)}(g) \equiv K_i^{(p)} \tag{8.57}$$

Using the class multiplication rule in (8.56) and replacing each group element g by $M^{(p)}(g)$

yields

$$\Big(\sum_{g\in C_i} M^{(p)}(g)\Big)\Big(\sum_{g'\in C_j} M^{(p)}(g')\Big) = \sum_k c_{ij}{}^k \sum_{g''\in C^k} M^{(p)}(g'')$$

$$K_i^{(p)}K_j^{(p)} = \sum_k c_{ij}{}^k K_k^{(p)} \tag{8.58}$$

We claim that all matrices $K_i^{(p)}$ are proportional to the unit matrix: $K_i^{(p)} = \gamma_i^{(p)} I^{(p)}$. This follows from

$$M^{(p)}(g_0)\sum_{g\in C_i} M^{(p)}(g)M^{(p)}(g_0^{-1}) = \sum_{g\in C_i} M^{(p)}(g) \tag{8.59}$$

where we used that for any class C_i one has $g_0 C_i g_0^{-1} = C_i$. So $K_i^{(p)}$ commutes with all $M^{(p)}(g_0)$, and then Schur's lemma says that $K_i^{(p)}$ is proportional to the unit matrix

$$K_i^{(p)} = \gamma_i^{(p)} I^{(p)} \tag{8.60}$$

Then (8.58) yields

$$\gamma_i^{(p)}\gamma_j^{(p)} = \sum_k c_{ij}{}^k \gamma_k^{(p)}\,. \tag{8.61}$$

Having obtained these four properties of $c_{ij}{}^k$, we now complete the proof that n_{irreps} equals n_C. First we take the trace of the matrices $K_i^{(p)}$ yielding $\operatorname{tr} K_i^{(p)} = \gamma_i^{(p)} \dim R^{(p)}$, but from its definition as a sum over matrices $M^{(p)}(g)$ with g in C_i we also have $\operatorname{tr} K_i^{(p)} = |C_i|\chi^{(p)}(C_i)$. Hence

$$\gamma_i^{(p)} = \frac{|C_i|\chi^{(p)}(C_i)}{\dim R^{(p)}} \tag{8.62}$$

Then (8.61) yields

$$|C_i|\chi^{(p)}(C_i)|C_j|\chi^{(p)}(C_j) = \dim R^{(p)} \sum_k c_{ij}{}^k |C_k|\chi^{(p)}(C_k) \tag{8.63}$$

Our analysis of the regular representation gave us a relation involving $\dim R^{(p)}\chi^{(p)}(g)$

$$\chi^{reg}(g) = \sum_p \dim R^{(p)}\chi^{(p)}(g) = \begin{cases} |G| & \text{if } g = e \\ 0 & \text{if } g \neq e\,. \end{cases} \tag{8.64}$$

Summing (8.63) over p, and substituting this relation, we obtain

$$\sum_p |C_i|\chi^{(p)}(C_i)|C_j|\chi^{(p)}(C_j) = |G|c_{ij}{}^1|C_1| = |G||C_i|\delta_{ij^{-1}}\,. \tag{8.65}$$

where we used $c_{ij}{}^1 = |C_i|\delta_{ij^{-1}}$ and $|C_1| = 1$ since the class C_1 contains only one element (e).

We may assume that the matrices $M^{(p)}(g)$ are unitary. In that case

$$\chi^{(p)}(C_j) = \left(\chi^{(p)}(C_{j^{-1}})\right)^* \tag{8.66}$$

because the class $C_{j^{-1}}$ contains the inverses of the group elements of C_j. Note that $|C_{j^{-1}}|$ is equal to $|C_j|$. Setting $j^{-1} = k$ leads then to

$$\sum_p |C_i|\chi^{(p)}(C_i)|C_k|\left(\chi^{(p)}(C_k)\right)^* = |G||C_i|\delta_{ik} = |G||C_k|\delta_{ik}\,. \tag{8.67}$$

Dividing by $|C_k|$, setting $i = j$, and summing over classes yields

$$\sum_{i=1}^{n_C} \sum_{p=1}^{n_{irreps}} |C_i|\chi^{(p)}(C_i)\left(\chi^{(p)}(C_k)\right)^* = |G|n_C\,. \tag{8.68}$$

The orthogonality relation for characters yields

$$\sum_{p=1}^{n_{irreps}} \sum_{i=1}^{n_C} |C_i|\left(\chi^{(p)}(C_i)\right)^*\chi^{(p)}(C_i) = |G| \sum_{p=1}^{n_{irreps}} \delta^{pp} = |G|n_{irreps}\,. \tag{8.69}$$

Comparing both equations proves the assertion

$$n_C = n_{irreps}\,. \tag{8.70}$$

Chapter 9

Real, pseudoreal and complex representations

If a set of matrices $M(g)$ forms a matrix representation of a group G, $M(g_1)M(g_2) = M(g_1g_2)$, then also the set of matrices $M(g)^*$ forms a matrix representation. Should one include $M(g)^*$ in the list of irreps if $M(g)$ is an irrep? Only if $M(g)^*$ is inequivalent, not if $M(g)^* = SM(g)S^{-1}$. This leads to the following classification of irreps:

1) If $M(g)^* = SM(g)S^{-1}$ **and** if there exist another matrix R such that all matrix elements $RM(g)R^{-1}$ are real for all g, then the irrep is called a **real** irrep.

2) If $M(g)^* = SM(g)S^{-1}$ but there is **no matrix *R*** such that $RM(g)R^{-1}$ is real for all g, then the irrep is called a **pseudoreal** irrep.

3) If $M(g)$ is not equivalent to $M(g)^*$, it is called a **complex** irrep.

We consider irreps because for a reducible rep in block form, different blocks could have different reality properties. So for a real irrep one can find a basis (make a similarity transformation) such that in this basis all matrix elements of all matrices $M(g)$ are real numbers. For a pseudoreal representation the matrices $M(g)$ and $M(g)^*$ give in physical applications the same results ($M(g)^*$ is just $M(g)$ in a different basis, $M(g)^* = SM(g)S^{-1}$). But for a complex representation the physics of $M(g)$ is physically different from $M(g)^*$.

We consider here only finite groups, but the notions of real, pseudoreal and complex matrix representations hold also for Lie groups. The most famous example is the two-dimensional (vector, defining) matrix representation of $SU(2)$ which is pseudoreal[1]. We shall later analyze the reality properties of matrix representations of Lie algebras in great detail. Reality plays an important role for Majorana spinors; as we discuss in the next chapter. Majorana spinors in Minkowski or Euclidean space only exists if the representation of the Dirac matrices is real, but not if it is pseudoreal or complex. (If it is pseudoreal, one can define so-called symplectic Majorana spinors.)

[1] The generators $T_j = -\frac{i}{2}\sigma_j$ with σ_j the three Pauli matrices satisfy the relation $T_j^* = ST_jS^{-1}$ with $S = \sigma_2 = S^{-1}$.

Another area in particle physics where the reality or complexity of a representation plays a crucial role are the chiral anomalies in 3 (or higher) dimensions. In quantum field theory, if particles form a multiplet that transforms according to a representation R^i, then their complex conjugates (the antiparticles) transform in the complex conjugate representation. Only if the representation R^i is complex (if its complex conjugate $(R^i)^*$ is not related by a similarity transformation to R^i) do chiral anomalies in 3-dimensions exist.

If a representation $M(g)$ of a finite group G is real or pseudoreal, its characters are real.

$$\chi(g) = \operatorname{tr} M(g) = \operatorname{tr} SM(g)S^{-1} = \operatorname{tr} M(g)^* = \chi(g)^* \,. \tag{9.1}$$

The converse holds as well.

Theorem: If $\chi(g) = \chi(g)^*$ then $M(g)$ is equivalent to $M(g)^*$. So $\chi(g)$ is complex iff $M(g)$ is complex.

Proof: We prove a more general statement: if two representations $M_I(g)$ and $M_{II}(g)$ (of the same group[2]) have the same set of characters, $\chi_I(g) = \chi_{II}(g)$, then M_I and M_{II} are equivalent: $M_I = SM_{II}S^{-1}$. (This covers the case that $\chi(g) = \chi(g)^*$ because in this case $M_I(g) = M(g)$ and $M_{II}(g) = M(g)^*$.) To prove this claim, we use the orthogonality relations for characters. Assume that the irreps M_I and M_{II} are inequivalent, then we run into a contradiction. On the one hand, because M_I and M_{II} are inequivalent irreps, the orthogonality relations of character table tell us that

$$\sum_g \chi_I(g)^* \chi_{II}(g) = 0 \,. \tag{9.2}$$

On the other hand, for an irrep one always has

$$\sum_g \chi_I(g)^* \chi_I(g) = |G| \,. \tag{9.3}$$

If $\chi_I(g) = \chi_{II}(g)$ these two equations contradict each other. Hence the irreps are equivalent, $M_I = SM_{II}S^{-1}$. In particular for $M_I = M$ and $M_{II} = M^*$ we find $M^*(g) = SM(g)S^{-1}$.

9.1 Frobenius-Schur criterion

Criterion (Frobenius-Schur): A **unitary** irrep is

$$\left.\begin{array}{r} \text{real} \\ \text{pseudoreal} \\ \text{complex} \end{array}\right\} \text{ if } \sum_g \chi(g^2) = \left\{\begin{array}{r} |G| \\ -|G| \\ 0 \end{array}\right.$$

[2] The characters of D_4 and Q_4 are equal, but the corresponding representations are not equivalent. This does not contradict the theorem because in this case we are dealing with different groups.

Note the g^2 in $\chi(g^2)$. We shall prove this theorem later, but first we give some examples.

Examples:

1) A_5. Referring to (6.11)–(6.14), and using that the 60 rotations of an icosahedron form the group A_5 and permute the 6-diagonals, one finds a reducible 6-dimensional representation of A_5. Extracting the unit dimensional representation, one ends up with $\chi_{\text{5-dim}} = (5, 1, -1, 0, 0)$, corresponding to the 5 classes $\{e\,[1]$, twins $(12)\,[15]$, 3-cycles $(123)\,[20]$, and two classes of 5-cycles $(12345)\,[12]$ and $(12354)\,[12]\}$.[3] See table 12.4. We use $e^2 = e$, $(\text{twin})^2 = e$, $(123)^2 = (132)$ and $(12345)^2 = (13524)$. Then

$$\sum_g \chi(g^2) = 1 \times 5 + 15 \times 5 + 20 \times (-1) + 0 + 0 = 60 : \ \textbf{real} \tag{9.4}$$

Indeed, the 5×5 matrices $M(g)$ permuting the 5 cross-triplets of an icosahedron are all real.

2) $Z_3 = (e, a, a^2)$. This is an abelian group hence all its irreps are one-dimensional. The 3 irreps are composed of phases as follows

Z_3	e	a	a^2
χ_1	1	1	1
χ_1'	1	ω	ω^2
χ_1''	1	ω^2	ω

$\omega = e^{\frac{2\pi i}{3}}$

It is easy to check that the orthogonality relations are satisfied. Let us apply the Frobenius-Schur criterion to the irrep with χ_1'. We obtain

$$\sum_g \chi_1'(g^2) = 1 + e^{\frac{4\pi i}{2}} + e^{\frac{2\pi i}{3}} = 0 : \ \textbf{complex} \tag{9.5}$$

The 1×1 matrices $1, \omega, \omega^2$ are indeed complex, and similarity transformations of 1×1 matrices have no effect.

3) Q_4 (quaternion group) with the 5 classes $(E, -E, \pm I, \pm J, \pm K)$. For the 2×2 irrep (with I, J, K represented by the Pauli matrices $-i\sigma_j$) we get

$$\sum_g \chi_{\mathbf{2}}(g^2) = 2 \times 1 + 2 \times 1 + 2 \times (-2) + 2 \times (-2) + 2 \times (-2) = -8 : \ \textbf{pseudoreal} \tag{9.6}$$

Then there should be a matrix C such that $CM(g)C^{-1} = M(g)^*$. (We write C instead of S because for $SU(2)$ the matrix S is the charge conjugation matrix, which is usually denoted

[3] The set of 5-cycles does not form one class but two classes. This can be verified by explicit evaluation of $g(12345)g^{-1}$, but it is already clear from the fact that the order of a class should be a divisor of the order of the group (24 is not a divisor of 60, but 12 is a divisor). The group elements (12354) and (13524) are obtained from (12345) by an odd number of permutations of the form $(ab)(12345)(ab)$, hence they form a separate class.

by C.) This gives 8 relations for the matrix C

$$\begin{aligned} CEC^{-1} &= E \qquad C(-i\sigma_j)C^{-1} = (-i\sigma_j)^* \\ C(-E)C^{-1} &= -E \qquad C(i\sigma_j)C^{-1} = (i\sigma_j)^* \end{aligned} \tag{9.7}$$

where E is the unit matrix. There is indeed a solution: C is proportional to $\sigma_2 = \sigma_2^{-1}$.

$$\begin{aligned} \sigma_2(i\sigma_1)\sigma_2 &= -i\sigma_1 = (i\sigma_1)^* \\ \sigma_2(i\sigma_2)\sigma_2 &= i\sigma_2 = (i\sigma_2)^* \\ \sigma_2(i\sigma_3)\sigma_2 &= -i\sigma_3 = (i\sigma_3)^* \,. \end{aligned} \tag{9.8}$$

The proportionality constant cancels in these relations, and we set

$$C = i\sigma_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{9.9}$$

The matrix C is antisymmetric. This is a general feature for pseudoreal irreps as we shall now discuss.

We shall first prove that the matrix S in $M(g)^* = SM(g)S^{-1}$ is an invariant matrix, and is either symmetric or antisymmetric. Then we shall prove that S is symmetric for real irreps and antisymmetric for pseudoreal irreps. Finally we shall prove the Frobenius-Schur algorithm.

Theorem: If **for a unitary rep** $M(g)$ one has $M(g)^* = SM(g)S^{-1}$, then the matrix S is either antisymmetric or symmetric, and it is an invariant tensor. (This relation does not hold if the representation is not unitary. Any representation can be made unitary by a similarity transformation, but that similarity transformation is in general not unitary, see (7.16).)

Proof: Unitarity states that $M^*(g) = (M^T)^{-1}$. Then if $M^* = SMS^{-1}$ we get $SMS^{-1} = (M^T)^{-1}$, or $M^T SM = S$. Taking the transpose and then the inverse, yields

$$(S^T)^{-1} = M^{-1}(S^T)^{-1}(M^T)^{-1} = M^{-1}(S^T)^{-1}SMS^{-1} \tag{9.10}$$

Hence

$$(S^{T,-1}S)M = M(S^{-1,T}S) \tag{9.11}$$

Then Schur's lemma says:

$$\begin{aligned} &S^{-1,T}S = \alpha I \\ &\qquad S = \alpha S^T \;\Rightarrow\; S^T = \alpha S \\ &(S^T)^T = S = \alpha S^T = \alpha^2 S \\ &\Rightarrow \alpha^2 = 1 \Rightarrow \alpha = \pm 1 \end{aligned}$$

$$\boxed{S^T = \pm S} \tag{9.12}$$

Next we want to show that S is an invariant tensor, but for that we first need the definition of a tensor. So how does one introduce tensors in group theory? One begins with contravariant vectors v^α and covariant vectors w_α. We define that w_α transforms under finite (not infinitesimal) group transformations as follows

$$(w')_\alpha = w_\beta M^\beta{}_\alpha(g) \tag{9.13}$$

The vectors w_α form a representation space (carrier space) on which the group acts[4]

$$((w_\alpha)_I)_{II} = \left(w_{\beta'} M(g_I)^{\beta'}{}_\alpha\right)_{II} = \left(w_{\beta'} M(g_I)^{\beta'}{}_{\beta''}\right) M(g_{II})^{\beta''}{}_\alpha = w_{\beta'} M(g_I g_{II})^{\beta'}{}_\alpha \,. \tag{9.14}$$

Given the transformation rule of w_α, we require that $w_\alpha v^\alpha$ is a scalar, namely that $w'{}_\alpha v'^\alpha = w_\alpha v^\alpha$. This yields the following transformation rule for v^α

$$v'^\alpha = M^{-1}(g)^\alpha{}_\beta v^\beta \tag{9.15}$$

because $w' \cdot v' = w'_\alpha v'^\alpha = w_\beta M(g)^\beta{}_\alpha M^{-1}(g)^\alpha{}_{\beta'} v^{\beta'} = w_\beta v^\beta$. For transformations in group theory we can replace $M^{-1}(g)^\alpha{}_\beta$ by $M(g^{-1})^\alpha{}_\beta$. Then

$$v'^\alpha = M(g^{-1})^\alpha{}_\beta v^\beta \tag{9.16}$$

Also v^α carries a representation of G as is clear from the following steps, using again the active point of view,

$$((v^\alpha)_I)_{II} = \left(M(g_I^{-1})^\alpha{}_\beta v^\beta\right)_{II} = M(g_{II}^{-1})^\alpha{}_{\beta'} \left(M(g_I^{-1})^{\beta'}{}_\beta v^\beta\right) = M\left((g_I g_{II})^{-1}\right)^\alpha{}_\beta v^\beta \,. \tag{9.17}$$

Having defined vectors in group theory, we can now build tensors with any number of contravariant and covariant indices. A general tensor transforms as follows

$$T'{}_{\alpha_1 \cdots \alpha_n}{}^{\beta_1 \cdots \beta_n}(g) = M(g^{-1})^{\beta_1}{}_{\beta'_1} \cdots M(g^{-1})^{\beta_n}{}_{\beta'_n} T_{\alpha'_1 \cdots \alpha'_m}{}^{\beta'_1 \cdots \beta'_n} M(g)^{\alpha'_1}{}_{\alpha_1} \cdots M(g)^{\alpha'_n}{}_{\alpha_n} \,. \tag{9.18}$$

Having defined tensors, we can clean up a problem that may have puzzled the reader. The orthogonality relations for matrix elements of unitary irreps

$$\sum_g \left(M^{(i)}(g)^\mu{}_\nu\right)^* M^{(j)}(g)^\alpha{}_\beta = \delta_i^j \delta_\mu^\alpha \delta_\beta^\nu \frac{|G|}{\dim R^{(i)}} \tag{9.19}$$

do not seem consistent: the indices on the left-hand side do not appear in the same position as on

[4] This is the active point of view: $((w_\alpha)_I)_{II} = (w'_\alpha)_{II} = w'_\beta M_{II}{}^\beta{}_\alpha$ with $w'_\beta = w_\gamma M_I{}^\gamma{}_\beta$. For the passive point of view one must use M^{-1} in the definition of $w'_\alpha = w_\beta (M^{-1})^\beta{}_\alpha$, because only then we get a representation: $((w_\alpha)_I)_{II} = (w_\beta (M_I^{-1})^\beta{}_\alpha)_{II} = (w_\beta)_{II} (M_I^{-1})^\beta{}_\alpha = w_\gamma (M_{II}^{-1})^\gamma{}_\beta (M_I^{-1})^\beta{}_\alpha = w_\gamma M^{-1}(g_I g_{II})^\gamma{}_\alpha$.

the right-hand side, so this relation does not seem to be covariant (by which is meant that the left-hand side transforms the same way the right-hand side does). However, for unitary transformations (to which this relation applies) the noncovariance is only apparent but not real because for unitary matrices $M^\alpha{}_\beta$ one has the relation (see (7.24))

$$(M^\mu{}_\nu)^* = (M^{-1})^\nu{}_\mu \tag{9.20}$$

Using this relation in (9.19), the equation becomes covariant (a tensor equation). A useful notation, but not more than that, is to introduce a matrix $(M^*_{(i)})_\mu{}^\nu$ whose matrix elements are equal to the compex conjugate of the matrix elements of M: $(M^{(i)\mu}{}_\nu)^* \equiv (M^*_{(i)})_\mu{}^\nu$. Using M^*, the covariance of tensor relations becomes manifest.

$$\sum_g (M^*_{(i)}(g))_\mu{}^\nu (M^{(j)}(g))^\alpha{}_\beta = \delta^j_i \delta^\alpha_\mu \delta^\beta_\nu \frac{|G|}{\dim R^{(j)}} \,. \tag{9.21}$$

Let us now come back to the matrix S in $M^*(g) = SM(g)S^{-1}$. We begin by putting indices

$$(M^\alpha{}_\beta)^* = (M^*)_\alpha{}^\beta = S_{\alpha\alpha'} M(g)^{\alpha'}{}_{\beta'} (S^{-1})^{\beta'\beta} \tag{9.22}$$

Thus S has both indices down, and its inverse has both indices up. The relation $S_{\alpha\beta}(S^{-1})^{\beta\gamma} = \delta_\alpha{}^\gamma$ is a true tensor relation because $\delta_\alpha{}^\gamma$ is a tensor. In fact, $\delta_\alpha{}^\beta$ is an **invariant tensor** by which is meant it does not transform

$$(\delta')_\alpha{}^\beta = M(g^{-1})^\beta{}_{\beta'} \delta_{\alpha'}{}^{\beta'} M(g)^{\alpha'}{}_\alpha = M(g^{-1})^\beta{}_{\beta'} M(g)^{\beta'}{}_\alpha = M(e)^\beta{}_\alpha = \delta^\beta{}_\alpha \,. \tag{9.23}$$

We are now ready to prove that $S_{\alpha\beta}$ is an invariant tensor. We start from

$$(M(g)^\alpha{}_\beta)^* = S_{\alpha\alpha'} M(g)^{\alpha'}{}_{\beta'} (S^{-1})^{\beta'\beta} = M(g^{-1})^\beta{}_\alpha = (M^{-1}(g))^\beta{}_\alpha \,. \tag{9.24}$$

We rearrange this equation by multiplying with $M(g)^\alpha{}_\gamma$ and $S_{\beta\delta}$

$$M(g)^\alpha{}_\gamma S_{\alpha\alpha'} M(g)^{\alpha'}{}_\delta = S_{\gamma\delta} \tag{9.25}$$

which can be rewritten in a more revealing way as follows

$$S_{\alpha'\beta'} M(g)^{\alpha'}{}_\alpha M(g)^{\beta'}{}_\beta = S_{\alpha\beta} \tag{9.26}$$

The left-hand side is the transformation law of a tensor $S_{\alpha\beta}$, and the right hand-side states that the transformed tensor is equal to itself. Hence, indeed, $S_{\alpha\beta}$ is an invariant tensor. In the same way one may prove that $(S^{-1})^{\alpha\beta}$ is an invariant tensor. Another invariant tensor is the matrix

$M(g)^\alpha{}_\beta$ itself. Indeed, transforming $M(g)^\alpha{}_\beta$ the same way as $v^\alpha w_\beta$ one obtains

$$M'(g)^\alpha{}_\beta = M(g^{-1})^\alpha{}_{\alpha'}\big(M(g)^{\alpha'}{}_{\beta'}\big)M(g)^{\beta'}{}_\beta = M(g)^\alpha{}_\beta \tag{9.27}$$

which proves the assertion.

Application: Using invariant tensors T one can construct **invariants** I

$$I = v^{\alpha^1}\cdots v^{\alpha^n} T_{\alpha^1\cdots\alpha^n}{}^{\beta^1\cdots\beta^m} w_{\beta^1}\cdots w_{\beta^m} \tag{9.28}$$

If T were an ordinary tensor and one would transform v, T and w, this expression would not transform, I would be a scalar. But if T is an invariant tensor and one does not transform T but only v and w, this expression will still be a scalar because one could act with the matrices for v and w on T, and T is an invariant tensor. An obvious example is $I = v^\alpha \delta_\alpha{}^\beta w_\beta = v^\alpha w_\alpha$.

9.2 Proof of the Frobenius-Schur criterion

We shall now first prove that the matrix S in $M(g)^* = SM(g)S^{-1}$ is symmetric iff (if and only if) $M(g)$ is real. It then follows that S is antisymmetric iff $M(g)$ is pseudoreal. This will allow us to also prove the Frobenius-Schur criterion. First we show that if for unitary $M(g)$ one has $M(g)^* = SM(g)S^{-1}$ and $RM(g)R^{-1} = D(g) =$ real, then S, $D(g)$ and R may all be assumed to be unitary.

The unitarity of S follows straightforwardly from the unitarity of $M(g)$ and $M(g)^*$: $M(g)^* = SM(g)S^{-1}$ so, taking the hermitian conjugate, $M(g)^{-1,*} = S^{-1,\dagger}M(g)^{-1}S^\dagger$ hence $M(g)^* = S^{\dagger,-1}$ $M(g)S^\dagger$. The two equations for $M(g)^*$ imply that $S^\dagger S$ commutes with $M(g)$, hence, according to Schur's lemma, $S^\dagger S = \alpha I$. Clearly α is positive. We can rescale S such that $S^\dagger S = I$, and thus S may be taken to be unitary.

To prove the unitarity of $D(g)$ define $D = \sum_g D(g)D(g)^\dagger$ which is real, hermitian, positive definite, hence symmetric. Then we can diagonalize D: $ODO^{-1} = \Lambda$ with orthogonal O is real, diagonal, positive definite, and $D = O^T\Lambda O$. Define $\widehat{R} = \Lambda^{-\frac{1}{2}}O$. Then $\widehat{D}(g) = \widehat{R}D(g)\widehat{R}^{-1}$ is real because $\widehat{R}$ is real. It is also unitary since

$$\begin{aligned}\widehat{D}(g)\widehat{D}(g)^\dagger &= \Big[\Big(\Lambda^{-\frac{1}{2}}O\Big)\, \underbrace{D(g)\,\underbrace{\Big(O^{-1}\Lambda^{\frac{1}{2}}\Big)\Big]\Big[\Lambda^{\frac{1}{2}}O}_{D}\, D(g)^\dagger}_{D(g)DD(g)^\dagger = D}\, O^{-1}\Lambda^{-\frac{1}{2}}\Big] \\ &= \Lambda^{-\frac{1}{2}}\big(ODO^{-1}\big)\Lambda^{-\frac{1}{2}} = \Lambda^{-\frac{1}{2}}\Lambda\Lambda^{-\frac{1}{2}} = I\,. \end{aligned} \tag{9.29}$$

So $\widehat{D}(g)$ is unitary. At this point we have shown that $M(g)^* = SM(g)S^{-1}$ with unitary S, and $\widehat{D}(g) = \widehat{R}D(g)\widehat{R}^{-1} = \widehat{R}RM(g)R^{-1}\widehat{R}^{-1} = \widetilde{R}M(g)\widetilde{R}^{-1}$ is real and unitary with $\widetilde{R} = \widehat{R}R$.

But if $\widetilde{R}M(g)\widetilde{R}^{-1} = \widehat{D}(g)$ and $M(g)$ and $\widehat{D}(g)$ are both unitary, then also $\widetilde{R}$ is unitary. This is easily proven: $\widetilde{R}M(g)\widetilde{R}^{-1} = \widehat{D}(g)$ and $\widehat{D}(g)^\dagger = \widehat{D}(g)^{-1} = \widetilde{R}^{-1,\dagger}M(g)^{-1}\widetilde{R}^\dagger$ so $\widetilde{R}M(g)\widetilde{R}^{-1} = \widetilde{R}^{\dagger,-1}M(g)\widetilde{R}^\dagger$. Thus $\widetilde{R}^\dagger\widetilde{R}$ commutes with all $M(g)$, hence according to Schur's lemma, $\widetilde{R}^\dagger\widetilde{R} = \alpha I$ with $\alpha > 0$. Rescaling $\widetilde{R}$ makes it unitary. So from now on we assume without loss of generality that $M(g)^* = SM(g)S^{-1}$ with unitary $M(g)$ and S, and $RM(g)R^{-1} = D(g) =$real and unitary, with unitary R.

We now prove the following steps for unitary irreps $M(g)$

1) if $M(g)$ is real, then S in $M(g)^* = SM(g)S^{-1}$ is symmetric.

2) if S in $M(g)^* = SM(g)S^{-1}$ is symmetric, then $M(g)$ is real.
At this point we also know that S is antisymmetric iff $M(g)$ is pesudoreal.

3) if $M(g)$ is real, then $\sum_g \chi(g^2) = |G|$.

4) if $M(g)$ is pseudoreal, then $\sum_g \chi(g^2) = -|G|$ (here we use that S is antisymmetric).

5) finally we prove for complex $M(g)$ that $\sum_g \chi(g^2) = 0$.

1) If $M(g)$ is real, then $RM(g)R^{-1} = D(g) =$ real for some unitary R. We also have $M(g)^* = SM(g)S^{-1}$ with unitary S, and we must show that S is symmetric. We have

$$\begin{aligned} D(g) = D(g)^* = R^*M(g)^*R^{*,-1} = RM(g)R^{-1} \\ \Rightarrow M(g)^* = R^{*,-1}(RM(g)R^{-1})R^* = SM(g)S^{-1} \end{aligned} \tag{9.30}$$

with $S = R^{*,-1}R$. Since R is unitary, $S = R^TR$ is symmetric (and unitary).

2) Now we show the converse: we assume that S is symmetric and unitary, and must prove that $M(g)$ can be made real. If S is symmetric and unitary, one can take a square root B of S which is again symmetric and unitary: $S = B^2$ and $B^\dagger = B^{-1}$, $B^T = B$. We prove this later. Then

$$M(g)^* = SM(g)S^{-1} = B^2M(g)B^{-2}. \tag{9.31}$$

Hence $B^{-1}M(g)^*B = BM(g)B^{-1}$. Since $B^{-1} = B^{*T}$ we get $B^{-1}M(g)^*B = B^*M(g)^*B^{*,-1}$ which implies that $BM(g)B^{-1} \equiv D(g)$ is real (and unitary). Hence B is the matrix R, and we have proven the reality of $M(g)$.

3) If $M(g)$ is real, then $\sum_g \chi(g^2) = |G|$. This follows from the orthogonality relations for matrix elements

$$\begin{aligned} &\sum_g \chi(g^2) = \sum_g M(g^2)^\mu{}_\mu = \sum_g M(g)^\mu{}_\nu M(g)^\nu{}_\mu = \sum_g M(g)^\mu{}_\nu S^{-1,\nu\rho}(M(g)^*)_\rho{}^\sigma S_{\sigma\mu} \\ &= S^{-1,\nu\mu}S_{\nu\mu}\frac{|G|}{\dim R} = \frac{|G|}{\dim R}\,\mathrm{tr}\, S^{-1}S^T = \frac{|G|}{\dim R}(+\,\mathrm{tr}\, S^{-1}S) = \frac{|G|}{\dim R}(\dim R) = |G|\,. \end{aligned} \tag{9.32}$$

4) If $M(g)$ is pseudoreal, we use that $S^T = -S$

$$\sum_g \chi(g^2) = \sum_g M(g)^\mu{}_\nu M(g)^\nu{}_\mu = \sum_g M(g)^\mu{}_\nu S^{-1,\nu\rho}(M(g)^*)_\rho{}^\sigma S_{\sigma\mu} = \frac{|G|}{\dim R} S^{-1,\nu\mu} S_{\nu\mu}$$
$$= \frac{|G|}{\dim R} \operatorname{tr} S^{-1} S^T = \frac{|G|}{\dim R}\left(-\operatorname{tr} S^{-1} S\right) = \frac{|G|}{\dim R}(-\dim R) = -|G|\,. \quad (9.33)$$

5) Finally consider complex $M(g)$. Then

$$\sum_g \chi(g^2) = \sum_g M(g)^\mu{}_\nu M(g)^\nu{}_\mu = \sum_g M(g)^\mu{}_\nu N(g)^\nu{}_\mu \quad (9.34)$$

where $N(g) = M(g)^*$ is an inequivalent irrep. The orthogonality relations for the matrix elements of two inequivalent irreps then yield $\sum_g \chi(g^2) = 0$.

9.I Taking the square root of a symmetric unitary matrix

It remains to be proven that one can take a square root of a symmetric unitary matrix which is again symmetric and unitary.[5]

Proof: $\mathcal{U}^T = \mathcal{U}$ and $\mathcal{U}\mathcal{U}^\dagger = I$, hence $\mathcal{U}\mathcal{U}^* = I$. Take real and imaginary parts of $\mathcal{U}$

$$A = \mathcal{U} + \mathcal{U}^*\,; \qquad B = \tfrac{1}{i}(\mathcal{U} - \mathcal{U}^*)\,. \quad (9.35)$$

A and B are both real and symmetric, and since $\mathcal{U}^* = \mathcal{U}^{-1}$, A and B commute. Hence they can be diagonalized simultaneously by an orthogonal matrix O, and since $\mathcal{U} = A + iB$ is unitary, the matrix elements of the diagonal matrix are phases.

$$O^T(A + iB)O = \Lambda = e^{i\phi} \quad (9.36)$$

where ϕ is a diagonal real matrix. Then

$$\left.\begin{aligned} \mathcal{U} &= O e^{i\phi} O^T \\ V &= O e^{\frac{i}{2}\phi} O^T \end{aligned}\right\} \quad V^2 = \mathcal{U} \quad (9.37)$$

The matrix V is a symmetric and unitary square root of $\mathcal{U}$.

[5] I thank Prof. W. Weisberger for constructing this proof.

Chapter 10

All subgroups of $\boldsymbol{SO(3)}$ and $\boldsymbol{SU(2)}$, and the groups $\boldsymbol{SL(2,3)}$ and $\boldsymbol{GL(2,3)}$.

Given a group G, one may ask what are its infinite or finite subgroups. We shall first enumerate the Lie subgroups and the finite subgroups of $SO(3)$ and $SU(2)$. For $SU(2)$ we shall encounter three new finite subgroups: the binary tetrahedral group $SL(2,3)$, the binary octahedral group $GL(2,3)$ and the binary icosahedral group $SL(2,5)$. They are the covering groups[1] of the rotation groups A_4, S_4 and A_5 of a tetrahedron, octahedron, and icosahedron, respectively, so

$$SL(2,3)/Z_2 = A_4\,; \quad GL(2,3)/Z_2 = S_4\,; \quad SL(2,5)/Z_2 = A_5\,. \tag{10.1}$$

We shall discuss $SL(2,3)$ and $GL(2,3)$ in detail, but leave $SL(2,5)$ as an exercise.

Warning: These groups are **not** the full isometry groups S_4, $S_4 \times Z_2$, and $A_5 \times Z_2$ of the tetrahedron, cube and icosahedron (where $Z_2 = (e,\sigma)$ with σ space inversion). It is also **not** true that $SL(2,3) = A_4 \times Z_2$ or $A_4 \rtimes Z_2$, or $GL(2,3) = S_4 \times Z_2$ or $S_4 \rtimes Z_2$, or $SL(2,5) = A_5 \times Z_2$ or $A_5 \rtimes Z_2$. For example, $SL(2,3)$ has no subgroup A_4, as we shall discuss.

The nontrivial subgroups of $\boldsymbol{SO(3)}$ are the Lie groups $SO(2)$ and $O(2)$[2] with group elements

$$\begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \text{ and } \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

[1] The covering group G' of a (finite or infinite) group G satisfies $G'/K \simeq G$, where K is the center (or a subgroup of the center) of G'. For a Lie group G the covering group G' is simply connected, while for a finite group G it yields the projective representations of G (representations up to a phase, as in quantum mechanics). We shall later discuss in detail the covering groups of $SO(N)$, $SU(2)$ and $Sp(2N,R)$.

[2] If O in $O(2)$ has $\det O = -1$, multiply by $\begin{pmatrix} 1 & & \\ & 1 & \\ & & -1 \end{pmatrix}$ to obtain $\det O = +1$ for $O \in SO(3)$.

$$= \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ \sin\theta & -\cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix} = \begin{pmatrix} \cos\theta & \sin\theta & 0 \\ \sin\theta & -\cos\theta & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{10.2}$$

The latter are inequivalent to the former (their traces differ). The finite subgroups are

$\boldsymbol{Z_n}$**:** the cyclic groups of order n

$\boldsymbol{D_n}$**:** the dihedral groups of order $2n$ (a discretized version of (10.2))

$\boldsymbol{A_4}$**:** the rotation group of a tetrahedron of order 12

$\boldsymbol{S_4}$**:** the rotation group of a cube of order 24

$\boldsymbol{A_5}$**:** the rotation group of an icosahedron of order 60.

The nontrivial subgroups of $\boldsymbol{SU(2)}$ are the following: the Lie group $U(1) = \left(\begin{smallmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{smallmatrix}\right)$, which is the maximal torus T and the Lie group $N(T)$ which is its normalizer with group elements

$$\left\{ g(\theta) = \begin{pmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{pmatrix};\ 0 \le \theta < 2\pi \right\} \cup \left\{ g'(\theta) = \begin{pmatrix} 0 & ie^{-i\theta} \\ ie^{i\theta} & 0 \end{pmatrix};\ 0 \le \theta < 2\pi \right\} \tag{10.3}$$

$N(T)$ is the set of elements g of $SU(2)$ such that $gtg^{-1} = t'$ with t and t' in T (one finds $g'(\theta)g(\eta)g'(\theta)^{-1} = g(-\eta)$). Further there is the following set of **finite subgroups of** $\boldsymbol{SU(2)}$ given by the ADE classification

$\boldsymbol{A_n}$**:** Z_n, the cyclic groups (order n)

$\boldsymbol{D_n}$**:** Q_{2n}, the binary dihedral (dicyclic) groups (order $4n$)

$\boldsymbol{E_6}$**:** $SL(2,3)$, the binary tetrahedral group (order 24)

$\boldsymbol{E_7}$**:** $GL(2,3)$, the binary octahedral group (order 48)

$\boldsymbol{E_8}$**:** $SL(2,5)$, the binary icosahedral group (order 120).

The binary dihedral groups of order $4n$ are defined by the following matrix representations

$$\left\{ q_n(k) = \begin{pmatrix} e^{\frac{2\pi ik}{2n}} & 0 \\ 0 & e^{-\frac{2\pi ik}{2n}} \end{pmatrix} \cup \begin{pmatrix} 0 & ie^{-\frac{2\pi ik}{2n}} \\ ie^{\frac{2\pi ik}{2n}} & 0 \end{pmatrix} \right\} = \left\langle Z_{2n}; i\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right\rangle, \tag{10.4}$$

with $0 \le k < 2n$. Z_n are the rotation groups of a regular n-gon, but, as we already mentioned, $\boldsymbol{E_6}$ **is not isomorphic to the isometry group of a tetrahedron**. (As we shall see, E_6 has a nontrivial center, while S_4 is the isometry group of a tetrahedron which has no nontrivial center.)

We shall discuss the binary tetrahedral group in some detail. This is a quite interesting topic as various new concepts will arise, but (so far[3]) this group has not played a major role in physics, hence for a first reading one may skip the following discussion.

*10.1 $SL(2,3)$

The group $SL(2,3)$ has order 24 and is the dihedral tetrahedron group which is the double cover of the rotation group A_4 of a tetrahedron: $SL(2,3)/Z_2 = A_4$. It is also the special linear group of 2×2 matrices with determinant $+1$ whose entries are elements of a field of characteristic 3, meaning that its entries can only be $(0,1,2)$ modulo 3, or equivalently and nicer to work with $(-1,0,1)$ modulo 3. This group has 24 elements.[4] One can systematically find the 24 group elements by first considering matrices with two zeros, then matrices with one zero in a particular entry, and finally no zeros. The following set of 24 2×2 matrices forms a group if one defines group multiplication as matrix multiplication modulo 3. There are **7 classes**:

$$\begin{array}{c|ccccccc}
\text{order of } g & 1 & 2 & 3 & & 3 & 6 & 6 & 4 \\
 & \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} & \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} & \leftrightarrow & \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} & \begin{pmatrix} -1 & 1 \\ 0 & -1 \end{pmatrix} & \begin{pmatrix} -1 & -1 \\ 0 & -1 \end{pmatrix} & \pm\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} = \pm I \\
\text{group} & & & \begin{pmatrix} -1 & 1 \\ -1 & 0 \end{pmatrix} & \leftrightarrow & \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix} & \begin{pmatrix} 0 & 1 \\ -1 & 1 \end{pmatrix} & \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix} & \pm\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \pm J \\
\text{elements} & & & \begin{pmatrix} 1 & 0 \\ -1 & 1 \end{pmatrix} & \leftrightarrow & \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} & \begin{pmatrix} -1 & 0 \\ -1 & -1 \end{pmatrix} & \begin{pmatrix} -1 & 0 \\ 1 & -1 \end{pmatrix} & \pm\begin{pmatrix} -1 & 1 \\ 1 & 1 \end{pmatrix} = \pm K \\
 & & & \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix} & \leftrightarrow & \begin{pmatrix} -1 & -1 \\ 1 & 0 \end{pmatrix} & \begin{pmatrix} 1 & 1 \\ -1 & 0 \end{pmatrix} & \begin{pmatrix} 0 & -1 \\ 1 & 1 \end{pmatrix} & \\
\text{order of } C & 1 & 1 & 4 & & 4 & 4 & 4 & 6
\end{array} \tag{10.5}$$

By order of g we mean the order of each group element, and by order of C we mean the number of group elements in each class. All 24 matrices have determinant $+1$, for example $\det\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = -2 \bmod 3 = 1$. The arrows will be discussed later; they connect group elements in the same subgroup Z_3. So there are at least 4 subgroups Z_3. There are also at least 4 subgroups Z_6: all group elements in the same row of the first six columns form a Z_6. And the quaternions give, of course, 3 subgroups Z_4. None of these subgroups is normal. We shall later present the complete list of nontrivial subgroups of $SL(2,3)$.

One can also define $SL(2,3)$ in terms of 24 unit quaternions[5] ($I^2 = J^2 = K^2 = -e$; $IJ = -JI = K$ and cyclically). There are 8 group elements of the quaternion group, a further set of 8

[3] For an attempt to use $SL(2,3)$ as classification group of elementary particles, see K. M. Case, R. Karplus and C. N. Yang, *Phys. Rev.* **101** (1956) 874.

[4] The order of $SL(2,n)$ is $\frac{1}{2}(n^2-1)(n^2-3)$ because in $\begin{pmatrix} a & b \\ c & d \end{pmatrix}$ one can pick a,b in n^2-1 ways (only the case $a=b=0$ is excluded), while one can pick (c,d) in n^2-3 ways (the cases $c,d=a,b$ and $c,d=-a,-b$ and $c,d=0,0$ are excluded). The determinant can be $+1$ or -1, hence the prefactor $\frac{1}{2}$.

[5] A unit quaternion is a quaternion $ae+bI+cJ+dK$ with unit norm: $|a|^2+|b|^2+|c|^2+|d|^2=1$.

quaternions of order 6, and a third set of 8 quaternions of order 3:

$$SL(2,3): \begin{cases} (\pm e, \pm I, \pm J, \pm K) & \text{the quaternionic group } Q \\ \frac{1}{2}(e \pm I \pm J \pm K) & \text{the 8 group elements of order 6} \\ \frac{1}{2}(-e \pm I \pm J \pm K) & \text{the 8 group elements of order 3} \end{cases} \tag{10.6}$$

These 24 quaternions define a finite group, which is isomorphic to $SL(2,3)$. To prove this isomorphism[6], consider the following presentation of $SL(2,3)$ (see the comment at the end for further discussion of this presentation)

$$SL(2,3) = \{s, t \,|\, s^6 = t^6 = e, (st)^4 = e\} \tag{10.7}$$

Choose s and t as follows: for the quaternions

$$s_q = \tfrac{1}{2}(e + I + J + K) \qquad t_q = \tfrac{1}{2}(e + I + J - K), \tag{10.8}$$

with Pauli matrices $I = i\sigma_3$, $J = i\sigma_2$, $K = i\sigma_1$ this becomes

$$s_P = \frac{1}{2}\begin{pmatrix} 1+i & 1+i \\ -1+i & 1-i \end{pmatrix} \qquad t_P = \frac{1}{2}\begin{pmatrix} 1+i & 1-i \\ -1-i & 1-i \end{pmatrix}. \tag{10.9}$$

For $SL(2,3)$ we choose the Chevalley matrices

$$s_C = \begin{pmatrix} -1 & 1 \\ 0 & -1 \end{pmatrix} \qquad t_C = \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix} \tag{10.10}$$

All 3 pairs (s_q, t_q), (s_P, t_P) and (s_C, t_C) satisfy $s^6 = t^6 = e$ and $(st)^4 = e$. $(st)_q$ is given by $\frac{1}{4}(2I + 2J - 2IK - 2JK) = J$, $(st)_P = i\sigma_2$ and $(st)_C = \left(\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right)$. Clearly $(st)^4 = e$. So the groups they generate are isomorphic. ((s_q, t_q) generate are subgroup of the quaternions, (s_P, t_P) a subgroup of $SU(2)$, and (s_C, t_C) a subgroup of $GL(2,3)$.)

$SL(2,3)$ can also be written as the semidirect product $SL(2,3) = Q_4 \rtimes Z_3$ where Q_4 is the quaternion group and Z_3 the cyclic group generated by $x = \frac{1}{2}(-e + I + J + K)$. The quaternion group is a normal subgroup.

There are two nontrivial normal subgroups:

$$N_1 = (e, -e) = Z_2\,; \quad N_2 = (\pm e, \pm I, \pm J, \pm K) = Q_4 = C(G)\,. \tag{10.11}$$

Since $SL(2,3)/Q_4 = Z_3$ and Q_4 is the commutator subgroup, there are 3 one-dimensional irreps,

[6] We thank José Figueroa for discussions.

and since there are 7 classes, we can only have

$$|SL(2,3)| = 24 = 1^2 + 1^2 + 1^2 + 2^2 + 2^2 + 2^2 + 3^2 \,. \tag{10.12}$$

The characters of the three two-dimensional irreps can be obtained from the character of the 2-dimensional irrep in terms of quaternions by multiplication with the 3 one-dimensional irreps, and the character of the 3-dim. irrep is obtained from the character of $SL(2,3)/N_1 \simeq A_4$ by lifting to $SL(2,3)$. The character table is then easy to compute and one may check that the orthogonality relations for characters are satisfied.

$SL(2,3)$	$e[1]$	$-e[1]$	$\pm I[6]$	$\left(\begin{smallmatrix}1&1\\0&1\end{smallmatrix}\right)[4]$	$\left(\begin{smallmatrix}-1&-1\\0&-1\end{smallmatrix}\right)[4]$	$\left(\begin{smallmatrix}1&-1\\0&1\end{smallmatrix}\right)[4]$	$\left(\begin{smallmatrix}-1&1\\0&-1\end{smallmatrix}\right)[4]$
χ_1	1	1	1	1	1	1	1
$\chi_{1'}$	1	1	1	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{4\pi i}{3}}$	$e^{\frac{4\pi i}{3}}$
$\chi_{1''}$	1	1	1	$e^{\frac{4\pi i}{3}}$	$e^{\frac{4\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$
χ_2	2	-2	0	-1	1	-1	1
$\chi_{2'} = \chi_2\chi_{1'}$	2	-2	0	$-e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	$-e^{\frac{4\pi i}{3}}$	$e^{\frac{4\pi i}{3}}$
$\chi_{2''} = \chi_2\chi_{1''}$	2	-2	0	$-e^{\frac{4\pi i}{3}}$	$e^{\frac{4\pi i}{3}}$	$-e^{\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$
χ_3	3	3	-1	0	0	0	0

Table 10.1: The seven classes of $SL(2,3)$ combine into the four classes of $SL(2,3)/N_1 = A_4$ as indicated by the vertical bars. The first three rows of χ_1's are from $SL(2,3)/N_2 = Z_3$, χ_2 is from the quaternions and χ_3 is from $SL(2,3)/N_1 = A_4$.

Subgroups of $SL(2,3)$: The number of nontrivial subgroups of $SL(2,3)$ is 13. We enumerate them:

1) one Z_2: $(e, -e)$;

2) three Z_4 generated by I or J or K;

3) one $Q = (\pm e, \pm I, \pm J, \pm K)$, the quaternion group (a Sylow 2-group);

4) four Z_3 generated[7] by group elements of order 3 (Sylow 3-groups);

5) four $Z_6 = Z_3 \times Z_2$ generated by the four pairs of Z_3 times $Z_2 = N_1$.

This yields the $1 + 3 + 1 + 4 + 4 = 13$ proper subgroups of $SL(2,3)$.

Warning: Note that there is no subgroup of order 12, even though the order of A_4 is 12, and $SL(2,3)/Z_2 = A_4$. Indeed, none of the group elements in (10.5) has order 12. In other words, although the 24 group elements in (10.5) form 12 pairs $+m$ and $-m$, it is not possible to choose from each pair either a $+m$ or $-m$ in such a way that one gets a group.

[7] For example $\left(\begin{smallmatrix}1&1\\0&1\end{smallmatrix}\right)$ generates the Z_3 group $\left(e, \left(\begin{smallmatrix}1&1\\0&1\end{smallmatrix}\right), \left(\begin{smallmatrix}1&-1\\0&1\end{smallmatrix}\right)\right)$ and we have connected $\left(\begin{smallmatrix}1&1\\0&1\end{smallmatrix}\right)$ and $\left(\begin{smallmatrix}1&-1\\0&1\end{smallmatrix}\right)$ in (10.5) by an arrow to indicate that they are part of the same Z_3. It is then clear that there are four Z_3 groups of this kind.

To avoid confusion. The group $G = SL(2,3)$ has 15 **subgroups** as we have seen (the two trivial subgroups are of course e and G), and $SL(2,3)$ has order 24, but there are also 15 **different groups** of order 24. To enumerate them is a nice exercise: there are 3 abelian groups and 12 nonabelian groups, one of which is of course $SL(2,3)$:

$$\begin{gathered} Z_2 \times Z_2 \times Z_2 \times Z_3\,; \quad Z_3 \times Z_8 = Z_{24}\,; \quad Z_3 \times Z_4 \times Z_2 = Z_6 \times Z_4 = Z_{12} \times Z_2\,; \\ S_3 \times Z_4\,; \quad D_4 \times Z_3\,; \quad Q_4 \times Z_3\,; \quad D_4 \rtimes Z_3\,; \quad Z_8 \rtimes Z_3\,; \\ A_4 \times Z_2\,; \quad Q_6 \times Z_2\,; \quad D_6 \times Z_2 = S_3 \times V_4\,; \\ SL(2,3)\,; \quad S_4\,; \quad Q_{12}\,; \quad D_{12}\,. \end{gathered} \tag{10.13}$$

*10.2 $GL(2,3)$

The group $GL(2,3)$ can be defined as the group of 2×2 matrices with nonzero determinant whose entries lie again in $F(3)$ (whose entries are $-1, 0, +1$ modulo 3). In addition to the 24 2×2 matrices of $SL(2,3)$ with determinant $+1$ we now have a further set of 24 group elements with determinant -1. We shall show that these new 24 group elements consist of a set of 12 group elements of order 2, and another set of 12 group elements of order 8. Whereas $SL(2,3)$ has 7 classes, $GL(2,3)$ has 8 classes. The two classes of $SL(2,3)$ which contain 4 group elements of order 3 each, become one class of $GL(2,3)$ of order 8. Similarly the two classes of $SL(2,3)$ which contain 4 group elements of order 6 each, become one class of $GL(2,3)$ of order 8. So the 7 classes of $SL(2,3)$ combine into 5 of the 8 classes of $GL(2,3)$.

The remaining 24 group elements of $Gl(2,3)$ with determinant -1 belong (of course) to different classes than the 24 group elements of $GL(2,3)$ with determinant $+1$, and they yield 3 new classes (in addition to the 5 classes formed by the 24 group elements of $SL(2,3)$), namely: one class with 12 group elements of order 2, and two classes of 6 group elements each of order 8.

$GL(2,3)$ has order 48. The 24 group elements with determinant $+1$ form the subgroup $SL(2,3)$. The 12 group elements of $GL(2,3)$ with determinant -1 and order 2 are given by

$$\begin{gathered} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} -1 & -1 \\ 0 & 1 \end{pmatrix} \\ \begin{pmatrix} -1 & 0 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} -1 & 0 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} 1 & -1 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} -1 & 1 \\ 0 & 1 \end{pmatrix} \end{gathered} \tag{10.14}$$

The 12 group elements of $GL(2,3)$ with determinant -1 and order 8 form two classes, one with trace +1 and the other with trace −1

$$\begin{pmatrix}-1 & 1\\ -1 & -1\end{pmatrix}\begin{pmatrix}-1 & -1\\ 1 & -1\end{pmatrix}\begin{pmatrix}0 & -1\\ -1 & 1\end{pmatrix}\begin{pmatrix}1 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 1\end{pmatrix}\begin{pmatrix}1 & -1\\ -1 & 0\end{pmatrix}$$
$$\begin{pmatrix}1 & -1\\ 1 & 1\end{pmatrix}\begin{pmatrix}1 & 1\\ -1 & 1\end{pmatrix}\begin{pmatrix}-1 & -1\\ -1 & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}-1 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0 & -1\\ -1 & -1\end{pmatrix} \qquad (10.15)$$

The 8 classes of $GL(2,3)$ are as follows

$$\begin{array}{c|cccccccc} \text{order of } g & 1 & 2 & 3 & 6 & 4 & 2 & 8 & 8 \\ \text{coset representative} & e & -e & \left(\begin{smallmatrix}1&1\\0&1\end{smallmatrix}\right) & \left(\begin{smallmatrix}-1&-1\\0&-1\end{smallmatrix}\right) & \left(\begin{smallmatrix}0&-1\\1&0\end{smallmatrix}\right) & \left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right) & \left(\begin{smallmatrix}-1&1\\-1&-1\end{smallmatrix}\right) & \left(\begin{smallmatrix}1&-1\\1&1\end{smallmatrix}\right) \\ \text{order of } C & 1 & 1 & 8 & 8 & 6 & 12 & 6 & 6 \end{array} \qquad (10.16)$$

There are 3 nontrivial normal subgroups of $GL(2,3)$:

$$N_1 = (e, -e) \text{ of order } 2; \quad N_2 = Q \text{ of order } 8; \quad N_3 = SL(2,3) \text{ of order } 24. \qquad (10.17)$$

- The commutator subgroup is $C_2(G) = N_3 = SL(2,3)$, so there will be two one-dimensional irreps.
- $GL(2,3)/Q$ has order 6, and is nonabelian, so it must be S_3. The irreps of S_3 have dimensions $\mathbf{1}, \mathbf{1}, \mathbf{2}$, and we can lift the 2-dimensional irrep of S_3 to $GL(2,3)$.[8]
- Similarly, we can use that $GL(2,3)/N_1 \simeq S_4$, and lift the irreps of S_4 of dimensions $\mathbf{1}, \mathbf{1}, \mathbf{2}, \mathbf{3}, \mathbf{3}$ to irreps of $GL(2,3)$. This produces the 3-dimensional irreps.
- We can multiply these irreps by the two 1-dim. characters.

At this point we know that

$$|GL(2,3)| = 48 = 1^2 + 1^2 + 2^2 + x^2 + y^2 + 3^2 + 3^2 + z^2 \,. \qquad (10.18)$$

There is only one solution to this Diophantine equation: $x = y = 2$ and $z = 4$. From the orthogonality relations we find then a unique solution for the character χ_4. That leaves the two characters $\chi_{2'}$ and $\chi_{2''}$. They are complex, hence each other's complex conjugates. One can use the orthogonality relations to fix them partially, but we have not found a nice physical way to fix them completely and simply.

The character table for $GL(2,3)$ can now be written down

[8] The 6 elements of $GL(2,3)/Q$ form 3 classes of S_3. One class of S_3 consists of Q, the largest class of S_3 contains all group elements with det $= -1$, and the third class contains all remaining group elements with det $= +1$.

$GL(2,3)$	$e[1]$	$-e[1]$	order 3[8]	order 6[8]	order 4[6]	order 2[12]	order 8[6]	order 8[6]
χ_1	1	1	1	1	1	1	1	1
$\chi_{1'}$	1	1	1	1	1	-1	-1	-1
χ_2	2	2	-1	-1	2	0	0	0
$\chi_{2'}$	2	-2	-1	1	0	0	$i\sqrt{2}$	$-i\sqrt{2}$
$\chi_{2''}$	2	-2	-1	1	0	0	$-i\sqrt{2}$	$i\sqrt{2}$
χ_3	3	3	0	0	-1	1	-1	-1
$\chi_{3'} = \chi_3\chi_{1'}$	3	3	0	0	-1	-1	1	1
χ_4	4	-4	1	-1	0	0	0	0

Table 10.2: χ_2 is from $GL(2,3)/N_2 = S_3$ and χ_3 is from $GL(2,3)/N_1 = S_4$.

Comment about the 4th representation theorem. The groups $SL(2,3)$ and $GL(2,3)$ have nontrivial abelian normal subgroup (the group elements $\pm e$), hence they are non-semisimple. Thus we can apply the fourth theorem on representations, which states that the dimension of any irrep of G should be a divisor of the index of each maximal normal abelian subgroup of G. There is only one maximal abelian normal subgroup of $SL(2,3)$ and $GL(2,3)$, namely $N_1 = (e, -e)$, and its index is 12 and 24, respectively. So $SL(2,R)$ can only have irreps with dimensions $1,2,3,4,6$, and $GL(2,3)$ with dimensions $1,2,3,4,6,12$. This is indeed what we found, but we already knew this from Lagrange's theorem, so the fourth theorem is not useful is these two cases.

Comment about the presentations of $\boldsymbol{A_4}$ and $\boldsymbol{SL(2,3)}$. For A_4 a presentation is given by $G = \{s, t \,|\, s^3 = t^2 = e, aba = ba^2b\}$. It is straightforward to show that the constraint $aba = ba^2b$ is equivalent to the constraint $(ab)^3 = 1$. One can take for a any 3-cycle, for example (123), and for b any twin, for example (12)(34). To prove that this is a correct presentation, we must show that products of a and b yield 12 group elements, that this set is closed, and that it agrees with the group multiplication table of A_4. The complete set of products of a and b can be written as

$$\big(e, a, a^2\big)\,, \quad \big(b, ab, a^2b\big)\,, \quad \big(ba, aba, a^2ba\big)\,, \quad \big(bab, abab = ba^2, a^2bab = aba^2\big) \tag{10.19}$$

Other combinations can be reduced to this set, using various identities such as

$$abab = ba^2, \quad a^2bab = aba^2, \quad a^2ba^2 = bab, \quad (ab)^3 = (ba)^3\,. \tag{10.20}$$

One can draw a picture of the construction of group elements as in figure 10.1.

For $SL(2,3)$ a presentation is given in (10.7). To prove that this presentation yields the group $SL(2,3)$, one may proceed in the same way as A_4. Other, equivalent, presentations of $SL(2,3)$ are as follows

$$\begin{aligned} &G = \big\{s, t \,|\, s^3 = t^3 = (st)^2\big\} \\ &G = \big\{a, b, c \,|\, a^4 = c^3 = e, b^2 = a^2, bab^{-1} = a^{-1}, cac^{-1} = b, cbc^{-1} = ab\big\}\,. \end{aligned} \tag{10.21}$$

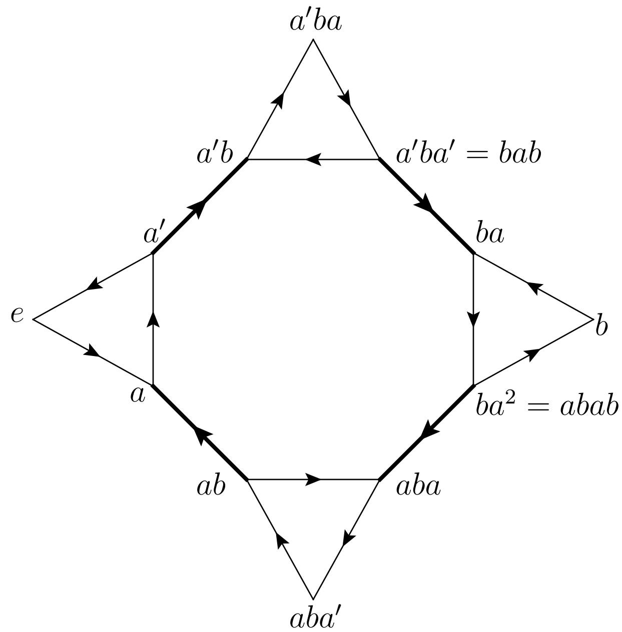


Figure 10.1: Right multiplication by a is indicated by ➝, while right multiplication by b is indicated by ➞. Reversal of arrows replaces a by $a' = a^2$, and keeps b (because $a^{-1} = a^2$ and $b^{-1} = b$).

Chapter 11

Application I: Dirac matrices, charge conjugation matrices and Majorana spinors

11.1 The Dirac equation

The Dirac equation $(\gamma^\mu \partial_\mu + m)\psi = 0$ contains Dirac matrices whose properties can be deduced from finite group theory. We first review how the Dirac equation was obtained, and then discuss the properties of Dirac matrices in $s+t$ dimensions (s space coordinates and t time coordinates).

Soon after quantum mechanics was constructed in late 1925 and early 1926, the question arose of a relativistic equation for the electron. Schrödinger and others took in 1926 the wave equation for a free complex one-component[1] field ϕ

$$\left[\partial_x^2 + \partial_y^2 + \partial_z^2 - \frac{1}{c^2}\partial_t^2 - \left(\frac{mc}{\hbar}\right)^2\right]\phi = 0 \tag{11.1}$$

but this seemed to lead to a fatal problem[2]: there was a currrent

$$j_\mu \sim \phi^\star \partial_\mu \phi - (\partial_\mu \phi^\star)\phi \tag{11.2}$$

which was on-shell conserved ($\partial^\mu j_\mu = 0$ if (11.1) holds). Believing (incorrectly) that the time component $j^0 \sim \left(\dot{\phi}^\star \phi - \phi^\star \dot{\phi}\right)$ was the probability density for an electron to be at a point x, it would imply that there could be negative probabilities. That made of course no sense. Later it was realized that ej_μ is the electric current, and $\frac{e}{c}j^0$ is the charge density which can, of course, be negative. But at the time, the wave equation did not seem correct, and the search was on for a better equation.

[1] E. Schrödinger, Annalen der Physik **81** (1926) 102. Section 6 contains a brief statement that he considered formally the wave function for an electron, but that he would withhold his calculations for the incorporation of spin.

[2] Another equally fatal problem with this equation for the electron in the hydrogen atom was that it did not yield the correct hydrogen spectrum. However, this is less relevant for our discussion of the origin of the Dirac equation.

Dirac studied this problem in 1928, and believed that if he could get rid of the $\frac{\partial}{\partial t}$ in j^0, the density problem could be cured. He therefore considered a field equation for a relativistic electron which was linear in time derivatives, and then the theory of special relativity of 1905 also required that the field equation be linear in space derivatives. That would lead to a Schrödinger equation of the form $i\hbar\frac{\partial\psi}{\partial t} = H\psi$ with H linear in space derivatives. Thus he considered the following field equation for a free electron

$$\left(\gamma^\mu\partial_\mu + \frac{mc}{\hbar}\right)\psi = 0 \tag{11.3}$$

where $\left(\frac{mc}{\hbar}\right)^{-1}$ is the Compton wavelength of the electron which A.H. Compton had encountered in his studies of Compton scattering in 1924. What was the meaning of the objects γ^μ? Dirac took them to be dimensionless matrices which would act on a multi-component ψ. In order that the relativistic mass relation $cp^\mu \cdot cp_\mu + (mc^2)^2 = 0$ would follow from his field equation, he multiplied the latter by $\gamma^\nu\partial_\nu - \frac{mc}{\hbar}$ and required that the result should be proportional to the wave equation. This led to a constraint on the matrices γ^μ

$$\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu} \tag{11.4}$$

Such a relation between three 2×2 matrices had been used by Pauli in 1927 for his nonrelativistic two-component spinor theory, but Dirac needed four matrices. He may have seen such an equation before because in 1843 Hamilton had discovered quaternions with imaginary units I, J, K which satisfy $\{I, J\} = \{J, K\} = \{K, I\} = 0$, $\{I, I\} = \{J, J\} = \{K, K\} = -2$, and there was much interest in quaternions in England. Later, a 2×2 matrix representation for quaternions was found in terms of "Pauli matrices"[3] ($I = -i\sigma_1, J = -i\sigma_2, K = -i\sigma_3$) which indeed satisfy (11.4) (and more: $\sigma_1\sigma_2 = i\sigma_3$ and cyclic relations). In fact, the more general problem of finding a solution of the equation $\{\gamma^\mu, \gamma^\nu\} = 2\delta^{\mu\nu}$ for any number of γ^μ in terms of matrices had been studied by the English mathematician William Clifford in 1878. Clifford had seen the work of 1844 of the German mathematician Hermann Grassmann who had studied anticommuting numbers ($ab = -ba$ so $\{a, b\} = 0$) but he added the requirement that $(\gamma^\mu)^2 = 1$. Thus there were some mathematical studies available for someone who would like to solve (11.4).

Dirac just tried. He could not use the 3 Pauli matrices because he needed 4 of them. He may first have tried 3×3 matrices but that does not work. Then he tried 4×4 matrices. That did

[3] These matrices were already known to the mathematician Felix Klein around 1850.

work, and the rest is history.[4] We usually do not need any explicit form of the Dirac matrices γ^m, but we mention here the representation most often used in 4-dimensional Minkowski space[5]

$$\gamma^k = \begin{pmatrix} 0 & -i\sigma^k \\ i\sigma^k & 0 \end{pmatrix} \quad \text{for } k = 1,2,3; \quad \gamma^0 = \begin{pmatrix} 0 & -iI \\ -iI & 0 \end{pmatrix} \tag{11.5}$$

It is obvious that they satisfy the Clifford algebra if one writes them as $\sigma^k \otimes \sigma^2$ and $-i\mathbb{I} \otimes \sigma^1$.

As we shall discuss when we reach the spinor representations of the Lie group $SO(3,1)$, the 4-component spinors transform under rigid Lorentz transformations as

$$\delta\psi = \tfrac{1}{2}\lambda^{mn}\left(\tfrac{1}{2}\gamma_{mn}\right)\psi - \lambda^{\rho}{}_{\sigma}x^{\sigma}\partial_{\rho}\psi \tag{11.6}$$

where $\frac{1}{2}\gamma_{mn} = \frac{1}{4}(\gamma_m\gamma_n - \gamma_n\gamma_m)$ are the Lorentz generators in the spinor representation. (The first term is a "spin-term" which acts on the indices of ψ, while the second term is an "orbital term" which acts on the coordinates x^μ of the field. The relative minus sign is needed for the Lorentz invariance of the Dirac action.) Using the explicit representations given the (11.5) one find that the 6 matrices $\gamma_{mn} = (\gamma_{kl}, \gamma_k\gamma_0)$ are given by

$$\gamma_{kl} = \begin{pmatrix} \sigma_{kl} & 0 \\ 0 & \sigma_{kl} \end{pmatrix}; \quad \gamma_{k0} = \begin{pmatrix} \sigma_k & 0 \\ 0 & -\sigma_k \end{pmatrix} \tag{11.7}$$

where $\sigma_{kl} = i\epsilon_{klm}\sigma^m$. Hence the set of matrices γ_{mn} are block-diagonal, and thus the Dirac spinors form (in $d = 3+1$ dimensions) a reducible representation of the Lorentz group.

The Dirac equation in (11.3) can be obtained from an action by the Euler-Lagrange variational principle. This action is called the Dirac action, and is given by $S = \int d^3x dt\, \mathcal{L}$ with

$$\mathcal{L} = -\overline{\psi}\left(\gamma^\mu\partial_\mu + \frac{mc}{\hbar}\right)\psi \tag{11.8}$$

Here $\overline{\psi} = \psi^\dagger i\gamma^0$ with $(\gamma^0)^2 = -I$. One needs the factor $i\gamma^0$ for rigid Lorentz invariance of the action. If one varies with respect to $\overline{\psi}$ one retrieves the Dirac equation in (11.3), and if one varies

[4] The Dirac equation was spectacularly successful: spin came out instead of having to be put in by hand, and also the famous (or notorious) Thomas factor 2 for spin-orbit coupling came out. But of course the new equation also led to new problems. For example, how did the 4-component $\psi^\alpha(\vec{\boldsymbol{x}}, t)$ transform under Lorentz rotations and boosts? In $\left(\gamma^\mu\partial_\mu + \frac{mc}{\hbar}\right)\psi = 0$, the $\frac{\partial}{\partial x^\mu}$ transformed as a vector, but the γ^μ were constant matrices and thus did not transform, so how could the equation still be Lorentz-covariant? Clearly, the four component ψ^α did not transform as a vector, but were there other four-component objects which transformed in an other but still well-defined way? What was that way? Ehrenfest in Leiden was confused, and asked van der Waerden (a Dutch mathematician in Göttingen with a knack for helping physicists with mathematics). He asked if there was a "spinor calculus" similar to the vector calculus of relativity. van der Waerden took up the challenge and created in 1929 the nowadays standard "dotted and undotted" spinor formalism with two-component spinors ψ^a and $\chi_{\dot{a}}$ where $a = 1,2$ and $\dot{a} = 1,2$.

[5] In flat space there is no distinction between curved indices μ and flat indices m, so in flat space we shall use them interchangeably.

with respect to ψ one finds the Dirac equation for $\overline{\psi}$

$$\left[(\partial_\mu \overline{\psi})\gamma^\mu - \frac{mc}{\hbar}\overline{\psi}\right] = 0 \tag{11.9}$$

One can also obtain the Dirac equation for $\overline{\psi}$ from (11.3) by taking the hermitian conjugate of (11.3) and multiplying by $i\gamma^0$.

The Dirac action is hermitian

$$\begin{aligned}\left[\overline{\psi}\left(\gamma^\mu \partial_\mu + \frac{mc}{\hbar}\right)\psi\right]^\dagger &= \psi^\dagger\left(\gamma_\mu \overleftarrow{\partial}_\mu + \frac{mc}{\hbar}\right) i\gamma^0\psi \\ &= \overline{\psi}\left(-\gamma^\mu \overleftarrow{\partial}_\mu + \frac{mc}{\hbar}\right)\psi \\ &= \overline{\psi}\left(\gamma^\mu \partial_\mu + \frac{mc}{\hbar}\right)\psi + \text{total derivative}\end{aligned} \tag{11.10}$$

(We used a useful notation: $(\gamma^\mu)^\dagger = \gamma_\mu$, which contains both $(\gamma^k)^\dagger = \gamma^k = \gamma_k$ and $(\gamma^0)^\dagger = -\gamma^0 = \gamma_0$.) It is also invariant under rigid Lorentz transformations. Minimal electromagnetic coupling is introduced by replacing ∂_μ by $\partial_\mu - \frac{ie}{\hbar c}A_\mu$ with $e < 0$ for an electron, and together with the Maxwell action, this yields the action for QED.

One can easily generalize these arguments to n-dimensional Minkowski space. All one needs is matrices γ^μ again satisfying $\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}$, but where now μ runs from 0 to $n-1$. In the next section we show that such matrices exist for any n, and we use group theory to determine whether the set of these matrices is unique. As we shall see, in n-dimensions the Dirac matrices are $2^{[\frac{n}{2}]} \times 2^{[\frac{n}{2}]}$ matrices. For example, 4×4 matrices in 4 or 5 spacetime dimensions and 2×2 matrices in 2 or 3 spacetime dimensions. (The symbol $[\frac{n}{2}]$ denotes the integer that is equal or less than $\frac{n}{2}$. So for $n = 3$ the symbol $[\frac{n}{2}]$ is equal to 1.) We shall also consider n-dimensional Euclidean space.

11.2 Clifford algebras and Dirac groups

We shall now study whether the solution Dirac found for the matrices γ^m is unique, and also discuss similar questions in higher (and lower) dimensions, both for Euclidean, and Minkowski spaces, in fact for spaces with s space coordinates and t time coordinates. To study the reality properties of the Dirac matrices, we could use the Frobenius-Schur theorem for the reality properties of irreducible representations (irreps) of finite groups, but a much simpler method is to consider a particular explicit matrix representations. Since the reality properties of Dirac matrices are unchanged by similarity transformations (as we shall discuss) it is sufficient to study one particular representation. For applications to Kaluza-Klein dimensional reduction, it simplifies the analysis greatly if one uses a particular representation. We shall define Majorana, Weyl, Majorana-Weyl, symplectic Majorana, and symplectic Majorana-Weyl spinors. To define Majorana spinors we must impose a reality condition on spinors, and for that we need the charge conjugation matrix (actually, two matrices in even dimensions as we shall see).

What has all this to do with group theory? The connection is as follows: To define an abstract Dirac group one needs a set of group elements and a group multiplication. The group elements are obtained by forming products of γ^μ, and products of these products, etc., simplifying the expressions we get by using the Clifford algebra, until the process closes (until we find no more new elements). This defines both the set of abstract group elements and the multiplication table of all these elements. The set of all these elements forms a finite group (perhaps not known to Dirac, but certainly to Pauli) which we call the Dirac group.

We begin in Euclidean space, and assume that there exist matrices γ^μ satisfying $\gamma^\mu\gamma^\nu+\gamma^\nu\gamma^\mu = 2\delta^{\mu\nu}I$. We view these γ^μ as abstract elements of a group. We take I as the unit element e of the group and γ^μ as the first n elements. The products $\gamma^\mu\gamma^\nu$ for $\mu<\nu$ are $\frac{1}{2}n(n-1)$ new elements, and $\gamma^\nu\gamma^\mu=-\gamma^\mu\gamma^\nu$ for $\mu\neq\nu$ are different elments from $+\gamma^\mu\gamma^\nu$. (In an algebra one can add and multiply, but in a group one can only multiply, thus $-\gamma^\mu\gamma^\nu$ is a different element from $\gamma^\mu\gamma^\nu$. For simplicity though, we keep writing $-\gamma^\mu\gamma^\nu$ instead of inventing new names like $(\gamma^\mu\gamma^\nu)'$.) Having obtained the element $\gamma^1\gamma^2$, we can multiply it with γ^1 in two ways: $\gamma^1\gamma^1\gamma^2=(\gamma^1\gamma^1)\gamma^2=\gamma^2$ and $\gamma^1\gamma^2\gamma^1=\gamma^1(-\gamma^1\gamma^2)=-\gamma^2$. Thus we find also a new set of n elements $-\gamma^\mu$. Going on in this way we get the following set of elements

$$G=\{\pm e, \pm\gamma^\mu, \pm\underset{\mu<\nu}{\gamma^\mu\gamma^\nu}, \pm\underset{\mu_1<\mu_2<\mu_3}{\gamma^{\mu_1}\gamma^{\mu_2}\gamma^{\mu_3}}, \cdots, \pm\gamma^1\gamma^2\cdots\gamma^n\} \tag{11.11}$$

Products with more than n γ-symbols can be reduced to expressions with less than (or equal to) n γ-symbols using the Clifford algebra. This set of elements forms a group, with e the unit element. Closure holds by construction. Since $(\gamma^\mu)^2=+I=e$, $(\gamma^\mu)^{-1}$ is equal to γ^μ (so the group elements γ^μ have order 2). We shall look for matrix representations, and matrix multiplication is associative, so we also assume that the multiplication of the abstract objects γ^μ is associative. (In fact, we already tacitly used associativity to obtain (11.11).) Thus we have a group and it is of order 2^{n+1} $\Big($namely order $G=2\left(1+\binom{n}{1}+\binom{n}{2}+\cdots+\binom{n}{n}\right)=2^{n+1}\Big)$

$$\text{Order } G = 2^{n+1}.$$

The first question to be settled is: what are the classes of this group? Since $\gamma^1\gamma^2\gamma^1=-\gamma^2$, a class with γ^2 contains also $-\gamma^2$. Going on in this way one finds that all classes, except the classes with e and $-e$, and $\pm\gamma^1\gamma^2\cdots\gamma^n$, contain two elements

$$+\gamma^{\mu_1}\cdots\gamma^{\mu_k} \text{ and } -\gamma^{\mu_1}\cdots\gamma^{\mu_k} \quad \text{for } \mu_1<\mu_2<\cdots<\mu_k \text{ with } 1<k<n.$$

The exceptions are the maximal elements $\pm\gamma^1\cdots\gamma^n$. Here it matters whether n is even or odd. If n is even one has for any γ^k that $\gamma^k\gamma^1\cdots\gamma^n\gamma^k=-\gamma^1\cdots\gamma^n$, hence both elements form one class.

But if n is odd, one has $\gamma^k\gamma^1\cdots\gamma^n\gamma^k = \gamma^1\cdots\gamma^n$. (Example: if $n=2$ one has $\gamma^k\gamma^1\gamma^2\gamma^k = -\gamma^1\gamma^2$ for any $k=1,2$, but for $n=3$ one has $\gamma^k\gamma^1\gamma^2\gamma^3\gamma^k = \gamma^1\gamma^2\gamma^3$ for any $k=1,2,3$.) Hence the class structure is as follows

$$\begin{aligned}\text{Even } n &: G = \{e, -e, \pm\gamma^\mu, \pm\gamma^\mu\gamma^\nu, \cdots, \pm\gamma^1\cdots\gamma^n\} : 2^n+1 \text{ classes} \\ \text{Odd } n &: G = \{e, -e, \pm\gamma^\mu, \cdots, \gamma^1\cdots\gamma^n, -\gamma^1\cdots\gamma^n\} : 2^n+2 \text{ classes}\end{aligned}$$

The next question to be settled is: what is the commutator subgroup $C(G)$? (The group generated by all elements of the form $g_1g_2g_1^{-1}g_2^{-1}$.) Since all group elements square to $\pm e$ one has for $k\neq l$ that $\gamma^k\gamma^l(\gamma^k)^{-1}(\gamma^l)^{-1} = \gamma^k\gamma^l\gamma^k\gamma^l = -\gamma^k\gamma^l\gamma^l\gamma^k = -e$. Hence $C(G)$ contains only two elements

$$C(G) = \{e, -e\} \tag{11.12}$$

Then $\frac{\text{order}G}{\text{order } C(G)} = \frac{2^{n+1}}{2} = 2^n$, and group theory tells us that there are 2^n one-dimensional irreps of the group. These one-dimensional irreps of the Dirac **group** do not satisfy $\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 0$ for $\mu\neq\nu$ (because for numbers a and b the relation $ab+ba=0$ implies $a=0$ and/or $b=0$), hence they are not a representation of the Clifford **algebra**. **Only the higher-than-one-dimensional irreps can be used in the Dirac equation.**

Using another group formula, order $G = \sum_i (\dim R^i)^2$, where R_i are the dimensions of the irreducible matrix representations (irreps) of G, and a third group formula: the number n_I of irreps is equal to the number n_C of classes, we find

$$\begin{aligned}\text{Even n} &: 2^{n+1} = \underbrace{1^2+\cdots+1^2}_{2^n \text{ squares}} + x^2 \quad \text{since} \quad n_C = n_I = 2^n+1 \\ \text{Odd n} &: 2^{n+1} = \underbrace{1^2+\cdots+1^2}_{2^n \text{ squares}} + x^2 + y^2 \quad \text{since} \quad n_C = n_I = 2^n+2\,.\end{aligned}$$

There is only one solution: $x = 2^{\frac{n}{2}}$ for even n and $x = y = 2^{\frac{n-1}{2}}$ for odd n. Thus for even $n=2k$ there is a unique $2^k\times 2^k$ matrix representation (up to equivalence), but for odd $n=2k+1$, there are two inequivalent irreps, both of dimension $2^k\times 2^k$. It is actually easy to find these two irreps in odd $2k+1$ dimensions from the unique irrep in even $n=2k$ dimensions. Denoting in even dimensions the matrix $\alpha\gamma^1\cdots\gamma^n$ by γ_c (c for chiral; for $n=4$ one often calls this matrix γ_5) and fixing α (up to a sign) by requiring that $\gamma_c^2 = +I$, we get the two irreps of the next odd dimension by adding $+\gamma_c$ or $-\gamma_c$ to the set of $n=$ even matrices γ^μ. The set $\{\gamma^\mu, -\gamma_c\}$ is inequivalent to the set $\{\gamma^\mu, \gamma_c\}$ as we shall shortly show. Thus these are the two inequivalent irreps for odd n. For example, if for $n=2$ we have γ^1, γ^2 (for example σ^1,σ^2 or σ^1,σ^3) then $\gamma_c = -i\gamma^1\gamma^2$ is a new abstract group element for $n=3$, and one gets two irreps for $n=3$, namely the irrep generated by $\{\gamma^1,\gamma^2,\gamma_c\}$ and the irrep generated by $\{\gamma^1,\gamma^2,-\gamma_c\}$.

Why are these two irreps inequivalent in odd dimensions? Suppose they were equivalent, then there should be a matrix S such that $\gamma^k = S\gamma^k S^{-1}$ for $k = 1, \cdots, n$ (even n) and also $S\gamma_c S^{-1} = -\gamma_c$. But since $\gamma_c = \alpha\gamma^1 \cdots \gamma^n$, one gets $S\gamma_c S^{-1} = \alpha(S\gamma^1 S^{-1}) \cdots (S\gamma^n S^{-1}) = \alpha\gamma^1 \cdots \gamma^n = +\gamma_c$. This contradicts the assumption. Thus they are inequivalent. In the same way one may prove that the irreps generated by $\{\gamma^1, \cdots, \gamma^n, \gamma_c\}$ and $\{-\gamma^1, \cdots, -\gamma^n, -\gamma_c\}$ are inequivalent. (So the set $(-\gamma^1, \cdots, -\gamma^n, -\gamma_c)$ should be related to the set $(\gamma^1, \cdots, \gamma^n, -\gamma_c)$ by a similarity transformation. It is clear that the similarity matrix is γ_c.)

In practice one can build explicit irreps in higher dimensions from known irreps in lower dimensions. A most useful construction starts in 7-dimensional Euclidean space with a set of seven 8×8 purely imaginary Dirac matrices which we denote by $\gamma^{(7)}$ (so $\gamma^{(7)}$ denotes the whole set). We shall prove that such a representation exists, and present an explicit representation below. Then the matrices $\gamma^{(7)} \times \sigma_2$ and $I \times \sigma_1$ form a set of 8 real 16×16 block off-diagonal Dirac matrices, which we denote by $\gamma^{(8)}$

$$\gamma^{(8)} = \left\{ \begin{pmatrix} 0 & -i\gamma^{(7)} \\ i\gamma^{(7)} & 0 \end{pmatrix}_{16\times16} , \quad \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}_{16\times16} \right\} \tag{11.13}$$

The chirality matrix $\gamma_c^{(8)}$ for the set $\gamma^{(8)}$ is given by $\left(\begin{smallmatrix} I & 0 \\ 0 & -I \end{smallmatrix}\right)$.[6] Then the matrices $\gamma^{(8)}$ and $\gamma_c^{(8)}$ form a set of 9 real 16×16 Dirac matrices in 9-dimensional Euclidean space (a Majorana representation), which we denote by $\gamma^{(9)}$. In 10 Euclidean dimensions we take $\gamma^{(9)} \times \sigma_1$ and $I \times \sigma_3$ which forms a set $\gamma^{(10)}$ of 10 real 32×32 matrices. In $d = 9+1$ dimensional Minkowski space we take instead $\gamma^{(9)} \times \sigma_1$ and $I \times i\sigma_2$ which yields again a real (Majorana) representation of the ten Dirac matrices. The 32×32 chirality matrix $\gamma_c^{(10)}$ in ten (Euclidean or Minkowskian) dimensions is real and diagonal $\left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$. Then the set $\gamma^{(9)} \times \sigma_1$, $I \times i\sigma_2$ and $\gamma_c^{(10)}$ gives a real (Majorana) irrep of the Dirac matrices in 11-dimensional Minkowski space. We stop at 11 dimensions because the highest dimension where a supersymmetric field theory exists is 11 (this theory is 11-dimensional supergravity).

For Euclidean dimensions $n = 2, 3, 4, 5, 6$ it is easy to directly construct explicit expression for the Dirac matrices. In $n = 2$ we take two Pauli matrices (σ_1 and σ_2, or σ_1 and σ_3, or σ_2 and σ_3). In $n = 3$ we have $\sigma_1, \sigma_2, \sigma_3$ where $\sigma_3 = \gamma_c^{(2)} = -i\sigma_1\sigma_2$. (So $\alpha = -i$ in $\gamma_c^{(2)} = \alpha\gamma^1\gamma^2$. One needs the factor $-i$ to satisfy $\sigma_3^2 = I$.) In $n = 4$ we may use

$$\gamma^k = \begin{pmatrix} 0 & -i\sigma^k \\ i\sigma^k & 0 \end{pmatrix} \quad \text{for } k = 1, 2, 3\,; \qquad \gamma^4 = \begin{pmatrix} 0 & I \\ I & 0 \end{pmatrix}, \tag{11.14}$$

and in $n = 5$ we use the $\{\gamma_\mu^{(4)}, \gamma_c^{(4)}\}$ where $\gamma_c^{(4)} = \gamma^1\gamma^2\gamma^3\gamma^4 = \left(\begin{smallmatrix} I & 0 \\ 0 & -I \end{smallmatrix}\right)$. Finally, in $n = 6$ Euclidean space we can either take $\gamma_\mu^{(5)} \times \sigma_1$ and $I \times \sigma_2$, or we may drop one of the matrices in the set $\gamma_\mu^{(7)}$ to obtain $\gamma_\mu^{(6)}$.

So far we discussed Euclidean space. To obtain the Dirac matrices for Minkowski space one

[6] Define in $d = 7$ $\gamma^7 = -i\gamma^1 \cdots \gamma^6$, then $\gamma_7^2 = I$ and $\gamma^1 \cdots \gamma^7 = iI$. Then in $d = 8$ we get $\gamma_c^{(8)} = (\gamma^1 \otimes \sigma_2) \cdots (\gamma^7 \otimes \sigma_2)(I \otimes \sigma_1) = \gamma^1 \cdots \gamma^7 \otimes \sigma_2\sigma_1 = I \otimes \sigma_3$.

can multiply one of the Dirac matrices by $\pm i$; this becomes then the Dirac matrix γ^0 associated with the time coordinate, satisfying $(\gamma^0)^2 = -I$. If there are t time coordinates, one multiplies t Dirac matrices by $\pm i$.

It remains to prove that in $n = 7+0$ (seven-dimensional Euclidean space) a completely imaginary representation (irrep) of the Clifford algebra exists, and then to construct such an irrep. The Frobenius-Schur criterion for finite groups G states that

$$\sum_{g\in G} \chi(g^2) = \sigma \text{ order } G \qquad \text{with } \sigma = \pm 1, 0 \tag{11.15}$$

and for $\sigma = +1$ the irrep is real, for $\sigma = -1$ it is pseudoreal, while for $\sigma = 0$ it is complex. The symbol χ denotes the trace of the matrices. Now note that if the irrep is purely imaginary, then $i\gamma_\mu$ (with $\mu = 1, \cdots, 7$) is real. The Dirac group generated by $i\gamma_\mu$ has in seven dimensions the following $2 \times 2^7 = 256$ elements.

$$\begin{gathered} G = \{\pm e, \pm i\gamma_\mu, \pm\gamma_{\mu\nu}, \pm i\gamma_{\mu\nu\rho}, \pm\gamma_{\mu\nu\rho\sigma}, \pm i\gamma_{\mu\nu\rho\sigma\tau}, \pm\gamma_{\mu\nu\rho\sigma\tau\upsilon}, \pm\gamma_1\cdots\gamma_7\} \\ \text{order } G = 2(1+7+21+35)\times 2 = 256\,. \end{gathered} \tag{11.16}$$

The square of all these group elements is $+I$ or $-I$.

$$\begin{gathered} (i\gamma^\mu)^2 = -I\,, \qquad (\gamma_{\mu\nu})^2 = -I\,, \qquad (i\gamma_{\mu\nu\rho})^2 = +I\,, \qquad (\gamma_{\mu\nu\rho\sigma})^2 = +I\,, \\ (i\gamma_{\mu\nu\rho\sigma\tau})^2 = -I\,, \qquad (\gamma_{\mu\nu\rho\sigma\tau\upsilon})^2 = -I\,, \qquad (\gamma_1\cdots\gamma_7)^2 = +I\,. \end{gathered} \tag{11.17}$$

Then, since the Dirac matrices in 7 dimensions are 8×8 matrices we obtain

$$\sum_g \chi(g^2) = 2\times 8\times(1-7-21+35+35-21-7+1) = 256\,. \tag{11.18}$$

So, $\sigma = +1$, and the matrices $i\gamma_\mu$ generate a real representation of the Dirac group. Then the matrices γ_μ are indeed equivalent to purely imaginary matrices. The representation they generate is complex because the Frobenius-Schur criterion yields now

$$\sum_g \chi(g^2) = 2\times 8\times(1+7-21-35+35+21-7-1) = 0\,. \tag{11.19}$$

To construct an explicit representation (not needed, but a good exercise and in practice very useful), we proceed as follows. First we construct a real irrep in $d = 3+1$ (a Majorana irrep in 4-dimensional Minkowski space), then a real irrep in $d = 3+2$, and finally an imaginary irrep in $d = 6+0$. The 7th Dirac matrix is then obtained as $-i\gamma^1\gamma^2\cdots\gamma^6$.

A Majorana irrep of the Dirac matrices in $d = 3+1$ spacetime (unique up to similarity transformations) is given by

$$\gamma^1 = \sigma^2\times\sigma^2\,, \quad \gamma^2 = I\times\sigma^1\,, \quad \gamma^3 = I\times\sigma^3\,, \quad \gamma^0 = \sigma^1\times(-i\sigma^2)\,. \tag{11.20}$$

One may check that they satisfy the Clifford algebra $\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}$. It is easily extended to the case $d = 3+2$ by adding

$$\gamma^5 = \sigma^3 \times (-i\sigma^2) \qquad \big(\text{real, and } (\gamma^5)^2 = -1\big) \tag{11.21}$$

(In fact, $\pm\gamma^5$ give the two inequivalent irreps; we continue with $+\gamma^5$.) We can use these five real matrices to obtain 5 of the 6 purely imaginary Dirac matrices Γ^M in $d = 6+0$: just tensor $\gamma^1, \gamma^2, \gamma^3$ with σ^2, and γ^0, γ^5 with iI

$$\Gamma^1 = \gamma^1 \times \sigma^2\,, \quad \Gamma^2 = \gamma^2 \times \sigma^2\,, \quad \Gamma^3 = \gamma^3 \times \sigma^2\,, \quad \Gamma^4 = \gamma^0 \times iI\,, \quad \Gamma^5 = \gamma^5 \times iI\,. \tag{11.22}$$

They all square to unity and are imaginary. There should be a sixth completely imaginary matrix Γ^6 which also squares to unity, and which anticommutes with the five Γ's obtained so far. By some trial and error one finds

$$\Gamma^6 = \sigma^2 \times I \times \sigma^3 \tag{11.23}$$

(The part $\sigma^2 \times I$ commutes with $\gamma^1, \gamma^2, \gamma^3$ but anticommutes with γ^0 and γ^5, while the part σ^3 anticommutes with the σ^2 in (11.22) and commutes with the iI in (11.22).) Having obtained 6 of the 7 imaginary Dirac matrices for $d = 7+0$, the seventh matrix is automatically obtained: it is proportional to the chirality matrix in six dimensions

$$\Gamma^7 = -i\Gamma^1 \cdots \Gamma^6 \tag{11.24}$$

We need the i in $-i\Gamma^1 \cdots \Gamma^6$ in order that $(\Gamma^7)^2 = I$, and with this factor i the matrix Γ^7 is also purely imaginary. Thus we have indeed constructed an explicit imaginary representation of the Dirac matrices in 7 Euclidean dimensions. For convenience we summarize it here

$$\begin{gathered}\Gamma^1 = \sigma^2 \times \sigma^2 \times \sigma^2\,, \qquad \Gamma^2 = I \times \sigma^1 \times \sigma^2\,, \qquad \Gamma^3 = I \times \sigma^3 \times \sigma^2\,, \qquad \Gamma^4 = \sigma^1 \times \sigma^2 \times I\,, \\ \Gamma^5 = \sigma^3 \times \sigma^2 \times I\,, \qquad \Gamma^6 = \sigma^2 \times I \times \sigma^3\,, \qquad \Gamma^7 = \sigma^2 \times I \times \sigma^1\,.\end{gathered} \tag{11.25}$$

Any other representation of the Dirac matrices in 7 Euclidean dimensions is obtained from this by a similarity transformation, and adding or not adding a minus sign to Γ^7.

Exercise. In which Minkowskian or Euclidean dimensions does a completely imaginary representation of the Dirac matrices exist?

11.2.1 D_4, Q_4 and the Dirac group in $d = 2$

The group D_4 and Q_4 are the only nonabelian groups of order 8. The Dirac group in two Euclidean dimensions $Dir(2)$ is the group generated by σ_1 and σ_2 it is also nonabelian and of order 8, hence $Dir(2)$ is isomorphic to either D_4 or Q_4. Further, the Dirac group in two-dimensional Minkowski space $Dir(1,1)$ is generated by σ_1 and $i\sigma_2$, and we want to find out whether $Dir(1,1)$ is equivalent to D_4 or Q_4. All four groups D_4, Q_4, $Dir(2)$ and $Dir(1,1)$ have a faithful two-dimensional irrep. We shall use these irreps to establish the isomorphisms.

The group elements and their 2×2 matrix irrep are as follows.

***D*₄.**

$$\begin{array}{cccccccc} e & R(\pi) & \big(R(\frac{\pi}{2}) & R(-\frac{\pi}{2})\big) & \big(\sigma_x & \sigma_y\big) & \big(\sigma_d & \sigma_{ad}\big) \\ I & -I & -i\sigma_2 & i\sigma_2 & \sigma_3 & -\sigma_3 & \sigma_1 & -\sigma_1 \end{array} \tag{11.26}$$

Here $R(\phi)$ denotes a rotation over an angle ϕ, σ_x and σ_y denote reflections about the x- and y-axis, and σ_d (σ_{ad}) denote a reflection about the diagonal (anti-diagonal) in the xy plane. We have indicated the classes by parentheses, so D_4 has 5 classes. This representation is clearly unitary and faithful.

Q_4. The quaternion group with group elements $(\pm E, \pm I, \pm J, \pm K)$ satisfying $I^2 = J^2 = K^2 = -E$ and $IJ = K$, $JK = I$, $KI = J$ is represented by the following 2×2 matrices

$$\begin{array}{cccccccc} E & -E & I & -I & J & -J & K & -K \\ I & -I & -i\sigma_1 & i\sigma_1 & -i\sigma_2 & i\sigma_2 & -i\sigma_3 & i\sigma_3 \end{array} \tag{11.27}$$

This representation is also unitary and faithful. The 8 group elements form a finite subgroup of $SU(2)$.

$Dir(2)$. The Dirac group in two Euclidean dimensions is generated by σ_1 and σ_2 and has the following group elements and representation

$$\begin{array}{cccccccc} e & -e & \gamma_1 & -\gamma_1 & \gamma_2 & -\gamma_2 & \gamma_1\gamma_2 & -\gamma_1\gamma_2 \\ I & -I & \sigma_3 & -\sigma_3 & \sigma_1 & -\sigma_1 & i\sigma_2 & -i\sigma_2 \end{array} \tag{11.28}$$

It is unitary and faithful.

$Dir(1,1)$. Finally the Dirac group in two-dimensional Minkowski space is generated by σ_1 and $i\sigma_2$ and we obtain

$$\begin{array}{cccccccc} e & -e & \gamma_1 & -\gamma_1 & i\gamma_2 & -i\gamma_2 & \gamma_1 i\gamma_2 & \gamma_1(-i\gamma_2) \\ I & -I & \sigma_1 & -\sigma_1 & i\sigma_2 & -i\sigma_2 & -\sigma_3 & \sigma_3 \end{array} \tag{11.29}$$

By inspection we see that D_4, $Dir(2)$ and $Dir(1,1)$ all contain the same set of 8 matrices, and after establishing which group elements of D_4 correspond to which group elements of $Dir(2)$ and $Dir(1,1)$, we see that both $Dir(2)$ and $Dir(1,1)$ are isomorphic to D_4.

The group Q_4 is a finite subgroup of $SU(2)$, but D_4 is not a subgroup of $SU(1,1)$. (For example, the determinant of σ_3 and σ_1 is not equal to $+1$. The matrix σ_3 is a generator of $SU(1,1)$ and a group element of Q_4.) Several interesting questions now arise: what are all finite subgroups of

$SU(2)$; is also D_4 a finite subgroup of a Lie group; what are the finite subgroups of other (simple) Lie groups?

11.3 Charge conjugation matrices and Majorana spinors

In this section we define and discuss the charge conjugation matrices and Majorana spinors in a spacetime with d dimensions, of which n_s dimensions are spacelike and n_t dimensions are timelike. The reader only interested in the results may consult table 11.1 below and the discussion after it.

A Majorana spinor λ is a spinor whose Majorana conjugate is equal to its Dirac conjugate. To use this definition of a Majorana spinor we must thus first define and discuss what the Majorana conjugate and the Dirac conjugate of a spinor are.

We shall begin by considering massless spinors λ, whose field equations read $\gamma^\mu \partial_\mu \lambda = 0$, because this is what one usually needs in supersymmetry, supergravity and string theory. Afterwards, we shall consider massive spinors. Although we will only discuss the case of spinors, the same results hold for spin $\frac{3}{2}$ vector-spinors, etc. Because of the masslessness of the spinors, there is a more general definition for the charge conjugation matrix than one usually encounters outside supersymmetric environments. This more general definition is only possible for massless spinors, just as one can only impose the Weyl condition for massless spinors. In fact, we shall also determine in which dimensions $d = (n_s, n_t)$ one can have Majorana-Weyl spinors.

The Dirac conjugate of a spinor λ is given by

$$\overline{\lambda}_D = \lambda^\dagger (i^\sigma \gamma^1 \cdots \gamma^{n_t}) \,, \quad \sigma = \tfrac{1}{2} n_t (n_t - 1) + 1 \tag{11.30}$$

if there are n_t time coordinates, and $(\gamma^1)^2 = \cdots = (\gamma^{n_t})^2 = -1$. The usual definition $\overline{\lambda}_D = \lambda^\dagger i \gamma^0$ in 4-dimensional Minkowski spacetime is the case $n_t = 1$ and in Euclidean space this formula gives $\overline{\lambda}_D = i\lambda^\dagger$.[7] This definition of $\overline{\lambda}_D$ follows from requiring that the Dirac action be hermitian and $\overline{\lambda}_D \chi$ for two spinors λ and χ should transform as a scalar under rigid Lorentz transformations, or, equivalently, that $\overline{\lambda}_D$ transforms as follows under infinitesimal rigid Lorentz transformations

$$\delta_L \overline{\lambda}_D = -\tfrac{1}{4} \overline{\lambda}_D \gamma^m \gamma^n \omega_{mn} + \text{orbital part} \tag{11.31}$$

if $\delta_L \lambda = \frac{1}{4} \omega_{mn} \gamma^m \gamma^n \lambda + \text{orbital part}$. Since the matrices $\gamma^1, \cdots, \gamma^{n_t}$ are antihermitian, one needs the matrices $\gamma^1 \gamma^2 \cdots \gamma^{n_t}$ in $\overline{\lambda}_D$ to achieve this.[8]

The Majorana conjugate $\overline{\lambda}_M$ of a spinor is given by $\overline{\lambda}_M = \lambda^T C$ where C is a constant matrix, called the charge conjugation matrix. In order that $\overline{\lambda}_M$ satisfies the same Dirac equation as the

[7] To keep the notation simple, we write $\lambda^\dagger i \gamma^1 \cdots \gamma^{n_t}$ for the general case and $\lambda^\dagger i \gamma^0$ for the Minkowski case.

[8] Requiring that the Dirac action be hermitian up to boundary terms one obtains $[-\lambda^\dagger i^\sigma \gamma^1 \cdots \gamma^{n_t} \gamma^\mu \partial_\mu \lambda]^\dagger = \lambda^\dagger (i^\sigma)^* \gamma^{n_t} \cdots \gamma^1 \gamma^\mu \partial_\mu \lambda +$ total derivative. Using $\gamma^{n_t} \cdots \gamma^1 = (-1)^{\frac{1}{2} n_t (n_t - 1)} \gamma^1 \cdots \gamma^{n_t}$, one obtains $\sigma = \frac{1}{2} n_t (n_1 - 1) + 1$.

Dirac conjugate $\overline{\lambda}_D$, namely $(\overline{\lambda}_M)\gamma^m\overleftarrow{\partial}_m = 0$, the matrix C must satisfy

$$C\gamma^m C^{-1} = \alpha(\gamma^m)^T \tag{11.32}$$

where α is a constant. To see this, one transposes $\gamma^m\partial_m\lambda$, inserts CC^{-1} and multiplies by C from the right, to obtain $\overline{\lambda}_M(C^{-1}\gamma^{m,T}C)\overleftarrow{\partial}_m = 0$, from which one deduces (11.32). Actually, by squaring (11.32) and using $\gamma^m\gamma^m = \gamma^{m,T}\gamma^{m,T} = \pm 1$ (no sum over m) one deduces that $\alpha^2 = +1$. Thus, there seem **two** charge conjugation matrices possible, for $\alpha = +1$ and $\alpha = -1$. We shall denote them by C_+ and C_- and thus

$$C_+\gamma^m C_+^{-1} = +(\gamma^m)^T, \quad C_-\gamma^m C_-^{-1} = -(\gamma^m)^T \tag{11.33}$$

We shall see that in even d there exist both a C_+ and a C_-, but in odd d there exists either a C_+ or a C_-, but not both.

It is clear that working with massive spinors leads to fewer possibilities for the charge conjugation matrix. Namely, if one requires that the Majorana conjugate spinor $\overline{\lambda}_M = \lambda^T C$ satisfies the same Dirac equation as the Dirac conjugate spinor $\overline{\lambda}_D = \lambda^\dagger(i\gamma^1\cdots\gamma^{n_t})$, and if λ satisfies $(\gamma^m\partial_m + M)\lambda = 0$, then one finds that

$$C\gamma^m C^{-1} = (-)^{n_t}(\gamma^m)^T \quad \text{(massive case)} \tag{11.34}$$

In particular, in Euclidean space ($n_t = 0$) only C_+ is allowed, while in Minkowski spacetime ($n_t = 1$) one can only use C_-.

We shall prove that in even d one has both a C_+ and a C_-, but in odd d one has either a C_+ or a C_-, but never both, by analyzing the finite group generated by products of the γ^m [1]. If one has in even d obtained C_+ or C_-, the other one is obtained by multiplication by γ_c, where γ_c is the chirality matrix, which is proportional to the product of all Dirac matrices and has a unit square, $\gamma_c^2 = +I$. (In $d = 4$, γ_c is often denoted by γ_5.) Moreover, in even d there is only one inequivalent irreducible representation (irrep) of the Clifford algebra whereas in odd d there are two irreps, which differ in the sign of one of the Dirac matrices. If $d = 2n + 1$, one obtains these irreps by taking the matrices γ^m for $d = 2n$ and adding plus or minus the chirality matrix γ_c for $d = 2n$. For example, in $d = 5$ the two irreps are $\{\gamma^m, \gamma_5\}$ and $\{\gamma^m, -\gamma^5\}$ where $m = 1, 2, 3, 4$ in the Euclidean case, and $m = 0, 1, 2, 3$ in the Minkowski case. The proofs of these facts were given before.

It is not always appreciated that one can always assume without loss of generality that the Dirac matrices satisfy $\{\gamma^m, \gamma^n\} = 2\eta^{mn}$ with the s spacelike matrices **hermitian** and the t timelike matrices **anti-hermitian**. The reason that this is possible is as follows [1]. First, consider d matrices satisfying $\{\gamma^m, \gamma^n\} = 2\delta^{mn}$. They generate a finite group, and can be taken to be unitary, because, as we have shown, any representation of a finite group can be made unitary by a similarity transformation. These unitary γ^m then still satisfy the Clifford algebra. Next, it follows from $(\gamma^m)^2 = +I$, that these unitary matrices γ^m are, in fact, hermitian. (If a unitary matrix is its own inverse, it is hermitian.) Finally, multiply t of the matrices by i, after which these matrices have become anti-hermitian.

One may now derive five properties

(i) $\overline{\lambda}_M$ and $\overline{\lambda}_D$ transform under Lorentz transformations in the same way, namely as $\delta\overline{\lambda} = \overline{\lambda}(-\frac{1}{2}\omega^{mn}\gamma_m\gamma_n) + \text{orbital part}$ when $\delta\lambda = \frac{1}{2}\omega^{mn}\gamma_m\gamma_n\lambda + \text{orbital part}$.

(ii) C_+ is either symmetric or antisymmetric. Similarly for C_-. (Proof: transpose (11.33) and iterate.)

(iii) C_+ can be scaled to be unitary. Idem for C_-. (Proof: complex conjugate (11.33) and iterate.)

(iv) $C_+\gamma^\mu$ is either symmetric or antisymmetric. Idem for $C_-\gamma^\mu$. (Proof: combine (11.33) with (ii).)

(v) The Dirac action for a massless anticommuting Majorana spinor is not a total derivative only if $C\gamma^\mu$ is symmetric. (For massive spinors a mass term is possible only if in addition C is antisymmetric.) Here C may be either C_+ or C_-. In addition there are the consistency conditions we shall now discuss.

We must now determine when we can satisfy the requirement that a spinor be a Majorana spinor, i.e., the requirement that $\overline{\lambda}_M = \lambda^T C$ is equal to $\overline{\lambda}_D$ in (11.30). Actually, one may replace this definition of a Majorana spinor by the weaker condition $\overline{\lambda}_M = \alpha\overline{\lambda}_D$ with α a constant; after some algebra one then discovers that $|\alpha| = 1$ and one may absorb the phase of α in λ such that one returns to $\overline{\lambda}_M = \overline{\lambda}_D$.

The definition of a Majorana spinor

$$\overline{\lambda}_D = \overline{\lambda}_M, \quad \overline{\lambda}_M = \lambda^T C, \quad \bar{\lambda}_D = \lambda^\dagger i^\sigma \gamma^1 \cdots \gamma^{n_t} \text{ with } \sigma = \tfrac{1}{2}n_t(n_t-1)+1 \tag{11.35}$$

with C either C_+ or C_- has a consistency condition. Namely, by solving (11.35) for λ^T ($\lambda^T = \overline{\lambda}_D C^{-1}$) and then complex conjugating one gets an expression for $\lambda^\dagger$. If one then uses (11.35) again to solve this time for $\lambda^\dagger$

$$\lambda^\dagger = \overline{\lambda}_M \gamma^{n_t} \cdots \gamma^1 (-1)^{n_t} (i^\sigma)^* \tag{11.36}$$

and equates this to $(\overline{\lambda}_D C^{-1})^*$, one obtains an equation relating C to C^*

$$C\gamma^{n_t} \cdots \gamma^1 = \gamma^{1,T} \cdots \gamma^{n_t,T} C^{-1,*} \tag{11.37}$$

Using a unitary C then relates C^T to C as follows

$$\begin{aligned} C_+^T &= (-)^{\frac{1}{2}n_t(n_t-1)} C_+ = (-)^{\left[\frac{1}{2}n_t\right]} C_+ \\ C_-^T &= (-)^{\frac{1}{2}n_t(n_t+1)]} C_- = (-)^{\left[\frac{1}{2}(n_t+1)\right]} C_- \end{aligned} \tag{11.38}$$

where the entire symbol "$[\cdots]$" denotes "take the integer part of $\cdots$". Thus, **massless Majorana spinors exist if and only if there exist either a C_+ or a C_- satisfying this condition**. In particular, in Euclidean space C_+ and/or C_- must be symmetric, while in Minkowski space C_+ must be symmetric but C_- must be antisymmetric. (If one has massive spinors, one must satisfy (11.38) and (11.34), instead of (11.38) and (11.33).)

If one requires that for these Majorana spinors an action exists, then, for anticommuting spinors, one must furthermore require that $C\gamma^\mu$ be symmetric, while for commuting spinors (which appear in Kaluza-Klein dimensional reduction) $C\gamma^\mu$ must be antisymmetric. (Otherwise the Lagrangian is a total derivative.) We shall below deduce for which $d = (n_s, n_t)$ these criteria can be met, but first we introduce the concept of Majorana-Weyl spinors.

In even d (with arbitrary n_s and n_t) Weyl spinors exist; they are defined by $\gamma_c\lambda = +\lambda$ (left-handed spinors), or $\gamma_c\lambda = -\lambda$ (right-handed spinors), where we recall that γ_c is the product of the d Dirac matrices multiplied by a phase such that $(\gamma_c)^2 = +I$. It is easy to show that chiral spinors are massless. Clearly, this condition is maintained in time: $\lambda(t + \Delta t) = \lambda(t) + \Delta t\gamma^0\gamma^k\partial_k\lambda(t)$ is again chiral if $\lambda(t)$ is chiral. Similarly one proves that the Majorana property is maintained in time. We note that these γ_c with square $+I$ are always hermitian. (For example, in $d = 2$ one has $\gamma_c = -i\tau^1\tau^2 = \tau^3$, in $d = 4$ one has $\gamma_c = \gamma^1\gamma^2\gamma^3\gamma^4$, etc.)

The consistency condition that a spinor be both a Majorana spinor and a Weyl spinor follows from $\overline{\lambda}_D = \overline{\lambda}_M$ by replacing on both sides λ by $\gamma_c\lambda$. One finds then $i\lambda^\dagger(\gamma_c)^\dagger\gamma^1\cdots\gamma^{n_t} = \lambda^T(\gamma_c)^T C$. Next one uses (11.36) to obtain

$$C\gamma^{n_t}\cdots\gamma^1(-)^{n_t}(\gamma_c)^\dagger\gamma^1\cdots\gamma^{n_t} = (\gamma_c)^T C \tag{11.39}$$

Using that γ_c is hermitian, we can move it to the left of $\gamma^1\cdots\gamma^{n_t}$, and contracting the $\gamma_1\cdots\gamma_t$ and using that their square is $-I$, yields $(-)^t C(\gamma_c)^\dagger = (\gamma_c)^T C$. Thus

$$\gamma_c = (-)^t C^{-1}(\gamma_c)^T C = \beta(-)^t\gamma_d\cdots\gamma_1 = (-)^{[\frac{d}{2}]+t}\gamma_c \tag{11.40}$$

because d is even (β is the phase which yields $(\gamma_c)^2 = +I$). We conclude that Majorana-Weyl spinors exist if (11.38) is satisfied and if further $[\frac{d}{2}]+t$ is zero modulo 2. The latter condition is satisfied in Euclidean space if $d = 1, 4, 5, 8, 9, \cdots$ and in Minkowski spacetime if $d = 2, 3, 6, 7, 10, 11, \cdots$. In fact, Majorana-Weyl spinors exist in Minkowski spacetime only if $d = 2$ mod 8, and in Euclidean space only in $d = 8$ mod 8.

We now determine in which $d = (s, t)$ one can have Majorana, or Majorana-Weyl spinors. Whereas we could in principle use abstract theorems to derive these results, we will use a property which makes it very easy to derive these results, and to remember the derivation. Namely, we shall use the fact that all results obtained so far are representation independent [1]. For example, if $\gamma'_m = S\gamma_m S^{-1}$, then $C = S^T C' S$ and C' and C have the same symmetry properties. Thus we shall in each dimension choose a particular convenient representation of the Dirac matrices, first with $(\gamma^m)^2 = +I$ in all d, and then multiply t of them by i to get the correct (anti)hermiticity properties and the correct η^{mn} in $\{\gamma^m, \gamma^n\} = 2\eta^{mn}$. Then we will explicitly check which properties hold.

In $d = 2$ and 3 dimensions, we will use two or all three Pauli matrices σ^i. The reader may practice their understanding of the results obtained so far by trying to reproduce the first two rows of table 11.1. (Taking as Dirac matrices in $d = 2$ the matrices σ_1 and σ_2, one finds $C_+ = \sigma_1$ and $C_- = \sigma_2$. In $d = 3$ one finds $C_- = \sigma_2$.) In $d = 4$ we will use the following representation

$$\vec{\gamma} = \begin{pmatrix} 0 & -i\vec{\sigma} \\ +i\vec{\sigma} & 0 \end{pmatrix}, \quad \gamma^4 = \begin{pmatrix} 0 & +I \\ +I & 0 \end{pmatrix}, \quad \gamma_c = \gamma_5 = \begin{pmatrix} +I & 0 \\ 0 & -I \end{pmatrix} \tag{11.41}$$

In $d = 5$ one then uses all these five matrices. In $d = 7$ there exists a purely imaginary representation (one could also use $\gamma^m \times \sigma^1$ with $m = 1, \cdots, 5$ and $I \times \sigma^2$ and $I \times \sigma^3$). An example of such a purely imaginary and hermitian representation of the Dirac matrices in $d = 7$ is given by the following set of 8×8 matrices

$$\Gamma(7) = \Big(\gamma_2 \times \sigma_2, \quad \gamma_4 \times \sigma_2, \quad \gamma_5 \times \sigma_2, \quad \gamma_1 \times I, \quad \gamma_3 \times I, \quad \gamma_1\gamma_3 \times i\sigma_1, \quad \gamma_1\gamma_3 \times i\sigma_3\Big) \tag{11.42}$$

We shall not use the explicit form of these matrices; it will be sufficient to know that such a purely imaginary irrep exists in $d = 7$. In $d = 6$ we drop one of these matrices, which then becomes the chirality matrix. In $d = 9$ we use

$$\Gamma(9) = \Big(\Gamma(7) \times \sigma_2, \quad I(7) \times \sigma_1, \quad I(7) \times \sigma_3\Big) \tag{11.43}$$

where $\Gamma(7)$ are the seven purely imaginary Dirac matrices of $d = 7$ and $I(7)$ is the unit 8×8 matrix in $d = 7$ spinor space. Thus, all matrices in $d = 9$ Euclidean space are real. Again, the same holds for $d = 8$ by dropping one of them. Finally, in $d = 11$ we use

$$\Gamma(11) = \Big(I(9) \times \sigma_2, \quad \Gamma(9) \times \sigma_1, \quad I(9) \times \sigma_3\Big) \tag{11.44}$$

while in $d = 10$ we drop the last matrix. Thus, in $d = 10$ we have in the Euclidean case one Dirac matrix purely imaginary and the rest real, whereas in the Minkowski case we have a Majorana representation where all Dirac matrices are real.

$$\Gamma(10) = \Big(I(9) \times \sigma_2, \quad \Gamma(9) \times \sigma_1\Big), \quad \gamma_c = I(9) \times \sigma_3 \tag{11.45}$$

It is now immediately clear that in $d = 11$ and $d = 10$ Minkowski spacetime real spinors exist (the Dirac operator is real). In this way one may derive the results in the table 11.1. Since all results are periodic with period 8, we have only given the results from $d = 2$ to $d = 11$ (we included both $d = 2$ and $d = 11$ for convenience).

When no Majorana spinors exist in a dimension $d = (s, t)$ (namely in $d = 3, 4, 5$ dimensional Euclidean space and in $d = 5, 6, 7$ dimensional Minkowski spacetime), one can always define

Dim.	Symmetry	Is $C\gamma_\mu$ symmetric?	Is C block diagonal?	Which spinors exist in which space? Eucl. M	Eucl. MW	Mink. M	Mink. MW	Irreps of γ^μ Eucl.	Irreps of γ^μ Mink.
2	$C_+^T = +C_+$	yes	no	yes	no	yes	yes	R	R
	$C_-^T = -C_-$	yes		no	–	yes	yes		
3	$C_-^T = -C_-$	yes		no	–	yes	–	C	R
4	$C_+^T = -C_+$	no	yes	no	–	no	–	P	R
	$C_-^T = -C_-$	yes		no	–	yes	no		
5	$C_+^T = -C_+$	no		no	–	no	–	P	C
6	$C_+^T = -C_+$	no	no	no	–	no	–	P	P
	$C_-^T = +C_-$	no		yes	no	no	–		
7	$C_-^T = +C_-$	no		yes	–	no	–	C	P
8	$C_+^T = +C_+$	yes	yes	yes	yes	yes	no	R	P
	$C_-^T = +C_-$	no		yes	yes	no	–		
9	$C_+^T = +C_+$	yes		yes	–	yes	–	R	R
10	$C_+^T = +C_+$	yes	no	yes	no	yes	yes	R	R
	$C_-^T = -C_-$	yes		no	–	yes	yes		
11	$C_-^T = -C_-$	yes		no	–	yes	–	C	R

Table 11.1: Majorana (M) and Majorana-Weyl (MW) spinors in Euclidean and Minkowski spacetimes. R, P, C denote a real, pseudoreal or complex irrep of the Dirac matrices.

modified Majorana spinors (also called symplectic Majorana spinors). For this one needs an even number of spinors, in pairs λ^i $(i = 1, 2)$, and one defines the Dirac conjugate as before, but the Majorana conjugate is now defined by

$$\overline{\lambda}^i_M \equiv (\lambda^j)^T \Omega_{ji} C, \quad \Omega_{ji} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{11.46}$$

where the matrix Ω is a symplectic matrix with two unit matrices off-diagonal. One may verify that with this definition the consistency condition for Majorana spinors gets an extra factor $\Omega^*\Omega = -I$ so that when no Majorana spinors exist in a given $d = (s, t)$, then symplectic Majorana spinors exist, and vice-versa. A Dirac action exists for anticommuting massless modified Majorana spinors if $C\gamma^\mu$ is antisymmetric, and mass term exists in the action if C is symmetric.

Suppose Majorana spinors exist in a given space with dimension $d = (s, t)$. Then, one can also define symplectic Majorana spinors **in the same space**. (This is useful to make the action of the R-symmetry group in the theory of supersymmetry on the spinors manifest. In particular, one can use this for $N = 2$ models in $d = (3, 1)$.) To prove this, assume that one has given an even number of Majorana spinors, say two, each satisfying the Majorana condition

$$\overline{\lambda}^i = (\lambda^i)^T C = (\lambda^i)^\dagger (i\gamma^1 \cdots \gamma^{n_t}) \tag{11.47}$$

Define next their chiral projections by

$$\lambda_L^i \equiv \tfrac{1}{2}(1+\gamma_c)\lambda^i, \quad \lambda_R^i \equiv \tfrac{1}{2}(1-\gamma_c)\lambda^i \tag{11.48}$$

For simplicity we from now on discuss the case of $d = (3,1)$. Then the Majorana condition can be rewritten on the chiral basis as follows

$$\begin{aligned} &(\zeta^i)^T C = (\zeta_i)^\dagger (i\gamma^0), \quad \zeta^i = \lambda_L^i, \quad \zeta_i = \lambda_R^i \\ &(\zeta_i)^T C = (\zeta^i)^\dagger (i\gamma^0) \quad \text{with} \quad C_\pm \gamma_5 = \gamma_5^T C_\pm \end{aligned} \tag{11.49}$$

Let us now define nonchiral spinors χ^i by

$$\chi^i \equiv \zeta^i + \epsilon^{ij}\zeta_j = \lambda_L^i + \epsilon^{ij}\lambda_R^j \tag{11.50}$$

It follows that χ^i are a pair of symplectic Majorana spinors but with the other charge conjugation matrix (namely $-C\gamma_5$ instead of C). The proof is straightforward, just substitute the definition of χ^i into

$$(\chi^i)^T \epsilon_{ij}(-C\gamma_5) = (\chi^j)^\dagger (i\gamma^0) \tag{11.51}$$

Summarizing, if in $d = (s,t)$ ordinary Majorana spinors exist using C, also symplectic Majorana spinors exist using $C\gamma_c$.

Finally, we come back to our promise to show that in even d always both a C_+ and a C_- exist, but in odd d only C_+ or C_-, while in even (odd) d there is one (two) irreducible representations (irreps) of the Clifford algebra. We begin by constructing a finite group G whose elements are $(+)$ or $(-)$ times products of Dirac matrices. For example in $d = 2$, this group has 8 elements and in $d = 4$ it has 32 elements. In general, G has order 2^{d+1}. We now use the following theorems of finite group theory [1]

(i) The number of irreps equals the number of classes.

(ii) The order of G equals the sum of the squares of the dimensions of all inequivalent irreps: $|G| = \sum_i (d_i)^2$.

(iii) The number of one-dimensional irreps of a finite group equals the order of G divided by the order of the commutator subgroup $C(G)$. (This is the group generated by all elements of the form $aba^{-1}b^{-1}$.)

We now apply these theorems separately to the cases d =even and d =odd.

$\boldsymbol{d} = \mathbf{even.}$ The number of classes is $2^d + 1$ ($+I$ and $-I$ are separate classes). The order of $C(G)$ is $+2$ (namely $C(G)$ contains $+I$ and $-I$). Hence

$$\text{order } G = 2^{d+1} = 2^d(1)^2 + (d_i)^2 \tag{11.52}$$

where d_i is the dimension of the unique irrep of G which is not one-dimensional. Clearly, $d_i = 2^{[\frac{d}{2}]}$.

$\boldsymbol{d} = \mathbf{odd.}$ The number of classes is now $2^d + 2$, because $+\gamma^1 \cdots \gamma^d$ and $-\gamma^1 \cdots \gamma^d$ both commute with all γ^m, hence with all group elements, hence form each separately a class. Again, order $C(G) = 2$. Thus the number of one-dimensional irreps is (again) 2^d. It follows that

$$\text{order } G = 2^{d+1} = 2^d(1)^2 + (d_i^1)^2 + (d_i^2)^2 \tag{11.53}$$

Clearly, there are **two** irreps which are not one-dimensional, each of dimension $2^{[\frac{d}{2}]}$. They can be obtained from each other by changing the sign in front of one of the Dirac matrices. (That these two irreps are inequivalent follows from Schur's lemma: if $S\gamma^m S^{-1} = \gamma^m$ for $m = 1, \cdots, d-1$, then S commutes with the irrep of $d-1$ dimensions, hence $S = I$, so that $S\gamma^d S^{-1}$ cannot be equal to $-\gamma^d$.) From a physicist's point of view, the changing of the sign in front of one of the Dirac matrices is equivalent to replacing the corresponding coordinate by minus itself which is the parity operation.

It may be noted that all one-dimensional irreps of the finite group G cease to be irreps of the Clifford algebra, since they do not satisfy $\gamma_m\gamma_n + \gamma_n\gamma_m = 0$ for $m \neq n$. On the other hand, the higher-dimensional irreps of G are faithful, and also form irreps of the Clifford algebra. The proof is straightforward: since the matrix $M(-e)$ which represents the group element $\gamma^1\gamma^2\gamma^1\gamma^2 =$"$-e$" commutes with all other matrices of the representation, $M(-e) = \alpha I$ according to Schur's lemma. Moreover, from $(-e)(-e) = e$ it follows that $\alpha = \pm 1$. If $M(-e) = +I$, then $M(\gamma_m)M(\gamma_n) = M(\gamma_n)M(\gamma_m)$, and hence the representation would be abelian and thus one-dimensional since it is irreducible. Thus $M(-e) = -M(e)$, and then one obtains indeed $M(\gamma_m)M(\gamma_n) + M(\gamma_n)M(\gamma_m) = 0$ if $m \neq n$.

Suppose the matrices γ^m form an irrep of the Clifford algebra in $d =$even dimensions then the matrices $A^m \equiv +(\gamma^m)^T$ and $B^m \equiv -(\gamma^m)^T$ also form a representation of the same abstract finite group G as is generated by the γ^m (because the group multiplication table is the same). It follows from the uniqueness of the irrep of G if $d =$even, that A^m and B^n are equivalent to γ^m,

$$C_+\gamma^m C_+^{-1} = +(\gamma^m)^T, \quad C_-\gamma^m C_-^{-1} = -(\gamma^m)^T \tag{11.54}$$

Thus in even d, both a C_+ and a C_- exist. In odd d, the situation is different because there are then two irreps, so $+(\gamma^m)^T$ or $-(\gamma^m)^T$ might be equivalent to $\overline{\gamma}^m$ (related to γ^m by switching the sign in front of one of the Dirac matrices) instead of being equivalent to γ^m. To study this further, start with the C_+ and C_- of the space with $d =$ even, and then evaluate

$$C_\pm \gamma_c C_\pm^{-1} = \gamma_1^T \cdots \gamma_d^T = \sigma \gamma_c \tag{11.55}$$

where $\sigma = +1$ or -1. If $\sigma = +1$, $C = C_+$ in $d+1 =$ odd dimensions, whereas if $\sigma = -1$ then $C = C_-$. Thus, in odd dimensions there is either a C_+ or a C_- but never both.

Since the $(\gamma^m)^*$ generate the same finite group as the γ^m both in Euclidean and in Minkowski space, they are in $d =$ even equivalent to the γ^m (because the irrep is unique in $d =$ even). Thus

$$S(\gamma^m)^* S^{-1} = \gamma^m \tag{11.56}$$

which shows that the Dirac matrices in even Euclidean or Minkowski d are what is called in group theory *pseudoreal* or *real*. Since in Euclidean space the γ^m are hermitian, S is in that case equal to C_+ if $C = C_+$. In Euclidean odd d without a C_+ (for example, in $d = 3$) the pseudoreality condition does not hold. Then the representation is what is called in group theory *complex*.

The spinor representation of the orthogonal groups can also be real, pseudoreal, or complex. In odd d, there is only one spinor irrep (up to similarity transformations), but in even d there are two spinor irreps, conventionally denoted by the super- or sub-scripts (s) and (c). In odd d, the spinor generators are $\frac{1}{2}\Gamma_{mn}$ where $\Gamma_{mn} = \frac{1}{2}(\Gamma_m\Gamma_n - \Gamma_n\Gamma_m)$ with Γ_m the Dirac matrices in odd dimensions. In even $d = 2k$, one may take as Dirac matrices in Euclidean space the set $\Gamma_M = (\gamma_m \otimes \sigma_2, I \otimes \sigma_1)$ where $M = 1, \cdots, 2k$ and $M = 1, \cdots, 2k-1$. Then the matrices $\frac{1}{2}\Gamma_{MN}$ form a reducible representation of the orthogonal group; in fact, they are block-diagonal with in one block the generators $(\frac{1}{2}\gamma_{mn}, -\frac{i}{2}\gamma_m)$ of the (s) representation, and in the other block the generators $(\frac{1}{2}\gamma_{mn}, \frac{i}{2}\gamma_m)$ of the (c) representation.

If the Dirac matrices in odd dimensions form a real or pseudoreal representation, also the spinor representation is real or pseudoreal, simply because the equation $(\gamma^m)^* = S^{-1}\gamma^m S$ implies $\frac{1}{2}(\gamma^{mn})^* = S^{-1}\frac{1}{2}\gamma^{mn}S$. But if the Dirac matrices in odd dimensions form a complex representation, the spinor representation can be complex or real; in $d = 3+0$ the Dirac irrep and the spinor irrep are both complex, but in $d = 7+0$ the Dirac irrep is complex but the spinor irrep is real.

To give another example, consider the cases $d = 5+0$, $4+1$, $3+2$. In $d = 5+0$, the Dirac irrep and the spinor irrep are both pseudoreal, but in $d = 4+1$ the Dirac irrep is complex and the spinor irrep in pseudoreal, while in $d = 3+2$ the Dirac irrep is real and hence the spinor irrep is also real.

11.3.1 Faithfulness of the representations of the Dirac group

The last issue we want to discuss is the faithfulness of the representations of the Dirac group. We shall go through the various dimensions case by case, which also allows a nice direct way and summary of the various reality properties discussed before.

- $d=2+0$: $\pm I, \pm\sigma_1, \pm\sigma_3, \pm\sigma_1\sigma_3 = \pm i\sigma_2$: faithful, real.
- $d=1+1$: $\pm I, \pm\sigma_1, \pm i\sigma_2, \pm\sigma_3$: faithful, real.
- $d=3+0$: $\pm I, \pm\sigma_1, \pm\sigma_2, \pm\sigma_3, \pm\sigma_1\sigma_2 = \pm i\sigma_3, \pm\sigma_2\sigma_3 = \pm i\sigma_1, \pm\sigma_3\sigma_1 = \pm i\sigma_2, \pm\sigma_1\sigma_2\sigma_3 = \pm iI$: faithful, complex ($\sum\chi(g^2) \sim 1+3-3-1=0$).
- $d=2+1$: $\pm I, \pm\sigma_1, \pm i\sigma_2, \pm\sigma_3, \pm\sigma_1 i\sigma_2 = \pm\sigma_3, \pm i\sigma_2\sigma_3 = \pm\sigma_1, \pm\sigma_1\sigma_3 = \pm i\sigma_2, \pm\sigma_1 i\sigma_2\sigma_3 = \pm I$: **not** faithful, real.
- $d=4+0$: faithful, pseudoreal ($\sum\chi(g^2) \sim 1+4-6-4+1<0$).
- $d=3+1$: faithful, real (see construction).
- $d=2+2$: faithful, complex ($\sum\chi(g^2) \sim 1+(1-1)+(2-4)+(1-1)+1=0$).
- $d=5+0$: not faithful, pseudoreal ($\sum\chi(g^2) \sim 1+5-10-10+5+1<0$).
- $d=4+1$: faithful, complex ($\sum\chi(g^2) \sim 1+(4-1)+(6-4)+(4-6)+(1-4)-1=0$).
- $d=3+2$: not faithful, real (see construction).
- $d=6+0$: faithful, pseudoreal ($\sum\chi(g^2) \sim 1+6-15-20+15+6-1<0$).
- $d=5+1$:
- $d=7+0$: faithful, complex (see construction).
- $d=6+1$:
- $d=8+0$: faithful, real (see construction).
- $d=7+1$: faithful, complex ($\sum\chi(g^2) \sim 1+(7-1)+(-21+7)+(-35+21)+(35-21)+(21-7)+(1-7)-1=0$).

Bibliography

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Chapter 12

Application II: Molecular Spectra

12.1 Introduction

Consider a molecule consisting of N atoms in 3-dimensional space. The atoms oscillate about their equilibrium positions (and absorb or emit electromagnetic radiation if certain conditions, to be discussed, are met). There are $3N$ coordinates to describe the positions of the N atoms, and thus also $3N$ normal modes with frequencies $\omega_1, \cdots, \omega_{3N}$. (Recall that by definition in a normal mode all atoms oscillate back and forth with the same frequency, and go through their equilibrium position at the same time). The three translations yield three zero frequencies, and the three rotations yield another three vanishing frequencies. Thus there are $3N-6$ genuine normal modes with nonzero frequencies. (For linear molecules in 3 dimensions there is one rotational zero mode less, so then there are $3N-5$ nonzero modes).

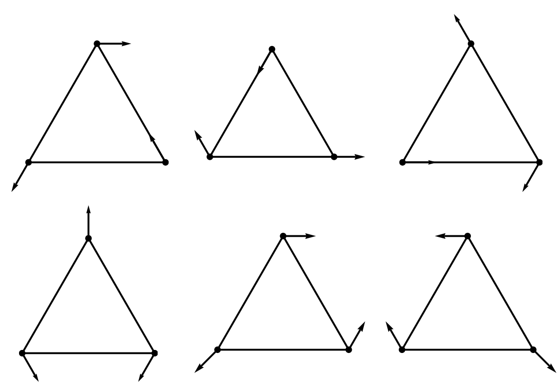


Figure 12.1: Top: three linearly dependent normal modes for a planar molecule with three identical atoms. The sum of all three motions vanishes, so any two of these normal modes can be used as a basis. For example, minus the sum of the last two yields the first one. All little arrows denote oscillations, and in the first three diagrams they are all parallel to a side of the triangle. Bottom: three other linear combinations whose sum again cancels. The frequency of the oscillations of all six diagrams is the same. In addition to any two of them, there is a third independent normal modes, the breather, where all atoms move radially in and out at the same time and with the same frequency, which is different from the frequency of the motion in the 6 diagrams.

Depending on the molecule, two or more frequencies may be degenerate. Group theory can be used to predict how many frequencies should be degenerate because normal modes form multiplets of the symmetry group of the molecule.[1] In principle, it is possible that the interatomic forces are precisely such that by accident more frequencies are degenerate, but in reality this finetuning will not happen if there is not a symmetry which enforces it. The normal modes are solutions of the linearized Lagrange equations of motion, but if one includes anharmonic terms (terms in the potential which are cubic and higher in the deviations from the equilibrium positions), there are interactions between the normal modes. It is known that for one single anharmonic pendulum the period of an oscillation starts depending on the amplitude. Furthermore, the time dependence is no longer a simple $\cos(\omega t)$ but rather a more complicated (but still periodic) function of time. If one has a molecule with N atoms and some of the normal modes are degenerate at the linearized level, it is no longer so clear whether degeneracy continues to hold at the nonlinear level; in fact, the whole concept of a normal mode may no longer exist. For example, the breather mode of a regular polyhedron will still have a periodic motion, but other modes will not be so symmetric, and periodicity may be lost. We enter here in the area of "chaos". We consider from now on only linearized equations of motion.

Let the positions of the atoms in an N atom molecule be given by $\vec{x}_j$ with $j = 1, ..., N$, and let $\vec{x}_j^{(0)}$ be their equilibrium positions. The N deviations $\vec{\xi}_j = \vec{x}_j - \vec{x}_j^{(0)}$ each lie in a 3-dimensional linear vector space $\mathbb{R}^3_j$ and their direct sum forms a vector $\vec{X} = (\vec{\xi}_1, ..., \vec{\xi}_N)$ in a $3N$ dimensional linear vector space which we call S. So $\vec{X}$ describes the deviations of the whole molecule. Normal modes labeled by J correspond to vectors $\vec{X}_J(t) = \cos(\omega_J t)\vec{X}_J^{(0)}$ which oscillate but whose direction $\vec{X}_J^{(0)}$ does not change.

Let us denote the $3N$ variables $\vec{\xi}_j$ with $j = 1, ..., N$ by ξ^α with $\alpha = 1, ..., 3N$. If the kinetic energy is given by $T = \sum_{\alpha=1}^{3N} \frac{1}{2} m_\alpha \dot{\xi}^\alpha \dot{\xi}^\alpha$ and the potential energy by $V = \sum_{\alpha,\beta} \frac{1}{2} k_{\alpha\beta} \xi^\alpha \xi^\beta$, we can rescale $\xi^\alpha = \frac{\eta^\alpha}{\sqrt{m_\alpha}}$, so that $T = \sum_{\alpha=1}^{3N} \frac{1}{2} (\dot{\eta}^\alpha)^2$. Then $V = \sum_{\alpha,\beta} \frac{1}{2} k'_{\alpha\beta} \eta^\alpha \eta^\beta$ (with $k_{\alpha\beta} = \sqrt{m_\alpha}\sqrt{m_\beta} k'_{\alpha\beta}$) can be diagonalized by an orthogonal transformation O:

$$\left(O^T\right)_I{}^\alpha k'_{\alpha\beta} \left(O\right)^\beta{}_J = \omega_J^2 \delta_{IJ} \text{ with } I, J = 1, ..., 3N. \tag{12.1}$$

Any orthogonal transformation keeps T diagonal, hence we have simultaneously diagonalized the

[1] To give a simple example, consider the motion of 3 identical atoms which form an equilaterial triangle in a plane. There are $3 \times 2 = 6$ degrees of freedom, with 2 translations and one rotation, so there are 3 genuine normal modes. These 3 modes form one singlet (one multiplet with one component) and one doublet (one multiplet with two components). So in this case there are two different nonzero frequencies. Physically it is clear what these modes are: the singlet is the "breather" where all atoms move simultaneously radially outward and inward. The doublet consists of any two of the motions depicted in figure 12.1. The sum of the three motions in figure 12.1 vanishes, thus two of them form a basis. The breather transforms into itself under all symmetry transformations of the triangle in its equilibrium position, but the two other modes transform into each other. Thus one gets one singlet and one doublet. Of course one can choose any basis for the doublet. For example, one could use the second diagram in figure 12.5 as a basis vector because it is a linear combination of the diagrams in figure 12.1 (namely the third diagram minus the second diagram).

two quadratic expressions T and V.

Since O is orthogonal, $\left(O^T\right)_I{}^\alpha = \left(O^{-1}\right)^I{}_\alpha$, we obtain $k'_{\alpha\beta}O^\beta{}_J = \omega_J^2 O^\alpha{}_J$, which can also be written as follows,

$$\left(k'_{\alpha\beta} - \omega_J^2\delta_{\alpha\beta}\right)O^\beta{}_J = 0 \tag{12.2}$$

The eigenvalues ω_J^2 are then given by the solutions of $\det\left(k' - \omega^2 I\right) = 0$, and the deviations of the atoms corresponding to a normal mode J with frequency ω_J are $\eta^\alpha_{(J)} = O^\alpha{}_J$, so $\xi^\alpha_{(J)} = \frac{1}{\sqrt{m_\alpha}}O^\alpha{}_J$. One can calculate the ω_J^2 and $O^\alpha{}_J$ by direct calculation, but this may be complicated, and the interactions between atoms may not be known exactly. Group theory yields information about the degeneracy of the ω_J^2, and also the symmetry or antisymmetry properties of the $\vec{X}_J$ under symmetry transformations, but not, of course, the values of ω_J^2 and $O^\alpha{}_J$. Some textbooks on molecular vibrations are given in references [1–6].

12.2 The spectrum of the H_2O molecule

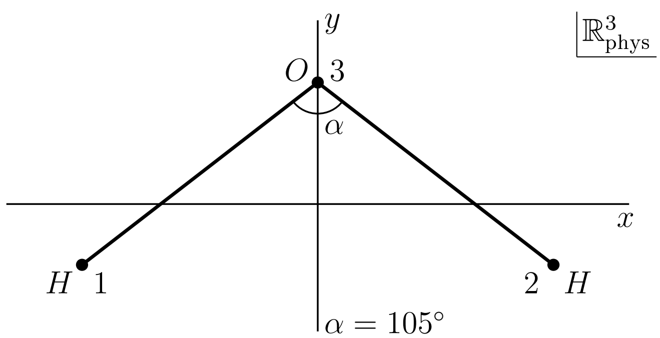


Figure 12.2: The H_2O molecule.

Consider as an example the H_2O molecule. This molecule has four symmetries at rest (when all deviations are set to zero): the transformation group G acting on the carrier space of the three atoms of the H_2O molecule contains four elements:

- $g_0 =$ identity.

- $g_1 = R_y(\pi) =$ a rotation over π along the y axis (the bissectix) through O and the center of mass. The latter we take as origin in the 3-dimensional space $\mathbb{R}^3_{\text{phys}}$ in which the molecule lies.

- $g_2 = \Sigma_{yz} =$ a reflection w.r.t. the y-z plane. (We take the z-axis perpendicular to the plane of the molecule in the equilibrium configuration.)

- $g_3 = \Sigma_{xy} =$ a reflection w.r.t the x-y plane.

We claim that these four elements form the group of four (sometimes written as V and called the Klein group, which is also the dihedral group D_2).[2] Clearly, $g_1^2 = g_2^2 = g_3^2 = g_0$. Note that g_1 maps a point (x, y, z) to $(-x, y, -z)$. Further $g_2(x, y, z) = (-x, y, z)$ and finally $g_3(x, y, z) = (x, y, -z)$. One may check the following relations by acting on points in the 3-dimensional space $\mathbb{R}^3_{\text{phys}}$ with coordinates (x, y, z)

$$g_1 g_2 = g_3 = g_2 g_1 \text{ , and cyclic equations} \tag{12.3}$$

This proves that G is the group of four ($V = (e, g_1) \otimes (e, g_2)$).

One can in general construct a matrix representation A of a symmetry group G in S as follows[3]. A given symmetry operation g moves atom s to atom $\pi_g s$, where the π_g are permutations of the N atoms. For example $\pi_{g_1} 1 = 2$, $\pi_{g_1} 2 = 1$, $\pi_{g_1} 3 = 3$. The deviation $\vec{\xi}_s$ of the atom at location s is mapped by g to a corresponding deviation $\vec{\xi'}_{\pi_g s}$ of the atom at the location $\pi_g s$. We defined g as a linear transformation on points with coordinates (x, y, z) in the 3-dimensional space $\mathbb{R}^3_{\text{phys}}$ in which the whole molecule is situated, but we can also define the action of g in a given subspace $\mathbb{R}^3_s$ of S by $g\vec{\xi}_s = \vec{\xi'}_{\pi_g s}$ where we view the vector $\vec{\xi'}_{\pi_g s}$ as a vector in $\mathbb{R}^3_s$. (So we put the infinitesimal vectors $\vec{\xi}_s$ and $\vec{\xi'}_{\pi_g s}$ at the origin of $\mathbb{R}^3_s$.) Then g acts simultaneously and the same way in all spaces $\mathbb{R}^3_s$ of the deviations $\vec{\xi}_s$ of each atom s. Consider a vector in the 3-dimensional space in which the molecule lies. We call this space the physical space $\mathbb{R}^3_{\text{phys}}$ and a vector with components $(x,\ y,\ z)$ in this space forms a representation. If we denote the 3×3 matrix representation of G in $\mathbb{R}^3_{\text{phys}}$ by $D^{\mathbb{R}^3_{\text{phys}}}(g)$, and in $\mathbb{R}^3_s$ by $D^{\mathbb{R}^3_s}(g)$, then for vectors $\vec{v}$ in $\mathbb{R}^3_s$ we have

$$D^{\mathbb{R}^3_{\text{phys}}}(g)\vec{v} = D^{\mathbb{R}^3_s}(g)\vec{v} \equiv D^{\mathbb{R}^3}(g)\vec{v} \quad \text{ with } \vec{v} \in \mathbb{R}^3_s \,. \tag{12.4}$$

We shall now construct the matrix representation A_g which acts in S. If before acting with a symmetry operation g on the molecule the deviations constitute the vector $\vec{X}$, and if after having made a symmetry operation on the molecule the new deviations constitute the vector $\vec{X}'$, we define

$$A_g \vec{X} = \vec{X}' \tag{12.5}$$

Since G is a transformation group acting on points in S, the set of $3N \times 3N$ matrices forms a (in general reducible) representation of G. This is intuitively clear: the result of a transformation of the deviations, followed by another transformation, yields a transformation of the deviations, but we shall give an explicit proof that one obtains a representation. We can also express this representation A_g in terms of the representation of g which acts in each $\mathbb{R}^3_s$. To do so, we introduce

[2]We define the dihedral group D_n of order $2n$ as the group of symmetries of a regular n-gon in the plane. Then the case $n = 2$ gives the symmetry of a line segment in the plane. The symmetry group of a line segment in 3 dimensions contains the continuous rotation group about the line segment, but we consider here the symmetry group of the H_2O molecule in 3 dimensions, which is V.

[3]We follow unpublished lectures by H. Freudenthal given at Utrecht University in 1959-1960.

projection operators P_s which project $\vec{X}$ onto $\vec{\xi}_s$

$$P_s\vec{X} = \vec{\xi}_s \tag{12.6}$$

Clearly $(P_1 \oplus \ldots \oplus P_N)\,\vec{X} = \vec{X}$. Here comes the definition of A_g:

$$P_{\pi_g s}A_g\vec{X} = D^{\mathbb{R}^3_s}(g)P_s\vec{X} \tag{12.7}$$

For example, for the H_2O molecule, a given configuration is given by the 3-dimensional deviation vectors $\vec{\xi}_I$,$\vec{\xi}_{II}$ and $\vec{\xi}_O$. The group element g_1 rotates the vector $\vec{x}^0_I + \vec{\xi}_I$ in $\mathbb{R}^3_{phys}$ to $\vec{x}^0_{II} + \vec{\xi}_{II}$ where $\vec{\xi}_{II} = \left(-\xi^1_I, \xi^2_I, -\xi^3_I\right)$. This can also be seen as first acting with g_1 on $\vec{\xi}_I$ in $\mathbb{R}^3_s$ as $D^{\mathbb{R}^3_s}(g_1)P_I\vec{X}$, and then interpreting the transformed deviation $D^{\mathbb{R}^3_s}(g_1)P_I\vec{X}$ as the deviation of the atom at location $\pi_{g_1}I = II$, which is $P_{II}\vec{X}'$ with $\vec{X}' = A_g\vec{X}$. So

$$P_{\pi_g s}A_g\vec{X} = D^{\mathbb{R}^3_s}(g)P_s\vec{X} \tag{12.8}$$

Let us now prove that the $3N \times 3N$ matrices A_g yield a (in general reducible) representation of G. We must show that, given that the 3×3 matrices $D^{\mathbb{R}^3_s}(g)$ form a representation of G, the matrices A_g satisfy the following relation

$$A_gA_h = A_{gh} \quad g, h \in G \tag{12.9}$$

We know that

$$\left.\begin{array}{r} P_{\pi_{gh}s}A_{gh}\vec{X} = D^{\mathbb{R}^3_s}(gh)P_s\vec{X} \\ P_{\pi_g s}A_g\vec{X} = D^{\mathbb{R}^3_s}(g)P_s\vec{X} \\ P_{\pi_h s}A_h\vec{X} = D^{\mathbb{R}^3_s}(h)P_s\vec{X} \end{array}\right\} \text{for each } s = 1, ..., N. \tag{12.10}$$

This is the definition of A. Using that the matrices $D^{\mathbb{R}^3_s}(g)$ form a representation, we have $D^{\mathbb{R}^3_s}(gh) = D^{\mathbb{R}^3_s}(g)D^{\mathbb{R}^3_s}(h)$, and then we obtain

$$\begin{aligned} P_{\pi_{gh}s}A_{gh}\vec{X} &= D^{\mathbb{R}^3_s}(g)D^{\mathbb{R}^3_s}(h)P_s\vec{X} = D^{\mathbb{R}^3_s}(g)\left(D^{\mathbb{R}^3_s}(h)P_s\vec{X}\right) \\ &= D^{\mathbb{R}^3_s}(g)P_{\pi_h s}A_h\vec{X} \equiv D^{\mathbb{R}^3_{s'}}(g)P_{s'}\vec{X}' \\ &= P_{\pi_g s'}A_g\vec{X}' = P_{\pi_g(\pi_h s)}A_g\left(A_h\vec{X}\right) \\ &= P_{\pi_{gh}s}A_gA_h\vec{X} \end{aligned} \tag{12.11}$$

To simplify the notation we introduced in the second line the symbols $s' = \pi_h s$ and $\vec{X}' = A_h\vec{X}$, but in the third time we substituted them back. We also used in the second line that $\mathbb{R}^3_s = \mathbb{R}^3_{s'}$, see (12.4). Summing over s and using $\sum_s P_s = I$ removes the projection operators, and we obtain

$$A_{gh}\vec{X} = A_gA_h\vec{X} \tag{12.12}$$

Since $\vec{X}$ is an arbitrary vector in S, this proves that indeed $A_{gh} = A_g A_h$.

The A_g form a group of linear transformations in S. Physically nothing changes if one acts with A_g on the deviation of the whole molecule in S. Thus a normal mode with frequency ω is mapped to a normal mode with the same ω. **All normal modes with a given frequency form an invariant subspace of S.** Some normal modes are nondegenerate - then the representation is a one-dimensional irreducible representation (irrep). If k normal modes have the same frequency, this yields a k-dim. invariant subspace, hence a k-dim. irrep. **So, S splits up into irreps of G.** If one finds twice a given irrep in S, the frequency of the normal modes in the first irrep will in general be different from the frequency in the other irrep.

To find these irreps, we clearly need to know the following characters:

1) the reducible character of G in $\mathbb{R}^3_{\text{phys}}$

2) the reducible character of G in S

3) the irreducible characters of G.

ad 1) The reducible character of G in $\mathbb{R}^3_{\text{phys}}$ is denoted by $\chi_{R^3}(g)$ and is given by

$$\begin{aligned} &\chi_{R^3}(g) = 1 && \text{for reflections} \\ &\chi_{R^3}(g) = \left(1 + 2\cos\varphi_g\right) && \text{for rotations} \end{aligned} \tag{12.13}$$

because the trace of a rotation matrix in 3 dimensions is $1 + 2\cos\varphi_g$ where φ_g is the rotation angle (π in our case), and for reflections the trace equals 1, for example

$$\operatorname{tr}\begin{pmatrix} -1 & & \\ & 1 & \\ & & 1 \end{pmatrix} = 1 \tag{12.14}$$

ad 2) To compute the character $\chi_S(g) = \operatorname{tr} A_g$, we note that only atoms which are not moved to another location by g can contribute to the trace. These atoms yield each the same contribution as $\chi_{R^3}(g)$. If c_g denotes the number of atoms which are not moved under g, we get

$$\chi_S(g) = c_g \chi_{R^3}(g) \tag{12.15}$$

ad 3) It is easy to calculate the characters of the group of four. Because G is abelian, there are 4 one-dimensional characters which we denote by χ_0, χ_1, χ_2 and χ_3.

The results for all these characters are found in table 12.1. By using $\chi_S = n_0\chi^0 + n_1\chi^1 + n_2\chi^2 + n_3\chi^3$, and the orthogonality relations $(\chi^i, \chi^j) \equiv \Sigma_g \chi^i(g)\left(\chi^j(g)\right)^* = \delta^i_j \operatorname{order}(G) = 4\delta^i_j$, we find out how many times an irrep is contained in χ_S. In the example of the H_2O molecule we get from (χ_S, χ^j)

$$n_0 = 3; \qquad n_1 = 1; \qquad n_2 = 2; \qquad n_3 = 3. \tag{12.16}$$

H_2O	χ^0	χ^1	χ^2	χ^3	χ_{R^3}	c_g	χ_S
g_0	1	1	1	1	3	3	9
g_1	1	1	-1	-1	-1	1	-1
g_2	1	-1	1	-1	1	1	1
g_3	1	-1	-1	1	1	3	3

Table 12.1: Character table for the Klein group V. Usually we write the classes in a horizontal row, but in this case we put them in a vertical column to get a character table which looks nicer (wider than deep).

However, the representation A contains still the translations and rotations, which form two invariant subspaces as we shall show, and whose contributions to χ_S we want to subtract. The matrices A_g map each of these spaces into itself, as we now show.

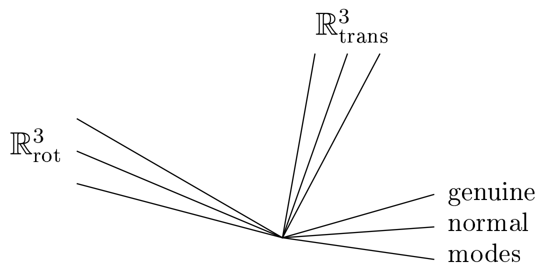


Figure 12.3: The normal modes in the space S.

An infinitesimal translation of the whole molecule maps the equilibrium positions $\vec{x}_s^0$ to $\vec{x}_s^0 + \vec{a}$. So $\vec{\xi}_s = \vec{a}$, independently of s. Then

$$\vec{X}_{\text{tr}} = (\vec{a}, \dots, \vec{a}) \in \mathbb{R}^3_{\text{trans}} \subset S \tag{12.17}$$

spans a 3-dimensional linear vector space $\mathbb{R}^3_{\text{trans}}$ in S. Since g maps each $\vec{\xi}_s = \vec{a}$ to $g\vec{\xi}_s = g\vec{a}$, we see that A maps the space $\vec{X}_{\text{trans}}$ into itself:

$$A_g\,(\vec{a}, \dots, \vec{a}) = (g\vec{a}, \dots, g\vec{a}) \in \mathbb{R}^3_{\text{trans}} \tag{12.18}$$

The contribution of this 3-dimensional subspace of the translations to the characters of G in S is thus the same as the character of g in $\mathbb{R}^3_{\text{phys}}$ or in $\mathbb{R}^3_s$

$$\chi_{\text{tr}}(g) = \chi_{R^3}(g) \tag{12.19}$$

Let us study this result for the character of translations in more detail. A basis for the deviations of the molecule which describe an overall translation, is given by

$$\vec{X}_{tr} = (\vec{a}, \vec{a}, \vec{a}) \Rightarrow \begin{array}{ll} X^1_{tr} = (1,0,0;1,0,0;1,0,0) & \text{times } a_x \\ X^2_{tr} = (0,1,0;0,1,0;0,1,0) & \text{times } a_y \\ X^3_{tr} = (0,0,1;0,0,1;0,0,1) & \text{times } a_z \end{array} \tag{12.20}$$

These vectors form a 3-dim. linear vector subspace $\mathbb{R}^3_{tr}$ of S. We claim that the action of A maps this space into itself in the same way as G acts in $\mathbb{R}^3_{phys}$, namely according to the 3×3 matrix representation whose character is χ_{R^3}. For an arbitrary vector $\vec{X}$ in S we find when we act with g_1

$$A_{g_1}\left(\vec{\xi}_1, \vec{\xi}_2, \vec{\xi}_3\right) = \left(g_1\vec{\xi}_2, g_1\vec{\xi}_1, g_1\vec{\xi}_3\right) = \left(-\xi_2^1, \xi_2^2, -\xi_2^3; -\xi_1^1, \xi_1^2, -\xi_1^3; -\xi_3^1, \xi_3^2, -\xi_3^3\right) \tag{12.21}$$

and similarly for A_{g_2} and A_{g_3}. So the vectors $(\vec{a}, \ldots, \vec{a})$ form a 3-dimensional subspace of S, and A_g maps a vector in this subspace to another vector in this subspace. For example the vector $\vec{X} = (a, 0, 0; a, 0, 0; a, 0, 0)$ is mapped by the rotation g_1 to the vector $A\vec{X} = (-a, 0, 0; -a, 0, 0; -a, 0, 0; -a, 0, 0)$. The trace of A_g in this 3×3 subspace is $\chi_{\mathrm{tr}}(g)$. On the basis $\vec{X}^1_{\mathrm{tr}}$, $\vec{X}^2_{\mathrm{tr}}$, $\vec{X}^3_{\mathrm{tr}}$ for this subspace the matrix A_{g_1} acts as

$$A_{g_1}\vec{X}^1_{\mathrm{tr}} = -\vec{X}^1_{\mathrm{tr}}; \qquad A_{g_1}\vec{X}^2_{\mathrm{tr}} = \vec{X}^2_{\mathrm{tr}}; \qquad A_{g_1}\vec{X}^3_{\mathrm{tr}} = -\vec{X}^3_{\mathrm{tr}} \tag{12.22}$$

Hence, $\chi_{\mathrm{tr}}(g_1) = -1$. In a similar way one can evaluate χ_{tr} on the other classes.

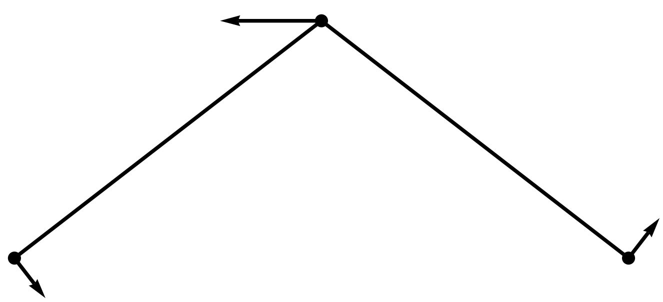


Figure 12.4: An infinitesimal rotation of the H_2O molecule along the z-axis. The three infinitesimal vectors are $\vec{X}^3_{\mathrm{rot}}$. There are also infinitesimal rotations along the x-axis and y-axis. Together they form a 3-dimensional subspace $\mathbb{R}^3_{\mathrm{rot}}$ in S. Under the finite rotations and reflections of the symmetry group V they are transformed to $\vec{\xi}'_{\mathrm{rot},\pi_g g'}$.

The infinitesimal rotations in $\mathbb{R}^3_{phys}$ map a vector $\vec{x}$ to $\vec{x} + \left(\vec{b} \times \vec{x}\right)$ with infinitesimal $\vec{b}$. So, at site s the vector $\vec{x}^{(0)}_s$ is mapped to $\vec{x}^0_s + \left(\vec{b} \times \vec{x}^0_s\right)$. Then $\vec{\xi}_s = \left(\vec{b} \times \vec{x}^0_s\right)$ and

$$\vec{X}^{\vec{b}}_{\mathrm{rot}} = \left(\vec{b} \times \vec{x}^0_1, \ldots, \vec{b} \times \vec{x}^0_N\right) \in \mathbb{R}^3_{rot} \subset S \tag{12.23}$$

This $\vec{X}^{\vec{b}}_{\mathrm{rot}}$ is a kind of "velocity field". How does A act on the three vectors $\vec{X}^{\vec{b}}_{\mathrm{rot}}$ (parametrized by the 3 rotation parameters $\vec{b}$)? The group G acts in $\mathbb{R}^3_s$ as

$$\vec{\xi}_s = \left(\vec{b} \times \vec{x}^0_s\right) \underset{g}{\rightarrow} g\left(\vec{b} \times \vec{x}^0_s\right) = \det\left(D_{R^3}(g)\right)\left(g\vec{b} \times g\vec{x}^0_s\right) \tag{12.24}$$

Namely, under proper rotations $\vec{b} \times \vec{x}^0_s$ transforms as a vector, but under reflections it acquires a minus sign, which is provided by $\det\left(D_{\mathbb{R}^3}(g)\right)$. So A acts in the 3-dimensional subspace $\mathbb{R}^3_{rot} \subset S$

the same way as g times $\det g$. In the character table we find then

$$\chi_{rot}(g) = \det(D_{R^3}(g))\chi_{R^3}(g) \tag{12.25}$$

Just as we did for the translations, we also check this result for the rotations, this time by constructing the representation matrix for two particular group elements. For g_1 the characters are claimed to be the same, $\chi_{\text{tr}}(g_1) = \chi_{\text{rot}}(g_1) = -1$, but for reflections they should differ by a sign, $\chi_{\text{tr}}(g_3) = 1$ and $\chi_{\text{rot}}(g_3) = -1$. Under g_1 we find $A_{g_1}\vec{X}^1_{\text{rot}} = -\vec{X}^1_{\text{rot}}$ where $\vec{X}^1_{\text{rot}}$ are the deviations due to an infinitesimal rotation about the x-axis. ($\vec{\xi}_I$ and $\vec{\xi}_{II}$ lie along the positive z-axis and $\vec{\xi}_O$ along the negative z-axis)[4]. Further, $A_{g_1}\vec{X}^2_{\text{rot}} = \vec{X}^2_{\text{rot}}$ and $A_{g_1}\vec{X}^3_{\text{rot}} = -\vec{X}^3_{\text{rot}}$. (The deviations corresponding to $\vec{X}^3_{\text{rot}}$ are exhibited in figure 12.4). Thus $\chi_{\text{rot}}(g_1) = -1$ which agrees with the expected result. For g_3 (reflections about the x-y plane) one has $A_{g_3}\vec{X}^1_{\text{rot}} = -\vec{X}^1_{\text{rot}}$, $A_{g_3}\vec{X}^2_{\text{rot}} = -\vec{X}^2_{\text{rot}}$ and $A_{g_3}\vec{X}^3_{\text{rot}} = \vec{X}^3_{\text{rot}}$. Thus $\chi_{\text{rot}}(g_3) = -1$, again in agreement with the expected result.

The character of the genuine normal modes is then

$$\chi_{genuine} = \chi_S - \chi_{tr} - \chi_{rot} = \begin{pmatrix} 9 \\ -1 \\ 1 \\ 3 \end{pmatrix} - \begin{pmatrix} 3 \\ -1 \\ 1 \\ 1 \end{pmatrix} - \begin{pmatrix} 3 \\ -1 \\ -1 \\ -1 \end{pmatrix} = \begin{pmatrix} 3 \\ 1 \\ 1 \\ 3 \end{pmatrix} = 2\chi_0 + \chi_3 \tag{12.26}$$

Taking inner product with χ_0, χ_1,χ_2 and χ_3 shows that $\boldsymbol{\chi_{genuine}}$ **contains** $\boldsymbol{\chi_0}$ **twice and** $\boldsymbol{\chi_3}$ **once.**

Each character χ_0, ... ,χ_3 corresponds to an irreducible rep, which is one-dimensional in this case. So the two normal modes corresponding to the two χ_0 form each separately an invariant subspace; they are not degenerate, and have different frequencies ω. In fact, all 3 normal modes are nondegenerate (the irreps of G are one-dimensional because G is abelian). There are two normal modes with the symmetry of χ_0 (illustrated in figure 12.5) and one normal mode with the symmetry of χ_3 (illustrated in figure 12.6).

Can the three singlets of normal modes of water be detected? (We use the theory of infrared and Raman spectroscopy which is explained in the next section. Readers unfamiliar with this theory are advised first to read the next section up to equation (12.30) and then to come back to this section.) It is clear that they all can absorb infrared radiation because their dipole moments are nonvanishing. But they are also Raman active. To see this we must reduce the 6-dimensional representation $r^i r^j$ into irreps of $G = V$. Let us begin with the 3-dimensional representation $r^i = (x, y, z)$ (which will confirm that all modes are infrared active). More precisely, we consider 3 vectors $\vec{e}_x, \vec{e}_y, \vec{e}_z$ along the x-, y- and z-axis, respectively, and determine how they transform under

[4] To avoid confusion, note that there are two groups involved. First there are the generators of rotations about the x, y and z axis which produce the three infinitesimal vectors $\vec{X}^1_{\text{rot}}, \vec{X}^2_{\text{rot}}$ and $\vec{X}^3_{\text{rot}}$. Then there is the Klein group of 4 finite rotations and reflections which acts on the infinitesimal vectors $\vec{X}^1_{\text{rot}}, \vec{X}^2_{\text{rot}}$ and $\vec{X}^3_{\text{rot}}$.

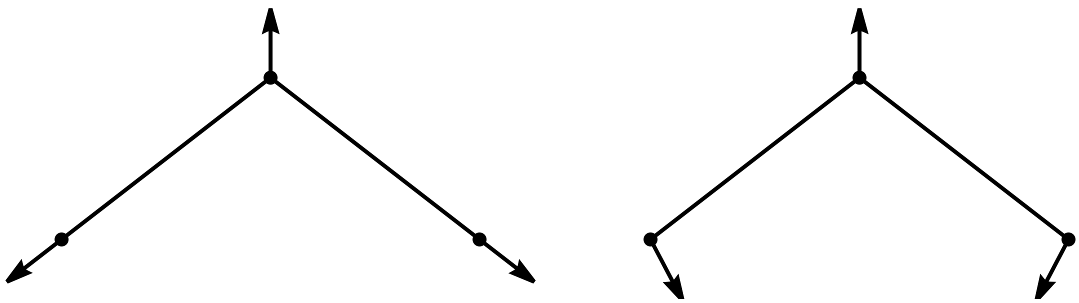


Figure 12.5: The two genuine modes with the same symmetry as χ_0 yield two singlets with different frequencies. Each of these two modes is symmetric under g_1, g_2, g_3 (one rotation, two reflections). The first mode is called the breather or the symmetric stretch mode, the second is called the bending mode.

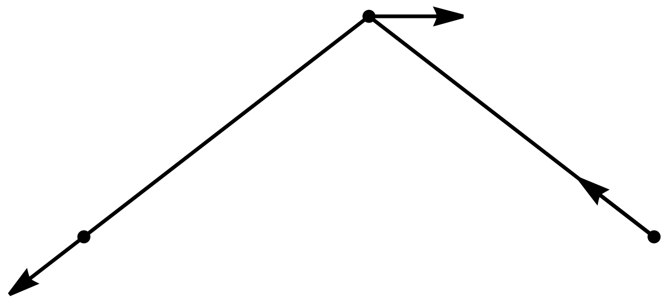


Figure 12.6: The third genuine mode is also a singlet. It has the same symmetry as χ_3. It is antisymmetric under rotation along the y-axis (g_1) and reflection w.r.t. the bisectrix plane (g_2), but symmetric under reflections w.r.t. molecule plane (g_3). This mode is called the asymmetric stretch mode.

G. One easily confirms that $\vec{e}_x$ is invariant under g_0 and g_3, but transforms into $-\vec{e}_x$ under g_1 and g_2. Hence $\vec{e}_x$ transforms like χ_3. (Equivalently, the operator x in quantum mechanics transforms like χ_3.) Similarly one finds that $\vec{e}_y$ transforms like χ_0, and $\vec{e}_z$ like χ_2. So both for the two modes with symmetry χ_0 and for the mode with symmetry of χ_3 there are operators among x, y, z which transform under G in the same way as these modes. All three modes are thus IR active.

The operators $r^i r^j$ transform like the products of the irreps of r^i

$$
\begin{aligned}
&xx \text{ as } \chi_3\chi_3 = \chi_0\,; \quad yy \text{ as } \chi_0\chi_0 = \chi_0\,; \quad zz \text{ as } \chi_2\chi_2 = \chi_0\,; \\
&xy \text{ as } \chi_3\chi_0 = \chi_3\,; \quad xz \text{ as } \chi_3\chi_2 = \chi_1\,; \quad yz \text{ as } \chi_0\chi_2 = \chi_2\,.
\end{aligned}
$$

The 3 physical modes formed 3 singlets, two with symmetry character χ_0 and one with symmetry character χ_3. So the operators xx and zz can produce Raman scattering for the first two modes, and xy and yz for the third mode. Thus all three physical modes are also Raman active.

H_2O	χ_0	χ_1	χ_2	χ_3	χ_{R^3}	c_g	χ_S	χ_{tr}	χ_{rot}	χ_{gen}
g_0	1	1	1	1	3	3	9	3	3	3
g_1	1	1	-1	-1	-1	1	-1	-1	-1	1
g_2	1	-1	1	-1	1	1	1	1	-1	1
g_3	1	-1	-1	1	1	3	3	1	-1	3
IR	y		z	x						
Raman	xx, yy, zz	xz	yz	xy						

Table 12.2: Character table for the Klein group V and for the zero modes and the genuine (nonzero) normal modes. (To simplify the notation, we have written the group elements in a column instead of a row.) The one-but-last row contains the irreducible characters into which x, y, z decompose. This row shows that the normal modes with the same symmetry as χ_0, χ_2 and χ_3 are infrared active. The last row contains the irreducible characters into which the 6 operators $xx, xy, \cdots, zz$ decompose. This row shoes that the normal modes with the same symmetry as χ_0, χ_1 and χ_3 are Raman active. The genuine normal modes of the H_2O molecule decompose into two singlets with the symmetry of χ_0 and one singlet with the symmetry of χ_3. Thus one expects to see three lines in the IR spectrum of water, and also 3 lines in the Raman spectrum of water. The IR lines are observed, see figure 12.10. The Raman lines are difficult to detect in water.

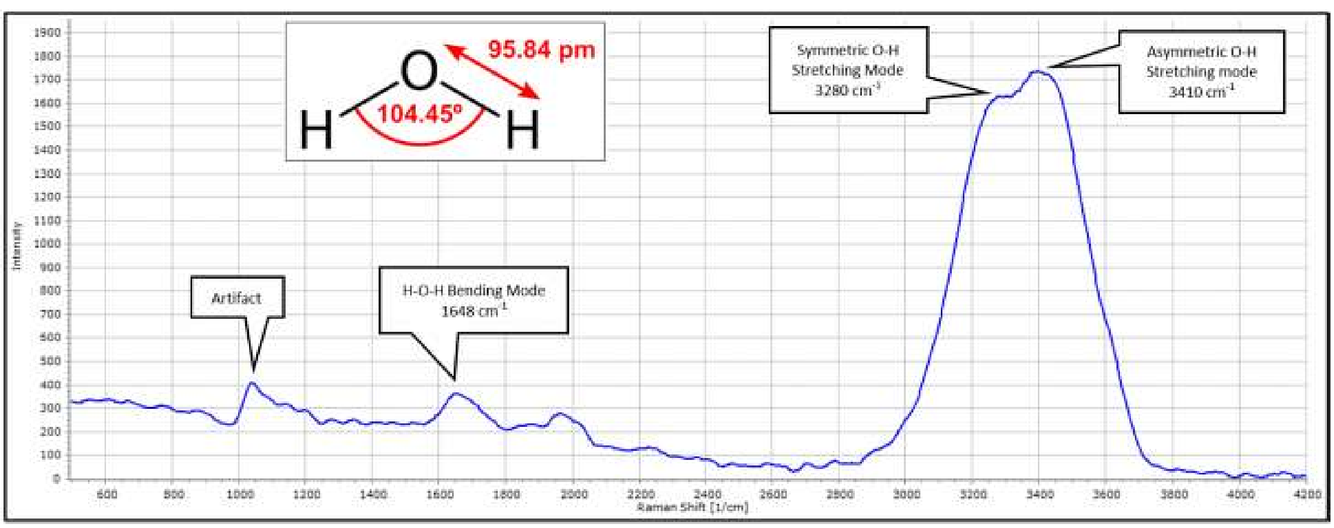


Figure 12.7: The Raman spectrum of H_2O molecule.

12.3 The spectrum of the CO_2 molecule

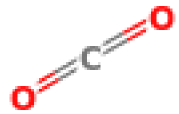


Figure 12.8: The CO_2 molecule.

The CO_2 molecule is a linear molecule, hence the number of nonzero normal modes is $3N - 5 = 4$. It is not difficult to find them, see figure 12.9. However, from a group theoretic point of view, there is a new complication: there is an infinite symmetry group of rotations about the axis connecting the 3 atoms. One can extend the analysis we have performed for finite groups to infinite groups of this kind, but we shall not do so, but refer to [1]. The result of this analysis is that the IR spectrum consists of 2 lines, namely a line due to the asymmetric stretch (a singlet), and another line due to the two bending modes (a doublet). The symmetric stretch mode does not produce an absorption line in the IR spectrum because its dipole moment is time-independent. The Raman spectrum consists of 3 lines (?).

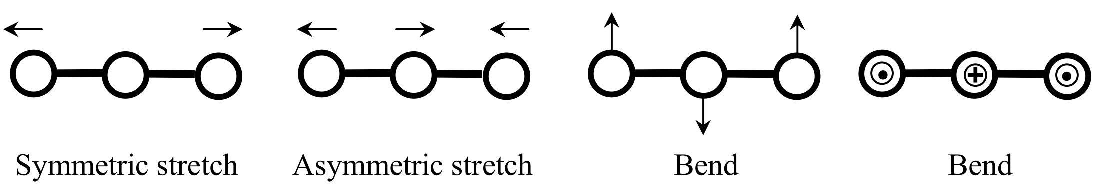


Figure 12.9: The normal modes of CO_2. A linear molecule has $3N - 5$ normal modes. There are four normal modes but only three frequencies in the vibrational spectrum because the last two normal modes are degenerate. The last normal mode is absent for H_2O. [7] For CO_2, the symmetric stretch mode is IR inactive, but the other modes (the asymmetric mode and the bend modes) are IR active, and produce two IR lines. There are also 3 Raman lines in the CO_2 spectrum.

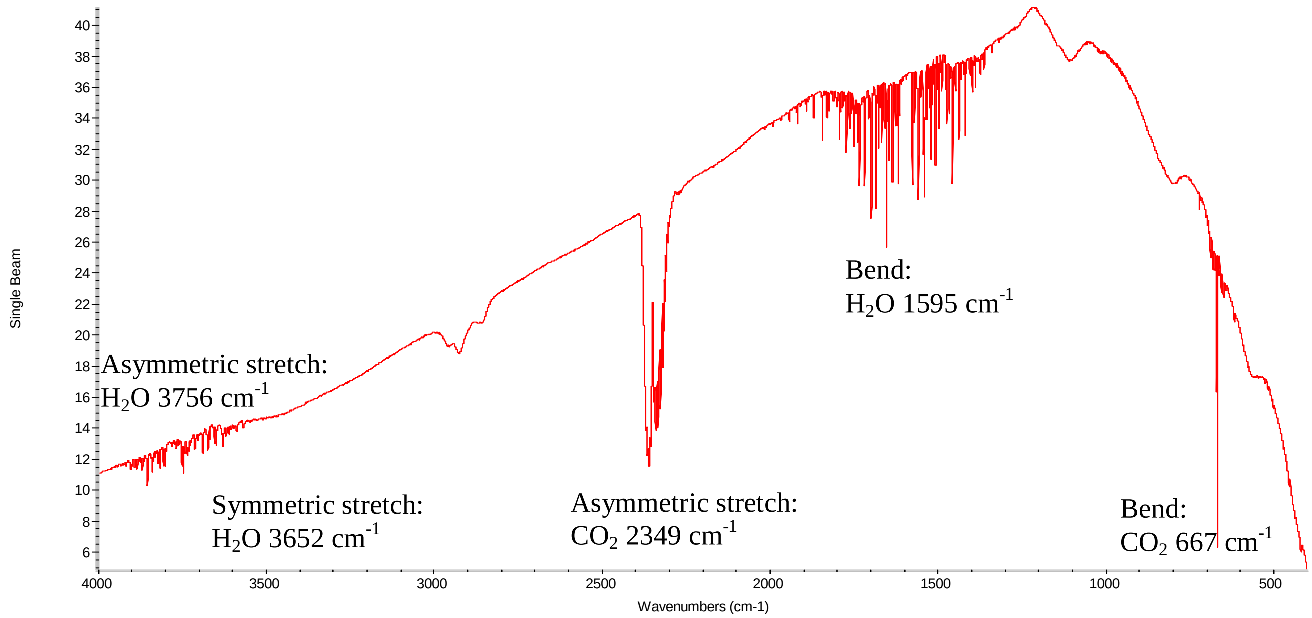


Figure 12.10: Experimental results for the infrared spectrum of air. [7] All three vibrational normal modes of water and two of the three frequencies in the spectrum of CO_2 are clearly visible. The symmetric stretch mode for CO_2 in figure 12.9 is not visible in this figure because it is not infrared active (the dipole moment does not change in time) but it appears in the Raman spectrum of CO_2. The wave numbers $k = \frac{2\pi}{\lambda}$ are given in cm^{-1}. Around each vibrational mode one sees many lines of the rotational spectrum. (The words 'Single Beam' in the figure indicate that a single laser beam was used to shine on air. One can also use two counter-moving laser beams; this allows to suppress the effects of Doppler broadening, but in infrared experiments Doppler broadening is not important.)

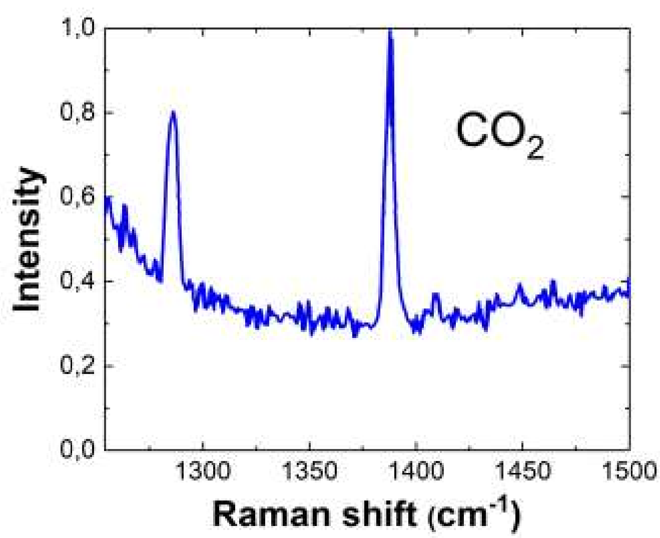


Figure 12.11: The Raman spectra of CO_2 molecule.

Exercises.

1) The molecule CCl_4 consists of four identical chlorine atoms in the shape of a tetrahedron, and one carbon atom C at the center of the tetrahedron. The symmetry group of this molecule is S_4. Derive "the spectrum", and draw pictures of the normal modes.

2) The ammonium molecule NH_3 has the form of a pyramid. The isometries consist of 3 rotations, and 3 reflections about planes through the atom N and one of the H atoms. The symmetry group is $D_3 = S_3$ with 3 classes. The character table is given in table 12.3. There are 6 genuine normal modes. Find them in the representation A. Identify them physically (for example, one normal mode is the "breather" where all 4 atoms move radially outward at the same time). See Cornwell, volume I, pages 182, 196, 338.

NH_3	(e)	$(12),(13),(23)$	$(123),(132)$
$\chi^{(0)}$	1	1	1
$\chi^{(1)}$	1	-1	1
$\chi^{(2)}$	2	0	-1

Table 12.3: Character table for NH_3.

12.4 Buckyballs

As another, less trivial, application of group theory to molecular spectra, we shall consider buckyballs [8] and derive the predictions to leading (lowest) order in perturbation theory for the infrared spectrum (4 lines) and the Raman spectrum (10 lines). Buckyballs[5] consist of 60 carbon atoms (^{12}C) and are usually denoted by C_{60}. Thus they contain $3 \times 60 - 6 = 174$ genuine (not zero modes) normal modes. Clearly, group theory is needed to analyze their spectra.

One can obtain it from an icosahedron (12 vertices, 30 edges, 20 triangular faces) by cutting off the tops around the vertices; then each vertex is replaced by a pentagon with 5 vertices, and thus a buckyball has 60 vertices. Its number of faces is 32 (the 20 triangles of the icosahedron become 20 hexagons of the buckyball, and there are 12 newly created pentagons). The number of edges is 90: there are 30 edges for an icosahedron, while cutting off the top around vertices creates $12 \times 5 = 60$ further edges. Euler's topological relation between the number of vertices (v), edges (e) and faces (f) is satisfied:

$$v - e + f = \begin{cases} 12 - 30 + 20 = 2 & \text{(icosahedron)} \\ 60 - 90 + 32 = 2 & \text{(buckyball)} \end{cases} \tag{12.27}$$

[5] The name refers to the architect Buckminster Fuller who constructed dome-like buildings which looked like part of a soccer ball. The molecules C_{60}, C_{70}, ... are often called fullerenes, and the ball-like C_{60} molecule is called a buckyball.

One can manufacture buckyballs in the lab by shining laser light on a plate of graphite and blowing He gas over the plate; the carbon atoms in the gas assemble into round C_{60} molecules, fewer into round C_{70} molecules, and other linear and ring-like structures. A much more efficient way to manufacture buckyballs is to produce strong electric discharges between two electrodes made of graphite.

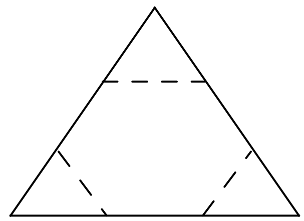


Figure 12.12: Cutting off the tops around 12 vertices of an icosahedron, the triangular faces become hexagons. At the vertices, 12 pentagons are created, yielding 32 faces for a buckyball.

We take the symmetry group of a buckyball the same as that of an icosahedron. (The symmetry group of a buckyball contains certainly the symmetry group of an icosahedron, but it may be larger. This does not affect the spectrum, as we discuss in a comment at the end of this section.) The latter is denoted by I_h.There are 60 rotations[6] forming the group A_5, and 60 isometries with $\det M(g)^{R^3} = -1$, yielding another 60 elements. The latter can be written as the product σA_5 where σ is the space inversion ($\sigma\vec{r} = -\vec{r}$). Hence

$$I_h = A_5 \cup \sigma A_5 \tag{12.28}$$

The group element σ commutes with all elements of A_5. Thus the symmetry group is not S_5 which has no central element. Because σ commutes with A_5, one can write I_h as a direct product: $I_h = A_5 \times C_2$ where $C_2 = \{e, \sigma\}$. Since the subgroups H_1 and H_2 in a direct product group $H_1 \times H_2$ are normal subgroups, the group A_5 is an invariant subgroup of I_h. Then I_h/A_5 is again a group, and it is isomorphic to Z_2 whose characters are $(1, 1)$ and $(1, -1)$. Because the product of characters is again a character, it follows that if the characters of A_5 are denoted by an $n \times n$ matrix K, then the characters of I_h are given by the following $2n \times 2n$ matrix.

$$\chi(I_h) = \begin{pmatrix} K & K \\ K & -K \end{pmatrix} \tag{12.29}$$

We shall see that $n = 5$, so we shall write the characters as 10-component rows. The first 5

[6]The 60 rotations consist of the unit element and further $4 \times 6 = 24$ rotations about icosaeder diagonals, $2 \times 10 = 20$ rotations about dodekaeder diagonals, and $1 \times 15 = 15$ rotations about the "cross-diagonals", which connect the middles of the 15 pairs of parallel opposite edges into which the 30 edges decompose. To show that these 60 rotations form the group A_5, note that **the 15 cross-diagonals form five triplets of mutually orthogonal cross-diagonals**. If one numbers these triplets by 1, 2, 3, 4 and 5, the 60 rotations correspond to the permutations of the group A_5. The 24 rotations about the icosaeder diagonals form two classes of 5-cycles, the 20 rotations about the dodekaeder diagonals form the 3-cycles, and the 15 rotations about the cross-diagonals form the twins. (The two classes of 5-cycles correspond to rotations over 72° and $2 \times 72°$.)

characters correspond to $\sigma = +1$, while the last 5 characters have $\sigma = -1$. Because A_5 is simple (as we shall prove below), its commutator subgroup is equal to A_5, and hence there is only one 1-dimensional irrep of A_5, and two 1-dimensional irreps of I_h.

We now construct the character table. We begin with the characters of A_5.[7] The group A_5 has 60 elements grouped into 5 classes: the unit element, 15 "twins" (such as (12)(34)), 20 3-cycles (such as (123)), 12 5-cycles (such as (12345) and those obtained from it by an even number of permutations), and another 12 5-cycles (for example (12354) and those obtained from it by an even number of permutations):

$$G = \{(e), 15\text{ twins}, 20\text{ 3-cycles}, 12\text{ 5-cycles}, 12\text{ 5-cycles}\} \tag{12.30}$$

(The 24 5-cycles cannot form one class because 24 is not a divisor of 60.) Let us first give a very simple proof that A_5 is simple. Any normal subgroup must be composed of entire classes, and its order should be a divisor of the order of A_5 which is 60. It is easy to check that there is no integer linear combination of the numbers $1, 15, 20, 12$ and 12 which contains 1 and which is a divisor of 60. Thus A_5 contains no normal subgroups: it is simple.

We already showed that the elements of the group A_5 correspond to the rotations of the icosaheder. For example, the first class of 5-cycles contains the rotations over $\pm\frac{2\pi}{5}$, while the second class contains the rotations over $\pm\frac{4\pi}{5}$[8]. There are thus 5 irreps of A_5, and only one 1-dimensional irrep (the unit irrep) as we explained before. Hence, we obtain the Diophantic equation

$$60 = 1^2 + x^2 + y^2 + z^2 + t^2 \tag{12.31}$$

of which there is only one solution:

$$60 = 1^2 + 3^2 + 3^2 + 4^2 + 5^2 \tag{12.32}$$

One can check by going through all possibilities that (12.32) is the only solution of (12.31). However, this is a laborious exercise, and it is easier to first identify a few of the higher-dimensional irreps, and then to solve (12.31). We now identify the four higher-dimensional irreps by various methods. First of all, as for any permutation group, the permutations of the 5 triplets of cross-diagonal (see footnote 6) define a reducible linear representation, in this case of 5×5 matrices. Its character (the number of crosslines that are kept fixed) is $(5, 1, 2, 0, 0)$. The unit irrep is contained

[7] We follow unpublished lecture notes from 1960 by Hans Freudenthal from Utrecht University.

[8] Rotations over $\frac{2\pi}{5}$ are physically equivalent to rotations over $-\frac{2\pi}{5}$, but they are physically different from rotations over $\frac{4\pi}{5}$ and $\frac{6\pi}{5}$. This explains geometrically why the 5-cycles form two classes. If (12345) denotes a rotation over $\frac{2\pi}{5}$, then $(13524) = (12345)(12345)$ corresponds to a rotation over $\frac{4\pi}{5}$. It is easy to check that $(12345) = \varphi(13524)\varphi^{-1}$ with $\varphi = (45)(35)(23)$. Thus these two rotations are conjugated in S_5 but not in A_5, which explains why there are two classes with 5-cycles in A_5. If one were to begin by assuming that A_5 has 4 instead of 5 classes, with only one instead of two classes with 5-cycles, one would soon discover an inconsistency: $60 = 1^2 + x^2 + y^2 + z^2$ has no integer solutions for x, y, z with x, y, z all larger than one.

in it only once because

$$1 \cdot 5 \cdot 1 + 1 \cdot 1 \cdot 15 + 1 \cdot 2 \cdot 20 + 1 \cdot 0 \cdot 12 + 1 \cdot 0 \cdot 12 = 60 \tag{12.33}$$

Substracting it, we find the character $(4, 0, 1, -1, -1)$ which is irreducible since

$$4^2 \cdot 1 + 0^2 \cdot 15 + 1^2 \cdot 20 + (-1)^2 \cdot 12 + (-1)^2 \cdot 12 = 60 \tag{12.34}$$

Next we view A_5 as the transformation group which permutes the 6 icosaeder diagonals. To find the character of this representation we must determine how many diagonals are kept fixed by the 5 types of rotations. One finds $(6, 2, 0, 1, 1)$. The unit character is contained in it once $(6 \cdot 1 \cdot 1 + 2 \cdot 1 \cdot 15 + 0 \cdot 1 \cdot 20 + 1 \cdot 1 \cdot 12 + 1 \cdot 1 \cdot 12 = 60)$, and subtracting it one finds the irreducible character of a 5-dimensional irrep, $(5, 1, -1, 0, 0)$. At this point one can solve the Diophantic equation in (12.32) and one finds that there are two further irreps of dimension 3.

To identify these two 3-dimensional irreps, we consider the rotations of the icosaeder in physical 3-dimensional space. The character of this irrep is according to (12.13):

$$\chi_{R^3} = \left(3, -1, 0, 1 + 2\cos\left(\tfrac{2\pi}{5}\right), 1 + 2\cos\left(\tfrac{4\pi}{5}\right)\right) \tag{12.35}$$

(The 0 is the character of the rotations that correspond to the 3-cycles: $1 + 2\cos\left(\frac{2\pi}{3}\right) = 0$.) One may show[9] that $1 + 2\cos(\frac{2\pi}{5}) = \frac{1}{2}(1 + \sqrt{5})$ and $1 + 2\cos(\frac{4\pi}{5}) = \frac{1}{2}(1 - \sqrt{5})$. It is amusing to note that $\frac{1}{2}(1 + \sqrt{5})$ is the golden ratio we mentioned in the first chapter.

The last character is obtained by interchanging the last two classes[10] (or by using the orthogonality relations) and reads

$$\left(3, -1, 0, 1 + 2\cos\left(\tfrac{4\pi}{5}\right), 1 + 2\cos\left(\tfrac{2\pi}{5}\right)\right) \tag{12.36}$$

It is customary in chemistry to denote the characters of 1-dim. irreps by A, 2-dim. irreps by E, 3-dim. irreps by F, 4-dim. irreps by G, and 5-dim. irreps by H. The irreps with $\sigma = +1$ have subscript g (for gerade = even in German), while the irreps with $\sigma = -1$ have subscript u (for ungerade = odd in German). With this notation, we display the ten characters for I_h in table 12.4. The first two rows give the 10 classes of I_h and their orders, the next 10 rows give the 10 irreducible characters, then comes the row with n_g (the number of atoms held fixed by group element g). Next comes the character χ_{R^3} of the representation $M(g)^{R^3}$ of I_h in physical 3-dimensional space. We obtain χ_S from $n_g \chi_{R^3}$. We then record the character $\chi_{\text{trans}} = \chi_{R^3}$ for

[9] If $\sigma = e^{\frac{2\pi i}{5}}$, then $t_1 \equiv 1+2\cos(\frac{2\pi}{5}) = 1+\sigma+\sigma^{-1} = 1+\sigma+\sigma^4$, and $t_2 \equiv 1+2\cos(\frac{4\pi}{5}) = 1+\sigma^2+\sigma^{-2} = 1+\sigma^2+\sigma^3$. Using $1 + \sigma + \sigma^2 + \sigma^3 + \sigma^4 = 0$ one easily checks that $t_1 + t_2 = 1$ and $t_1 t_2 = -1$. Hence $t_j = \frac{1}{2}(1 \pm \sqrt{5})$, and $t_1 > 0$ while $t_2 < 0$.

[10] The interchange of the class which contains (12345) and the class that contains (12354) can be achieved in the S_5 by the inner automorphism $(12354) = (45)^{-1}(12345)(45)^{-1}$. In the A_5 this is an outer automorphism. Physically this means interchanging the rotations over $\pm\frac{2\pi}{5}$ with the rotations over $\pm\frac{4\pi}{5}$.

translations, and $\chi_{\rm rot} = (\det M(g)^{R^3})\chi_{R^3}$ for rotations. And finally we get the character for the genuine normal modes from $\chi_{\rm gen} = \chi_S - \chi_{\rm trans} - \chi_{\rm rot}$. To reduce clutter in table 12.4 we have introduced the notation

$$\varphi_\pm \equiv \tfrac{1}{2}\big(1 \pm \sqrt{5}\,\big). \tag{12.37}$$

I_h	e 1	twins 15	C_3 20	$C_{5,I}$ 12	$C_{5,II}$ 12	σ 1	σ twins 15	σC_3 20	$\sigma C_{5,I}$ 12	$\sigma C_{5,II}$ 12	
A_g	1	1	1	1	1	1	1	1	1	1	$x^2+y^2+z^2$
F_{1g}	3	-1	0	φ_+	φ_-	3	-1	0	φ_+	φ_-	$(R_x,\,R_y,\,R_z)$
F_{2g}	3	-1	0	φ_-	φ_+	3	-1	0	φ_-	φ_+	
G_g	4	0	1	-1	-1	4	0	1	-1	-1	
H_g	5	1	-1	0	0	5	1	-1	0	0	$\big(2z^2-x^2-y^2,$ $x^2-y^2,$ $xy,\,yz,\,zx\big)$
A_u	1	1	1	1	1	-1	-1	-1	-1	-1	
F_{1u}	3	-1	0	φ_+	φ_-	-3	1	0	$-\varphi_+$	$-\varphi_-$	$(x,\,y,\,z)$
F_{2u}	3	-1	0	φ_-	φ_+	-3	1	0	$-\varphi_-$	$-\varphi_+$	
G_u	4	0	1	-1	-1	-4	0	-1	1	1	
H_u	5	1	-1	0	0	-5	-1	1	0	0	
n_g	60	0	0	0	0	0	4	0	0	0	
χ_{R^3}	3	-1	0	φ_+	φ_-	-3	1	0	$-\varphi_+$	$-\varphi_-$	
χ_S	180	0	0	0	0	0	4	0	0	0	
$\chi_{\rm trans}$	3	-1	0	φ_+	φ_-	-3	1	0	$-\varphi_+$	$-\varphi_-$	
$\chi_{\rm rot}$	3	-1	0	φ_+	φ_-	3	-1	0	φ_+	φ_-	
$\chi_{\rm gen}$	174	2	0	$-2\varphi_+$	$-2\varphi_-$	0	4	0	0	0	

Table 12.4: Character table for an icosahedron or a buckyball. In the first row the 10 classes of the symmetry group $I_h = A_5 \cup \sigma A_5$ are indicated. The second row contains the order of these classes. The next 10 rows contain the characters of the 10 irreps of I_h. In the literature one sometimes denotes triplets by T instead of F. There is no intrinsic distinction between F_1 and F_2, they only differ in the choice of basic angle for rotations of pentagons ($\frac{2\pi}{5}$ or $\frac{4\pi}{5}$). The decomposition of $\chi_{\rm gen} = \chi_S - \chi_{trans} - \chi_{rot}$ into irreps reads $\chi_{\rm gen} = 2A_g + 3F_{1g} + 4F_{2g} + 6G_g + 8H_g + A_u + 4F_{1u} + 5F_{2u} + 6G_u + 7H_u$. To first-order in quantum-mechanical perturbation theory, the 4 infrared absorption lines are due to F_{1u}, while two of the Raman lines come from A_g and another 8 from H_g. In the last column we have written the irreps into which the rep $(x,\,y,\,z)$ and the rep $x^i x^j$ decompose. Clearly $(x,\,y,\,z)$ is irreducible, but $x^i x^j$ decomposes into two irreps. We have also written the representation of the rotational zero modes R_x, R_y, R_z; it is clearly irreducible.

The entry 4 of χ_S in table 12.4 needs an explanation. Put a buckyball on a table, resting on one of its hexagons. On top is then another hexagon with the same orientation. Cut the buckyball in half by a vertical plane that bisects two opposite parallel edges of both hexagons. This plane contains then 4 vertices which form a parallelogram. The axis through the center of the buckyball and perpendicular to the vertical plane crosses two other parallel and opposite edges of the buckyball. A rotation over π along this axis is a symmetry of the icosahedron and hence of the buckyball. The 4 vertices of the parallelogram are fixed points if one first makes a rotation over π, and then a space inversion. This explains the value 4 for the class with σtwins.

The reducible representation of the symmetry group I_h in the $3N$ dimensional space of combined deviations $\vec{X} = (\vec{\xi}_1, \dots, \vec{\xi}_N)$ can be brought on block-diagonal form by a unitary transformation. The irreducible representations, denoted by $M(g)^{(i)}$, are then contained n_α times in it. To find the numbers n_α for the 10 irreps, we use characters[11]

$$n_\alpha = (\chi^{(\alpha)}, \chi_S) = \tfrac{1}{120}\left[180 \cdot 1\chi^{(\alpha)}(e) + 4 \cdot 15\chi^{(\alpha)}(\sigma\text{twins})\right] \tag{12.38}$$

It is easy to calculate the integers n_α, and one finds

$$\chi_S = 2A_g + 4F_{1g} + 4F_{2g} + 6G_g + 8H_g + A_u + 5F_{1u} + 5F_{2u} + 6G_u + 7H_u \tag{12.39}$$

As a check we add the dimensions of the irreps multiplied by how often they occur, and find 180. Subtracting the character for translations $\chi_{R^3} = F_{1u}$ and the character for rotations $(\det D^{R^3})\chi_{R^3} = F_{1g}$, we find

$$\chi_{\text{gen}} = 2A_g + 3F_{1g} + 4F_{2g} + 6G_g + 8H_g + A_u + 4F_{1u} + 5F_{2u} + 6G_u + 7H_u \tag{12.40}$$

In total there are 46 distinct nonzero frequencies. (As a check one may show that $(\chi_{\text{gen}}, \chi_{\text{gen}}) = 30720$ is equal to $120 \times \sum(n^\alpha)^2$.)

One can radiate light on buckyballs and study two kinds of spectra:

i) *Infrared spectra.* These are absorption spectra. Non-monochromatic light hits the C_{60} molecules, and for certain frequencies of the light, C_{60} levels can be excited. There is thus less light at that frequency behind the target, so one sees an absorption spectrum. The quantum-mechanical matrix element for infrared spectra due to absorption of a photon with polarization vector $\vec{\epsilon}$ is according to semiclassical radiation theory given by $\langle Q_J | \sum_{i=1}^N e_i \, \vec{\epsilon} \cdot \vec{r}_i | 0\rangle$ where $\vec{r}_i$ are the equilibrium positions of the atoms and e_i their effective charges. One can expand each of the $3N$ deviations of a molecule into the $3N$ normal modes. Call these normal modes $Q_J(t) = Q_J \cos(\omega_J t)$. The Q_J form harmonic oscillators (see the introduction) so we can write them in terms of creation and annihilation operators as $\frac{1}{\sqrt{2}}(a_J + i a_J^\dagger)$. The molecule is to begin with in the ground state (or some excited state, but we assume for simplicity that it is in the ground state). Also there is a photon with frequency ω_0 in the incoming state. After absorption of the photon the molecule is in an excited state $|Q_J\rangle = a_J^\dagger|0\rangle$. The matrix element that describes the absorption of an incoming photon is given according to first-order perturbation theory

$$M = \langle Q_J | \textstyle\sum_i e_i \, \vec{\epsilon} \cdot \vec{r}_i | 0 \rangle \tag{12.41}$$

and is only then nonvanishing if at least one of the $3N$ operators x_i, y_i, z_i has an operator $\widehat{Q}_J$

[11] It might seem more direct to decompose χ_{gen} into irreps than χ_S because the latter still contains χ_{trans} and χ_{rot}, but because χ_S is so much simpler than χ_{gen}, we begin with χ_S.

in its expansion into normal modes. The normal modes in terms of generalized coordinates Q_J become a set of $3N$ decoupled harmonic oscillators, and at the quantum level the wave function of the buckyball becomes a product of $3N$ Hermite functions. The ground state $|0\rangle$ transforms as a scalar under the group G but the wave function corresponding to the state $\langle Q_J|$ is linear in Q_J, and in the decomposition of x, y, z into irreps the coordinates Q_J must transform like one of these irreps in order that the matrix element is nonvanishing. Since x, y and z transform as $D_g^{R_3}$ under A_5 and as $\sigma = -1$ under space inversion, only the normal modes whose character appear also in the character of the x, y, z representation can give infrared spectra. In figure 12.13 we see 4 clear IR absorption lines, at angular frequencies $\frac{\omega}{c} = \frac{2\pi}{\lambda} = 526$, 576, 1182 and 1428 cm^{-1}. Our task is to explain why there are precisely 4 lines.

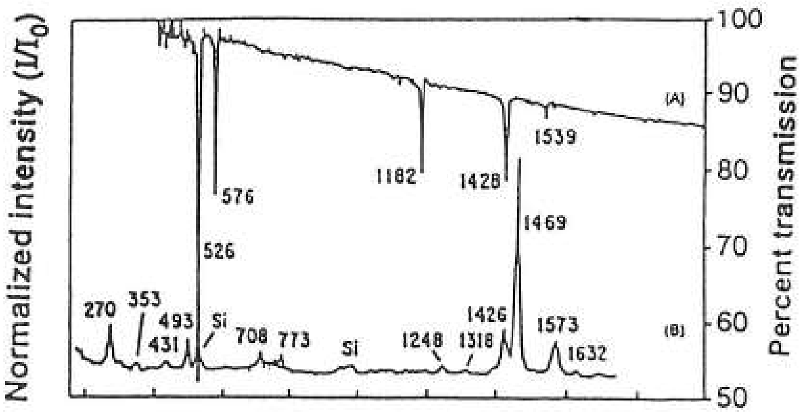


Figure 12.13: First-order infrared (A) and Raman (B) spectra for C_{60} taken with low incident optical power levels (< 50 mW/mm^2).

ii) *Raman spectra.* Monochromatic laser light with polarization vector $\vec{\epsilon}$ hits the C_{60} molecules, but now first one level (a) is excited, and then a transition to another level (b) occurs[12]. One observes then scattered light with polarization vector $\vec{\epsilon}\,'$ whose frequency is shifted. If the buckyball was in its ground state the final photon that comes out of the C_{60} molecule has a lower frequency ν' (less energy, red-shifted) $\nu' = \nu - \nu_{ab}$. If the molecule was in an excited state, the final photon that comes out can have higher frequenct (more energy, blue-shifted) $\nu' = \nu + \nu_{ab}$. The Raman spectrum is symmetric about the frequency ν of the incoming photon: on one side one finds the Raman lines which are red-shifted (Stokes lines), and on the other side one finds the lines that are blue-shifted (anti-Stokes lines). In semiclassical radiation theory, the matrix element for such a Raman line is according to second-order perturbation

[12] There are, of course, no lines in Raman spectra which correspond to the transition from the ground state directly to a final state, because in such transitions the incoming photon is absorbed, and so no scattered photon can be observed.

theory proportional to

$$\sum_i \frac{\langle Q_J| \sum_{j=1}^N e_j \vec{\epsilon'} \cdot \vec{r}_j |i\rangle\langle i| \sum_{k=1}^N e_k \vec{\epsilon} \cdot \vec{r}_k |0\rangle}{E_i - E_0} \tag{12.42}$$

where $|0\rangle$ is the ground state, $|i\rangle$ are all intermediate states and $\langle Q_J|$ is the final state with one quantum of the harmonic oscillator whose generalized coordinate is Q_J. If the energies E_i are not too different from each other[13], one can extract the factor $(E_i - E_0)^{-1}$, and using completeness $\sum_i |i\rangle\langle i| = I$ one is left with [2]

$$\sum_i \langle Q_J| \sum_{j=1}^N e_j \vec{\epsilon'} \cdot \vec{r}_j |i\rangle\langle i| \sum_{k=1}^N e_k \vec{\epsilon} \cdot \vec{r}_k |0\rangle = \langle Q_J| \left(\sum_{j=1}^N e_j \vec{\epsilon'} \cdot \vec{r}_j \right) \left(\sum_{k=1}^N e_k \vec{\epsilon} \cdot \vec{r}_k \right) |0\rangle \tag{12.43}$$

Thus only if the operator $\widehat{Q}_J$ appers in at least one of the decompositions of the quadrupole operators $x^i x^j$ (with $x^i = x, y, z$), there will be a Raman line in the spectrum. In figure 12.14 one sees the 10 lines in the Raman spectrum, namely two lines at 493, 1469 cm^{-1} (they are due to the irrep A_g in table 12.4), and eight lines at 270, 431, 708, 773, 1099, 1248, 1426 and 1572 cm^{-1} (they are due to the irrep H_g in table 12.4). Again, our task is to explain why there are 10 lines.

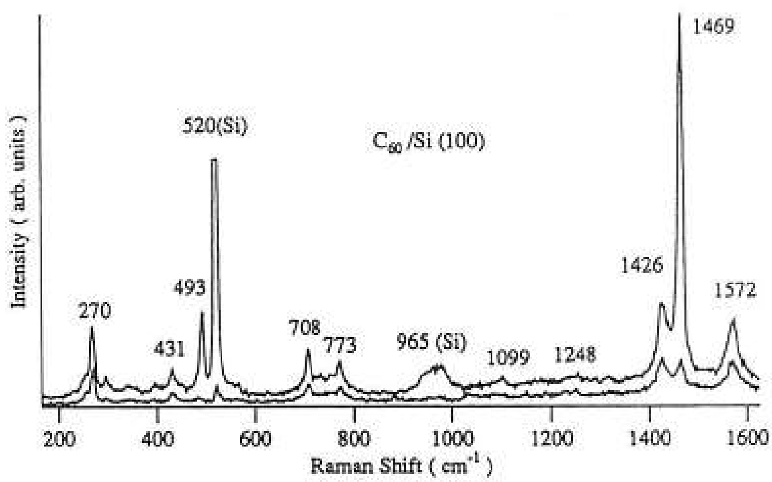


Figure 12.14: Polarized Raman spectra for C_{60}. The upper trace shows both A_g and H_g modes. The lower trace shows primarily H_g modes, the weak intensities for the A_g modes attributed to small polarization leakage. In the experiment on C_{60} there was also some contamination of Silicon, and one sees two Silicon lines.

Infrared radiation can only come from transitions to $\langle Q_J|$ where Q_J are irreps which are also contained in the representation $D^{\mathbb{R}^3}$. The representation $D^{\mathbb{R}^3}$ corresponds to the 3-dim. represen-

[13] A typical case where this happens is a semi-conductor which has an energy gap between the ground state and the set of closely-spaced excited states.

tation F_{1u}. We see from equation (12.40) that there should be 4 lines in the infrared spectrum, in agreement with experiment, see figure 12.13. The Raman spectrum can only come from Q_J with the same transformation properties under I_h as x^2 or $x_i x_j - \frac{1}{3}\delta_{ij}x^2$. Only A_g (a singlet) and H_g (a quintet) have these properties[14]. We see then from (12.40) that one should expect 2 Raman lines from A_g and 8 Raman lines from H_g, again in agreement with experiment, see figures 12.13 and 12.14.

Comment. The isometry group of the icosahedron is $A_5 \cup \sigma A_5 = A_5 \times (e, \sigma)$, where A_5 contains the 60 rotations and σ denotes the space inversion. We constructed the buckyball by cutting off little cones around the 12 vertices, and this created a surface with 12 newly created pentagons, while the 20 triangles of the icosahedron were changed into 20 hexagons. In this way we obtained a surface with $V = 12 \times 5 = 60$ vertices, $F = 20 + 12 = 32$ faces, and $E = 30 + 12 \times 5 = 90$ edges (check: V-E+F=2). The buckyball is certainly invariant under the isometry group of the icosahedron, but it has additional symmetries which the icosahedron did not possess (for example, the icosahedron has 60 rotational symmetries, while the buckyball has 180 rotational symmetries). If so, will multiplets of the normal modes of an icosahedron split into submultiplets of the buckyball? This would lead to more spectral lines in the spectrum of the buckyball than of the icosahedron and then taking only $G = A_5 \times (e, \sigma)$ into account would be wrong. As a toy model, we consider a triangle, of which we cut off little triangles near the vertices, yielding a hexagon. The triangle plays the role of icosahedron in this discussion, and the hexagon plays the role of the buckyball. Our aim is to compare the spectrum of the hexagon with the spectrum of the triangle.

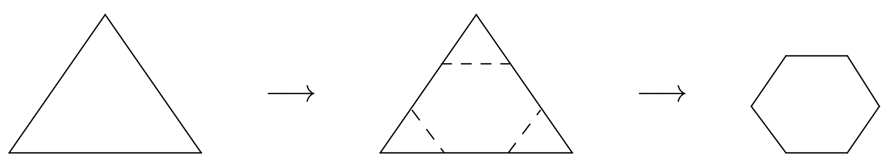


Figure 12.15:

The symmetry group in the plane of a triangle is D_3 of order 6, while the planar symmetries of the hexagon, excluding 3-dimensional symmetries, is D_6 of order 12. (We shall discuss the nonplanar symmetries later, but it is easy to count them: in the plane the hexagon has $2N - 3 = 9$ genuine normal modes, while in space it has $3N - 6 = 12$ genuine normal modes. Hence the hexagon has 9 planar and 3 nonplanar normal modes.)

To obtain the spectrum of the hexagon, we construct a table with the characters for the irreps of D_6, the character for "the physical representation" (the 2-dimensional representation $M_{R^2}(g)$ of D_6), the character χ_S for the deviation of all atoms in the space $S = R^{2N} = R^{12}$, and the

[14]One can also derive this result in a more formal way. The character of the tensor product $\mathbf{3} \times \mathbf{3}$ is $\chi^{3\times 3} = F_{1u}F_{1u} = \left(9, 1, 0, \varphi_+^2, \varphi_-^2, 9, 1, 0, \varphi_+^2, \varphi_-^2\right)$. It contains the trivial character A_g once, and this corresponds to the one-dimensional irrep $x^2 + y^2 + z^2$. It also contains the character $F_{1g} = (3, -1, 0, \varphi_+, \varphi_-, 3, -1, 0, \varphi_+, \varphi_-)$ once, and this corresponds to the 3-dimensional irrep $\vec{r} \times \vec{r}$. Finally it contains the character $H_g = (5, 1, -1, 0, 0, 5, 1, -1, 0, 0)$ once, and this corresponds to the symmetric traceless operator $r^i r^j - \frac{1}{3}\delta^{ij} r^2$.

character χ_{gen} for the genuine normal modes, namely all normal modes minus the 2 zero modes for translations in physical space, and also minus the one zero mode for rotations in the plane. Finally, we shall determine the spectrum of the hexagon: how many lines there are in the spectrum of the hexagon if $G = D_6$. Then we redo the whole calculation or $G = D_3$ and compare the results.

The various characters for D_6 are given in table 12.5 (the numbers in square brackets [] give the orders of the classes). There are 6 classes in total, namely 2 classes with 1 group element, 2 classes with 2 group elements, and 2 classes with 3 group elements obtained as follows

$$e \quad a \quad a^2 \quad a^3 \quad a^4 \quad a^5 \qquad b \quad ab \quad a^2b \quad a^3b \quad a^4b \quad a^5b$$

Hexagon, D_6	$e[1]$	$a^2[2]$	$a[2]$	$a^3[1]$	$b[3]$	$ab[3]$	
Cosets G/V	$C(D_6)$		$aC(D_6)$		$bC(D_6)$	$abC(D_6)$	
χ_1	1	1	1	1	1	1	$C(D_6) = \{e, a^2, a^4\}$
$\chi_{1'}$	1	1	-1	-1	-1	1	$G/C(D_6) = V$
$\chi_{1''}$	1	1	-1	-1	1	-1	The four 1-dim
$\chi_{1'''}$	1	1	1	1	-1	-1	characters of V.
χ_2	2	-1	1	-2	0	0	$\chi_2 = \chi_2\chi_1$
$\chi_{2'}$	2	-1	-1	2	0	0	$\chi_{2'} = \chi_2\chi_{1'} = \chi_2\chi_{1''}$
n_g	6	0	0	0	0	2	number of atoms held fixed
χ_{R^2}	2	-1	1	-2	0	0	tr $D_{\mathbb{R}^2}$ of physical space
χ_S	12	0	0	0	0	0	$\chi_S = n_g\chi_{R^2}$
χ_{tr}	2	-1	1	-2	0	0	$\chi_{\text{tr}} = \chi_{R^2}$
χ_{rot}	2	-1	1	-2	0	0	$\chi_{\text{rot}} = \chi_{R^3} \det D_{\mathbb{R}^3} = \chi_2\chi_{1'''}$
χ_{gen}	8	2	-2	4	0	0	$\chi_{\text{gen}} = \chi_S - \chi_{\text{tr}} - \chi_{\text{rot}}$

Table 12.5: a denotes rotation over 60° and b reflection about y-axis.

The commutator subgroup is $C(D_6) = (e, a^2, a^4)$. The 4 coset elements of $D_6/C(D_6)$ are

$$C = (e, a^2, a^4), \quad aC = (a, a^3, a^5), \quad bC = (b, a^2b, a^4b) \text{ and } abC = (ab, a^3b, a^5b). \tag{12.44}$$

and they form the group V. We then get four 1-dim irreps from $D_6/C(D_6) = V$, and $12 = 1^2 + 1^2 + 1^2 + 1^2 + x^2 + y^2$. There is only one solution: $x = y = 2$. The isometries in the plane give a 2-dimenaional irrep.

Using the orthogonality relations for characters, we find

$$\chi_{\text{gen}} = \sum_i n_i \chi^i$$
$$n_1 = 1\,, \quad n_{1'} = 2\,, \quad n_{1''} = 1\,, \quad n_{1'''} = 0\,, \quad n_2 = 1\,, \quad n_{2'} = 3 \Rightarrow \textbf{8 lines}. \tag{12.45}$$

As a check we evaluate

$$(\chi_{\text{gen}}, \chi_{\text{gen}}) = |D_6| \sum_{i=1}^{6} n_i^2 = 12 \times 16 \tag{12.46}$$

where $\chi_{\text{gen}} = \sum_i n_i \chi^i$ which agrees with $\sum_i n_i^2 = 16$. Also $(\chi_S, \chi_S) = 28 \times 12$ and $\chi_S = \sum_i m_i \chi^i$ agrees with $\sum_i m_i^2 = 28$ since $\chi_{tr} = \chi_2 + \chi_1$ and $\chi_{rot} = \chi_2 + \chi_{1'''}$, hence

$$m_1 = 1\,, \quad m_{1'} = 2\,, \quad m_{1''} = 1\,, \quad m_{1'''} = 1\,, \quad m_2 = 3\,, \quad m_{2'} = 3\,. \tag{12.47}$$

The hexagon yields then a spectrum with 8 lines.

Let us now determine the spectrum of a hexagon if we only take the symmetry group D_3 into account instead of D_6. We get table 12.6.

Hexagon, D_3	$e[1]$	$a^2[2]$	$b[3]$	Comments
χ_I	1	1	1	
$\chi_{I'}$	1	1	-1	
χ_{II}	2	-1	0	
n_g	6	0	1	
χ_{R^2}	2	-1	0	$\chi_{II} = \chi_{R^2} - \chi_I$
χ_S	12	0	0	
χ_{tr}	2	-1	0	
χ_{rot}	12	-1	0	
χ_{gen}	9	0	0	

Table 12.6: a^2 denotes rotation over 120° and b reflection about y-axis.

We now find $(\chi_{\text{gen}}, \chi_{\text{gen}}) = 144 = 24 \times 6$. Hence $\chi_{\text{gen}} = \sum_J n_J \chi^J$ with

$$n_I = 2\,, \quad n_{I'} = 2\,, \quad n_{II} = 4 \Rightarrow \mathbf{8\ lines}. \tag{12.48}$$

These multiplets split as follows under the larger symmetry group D_6

$$n_I = n_1 + n_{1''} = 1 + 1\,; \quad n_{I'} = n_{1'} + n_{1'''} = 2 + 0\,; \quad n_{II} = n_2 + n_{2'} = 1 + 3\,. \tag{12.49}$$

We see that each multiplet remains a multiplet, hence the spectrum is unchanged (although one gains more information about the symmetries of a given multiplet if the symmetry group is larger). We anticipate that the same holds for buckyballs.

*12.5 Case study 1: the spectrum of the $CO_3^=$ ion

As a third example of the role of finite group theory in the theory of molecular vibrations we consider the $CO_3^=$ ion [3], which forms an equilateral triangle of 3 oxygen atoms in the horizontal x-y plane with a carbon atom in the middle. If one views the triangle as a polygon in the plane, its isometries form the dihedral group D_3, but the deviations of the atoms from their equilibrium positions constitute of course a physical system in three dimensions, and its symmetry group is larger than D_3. In equilibrium this molecule is invariant under 12 symmetry operations, namely 6 rotations and 6 (generalized) reflections. The rotations are e, C_3^1, $C_3^2 = (C_3^1)^2$ around the z axis over angles 0, $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$, and further a rotation C' over π along an axis through vertex 1 and the center, another π-rotation C'' along the axis through vertex 2 and the center, and a third rotation C''' over π along the axis connecting vertex 3 and the center. The reflections are: σ_h with respect to the horizontal plane, and σ_v', σ_v'', σ_v''' with respect to vertical planes through the center and the vertices 1, 2 and 3. This only yields 4 reflections, but closure of the group[15] yields two more generalized reflections which are a product of a rotation C_3^1 or C_3^2 followed by the reflection σ_h. The element σ_h commutes with all other group elements. The total set of 12 group elements is called D_{3h} in the chemical literature. We discuss it further below.

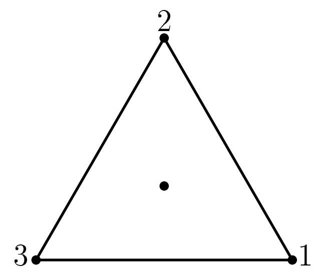


Figure 12.16: The structure of a $CO_3^=$ ion.

To obtain the class structure of this group, we begin with the element σ_h. It commutes with all other elements because all twelve 3×3 matrices are block-diagonal with a 2×2 block and a 1×1 block, and σ_h is the unit matrix in these subspaces. Hence σ_h forms a class by itself. Next consider the class to which σ_v' belongs. Since $C_3^2 \sigma_v' C_3^1 = \sigma_v'''$ and $C_3^1 \sigma_v' C_3^2 = \sigma_v''$ this class, denoted by σ_v, contains all 3 vertical reflections. This is as expected: physically these 3 reflections are equivalent. The rotations C_3^1 and C_3^2 form a separate class denoted by C_3, as do the rotations C', C'', C''' which form the class C_2. And finally the elements $\sigma_h C_3^1$ and $\sigma_h C_3^2$ form the class $\sigma_h C_3$. This yields the class structure as indicated in the first line of table 12.7.

The rotations form the group $D_3 = S_3$. Each rotation permutes the vertices 1, 2 and 3, for example $C_3^1 = (123)$, $C_3^2 = (132)$ and $C' = (23)$. The other 6 elements can be written as $\sigma_h S_3$ (note that $\sigma_v' = \sigma_h C'$, $\sigma_v'' = \sigma_h C''$ and $\sigma_v''' = \sigma_h C'''$. Thus $\sigma_v = \sigma_h C_2$.) Thus the group is $S_3 \cup \sigma_h S_3$, which can be rewritten as the direct product group $S_3 \times \{e, \sigma_h\}$.

We now summarize the results of the characters in table 12.7, and afterwards discuss this table. There are 6 classes, and thus also 6 irreps. We construct the character table using the methods discussed before, see for example (12.29), and the character table of D_3 was constructed in chapter 8. (In this case, the matrix K contains the characters of $D_3 = S_3$ and is a 3×3 matrix formed by the first 3 entries of A_g, A_u' and E_u). The reducible 3-dimensional representation

[15] Often one begins with $S_3^1 = \sigma_h C_3^1$, and then closure brings in $S_3^5 = \sigma_h C_3^2$. (Of course, $S_3^2 = C_3^2$, $S_3^3 = \sigma_h$ and $S_3^4 = C_3^1$ are not new group elements).

$(x,\, y,\, z)$ decomposes into two irreps as indicated in the one-but-last column, and the reducible 6-dimensional representation $x^i x^j + x^j x^i$ (with $i,\, j = 1,\, 2,\, 3$) decomposes into four irreps as indicated in the last column. It is rather obvious that $x^2 + y^2$ and z^2 are singlets under all symmetries, and (xz, yz) form a doublet which is odd under σ_h. We can check that $2xy$ and $x^2 - y^2$ form another doublet which is even under σ_h by substituting the explicit transformation rules of x, y and z under the rotations over $\frac{2\pi}{3}$. One may also prove the decomposition of $x^i x^j$ into four irreps by decomposing the square of the character $\chi_{R^3} = \chi_{\text{tr}}$ of the reducible 3-dimensional representation spanned by x, y and z.[16]

$CO_3^=$	e 1	C_3 2	C_2 3	σ_h 1	$\sigma_h C_3$ 2	σ_v 3	IR	Raman
A_g	1	1	1	1	1	1		$x^2+y^2,\, z^2$
A'_g	1	1	-1	-1	-1	1	z	
A_u	1	1	1	-1	-1	-1		
A'_u	1	1	-1	1	1	-1	R_z	
E_u	2	-1	0	2	-1	0	(x, y)	$(2xy, x^2-y^2)$
E_g	2	-1	0	-2	1	0	(R_x, R_y)	(xz, yz)
χ_{tr}	3	0	-1	1	-2	1		
χ_{rot}	3	0	-1	-1	2	-1		
n_g	4	1	2	4	1	2		
χ_S	12	0	-2	4	-2	2		
χ_{gen}	6	0	0	4	-2	2		

Table 12.7: Character table for the $CO_3^=$ ion. Decomposing the reducible reps χ_{tr}, χ_{rot} and χ_{gen} we find $\chi_{\text{tr}} = A'_g + E_u$, $\chi_{\text{rot}} = A'_u + E_g$ and $\chi_{\text{gen}} = A_g + A'_g + 2E_u$.

We have now enough information to deduce the infrared and Raman spectra, and the reader who has understood the discussion of the spectrum of C_{60} can go directly to below (12.83). For readers who prefer a more detailed discussion with all steps included, we now present such a discussion. It is on purpose verbose, and extends to (12.83).

There are $4 \times 3 - 3 - 3 = 6$ nonzero modes and $3 + 3$ zero modes. The motion of the two most symmetric nonzero normal modes is as follows: in the breather mode all O atoms move radially outward while the C atom is fixed (figure 12.17), while there is also a motion out of the plane where the C atom moves upward and all O atoms move downwards (figure 12.18).

One may check that acting with one of the symmetries from each of the 6 classes on the breather produces the character A_g, and acting on the up-down mode produces the character A'_g. The rest of the normal modes form two doublets. Each of these two doublets corresponds to 3 degenerate normal modes which are linearly dependent. In figure 12.19 we only depict one normal mode of each triplet. The other two normal modes of each triplet are obtained by rotation along the z-axis

[16] Squaring $\chi_{R^3} = \chi_{\text{tr}} = (3, 0, -1, 1, -2, 1)$ yields $\chi_{R^3 \otimes R^3} = (9, 0, 1, 1, 4, 1)$ which decomposes into the four characters in the column denoted by Raman, and two further characters which transform as R_z and (R_x, R_y) and which come from the antisymmetric part ($\vec{r}_1 \times \vec{r}_2$ is a pseudovector). So $(\chi_{R^3} \otimes \chi_{R^3})_{sym} = 2A_g + E_u + E_g$ and $(\chi_{R^3} \otimes \chi_{R^3})_{antisym} = A'_u + E_g$.

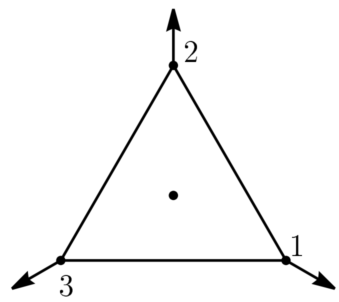


Figure 12.17: The breather A_g (this motion is in the x-y plane).

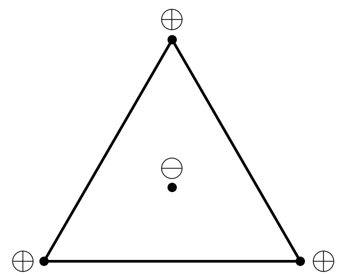


Figure 12.18: The up-down mode A'_g (here $\oplus$ indicates upward motion along the positive z-axis and $\ominus$ downward motion along the negative z-axis).

over $\frac{2\pi}{3}$ and $\frac{4\pi}{3}$. From symmetry alone it is clear that the sum of the deviations of each triplet of degenerate normal modes vanishes. A linearly independent set of degenerate modes consists then of any two of three degenerate modes. Acting with the symmetry operations on the first normal mode in figure 12.19 maps it into a linear combination of itself and the rotated normal mode. The same holds for the second normal mode in figure 12.19.

(If one would remove the C atom in the middle, one would be left with 3 atoms forming an equilateral triangle which has 3 nonzero normal modes, namely the breather and the second doublet in figure 12.19.)

Having obtained the character table of the $CO_3^=$ ion, and the multiplets of the 12 normal modes

$$\chi_{\text{gen}} = A_g + A'_g + 2E_u; \qquad \chi_{\text{tr}} = A'_g + E_u; \qquad \chi_{\text{rot}} = A'_u + E_g, \tag{12.50}$$

we now want to identify the IR and Raman spectra: which multiplets can absorb IR radiation, and which multiplets can emit Raman radiation. In particular, we want to find out whether some multiplets are both IR and Raman active.

IR radiation can be absorbed by the irreps that are present in the reducible rep of the coordinates x, y, z. If one views x as a unit vector along the x-axis, one can figure out how it transforms under the group elements into a linear combination of x, y, z representations of G. This is of course the representation D^{R^3} in physical 3-dim. space which is also the representation of the 3 translational zero modes.

$$D^{\mathbb{R}^3} = D^{\text{tr}} \tag{12.51}$$

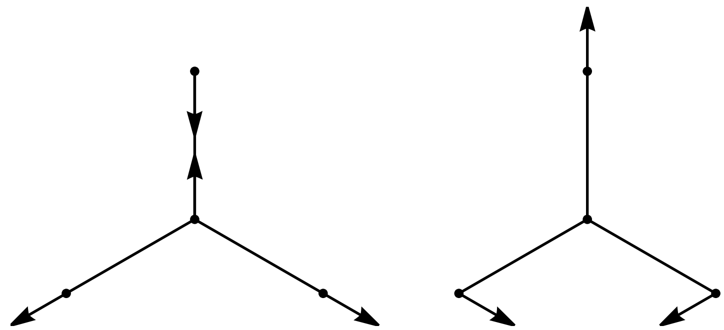


Figure 12.19: Motions of the doublets. A basis for the first doublet consists of the motion of the first figure together with the motion obtained by rotating the first figure over an angle $\frac{2\pi}{3}$ (or $\frac{4\pi}{3}$). These two motions transform into each other under the isometries, yielding a two-dimensional representation of the symmetry group. Taking the trace of the corresponding 2-dimensional matrices reproduces the character $E_u = (2, -1, 0, 2, -1, 0)$. For example, under the rotation C_3^1 the first motion transforms into the second motion, while the second motion transforms into a rotation which is minus the sum of the two motions, yielding the matrix $\left(\begin{smallmatrix} 0 & -1 \\ 1 & -1 \end{smallmatrix}\right)$ whose trace equals -1 which is indeed the character E_u for C_3. The same holds for the second doublet, but although the character of these two doublets are the same, the frequencies of these two doublets will be different.

For the characters one only needs one group element per class, and one can choose any suitable coordinate system. It is sufficient to only know the decomposition of $\chi_{\rm tr}$ into irreducible characters, but we shall also determine the matrices $D_g^{R^3}$ for a few group elements.

For the Raman spectrum similar selection rules hold, but now instead of x, y, z one needs the reducible representations of $x^i x^j$, so of the 6 combinations x^2, y^2, z^2, xy, xz, yz. Since x, y, z transform as $D_g^{R^3}$, one can take the direct product of the two representations $D_g^{R^3}$ and substract the antisymmetric part which transforms as $D_g^{\rm rot}$ (since $\vec{r} \times \vec{r}$ is an axial vector):

$$D^{\rm Raman} = D^{\rm tr} \otimes D^{\rm tr} - D^{\rm rot} \tag{12.52}$$

Decomposing the rep. of $x^i x^j$ into irreps, these are the irreps which can give rise to spectral lines in the Raman spectrum.

Let us first consider the transformations of x, y, z. Since the molecule lies in the x-y plane, we may anticipate that z transforms differently from the pair x, y, so we begin with z. It is clear that z (more precisely: a vector along the z-axis) is invariant under all group elements in e, C_3, σ_v but changes sign under C_2, σ_h, $\sigma_h C_3$. Thus z is a singlet, and should be one of the 1-dim. irreps. Scanning the character table one easily identifies this irrep

$$z \sim A'_g \tag{12.53}$$

Next we consider the pair x, y. From our study of characters we have already found that the reducible rep x, y, z decomposes into A'_g and E_u, and since we already identified $z \sim A'_g$, we know that $(x,\, y)$ should form a doublet which transforms according to 2×2 matrices whose trace is E_u. But for pedagogical reasons we still shall determine some of these matrices. Consider first how C_3^1 acts on x. Under an anticlockwise rotation over $2\pi/3$ the unit vector $\vec{e}_x$ along the x-axis transforms into a vector with components $(x',\, y')$, and the unit vector $\vec{e}_y$ along the y-axis transform into a vector with components $(x'',\, y'')$, given by

$$(x',\, y') = \left(-\frac{1}{2},\, \frac{1}{2}\sqrt{3}\right); \qquad (x'',\, y'') = \left(-\frac{1}{2}\sqrt{3},\, -\frac{1}{2}\right) \tag{12.54}$$

Hence the 2×2 matrix representation is given by

$$C_3^1 = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}, \qquad \chi^{(x,\, y)}(C_3) = -1 \tag{12.55}$$

The 2×2 matrices associated with the class C_2 are of course different for C_2', C_2'' or C_2''', but they will give the same character. It is easiest to construct the matrix for C_2'' (rotations along the y-axis over π), and one finds

$$C_2''(x,\, y) = (-x,\, y); \qquad C_2'' = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \chi^{(x,\, y)}(C_2) = 0 \tag{12.56}$$

Proceeding in this way with the other classes, one confirms that the pair x, y forms an irreducible 2×2 matrix representation of the symmetry group G whose trace is the character E_u

$$(x,\, y) \sim E_u \tag{12.57}$$

Let us now analyze the Raman spectrum. We need to determine how the symmetric tensor $x^i x^j$ transforms under G. We first use characters to find out how the reducible rep $x^i x^j$ decomposes into irreps, but then we shall, again for pedagogical reasons, construct some explicit matrices whose trace gives these characters. To obtain the reducible 6×6 rep $x^i x^j$, we take the direct product of two $(x,\, y,\, z)$ reps. As we already noted, one should substract the antisymmetric part of this direct product, but we shall first proceed with the direct product, and do the substraction later. Taking the trace we find $\chi^{x^i \otimes x^j} = \chi^{x^i}\chi^{x^j}$. Since

$$\chi^{x^i} = \chi^{(z)} + \chi^{(x,\, y)} = (1,\, 1,\, -1,\, -1,\, -1,\, 1) + (2,\, -1,\, 0,\, 2,\, -1,\, 0) = (3,\, 0,\, -1,\, 1,\, -2,\, 1) \tag{12.58}$$

which is of course equal to χ_{tr}, we obtain

$$\chi^{x^i \otimes x^j} = (9,\, 0,\, 1,\, 1,\, 4,\, 1), \tag{12.59}$$

which can be decomposed into irreps to yield

$$\chi^{x^i \otimes x^j} = 2A_g + A'_u + E_u + 2E_g \tag{12.60}$$

As a check we evaluate the inner product of this reducible rep with itself

$$\left(\chi^{x^i \otimes x^j},\, \chi^{x^i \otimes x^j}\right) = \frac{1}{12}(81 + 0 + 3 + 1 + 32 + 3) = 10, \tag{12.61}$$

which agrees with $2^2 + 1^2 + 1^2 + 2^2 = 10$. However, if we evaluate this character on the class e, we should find the dimension of the rep. of $x^i x^j$ which is 6, but we find $2 + 1 + 2 + 2 \times 2 = 9$. This discrepancy is of course due to the antisymmetric part of two vector reps. Denoting them by x_1^i and x_2^j, the antisymmetric part $x_1^i x_2^j - x_1^j x_2^i$ transforms as an axial vector, $\epsilon_{ijk} x^k$, hence we must substract the trace of D^{rot} which is $\chi_{\mathrm{rot}} = (3,\, 0,\, -1,\, -1,\, 2,\, -1) = A'_u + E_g$. This yields for the rep of the symmetric part of $x^i x^j$

$$\chi^{(x^i \otimes x^j)} = (6,\, 0,\, 2,\, 2,\, 2,\, 2) = 2A_g + E_u + E_g \tag{12.62}$$

So, characters tell us that the six-dimensional rep spanned by x^2, y^2, z^2, xy, xz, yz decomposes into two singlets and two doublets. Let us now explicitly construct these irreps.

The tensor component z^2 transforms under all elements of G into itself, hence it forms the irrep A_g

$$z^2 \sim A_g \tag{12.63}$$

Let us next consider x^2 and y^2. Since we already know how x and y transform, one can easily read off how x^2 and y^2 transform. Let us begin with $g = C_3^1$. Then we find from (12.54)

$$C_3^1 x^2 = \left(-\tfrac{1}{2}x - \tfrac{1}{2}\sqrt{3}y\right)^2; \qquad C_3^1 y^2 = \left(\tfrac{1}{2}\sqrt{3}x - \tfrac{1}{2}y\right)^2 \tag{12.64}$$

Taking the sum and difference yields

$$C_3^1(x^2 + y^2) = x^2 + y^2; \qquad C_3^1(x^2 - y^2) = -\tfrac{1}{2}(x^2 - y^2) + \sqrt{3}xy \tag{12.65}$$

Consider next C_2'' (the rotation along the y-axis over π). Then x transforms into $-x$ and y into y, so x^2 transforms into x^2 and y^2 into y^2, so

$$C_2''(x^2 + y^2) = x^2 + y^2; \qquad C_2''(x^2 - y^2) = x^2 - y^2 \tag{12.66}$$

In a similar way we find how particular group elements of the remaining classes act on x^2 and y^2:

$$\sigma_h(x^2 \pm y^2) = x^2 \pm y^2; \qquad \sigma_h C_3^1(x^2 \pm y^2) = \begin{cases} x^2 + y^2 \\ -\frac{1}{2}(x^2 - y^2) + \sqrt{3}xy \end{cases}; \qquad \sigma_v''(x^2 \pm y^2) = x^2 \pm y^2 \tag{12.67}$$

We already found that $x^2 - y^2$ transforms also into xy, so we compute also the action of these group elements on xy

$$C_3^1 xy = \left(-\tfrac{1}{2}x - \tfrac{1}{2}\sqrt{3}y\right)\left(\tfrac{1}{2}\sqrt{3}x - \tfrac{1}{2}y\right) = -\tfrac{1}{4}\sqrt{3}(x^2 - y^2) - \tfrac{1}{2}xy \tag{12.68}$$

$$C_2' xy = -xy; \qquad \sigma_h xy = xy; \qquad \sigma_h C_3^1 xy = \tfrac{1}{4}\sqrt{3}(x^2 - y^2) - \tfrac{1}{2}xy; \qquad \sigma_v'' xy = -xy \tag{12.69}$$

We thus reach the following conclusions:

- $x^2 + y^2$ is another singlet that transforms like A_g (and like z^2 as we already established)
- $x^2 - y^2$ and xy form a doublet, and transform as follows

$$C_3^1 \begin{pmatrix} x^2 - y^2 \\ xy \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \sqrt{3} \\ -\frac{\sqrt{3}}{4} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} x^2 - y^2 \\ xy \end{pmatrix}; \quad C_2' \begin{pmatrix} x^2 - y^2 \\ xy \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x^2 - y^2 \\ xy \end{pmatrix} \tag{12.70}$$

$$\sigma_h \begin{pmatrix} x^2 - y^2 \\ xy \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} x^2 - y^2 \\ xy \end{pmatrix}; \quad \sigma_h C_3^1 \begin{pmatrix} x^2 - y^2 \\ xy \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \sqrt{3} \\ -\frac{\sqrt{3}}{4} & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} x^2 - y^2 \\ xy \end{pmatrix} \tag{12.71}$$

$$\sigma_v'' \begin{pmatrix} x^2 - y^2 \\ xy \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} x^2 - y^2 \\ xy \end{pmatrix} \tag{12.72}$$

Taking the trace, we find the characters

$$\chi^{(x^2+y^2)} = (1,\, 1,\, 1,\, 1,\, 1,\, 1) = A_g \qquad \chi^{(x^2-y^2,\, xy)} = (2,\, -1,\, 0,\, 2,\, -1,\, 0) = E_u \tag{12.73}$$

So far we have discovered that z^2, $x^2 + y^2$, and $(x^2 - y^2,\, xy)$ form irreps. According to (12.62) we also must find a 2-dimensional linear subspace which transforms like E_g, and this suggests that xz and yz form a doublet. One may make a few checks. For example, under C_3^1, xz transforms into $\left(-\frac{1}{2}x - \frac{1}{2}\sqrt{3}y\right) z$ and yz into $\left(\frac{1}{2}\sqrt{3}x - \frac{1}{2}y\right) z$. Hence the 2×2 matrix representation of C_3^1 is

$$C_3^1 = \frac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \quad \Longrightarrow \quad \chi^{(xz,\, yz)}(C_3^1) = -1 \tag{12.74}$$

which agrees with E_g but also with E_u. However, under σ_h the doublet $(xz,\, yz)$ transforms into minus itself which agrees with E_u but not with E_g. Hence the doublet $(xz,\, yz)$ indeed transforms as E_u.

For completeness we also make a study of the transformation properties of the displacement vectors due to the three rotations along the x-axis, y-axis and z-axis. For each rotation, the vector sum of the displacement vectors vanishes, $\vec{x'} + \vec{y'} + \vec{z'} = 0$, as should be the case since the origin of the coordinate system is at the center of mass. The direct sum of these 3 displacement vectors gives the displacements vectors of the whole molecule.

$$\begin{aligned}
\vec{R}_x &= (0,\ 0,\ a;\ 0,\ 0,\ a;\ 0,\ 0,\ -2a) \\
\vec{R}_y &= (0,\ 0,\ -a;\ 0,\ 0,\ a;\ 0,\ 0,\ 0) \\
\vec{R}_z &= \left(\tfrac{1}{2}a,\ \tfrac{1}{2}\sqrt{3}a,\ 0;\ \tfrac{1}{2}a,\ -\tfrac{1}{2}\sqrt{3}a,\ 0;\ -a,\ 0,\ 0\right)
\end{aligned} \tag{12.75}$$

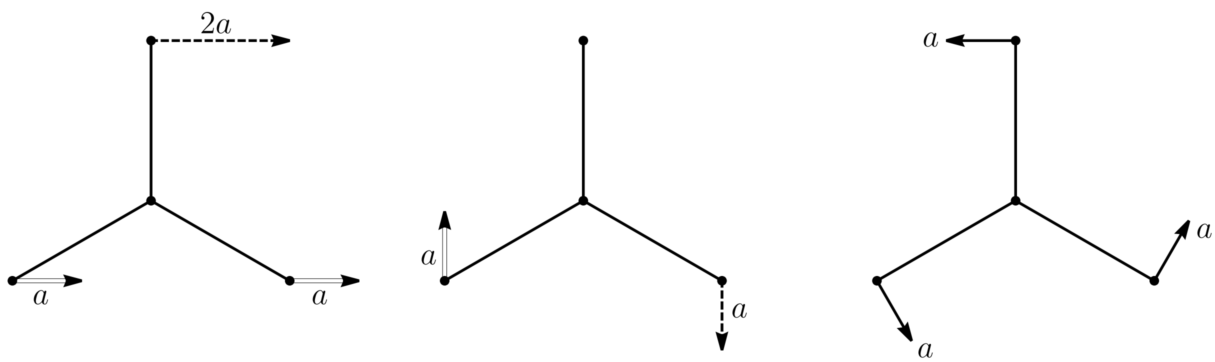


Figure 12.20: The motions due to the three rotations R_x, R_y and R_z. Dashed arrows go into the page and double arrows come out of the page. For the rotation along the x-axis we have $\vec{x'} = (0,\ 0,\ a)$, $\vec{y'} = (0,\ 0,\ a)$ and $\vec{z'} = (0,\ 0,\ -2a)$. For the rotation along the y-axis we have $\vec{x'} = (0,\ 0,\ -a)$, $\vec{y'} = (0,\ 0,\ a)$ and $\vec{z'} = (0,\ 0,\ 0)$. And for the rotation along the z-axis we have $\vec{x'} = (\tfrac{1}{2}a,\ \tfrac{1}{2}\sqrt{3}a,\ 0)$, $\vec{y'} = (\tfrac{1}{2}a,\ -\tfrac{1}{2}\sqrt{3}a,\ 0)$ and $\vec{z'} = (-a,\ 0,\ 0)$.

The three vectors $\vec{R}_x$, $\vec{R}_y$, $\vec{R}_z$ span a 3-dimensional subspace of the $3N = 12$ dimensional space S, and we want to find out into which irreducible invariant subspaces it decomposes. Consider first the 1-dim. subspace $\vec{R}_z$, corresponding to the third picture in figure 12.20. Looking at the picture, it is clear that $\vec{R}_z$ goes into itself under C_3^1, and

$$C_2''\vec{R}_z = -\vec{R}_z, \qquad \sigma_h\vec{R}_z = \vec{R}_z, \qquad \sigma_h C_3^1\vec{R}_z = \vec{R}_z, \qquad \sigma_v''\vec{R}_z = -\vec{R}_z \tag{12.76}$$

These are the transformation properties of the 1-dim character A_u', hence

$$R_z \sim A_u' \tag{12.77}$$

We are left with the two-dimensional linear vector space spanned by R_x and R_y, corresponding to the first two pictures in figure 12.20. The transformations under C_3^1 and $\sigma_h C_3^1$ are less obvious, but under the rest of the group elements one finds easily

$$\left.\begin{aligned} C_2''R_x &= -R_x \\ C_2''R_y &= R_y \end{aligned}\right\} \quad C_2'' = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}; \qquad \left.\begin{aligned} \sigma_h R_x &= -R_x \\ \sigma_h R_y &= -R_y \end{aligned}\right\} \quad \sigma_h = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \tag{12.78}$$

$$\left.\begin{aligned} \sigma_v''R_x &= R_x \\ \sigma_v''R_y &= -R_y \end{aligned}\right\} \quad \sigma_v'' = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{12.79}$$

$$\chi^{(R_x,\,R_y)}(C_2) = 0; \qquad \chi^{(R_x,\,R_y)}(\sigma_h) = -2; \qquad \chi^{(R_x,\,R_y)}(\sigma_v) = 0 \tag{12.80}$$

This is already enough information to conclude that the pair $(R_x,\, R_y)$ transforms as E_g, but for fun we work also out its transformation properties under C_3^1 and $\sigma_h C_3^1$. From the two first pictures in figure 12.20 one notes that under anticlockwise rotations over $\frac{2\pi}{3}$, R_x and R_y transform as follows

$$C_3^1 R_x = R_x' = -\frac{1}{2} R_x - \frac{3}{2} R_y \tag{12.81}$$

$$C_3^1 R_y = R_y' = \frac{1}{2}(R_x - R_y) \tag{12.82}$$

Hence

$$C_3^1 = \frac{1}{2}\begin{pmatrix} -1 & -3 \\ 1 & -1 \end{pmatrix} \qquad \text{and} \qquad \chi^{(R_x,\,R_y)}(C_3) = -1 \tag{12.83}$$

which agrees with E_u (or E_g). In a similar way we find that $(R_x,\, R_y)$ transforms under $\sigma_h C_3^1$ in agreement with E_g.

The results of our study of the transformation properties of $(x,\, y,\, z)$ and $x^i x^j$ are summarized in the last two columns in table 12.7. We see that $(x,\, y,\, z)$ contains the irreps A_g' and E_u, and since χ_{gen} contains the irreps $A_g + A_g' + 2E_u$, we expect 3 lines in the IR absorption spectrum of $CO_3^=$ (one from A_g' and two from E_u). On the other hand $x^i x^j$ contains the irreps A_g, E_u and E_g. Comparing with $\chi_{\text{gen}} = A_g + A_g' + 2E_u$, we expect 3 Raman emission spectrum lines (one from A_g and two from E_u). Two of these lines are both an IR and a Raman line but their frequencies are, of course, different. Hence experiment should produce the following spectrum:

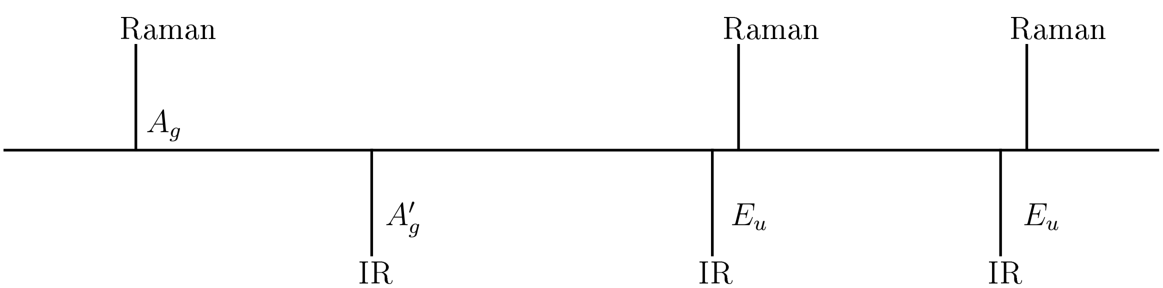


Figure 12.21: Spectral lines from $CO_3^=$.

*12.6 Case study 2: the spectrum of the XeF_4 molecule

The XeF_4 molecule [4] is believed to have the form of a square, with the four F atoms at the vertices and the Xe atom in the middle. There are $5 \times 2 - 2 - 1 = 7$ planar normal modes, and $5 \times 3 - 3 - 3 = 9$ planar and nonplanar modes, hence there are 2 nonplanar modes. The latter are easy to identify, see figure 12.23, but the planar modes require mode discussion which we provide later. We shall calculate the infrared and Raman spectrum as given by lowest order perturbation theory, and compare our predictions with the experimental results. There is agreement.

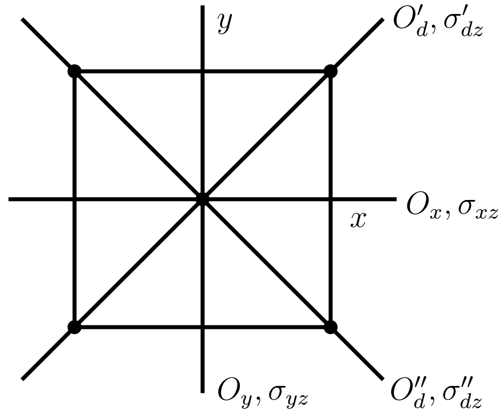


Figure 12.22: Some of the rotations and reflections of a XeF_4 molecule.

The symmetry group G of the molecule consists of 8 rotations which form a dihedral group, and 8 reflections (we define a reflection as an isometry with determinant -1). The 8 rotations are easily found: assuming that the molecule lies in the x-y plane, we have 3 rotations C^1, C^2, C^3 about the z-axis over angles $\frac{2\pi k}{4}$ with $k = 1, 2, 3$, and further 4 rotations over an angle π whose axes are the two diagonals and the x- and y-axis. We call these last 4 rotations O'_d, O''_d, O_x and O_y (see the figure 12.22). One can also easily spot 5 reflections with respect to the following planes: the vertical x-z plane with reflection σ_{xz}, the vertical y-z plane with reflection σ_{yz}, the two vertical planes containing one diagonal and the z-axis with reflections σ'_{dz} and σ''_{dz}, and finally the reflection σ_h with respect to the horizontal x-y plane. See again figure 12.22. In addition, the space inversion i (mapping $\vec{r}$ to $-\vec{r}$) is a symmetry. The two remaining reflections are less obvious and follow from requiring closure of the group G; they are $\sigma_h C^1$ and $\sigma_h C^3$.

The 8 rotations give the dihedral group[17] D_4 with presentation $a^4 = b^2 = e$ and $aba = b$. We take $a = C^1$ and $b = O_x$. Then all 8 rotations can be written as $a^m b^n$

$$\begin{array}{rcccccccc} R: & e, & C^1, & C^2, & C^3, & O_x, & O_y, & O'_d, & O''_d \\ & e, & a, & a^2, & a^3, & b, & a^2b, & ab, & a^3b \end{array} \tag{12.84}$$

The 8 reflections can be written as $\sigma_h R$. It is easy to check that σ_h commutes with a and b (σ_h and b are both represented by diagonal 3×3 matrices, and the group element a results in a rotation in the x-y plane while σ_h acts as the unit matrix in the x-y plane). One may check the following correspondence

$$\begin{array}{rcccccccc} \sigma_h R: & \sigma_h, & \sigma_h C^1, & \sigma_h C^2, & \sigma_h C^3, & \sigma_h O_x, & \sigma_h O_y, & \sigma_h O'_d, & \sigma_h O''_d \\ & \sigma_h, & \sigma_h C^1, & i, & \sigma_h C^3, & \sigma_{xz}, & \sigma_{yz}, & \sigma'_{dz}, & \sigma''_{dz} \end{array} \tag{12.85}$$

[17] The isometries of a square in the plane consists of 4 rotations and 4 reflections, yielding $G = D_4$, but in three dimensions these reflections can be viewed as rotations, and then the 8 rotations yield again D_4.

Since σ_h lies in the center of G, we can write G as a direct product group

$$G = R \otimes (e, \sigma_h) \tag{12.86}$$

Thus the classes of G consist of the classes of R, and σ_h times the classes of R. The classes of R are $\mathcal{C}_0 = \{e\}$, $\mathcal{C}_1 = \{a^2\}$, $\mathcal{C}_2 = \{a^1, a^3\}$, $\mathcal{C}_3 = \{b, a^2b\} = \{O_x, O_y\}$, $\mathcal{C}_4 = \{ab, ab^3\} = \{O_{d'}, O_{d''}\}$. This yields 10 classes of G. We record them in the first row of table 12.8.

G	$\mathcal{C}_0$	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\sigma_h\mathcal{C}_0$	$\sigma_h\mathcal{C}_1$	$\sigma_h\mathcal{C}_2$	$\sigma_h\mathcal{C}_3$	$\sigma_h\mathcal{C}_4$	IR	Raman
$a_{1g}\ \chi^{(1)}_{I+}$	1	1	1	1	1	1	1	1	1	1		$z^2,\ x^2+y^2$
$\chi^{(1)}_{II+}$	1	1	1	-1	-1	1	1	1	-1	-1	R_z	
$b_{1g}\ \chi^{(1)}_{III+}$	1	1	-1	1	-1	1	1	-1	1	-1		x^2-y^2
$b_{2g}\ \chi^{(1)}_{IV+}$	1	1	-1	-1	1	1	1	-1	-1	1		xy
$e_u\ \chi^{(2)}_{+}$	2	-2	0	0	0	2	-2	0	0	0	(x,y)	
$\chi^{(1)}_{I-}$	1	1	1	1	1	-1	-1	-1	-1	-1		
$a_{2u}\ \chi^{(1)}_{II-}$	1	1	1	-1	-1	-1	-1	-1	1	1	z	
$b_{2u}\ \chi^{(1)}_{III-}$	1	1	-1	1	-1	-1	-1	1	-1	1		
$b_{1u}\ \chi^{(1)}_{IV-}$	1	1	-1	-1	1	-1	-1	1	1	-1		
$\chi^{(2)}_{-}$	2	-2	0	0	0	-2	2	0	0	0	(R_x, R_y)	(zx, zy)
$\chi_{R^3} = \chi_{\text{tr}}$	3	-1	1	-1	-1	1	-3	-1	1	1		
χ_{rot}	3	-1	1	-1	-1	-1	3	1	-1	-1		
n_g	5	1	1	1	3	5	1	1	1	3		
χ_S	15	-1	1	-1	-3	5	-3	-1	1	3		
χ_{gen}	9	1	-1	1	-1	5	-3	-1	1	3		

Table 12.8: Character table for the XeF_4 molecule. In the first column we give the notation for characters used in [9, 10]. The subscript g and u denote "gerade" (even) and "ungerade" (odd) under space inversion ($\sigma_h\mathcal{C}_2$).

The character table for G has the structure

$$\begin{pmatrix} K & K \\ K & -K \end{pmatrix} \tag{12.87}$$

where K contains the characters of R. The commutator subgroup of R is $C(R) = \{e, C^2\}$ as follows from the fact that the relations $aba = b$ and $b^2 = e$ are even in a and b. Hence there are 4 one-dimensional irreps of R. Furthermore, since

$$\dim(R) = 8 = 1^2 + 1^2 + 1^2 + 1^2 + x^2, \tag{12.88}$$

there is one two-dimensional irrep for R. The 4 one-dimensional irreps can be constructed using that $N_{II} = \{e, a, a^2, a^3\}$, $N_{III} = \{e, a^2, b, a^2b\}$ and $N_{IV} = \{e, a^2, ab, a^3b\}$ are normal (invariant) subgroups. Then G/N are 2-dimensional subgroups whose characters are $(1, 1)$ and $(1, -1)$, and they induce the characters for R. The two-dimensional character of R is easily obtained by viewing R as linear transformations in the x-y plane (where $a = \left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$ and $b = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$). In this way one obtains the 10×10 character table in table 12.8.

The transformations of G in physical 3-dimensional space yield the character χ_{R^3}. The number of atoms held fixed by a given symmetry element of G[18] is written in the row labeled n_g, and multiplying χ_{R^3} with n_g gives the character χ_S of all 15 normal modes. To obtain the character for the nonzero modes we must substract from χ_S the characters for the translations and the rotations. The character χ_{tr} for translations is equal to χ_{R^3}, while the character χ_{rot} for rotations is obtained from χ_{tr} by multiplying the entries of χ_{tr} by a factor $\det(g) = -1$ which corresponds to reflections. Substracting χ_{tr} and χ_{rot} from χ_S we obtain the character χ_{gen} of the genuine (nonzero) normal modes of the molecule

$$\chi_{\text{gen}} = (9, 1, -1, 1, -1; 5, -3, -1, 1, 3) \tag{12.89}$$

We must decompose χ_{gen} into the 10 irreducible characters. First we take the product of χ_{gen} with itself, this yields

$$(\chi_{\text{gen}}, \chi_{\text{gen}}) = \sum_{\alpha=1}^{10} n_\alpha^2 \times |G| \tag{12.90}$$

where n_α is the number of times a given irreducible character χ_α appears in χ_{gen}. One finds

$$(\chi_{\text{gen}}, \chi_{\text{gen}}) = 81 + 1 + 2 + 2 + 2 + 25 + 9 + 2 + 2 + 18 = 144 = 9 \times 16 \tag{12.91}$$

Hence $\sum n_\alpha^2 = 9$. Next we find the number n_α that a given χ_α is contained in χ_{gen}. One finds in this way after some straightforward but tedious algebra

$$\chi_{\text{gen}} = \chi_{I+}^{(1)} + \chi_{III+}^{(1)} + \chi_{IV+}^{(1)} + 2\chi_{+}^{(2)} + \chi_{II-}^{(1)} + \chi_{III-}^{(1)} \tag{12.92}$$

As a check we note that this decomposition indeed satisfies $\sum n_\alpha^2 = 9$.

Our aim is to find the infrared and Raman spectrum. The infrared spectrum is due to matrix elements of the operators x_I, y_I, z_I (where I labels the atoms) which form the 3-dimensional reducible representation D_{R^3}. It is easy to see that (x, y) form a doublet under G, and z a singlet. In fact z transform like $\chi_{II-}^{(1)}$; for example, it is invariant under the rotations a^m, but it changes sign under the rotations O_x, O_y, O_d', O_d'' and the reflection σ_h. On the other hand (x, y) transforms like the doublet whose character is $\chi_+^{(2)}$. For example, under σ_h, the pair (x, y) does not change, which agrees with $\chi_+^{(2)}$ but not with $\chi_-^{(2)}$. Thus we have

$$\chi_{R^3} = \chi_+^{(2)} + \chi_{II-}^{(1)} \tag{12.93}$$

One can, of course, also obtain this decomposition from the orthogonality relations for characters.

[18] To check for example that $n_g = 3$ for the class with ab, begin with labeling the square as ${}^2_3\square^1_4$ and then act with b and afterwards with a as follows ${}^2_3\square^1_4 \xrightarrow{b} {}^3_2\square^4_1 \xrightarrow{a} {}^4_3\square^1_2$. Clearly the atoms at 1 and 3 and the atom at the center, are held fixed.

The infrared spectrum is due to those normal modes whose character appears both in $\chi_{\rm gen}$ and in χ_{R^3}. Those are the characters $\chi_+^{(2)}$ and $\chi_{II-}^{(1)}$. Since there are two characters $\chi_+^{(2)}$ in $\chi_{\rm gen}$, we predict 3 infrared lines

$$\chi_{\rm gen} = \chi_{I+}^{(1)} + \chi_{III+}^{(1)} + \chi_{IV+}^{(1)} + \underbrace{\chi_{II-}^{(1)} + 2\chi_+^{(2)}}_{\text{3 lines in the IR spectrum}} + \chi_{III-}^{(1)} \tag{12.94}$$

We now study the Raman spectrum. It is produced by the 6 operators $x_I^i x_J^j + x_I^j x_J^i$ with $i,j = 1,3$ (and $x^1, x^2, x^3 = x, y, z$). If we consider the direct product $\vec{r}\otimes\vec{r}$, we obtain the character $(\chi_{R^3})^2$, but we must substract the antisymmetric part

$$x_I^i x_J^j - x_I^j x_J^i = \epsilon^{ijk}(\epsilon_{klm} x_I^l x_J^m) \tag{12.95}$$

where $I, J = 1,5$ labels the atoms. The combination $\epsilon_{klm} x_I^l x_J^m$ transforms like an axial vector, and its character is thus the same as the character of the rotations $\chi_{\rm rot}$. (This $\chi_{\rm rot}$ is given in table 12.8, it is obtained from $\chi_{\rm tr}$ by multiplying the last 5 entries by -1. Decomposing it into irreducible characters, one finds that it contains a doublet (R_x, R_y) which transforms as $\chi_-^{(2)}$ and a singlet R_z which transforms as $\chi_{II+}^{(1)}$.) Hence, the character $\chi_{\rm Raman}$ of the operators $x_I^i x_J^j + x_I^j x_J^i$ is given by

$$\chi_{\rm Raman} = (\chi_{R^3})^2 - \chi_{\rm rot} \tag{12.96}$$

Using

$$(\chi_{R^3})^2 = (9,1,1,1,1;1,9,1,1,1) \tag{12.97}$$

$$\chi_{\rm rot} = (3,-1,1,-1,-1;-1,3,1,-1,-1) \tag{12.98}$$

we obtain

$$\chi_{\rm Raman} = (6,2,0,2,2;2,6,0,2,2) \tag{12.99}$$

We next decompose $\chi_{\rm Raman}$ into irreducible characters. First we take the inner product with itself

$$(\chi_{\rm Raman}, \chi_{\rm Raman}) = 36+4+0+8+8+4+36+0+8+8 = 112 = 7\times 16 \tag{12.100}$$

Hence $\sum n_\alpha^2 = 7$ for the decomposition of $\chi_{\rm Raman}$. Projecting out the χ^α from $\chi_{\rm Raman}$, one finds

$$\chi_{\rm Raman} = 2\chi_{I+}^{(1)} + \chi_{III+}^{(1)} + \chi_{IV+}^{(1)} + \chi_-^{(2)} \tag{12.101}$$

It indeed satisfies $\sum n_\alpha^2 = 7$. Only normal modes whose character appears both in $\chi_{\rm gen}$ and $\chi_{\rm Raman}$ can contribute to the Raman spectrum. This shows that there are also 3 lines in the Raman spectrum

$$\chi_{\text{gen}} = \underbrace{\chi^{(1)}_{I+} + \chi^{(1)}_{III+} + \chi^{(1)}_{IV+}}_{\text{3 lines in the Raman spectrum}} + 2\chi^{(2)}_{+} + \chi^{(1)}_{II-} + \chi^{(1)}_{III-} \tag{12.102}$$

Finally we compare the experimental result with the theoretical analysis. There are $5\times3-6=9$ nonzero normal modes for the XeF_4 molecule. We can get more detailed information as follows. The number of nonzero normal modes where motions lie in the x-y plane is $5\times2-3=7$. So there are only 2 nonzero normal modes which move out of the x-y plane. If the central Xe atom does not move in a given normal mode, that normal mode should correspond to a normal mode of a molecule without the central atom (which we might call an F_4 molecule for simplicity). Repeating the counting for such an F_4 molecule, we find $4\times2-3=5$ motions in the x-y plane, and $4\times3-6=6$ motions in the x-y-z space. Hence there is only one normal mode with motion outside the x-y plane which keeps the Xe atom fixed, and only one other normal mode whose motion is also outside the x-y plane but in which the Xe atom moves. We depict in figure 12.23 the motions of the 9 nonzero modes. The 7 nonzero normal modes whose motion lies in the x-y plane are shown in the first row, while the 2 nonzero normal modes which move out of the x-y plane are shown in the second row.

To become more familiar with these motions we perform a little thought-experiment. Suppose one removed the Xe atom from the molecule. Then the resulting F_4 molecule should have 5 nonzero normal modes in the plane and 1 out of the plane. Clearly the first three diagrams in the first row are also motions of an F_4 molecule, but the last two diagrams should be replaced by two other diagrams without the central atom. We can use table 12.8 to repeat the analysis for the F_4 molecule. Since now

$$n_g = (4,0,0,0,2;4,0,0,0,2) \tag{12.103}$$

one finds for $\chi_S = n_g\chi_{R^3}$ and χ_{gen}

$$\chi_S = (12,0,0,0,-2;4,0,0,0,2) \tag{12.104}$$

$$\chi_{\text{gen}} = (6,2,-2,2,0;4,0,0,0,2) \tag{12.105}$$

Then

$$(\chi_{\text{gen}},\chi_{\text{gen}}) = 36+4+8+8+16+8 = 80 = 5\times16 \tag{12.106}$$

Using the orthogonality relations for characters yields

$$\chi_{\text{gen}} = \chi^{(1)}_{I+} + \chi^{(1)}_{III+} + \chi^{(1)}_{IV+} + \chi^{(2)}_{+} + \chi^{(1)}_{III-} \tag{12.107}$$

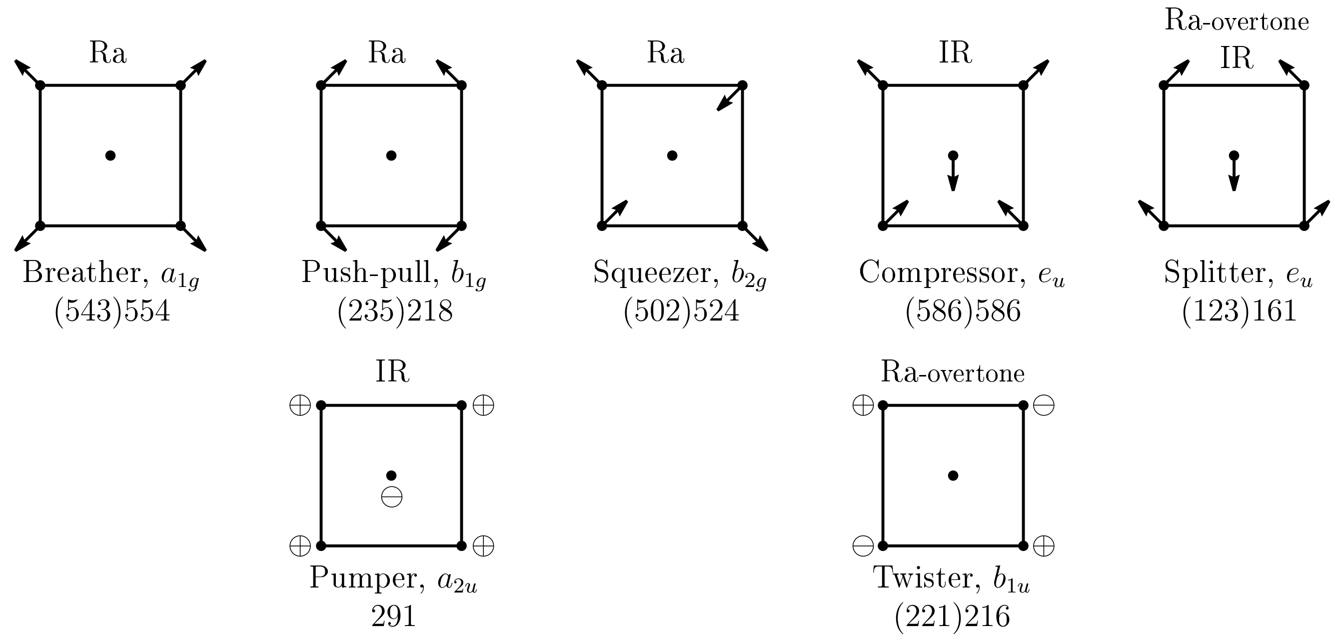


Figure 12.23: The 9 nonzero normal modes of the XeF_4 molecule. (The last two diagrams in the first line correspond to doublets and only one mode for each doublet is shown). The observed frequencies in cm^{-1} of [10] are given in parentheses, and precede those of [9]. Of the 3 predicted IR lines, those at 586 and 291 cm^{-1} are strongly visible in figure 12.24, but the IR line from e_u was seen in [10] at 123 cm^{-1}, but not in [9], while this same normal mode produces an overtone in the Raman spectrum of [9] at $2 \times 161 = 322$ cm^{-1}. Thus [9] indirectly sees the third IR line. The 3 predicted Raman lines are clearly visible in figure 12.24 as the lines at 554, 524 and 218 cm^{-1}. In addition, two very weak lines are seen at 322 and 433 cm^{-1}. The 322 line is an overtone as we already mentioned, while the 433 line is a second overtone which is attributed to the normal mode b_{1u} with frequency 216 cm^{-1}. Thus in this indirect way, the observed IR and Raman spectrum completely agree with the theoretical predictions.

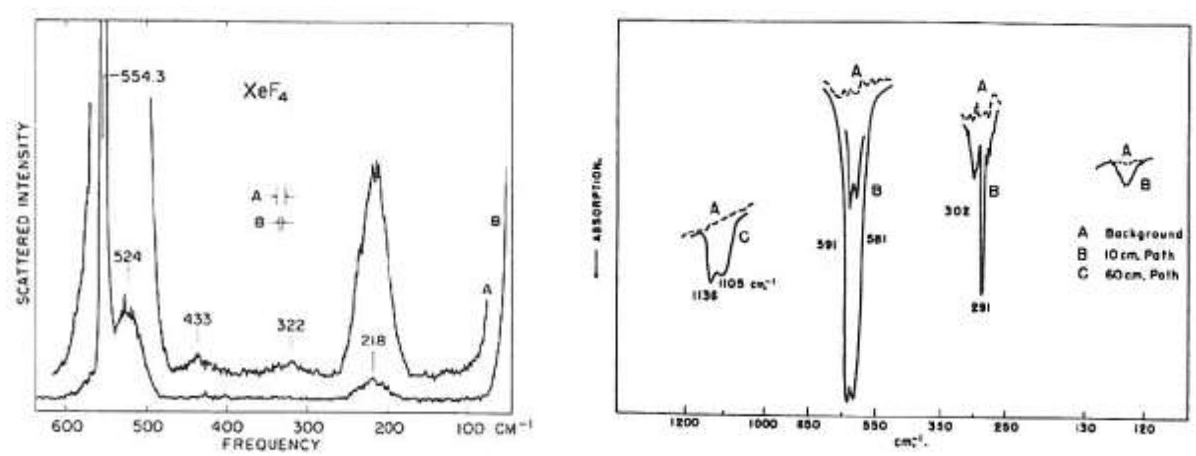
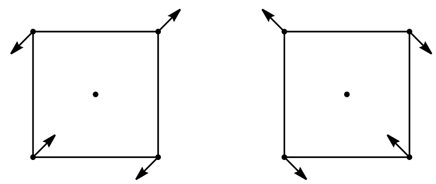


Figure 12.24: Raman [9] and IR [10] spectrum of XeF_4. There is agreement between theory and experiment, as discussed in the caption of figure 12.23.

This result agrees with $\sum n_\alpha^2 = 5$, and it also contains 6 nonzero normal modes. We find this time only one doublet, hence the two doublets of XeF_4 in the first row of figure 12.23 become one doublet of an F_4 molecule. We propose the following motions for this doublet:



Comment. The tedious part of the calculation of these spectra is the decomposition of the character χ_{gen} for the nonzero normal modes into irreducible characters. However, one can avoid this to some degree by directly computing the inner products $(\chi_{\text{gen}}, \chi_{IR})$ and $(\chi_{\text{gen}}, \chi_{\text{Raman}})$. One finds

$$(\chi_{\text{gen}}, \chi_{IR}) = 27 - 1 - 2 - 2 + 2 + 5 + 9 + 2 + 2 + 6 = 48 = 3 \times 16 \tag{12.108}$$

which suggests 3 or fewer[19] infrared lines. Similarly

$$(\chi_{\text{gen}}, \chi_{\text{Raman}}) = 54 + 2 + 4 - 4 + 10 - 18 + 4 + 12 = 64 = 4 \times 16 \tag{12.109}$$

which suggests 4 or fewer Raman lines.

*12.7 Case study 3: the spectrum of the SF_6 molecule

As a last example of the use of finite group theory for the unraveling of spectra, we consider the nonplanar molecule SF_6. The molecule sulfur-hexafluoride has the structure of an octahedron, with the sulfur atom at the center and the six fluorine atoms at the vertices. We shall first discuss the group O_h of isometries and present the character table. Then we shall discuss how the characters were obtained. Finally we shall derive the IR and Raman spectrum and compare with experiments.

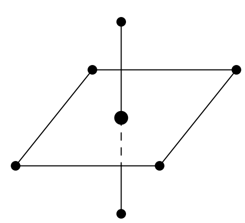


Figure 12.25: View from aside when the octahedron stands on one of its vertices. There are 8 faces, 6 vertices and 12 edges for an octahedron, but SF_6 has an extra S-atom at the center so that there are 15 genuine normal modes.

There are 24 rotations which form a group R. There are 3 kinds of rotations: (i) about an axis connecting two opposite vertices, (ii) about an axis connecting the centers of two opposite faces, and (iii) about an axis connecting the middles of two opposite edges.

[19]Fewer because it can happen (and does happen in our case) that a given character appears more than once in χ_{IR}, χ_{Raman} and/or χ_{gen}.

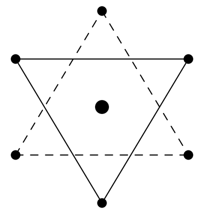


Figure 12.26: View from above when the octahedron lies on a table. The horizontal dotted triangle at the bottom is parallel to the horizontal solid triangle at the top.

(i) Consider the rotations about the vertical axis in figure 12.25 over angles $\pm\frac{\pi}{2}$, and over an angle π. All rotations over $\pm\frac{\pi}{2}$ are equivalent, but inequivalent to the rotations over π. Hence they belong to different classes. We denote these classes by $R_{vv}(\frac{\pi}{2})$ and $R_{vv}(\pi)$. There are 6 elements in $R_{vv}(\frac{\pi}{2})$ and 3 elements in $R_{vv}(\pi)$. (There are 3 axes connecting two opposite vertices.)

(ii) Next consider the rotations over angles $\pm\frac{2\pi}{3}$ about the vertical axis in figure 12.26. They belong to a class $R_{ff}(\frac{2\pi}{3})$ with 8 elements. (There are 4 axes connecting two opposite faces.)

(iii) Finally there are the rotations over an angle π about the axis connecting the middle of two opposite edges, for example, the $x-$axis or the $y-$axis in figure 12.25. They belong to a class $R_{ee}(\pi)$ and there are 6 of them (there are 12 edges).

For the 24 reflections and generalized reflections (other isometries with determinant -1) we take the following set

(i) Reflections σ_4, for example about the horizontal plane in figure 12.25 containing 4 vertices. There are 3 of them.

(ii) Reflections σ_2, for example about the two vertical planes in figure 12.25 which bisect two opposite horizontal edges. There are 6 of them.

(iii) Space inversion ($x \to -x$, $y \to -y$, $z \to -z$).

(iv) The product of rotations over $\pm\frac{\pi}{2}$ along the main diagonals (for example the vertical axis in figure 12.25) followed by a reflection about the plane orthogonal to the axis of rotation. Since there are 6 rotations, there are 6 of these generalized reflections.

(v) The last set of generalized reflections consists of rotations over an angle $\pm\frac{\pi}{3}$ (not $\pm\frac{2\pi}{3}$) along the diagonal connecting the centers of two opposite faces, followed again by a reflection about the plane orthogonal to the rotation axis. For example, in figure 12.26, a rotation over $\frac{\pi}{3}$ about the vertical axis is **not** a symmetry, because the 6 atoms lie alternatingly in the bottom triangle and the top triangle, but adding the reflections makes this operation an isometry. There are 8 of these.

This is the complete set of isometries. For example, rotation about the vertical axis in figure 12.25 about an angle π, followed by a reflection about the horizontal plane is equal to space inversion. The characters of this symmetry group of order 48 are given in table 12.9.

O_h	e 1	$R_{ff}(\frac{2\pi}{3})$ 8	$R_{ee}(\pi)$ 6	$R_{vv}(\frac{\pi}{2})$ 6	$R_{vv}(\pi)$ 3	i 1	$\sigma R_{vv}(\frac{\pi}{2})$ 6	$\sigma R_{ff}(\frac{\pi}{3})$ 8	σ_4 3	σ_2 6
A_{1g}	1	1	1	1	1	1	1	1	1	1
A_{2g}	1	1	-1	-1	1	1	-1	1	1	-1
E_g	2	-1	0	0	2	2	0	-1	2	0
$T_{1g}\,(R_x, R_y, R_z)$	3	0	-1	1	-1	3	1	0	-1	-1
T_{2g}	3	0	1	-1	-1	3	-1	0	-1	1
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1
A_{2u}	1	1	-1	-1	1	-1	1	-1	-1	1
E_u	2	-1	0	0	2	-2	0	1	-2	0
$T_{1u}\,(x, y, z)$	3	0	-1	1	-1	-3	-1	0	1	1
T_{2u}	3	0	1	-1	-1	-3	1	0	1	-1
n_g	7	1	1	3	3	1	1	1	5	3
χ_S	21	0	-1	3	-3	-3	-1	0	5	3
χ_{gen}	15	0	1	1	-1	-3	-1	0	5	3

Table 12.9: Characters of the symmetry group O_h of an octahedron which is also the symmtery group of SF_6. The group element i denotes space inversion, and the reflections σ in front of the rotations $R_{vv}(\frac{\pi}{2})$ and $R_{ff}(\frac{2\pi}{3})$ are about a plane that is orthogonal to the axes of these rotations. The numbers n_g are the numbers of atoms held fixed by the group elements of the corresponding class. The translations in R^3 form an irrep, namely T_{1u}, and the rotations in R^3 form also an irrep, namely T_{1g}.

Let us now discuss how the characters given in table 12.9 were obtained. The 24 rotations form a normal subgroup R of the group O_h with 48 elements, hence O_h/R is isomorphic to Z_2 whose characters are $(1, 1)$ and $(1, -1)$. Extending them to G yields A_{1g} and A_{1u}. The rotations $R_{ff}(\frac{2\pi}{3})$ and $R_{vv}(\pi)$ together with e form a normal subgroup N_R of the group of rotations R. (The only invariant subgroups of R have order $1+3$ or $1+3+8$. The $R_{vv}(\pi)$ and e form a normal subgroup isomorphic to V, and N_R is a normal subgroup of order 1+3+8.) This yields a character A_2 of R which is extended to the characters A_{2g} and A_{2u} of O_h. The 4 one-dimensional characters form the Klein group V if one multiplies them.

The 2-dimensional irrep can be obtained from a permutation representation of O_h. Because permutation representations are reducible (they have an eigenvector $(1, 1, \cdots, 1)$), we need a 3-dimensional permutation representation of O_h to obtain a 2-dimensional irrep. It is not difficult to spot 3 objects on which O_h can act as a transformation group: the 3 diagonals which connect the vertices. Acting with O_h on the three diagonals yield the character $(3, 0, 1, 1, 3, 3, 1, 0, 3, 1)$, and subtracting the unit character yields E_g. The product of E_g and A_{1u} yields E_u.

There are two 3-dimensional irreps. One of them is obvious: the 3-dimensional space in which the octahedron is situated. This is the irrep T_{1u}. One obtains T_{2u} as $T_{1u}A_{2g}$, and T_{1g} as $T_{1u}A_{1u}$, and T_{2g} as $T_{1u}A_{2u}$.

One obtains the character of all deviations by multiplying n_g by T_{1u}. This yields the reducible character χ_S. We must subtract the characters of infinitesimal translations and rotations. The representations of O_h due to infinitesimal translations has the character T_{1u} as we already discussed. The character for infinitesimal rotations is obtained from T_{1u} by multiplying the characters of all reflections by -1; this yields T_{1g}. Subtracting T_{1u} and T_{1g} from χ_S yields χ_{gen}.

The number of lines in the IR spectrum is the number of times T_{1u} is contained in χ_{gen}. This number is $(\chi_{gen}, \chi(T_{1u}))/|G|$, namely

$$\left[15{\cdot}3{\cdot}1 + 1(-1)6 + 1{\cdot}1{\cdot}6 + (-1)(-1)3 + (-3)(-3)1 + (-1)(-1)6 + 5{\cdot}1{\cdot}3 + 3{\cdot}1{\cdot}6\right] \tfrac{1}{48} = 2\,. \tag{12.110}$$

Hence there should only be **two lines in the IR spectrum**. Experiments see them at $\nu(^1T_{1u}) = 615\ \mathrm{cm}^{-1}$ and $\nu(^2T_{1u}) = 948\ \mathrm{cm}^{-1}$.

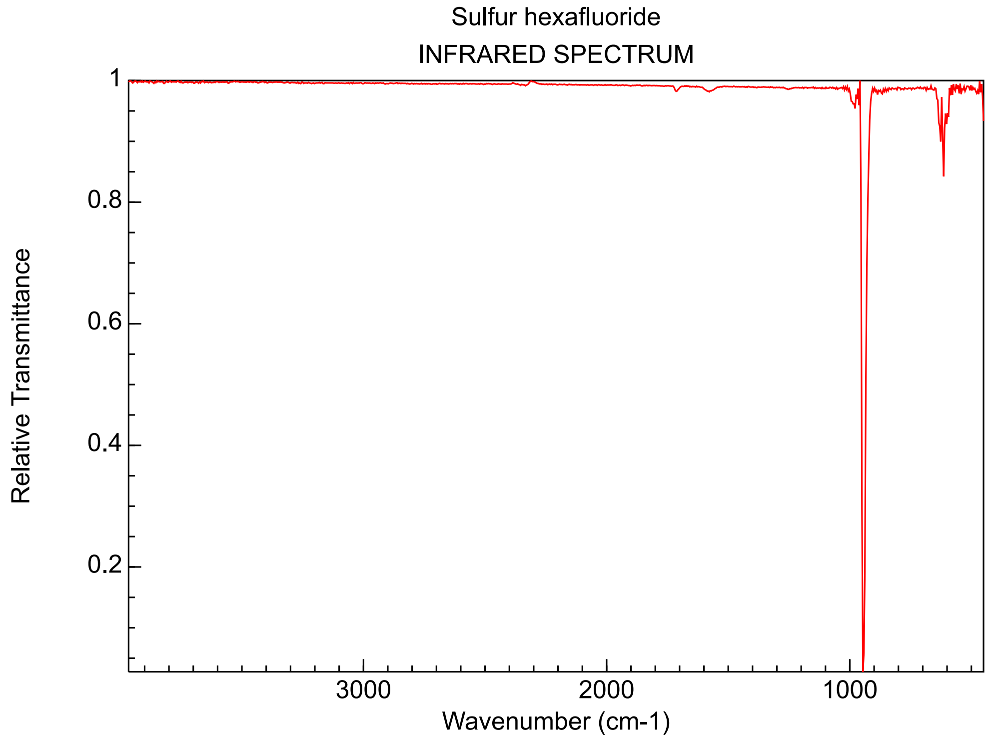


Figure 12.27: IR spectrum of SF_6. (Source: NIST Chemistry WebBook)

Finally we discuss the Raman spectrum. Using $\mathbf{3} \times \mathbf{3} = \mathbf{5} + \mathbf{3} + \mathbf{1}$ we find

$$\begin{aligned} \chi^{\mathbf{3}\times\mathbf{3}} &= T_{1u}T_{1u} = (9,0,1,1,1,9,1,0,1,1) \\ \chi^{\mathbf{5}} &= T_{1u}T_{1u} - T_{1g} - A_{1g} = (5,-1,1,-1,1,5,-1,-1,1,1) \end{aligned} \tag{12.111}$$

Since $\sum_g \chi^{\mathbf{5}}(g)\chi^{\mathbf{5}}(g)/$ Order $O_h = (25{\cdot}1+1{\cdot}8+1{\cdot}6+1{\cdot}6+1{\cdot}3+25{\cdot}1+1{\cdot}6+1{\cdot}8+1{\cdot}3+1{\cdot}6)/48 = 2$, the operators $r^ir^j - \frac{1}{3}\delta^{ij}r^2$ form a reducible representation. They can only contain one 3-dimensional irrep and one 2-dim irrep. One finds that it decomposes as

$$\begin{aligned} \chi^{\mathbf{1}} &= A_{1g}\,; \quad \chi^{\mathbf{5}} = E_g + T_{2g}\,; \\ \chi_{\text{Raman}} &= A_{1g} + E_g + T_{2g}\,. \end{aligned} \tag{12.112}$$

The character χ_{gen} splits up into irreducible characters as follows

$$\chi_{gen} = \underset{R}{A_{1g}} + \underset{R}{E_g} + \underset{R}{T_{2g}} + \underset{IR}{2T_{1u}} + T_{2u}\,. \tag{12.113}$$

As a first check, note that these irreps span a 15-dimensional space. As a second check, note that $\sum_g \chi_{gen}(g)\chi_{gen}(g) = 8{\cdot}48$ and $\sum_\alpha n_\alpha^2 = 1^2 + 1^2 + 1^2 + 2^2 + 1^2$ is indeed equal to 8.

We see that only A_{1g} (from the **1**) and E_g and T_{2g} (from the **5**) are Raman active. So we expect **three Raman lines**. Experiments find them at frequencies $\nu(A_{1g}) = 845$ cm^{-1}, $\nu(E_g) = 643$ cm^{-1} and $\nu(T_{2g}) = 547$ cm^{-1}.

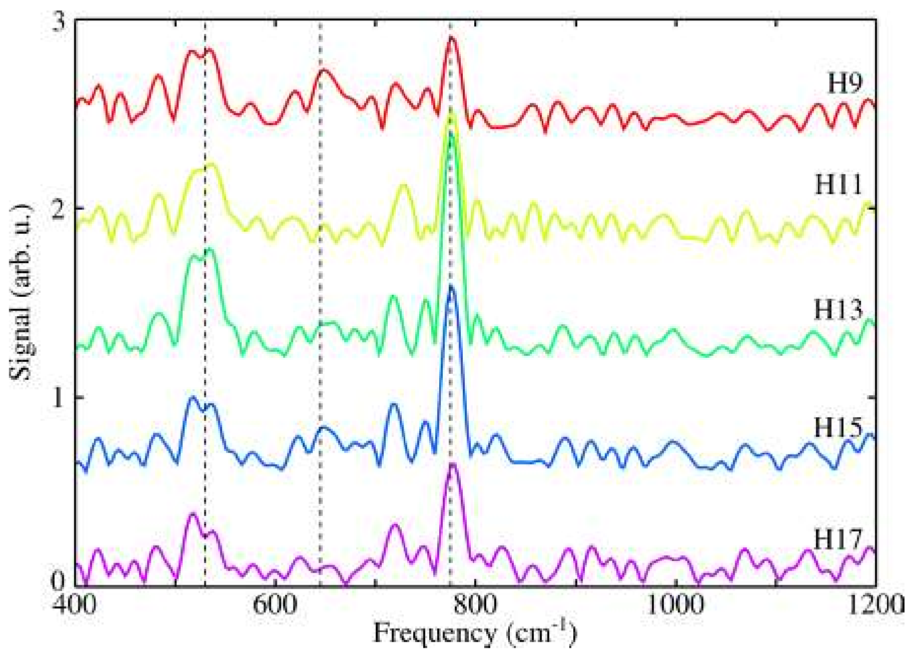


Figure 12.28: Raman spectrum of SF_6. [11]

For computer graphics of the 15 genuine normal modes of vibration for SF_6, search on Google "stretching modes of SF_6".

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