4.3 Examples of representations

4.3.1 The group $D_3$

In order to bring out the physical significance of a representation we will look now at the group $D_3$ introduced in subsection 2.2(6) and construct a matrix representation for it. We can form a faithful representation immediately by writing down the transformations induced by each operation in the ordinary three-dimensional Cartesian space. Let us choose basis vectors $e_x$ and $e_y$ as in figure 4.1, with $e_x$ pointing up out of the paper. Then, for example, the group element $R_1$ which rotates through 120° about the $x$-axis gives rise to the mapping

$$T(R_1)e_x = e'_x = -\frac{1}{2}e_x + (\frac{\sqrt{3}}{2})e_y,$$

$$T(R_1)e_y = e'_y = -\frac{1}{2}e_y - \frac{\sqrt{3}}{2}e_x,$$

$$T(R_1)e_z = e'_z = e_z$$

and hence, using equation (4.4), to the matrix

$$T(R_1) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$
In the same way, for the other group elements

\[
T(R_2) = \begin{pmatrix}
-2 & \sqrt{2} & 0 \\
-\sqrt{2} & -2 & 0 \\
0 & 0 & 1
\end{pmatrix}, \quad T(R_3) = \begin{pmatrix}
-1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & -1
\end{pmatrix}
\]

\[
T(R_4) = \begin{pmatrix}
\frac{1}{2} & -\sqrt{2} & 0 \\
-\sqrt{2} & -\frac{1}{2} & 0 \\
0 & 0 & -1
\end{pmatrix}, \quad T(R_5) = \begin{pmatrix}
\frac{1}{2} & \sqrt{2} & 0 \\
\sqrt{2} & -\frac{1}{2} & 0 \\
0 & 0 & -1
\end{pmatrix}
\]

with \( T(E) = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1
\end{pmatrix} \)

It is readily verified that these matrices possess the same multiplication table as the group elements. Thus for example we have

\[
T(R_1)T(R_4) = T(R_2)
\]

which is consistent with the entry \( R_1R_4 = R_2 \) in Table 2.5.

By taking the one-dimensional space of the vector \( e_z \), alone, we may generate a very simple one-dimensional representation which we denote by \( T^{(1)} \),

\[
T^{(1)}(R_1) = 1, \quad T^{(1)}(R_2) = 1, \quad T^{(1)}(R_3) = -1, \quad T^{(1)}(R_4) = -1, \quad T^{(1)}(R_5) = 1
\]

Notice that \( T^{(1)} \) is not the same as the identity representation which we denote by \( T^{(0)}(R_1) = 1 \), associating +1 with every group element. Notice also that the three numbers \(-1\) are associated with the three elements which belong to the same class \( \nu_3 \) (see section 2.7) of the group \( D_3 \). This is an example of a general feature. It will be explained in section 4.9 that representations of elements in the same class have some common properties.

Because of the presence of the zeros in the third row and third column of the matrices \( T(R_i) \) it is clear that the \( 2 \times 2 \) matrices formed by the first two rows and columns are themselves a representation of the group \( D_3 \), which we denote by \( T^{(0)} \).

### 4.3.2 The group \( \mathfrak{A}_2 \)

We may use the same space as in the previous example to generate a representation of the infinite group \( \mathfrak{A}_2 \) of rotations about the \( z \)-axis. The group elements \( R(\alpha) \) are now labelled by the continuous parameter \( \alpha \) in the
4.3.3 Group Representations

range $0 \leq a < 2\pi$ and the matrix was given in section 3.8 as

$$T(a) = \begin{pmatrix} \cos a & -\sin a & 0 \\ \sin a & \cos a & 0 \\ 0 & 0 & 1 \end{pmatrix}$$  \hspace{1cm} (4.6)

One immediately verifies that

$$T(a)T(b) = T(a + b)$$  \hspace{1cm} (4.7)

for any $a$ and $b$, consistent with the multiplication rule $R(a)R(b) = R(a + b)$ for the group elements.

4.3.3 Function spaces

The first two examples of representations were constructed in the familiar physical space of three dimensions and it may be difficult to visualize at this stage how representations of dimension greater than three may be constructed for groups like $D_3$ and $S_3$. To show how this may be achieved we consider the transformations of functions induced by such coordinate rotations as in equation (3.37), to form representations in function space. These will be most important in applications of group theory in quantum mechanics.

Suppose we have a space $L$ of functions $\psi(r)$ of some coordinates $r$ which is invariant under a group of coordinate transformations $G_a$ in the sense that if $\psi(r)$ belongs to the space $L$ then so also does $\psi(G_a^{-1}r)$ for all $G_a$ in the group. We can then define a representation $T$ in the function space $L$ by the transformations

$$T(G_a)\psi(r) = \psi(G_a^{-1}r)$$  \hspace{1cm} (4.8)

of the kind discussed in section 3.7. Again it is easily verified that this definition satisfies the condition (4.1) since, defining $\psi'(r) = \psi(G_a^{-1}r)$, we have

$$T(G_a)T(G_b)\psi(r) = T(G_a)\psi(G_b^{-1}r) = T(G_a)\psi'(G_b^{-1}r) = \psi'( (G_aG_b)^{-1}r) = T(G_aG_b)\psi'(r)$$

(It is vital in this proof to introduce the new function $\psi'(r) = \psi(G_a^{-1}r)$ since, in general, $T(G_a)\psi(G_b^{-1}r) \neq \psi(G_a^{-1}G_b^{-1}r)$.)

The matrix representation in function space is obtained from the general expression, equation (4.2), by introducing a basis $\psi_i(r)$ in function space and expanding

$$T(G_a)\psi_i(r) = \psi_i(G_a^{-1}r) = \psi_i'(r) = \sum_j T_{ij}(G_a)\psi_j(r)$$  \hspace{1cm} (4.9)

The $\psi_i(r)$ are particular examples of the abstract $e_i$.

As an example, the six-dimensional space $L$ of quadratic functions introduced in subsection 3.2.4 is clearly invariant under any rotation and in
4.4 The generation of an invariant subspace

If an operator $T$ is defined in a space $L$ then it may be possible to find some subspace $L_1$ of $L$ with the property that if $r_1$ is any vector in $L_1$ then the transformed vector $r_1' = Tr_1$ also lies in the subspace $L_1$. Such a subspace is called 'invariant' with respect to the operator $T$. More generally, given a set of operators $T(G_a)$ in $L$ which form a representation of a group $\mathcal{G}$, it may be possible to find a subspace $L_1$ which is invariant with respect to all $T(G_a)$ as $G_a$ runs through a group $\mathcal{G}$. The subspace $L_1$ is then said to be invariant with respect to the transformations induced by the group $\mathcal{G}$ and we generally use the term 'invariant subspace' in this latter sense.

In the example of subsection 4.3.1 it is clear from the matrices that the subspace defined by the vectors $e_3$ and $e_7$ is invariant as is its orthogonal complement (see section 3.1), the one-dimensional space defined by $e_8$. The six-dimensional function space of the example in subsection 4.3.3 is itself a subspace of the space of all continuous functions which has an infinite number of dimensions.

The main point of this section is to show how to generate an invariant subspace starting from a single vector of the space. Let $r$ be an arbitrary vector in $L$ and define the set of $g$ vectors $r_a$ by the equation

$$r_a = T(G_a)r$$

where $G_a$ runs through the $g$ elements of a group $\mathcal{G}$. It follows immediately that the set of vectors $r_a$ span an invariant subspace of $L$ since for any $b$,
4.4 Group Representations

\[ T(G_s) r_a = T(G_b) T(G_s) r = T(G_b G_s) r = T(G_s) r = r_a \]  
(4.11)

where the group element \( G_s \) is given by \( G_s = G_b G_a \).

If all the vectors \( r_a \) are linearly independent, they will form a basis for a \( g \)-dimensional representation of the group, since equation (4.11) is a particular form of the general equation (4.2) for a representation. In fact the matrix of \( T(G_s) \) would be given by \( T_{ij}(G_b) = 1 \) if the group elements labelled by those indices \( b_i \) and \( j \) satisfy the relation \( G_s G_j = G_j \). Otherwise, the matrix elements are all zero.

In general, the vectors \( r_a \) will not be linearly independent but it will always be possible to construct a number \( s \leq g \) of linearly independent basis vectors as linear combinations of the \( r_a \). It is usually convenient to make the independent basis vectors orthonormal by the Schmidt process. To illustrate this generation procedure we return to the example in subsection 4.3.3. In particular we generate from the single function \( \psi_1(r) = x^2 \) using the group \( D_2 \),

\[ T(E) \psi_1 = \psi_1 \]
\[ T(R_c) \psi_1 = \frac{1}{2} x^2 + \frac{1}{2} y^2 - \frac{\sqrt{2}}{2} x y \]
\[ T(R_d) \psi_1 = \frac{1}{2} x^2 + \frac{1}{2} y^2 + \frac{\sqrt{2}}{2} x y \]
\[ T(R_e) \psi_1 = \psi_1 \]
\[ T(R_f) \psi_1 = \frac{1}{2} x^2 + \frac{1}{2} y^2 - \frac{\sqrt{2}}{2} x y \]
\[ T(R_g) \psi_1 = \frac{1}{2} x^2 + \frac{1}{2} y^2 + \frac{\sqrt{2}}{2} x y \]

By inspection it is clear that the generated functions are not linearly independent, that the generated space has only three dimensions and that the three functions \( x^2, y^2 \) and \( xy \) will provide a basis, though not an orthonormal one. The matrix representation in this basis is then deduced using equation (4.2), giving

\[ T(R_1) = \begin{pmatrix}
\frac{1}{2} & \frac{1}{2} & -\frac{\sqrt{2}}{2} \\
\frac{1}{2} & -\frac{1}{2} & \frac{\sqrt{2}}{2} \\
-\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & \frac{1}{2}
\end{pmatrix}, \quad T(R_2) = \begin{pmatrix}
\frac{1}{2} & \frac{1}{2} & -\frac{\sqrt{2}}{2} \\
\frac{1}{2} & -\frac{1}{2} & \frac{\sqrt{2}}{2} \\
\frac{\sqrt{2}}{2} & \frac{\sqrt{2}}{2} & -\frac{1}{2}
\end{pmatrix}, \text{ etc.}
\]

The Schmidt procedure for finding an orthonormal basis (section 3.1) involves rather more arithmetic. One first writes \( \phi_1 = A x^2 \) with \( A \) chosen to normalise \( \phi_1 \) using the scalar product (3.13)

\[ \int \int \int \phi_1^* \phi_1 \, d\tau = 1 \]

giving

\[ \phi_1 = \left( \frac{35}{4\pi} \right) x^2 \]

Then put \( \phi_2 = B(y^2 - C \phi_1) \) and find \( C \) and \( B \) by insisting on the orthogonality
Group Representations

$(\phi_1, \phi_2) = 0$ and the normalisation $(\phi_2, \phi_2) = 1$. This gives

$$\phi_2 = \left( \frac{35}{32\pi} \right)^\frac{1}{2} (3y^2 - x^2)$$

It is soon verified that, because it is an odd function in $x$ and $y$, the function $xy$ is orthogonal to both $\phi_1$ and $\phi_2$. Normalising, we have

$$\phi_3 = \left( \frac{105}{4\pi} \right)^\frac{1}{2} xy$$

4.5 Irreducibility

The examples in section 4.4 show that it is possible to construct matrix representations of ever-increasing size by increasing the complexity of the function space. A study of the possible representations of even a simple group like $D_3$ would therefore seem a very daunting proposition. But we are saved by the following very remarkable property of group representations. For a finite group all representations may be 'built up' from a finite number of 'distinct' irreducible representations. The group $D_3$, for example, has only three distinct irreducible representations, two of which are one dimensional and one is two dimensional. We have introduced several new words here which will be carefully defined very soon but let us first look back at the example in subsection 4.3.1 for an illustration. In that example the representation had dimension three. However, a glance at the matrices reveals that the $2 \times 2$ matrices obtained by taking only the first two rows and columns form a two-dimensional representation, while the diagonal matrix elements in the third row and column form a one-dimensional representation. This is possible because of the zeros in the coupling positions between the first two rows and columns and the third. In terms of the vector space this means that the two vectors $e_x$ and $e_y$ form an invariant vector space, while the single vector $e_z$ forms a second invariant vector space which is orthogonal to the first. In such a situation we say that the three-dimensional representation has reduced into a 'sum' of a two-dimensional representation and a one-dimensional representation. It is obvious that the one-dimensional representation cannot be further reduced and by trial one could see that the two-dimensional representation also cannot be reduced. By this we mean that it is impossible to find a new basis $e_1 = \alpha e_x + \beta e_y$ and $e_2 = \alpha e_x - \beta e_y$ such that the matrix elements

$$T_{1,2}(R_\theta) = (e_1, T(R_\theta)e_2) \text{ and } T_{2,1}(R_\theta) = (e_2, T(R_\theta)e_1)$$

in the new basis are zero for all elements $R_\theta$ of the group $D_3$. Such a representation, which cannot be reduced, is called 'irreducible'.

From a physical point of view the concept of irreducibility is of crucial importance since, as we show in the next chapter, the wave functions
Group Representations

4.5

describing the stationary states of a symmetrical system with the same energy
will in general provide the basis functions for an irreducible representation
of the group of symmetry operations.

Let us now define the concept of reduction in more general terms. Let \( L \) be a
space which is invariant with respect to the transformations \( T(G_a) \) induced by
some group \( G \) of elements \( G_a \). Then if \( L_1 \) is a subspace of \( L \) which is invariant
and if \( L_2 \), the orthogonal complement (see section 3.1) of \( L_1 \), is also invariant
then the representation \( T \) is said to reduce. If it is impossible to find such a
subspace, then the representation \( T \) is said to be 'irreducible'. It is essential in
this definition of reducibility that both the subspace \( L_1 \) and its orthogonal
complement \( L_2 \) should be invariant. Once again there is a fortunate
simplification since, if the representation operators \( T(G_a) \) are unitary, the
invariance of \( L_1 \) implies the invariance of \( L_2 \). The proof is immediate. Let us
denote the basis vectors of \( L_1 \) by \( e_i \) and those of \( L_2 \) by \( e_j \), so that by definition
of \( L_2 \), \( (e_i, e_j) = 0 \). From the invariance of \( L_1 \) we have that \( (T(G_a)e_i, e_j) = 0 \)
for all \( G_a \) and from the unitarity of \( T \) this is equivalent to \( (e_i, T(G_a^{-1})e_j) = 0 \)
which implies also that \( (e_i, T(G_a)e_j) = 0 \) for all \( G_a \). This last equation shows that the
vectors \( T(G_a)e_j \) are orthogonal to the \( e_i \) and so must lie in \( L_2 \). Hence \( L_2 \) is
invariant, as required. The restriction to unitary representations is not severe
since, as we shall show in section 4.6, almost all of the representations of
interest in physical problems are unitary. It is therefore possible to divide any
space \( L \) into a sum of subspaces \( L_n \) (not necessarily only two in number) each
of which is invariant and irreducible, although this division is not necessarily
unique. We may write \( L = L_1 + L_2 + L_3 + \ldots \) where each \( L_n \) is irreducible
and invariant under the transformations \( T(G_a) \). Correspondingly, we write
the reduction of the representation as

\[
T(G_a) = T^{(1)}(G_a) + T^{(2)}(G_a) + T^{(3)}(G_a) + \ldots
\]  

(4.12)

where \( T^{(n)}(G_a) \) is the irreducible representation induced in the space \( L_n \). This
equation is to be interpreted as a sum of operators \( T^{(n)}(G_a) \) which operate in
different spaces \( L_n \) and the 'dot' over the plus sign reminds us of this fact.

In terms of matrices, if the ordering of the basis vectors is chosen so that
those belonging to \( L_1 \) are written first to be followed by those of \( L_2 \) and so on,
then the matrix will appear in a 'block diagonal' form with zeros elsewhere, as
illustrated below. Here, the matrix \( T^{(n)}(G_a) \) is a square matrix of dimension
equal to that of the subspace \( L_n \), while the entries 0 denote rectangular zero
matrices.

\[
\begin{pmatrix}
T^{(1)} & 0 & 0 & \ldots & 0 \\
0 & T^{(2)} & 0 & \ldots & 0 \\
0 & 0 & T^{(3)} & \ldots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & \ldots & 0
\end{pmatrix}
\]
Each $T^{(q)}(G_j)$ is an irreducible matrix representation of the group $G_j$. Given an arbitrary matrix representation $T$ it is, of course, necessary to transform carefully to the new basis appropriate to the subspaces $L_q$ in order to achieve the simple block diagonal form for the matrix. We write the equation

$$T(G_j) = T^{(1)}(G_j) \oplus T^{(2)}(G_j) \oplus T^{(3)}(G_j) + \ldots \quad (4.13)$$

for the matrix reduction, analogous to equation (4.12) for the operators. The 'dot' over the plus sign again reminds us that this is not the usual matrix addition but signifies that $T$ is composed of the square matrices $T^{(q)}(G_j)$ arranged down the diagonal.

Given an arbitrary vector $r$ we may construct an invariant space $L$ as described in section 4.4 by the operations $T(G_j)r$. If this space is then reduced into irreducible subspaces $L_q$ it follows that the vector $r$ may be written $r = \sum q r_q$, where $r_q$ lies in $L_q$. Thus the arbitrary vector $r$ is said to be analysed into irreducible components $r_q$.

### 4.6 Equivalent representations

The reduction process described in section 4.5 enables us in principle to reduce any representation to its constituent irreducible representations. Henceforth, therefore, we shall largely restrict our attention to the properties of irreducible representations, knowing that the properties of any reducible representation may be deduced from them. Even so, there will still be an infinite number of possible irreducible representations, as may be seen from the example in subsection 4.3.1. The space defined by the two vectors $e_x$ and $e_y$ was irreducible and provided a two-dimensional irreducible representation of $D_3$. However, a different choice of basis vectors within the space would give rise to a different set of matrices $T(G_j)$. One might hope that such a trivial change of basis would leave the essential properties of the representation unchanged and this is indeed true. We now introduce the concept of the equivalence of representations which puts this idea into precise form.

Let $T(G_j)$ denote a representation of a group $G_j$ in a space $L$. Then if $A$ is a mapping from $L$ on to a space $L'$ with the same dimension, it follows that the set of operators

$$T'(G_j) = AT(G_j)A^{-1} \quad (4.14)$$

which act in $L'$ also form a representation of $G_j$. This is readily proved, since

$$T'(G_j)T'(G_j) = AT(G_j)A^{-1}AT(G_j)A^{-1}$$

$$= AT(G_j)T(G_j)A^{-1}$$

$$= AT(G_j)A^{-1}$$

$$= T'(G_j)G_k$$

which is the defining property (4.10) for a representation. The two repre-
sentations $T'$ and $T$ are said to be 'equivalent'. It is vital that the mapping $A$ be the same for all group elements $G_a$. As a particular case $L$ and $L'$ may be the same space.

If $T'$ and $T$ are equivalent and if $T''$ and $T'$ are equivalent then it follows that $T''$ and $T$ are also equivalent, so that one has the concept of a class of mutually equivalent representations.

For matrix representations a change of basis produces an equivalent matrix representation. In detail, let $T(G_a)$ be a set of operators with matrices $T(G_a)$ in a basis $e_i$. Then if the new basis is given by $e'_i = A e_i$, the matrix of $T(G_a)$ in the new basis is given by the matrix product $A^{-1} T(G_a) A$, since

$$ T e'_i = T A e_i = \sum_j (T A)_{ij} e_j = \sum_j (T A)_{ij} (A^{-1})_{jk} e'_k $$

$$ = \sum_k (A^{-1} T A)_{ik} e'_k $$

The reason for the interchange of $A$ and $A^{-1}$ as compared with equation (4.14) is that whereas (4.14) described a new operator, the present discussion concerns the same operator $T(G_a)$ but referred to a new basis.

One might expect that the important properties of a representation would be common to any two equivalent representations and indeed this will be found to be the case. As a result, we may restrict our attention to only one representation from each class of equivalent representations. In particular, we need consider only unitary representations because of a result known as Maschke's theorem which states that, for finite groups, every class of equivalent representations contains unitary representations\(^1\). The theorem is also true for most infinite groups of interest in physics.

### 4.6.1 Proof of Maschke's theorem

We need to show that any representation is equivalent to a unitary representation. Given a representation $T(G_a)$ we must find an operator $S$ such that the equivalent representation $T'(G_a) = ST(G_a)S^{-1}$ is unitary. In fact we shall show that the operator $S = \{ \sum_b T(G_b) T(G_b) \}^{1/2}$ will suffice, although we shall not attempt to explain the inspiration which led to this choice. To prove unitarity we must show that

$$ T'(G_a) = T'(G_a)^{-1} $$  \hspace{1cm} (4.15)

The first step is to write

$$ T'(G_a)S^{-1} T(G_a) = \sum_b T'(G_b) T'(G_a) T(G_b) T(G_a) $$

$$ = \sum_b T'(G_b G_a) T(G_a) $$

$$ = \sum_b T'(G_b) T(G_a) $$

$$ = S $$  \hspace{1cm} (4.16)

\(^1\) This is not the form usually attributed to Maschke but it is most convenient for our purpose.
where \( G = G_x G_z \). We have used the group property that, if \( G_x \) is fixed and the element \( G_z \) runs through the group, covering each element once and once only then \( G_z \) also runs through the group elements once and once only—see section 2.9. Now, post-multiplying both sides of (4.16) by \( T^{-1} (G_z) S^{-1} \) and pre-multiplying by \( S^{-1} \) we have

\[
S^{-1} T \ (G_z) S = ST^{-1} (G_z) S^{-1}
\]

i.e.

\[
(ST (G_z S^{-1})^{-1} = (ST (G_z S^{-1})^{-1})^{-1}
\]

which is the required unitarity condition (4.15). We have used the fact that the operator \( S \) is Hermitian.

### 4.7 Inequivalent irreducible representations

Two representations \( T \) and \( T' \) are said to be 'inequivalent' if there exists no operator \( A \) which satisfies equation (4.14) for all \( G_a \) of the group. It is also convenient to refer to equivalent irreducible representations as the same representation. (So far as the matrix is concerned this implies that we shall always imagine the basis to be chosen so that the matrices are identical.) In terms of the reduction (4.12) of a reducible representation into its irreducible constituents this means that an irreducible representation may appear several times in the reduction. We therefore write the reduction as

\[
T = \sum_a m_a T^{(a)}
\]

where \( a \) runs only over the inequivalent irreducible representations and the integer \( m_a \) gives the number of times that the irreducible representation \( T^{(a)} \) occurs in the reduction. (The 'dot' over the summation sign has the same significance as in equation (4.13).)

For example, the six-dimensional representation in subsection 4.3.3 contains the identity representation twice in its reduction. The two independent functions \((x^2 + y^2)\) and \(z^2\) are both invariant under the group \( D_3 \), and each therefore is the basis function for the one-dimensional identity representation \( T^{(1)} \) which associates the number 1 with each group element. It can also be shown (see problem 4.9) that the two-dimensional representation \( T^{(2)} \) encountered in subsection 4.3.1 also appears twice in this reduction which may therefore be written \( T = 2T^{(1)} + 2T^{(3)} \).

### 4.8 Orthogonality properties of irreducible representations

Through the arguments of the previous three sections, the study of group representations has been reduced to the study of the inequivalent irreducible representations which, we now find, possess important 'orthogonality' proper-