1.2.4 Introduction

This simple problem completely. The coupled equations of motion are

\[ M\ddot{x}_1 = -\lambda x_1 - \lambda (x_1 + x_2) \]
\[ M\ddot{x}_2 = -\lambda x_2 - \lambda (x_1 + x_2) \]

which suggest the definition of new coordinates \( Q_1 = x_1 + x_2 \) and \( Q_2 = x_1 - x_2 \). Then by adding and subtracting the two coupled equations we find

\[ M\ddot{Q}_1 = -3\lambda Q_1 \quad \text{and} \quad M\ddot{Q}_2 = -\lambda Q_2 \]

which shows that the new coordinates \( Q_1 \) and \( Q_2 \) perform simple harmonic vibrations \( Q_i \propto \cos \omega_i t \) with frequencies \( \omega_1 = (3\lambda/M)^{1/2} \) and \( \omega_2 = (\lambda/M)^{1/2} \), respectively. The original coordinates \( x_1 \) and \( x_2 \) will be superpositions of the two pure oscillations since \( x_1 = \frac{1}{2}(Q_1 + Q_2) \) and \( x_2 = \frac{1}{2}(Q_1 - Q_2) \). The new coordinates \( Q_1, Q_2 \) and the two frequencies are usually referred to as 'normal' coordinates and 'normal' frequencies.

Notice that the new coordinates \( Q_1 \) and \( Q_2 \) are even and odd, respectively, under the symmetry reflection. If we denote this reflection by \( \sigma \), then \( \sigma Q_1 = Q_1 \) and \( \sigma Q_2 = -Q_2 \). In other words the new coordinates transform more simply under the reflection than do the original coordinates \( x_1 \) and \( x_2 \), and furthermore the equations of motion are uncoupled when written in terms of the new coordinates.

In some complicated problems it is not always possible to decouple all equations of motion from one another by such a simple step, but nevertheless by choosing new coordinates to transform 'simply' under the symmetry operations one is able to achieve considerable reduction in the extent of the coupling. Again, although it is clear in this example that \( Q_1 \) and \( Q_2 \) transform in the simplest possible way, in more complicated symmetries we shall have to define and examine this concept of 'simplicity'. This will be done in chapter 4. For example in the \( \text{NH}_3 \) molecule which, with four atoms, has altogether twelve degrees of freedom, the use of symmetry considerations can reduce the number of coupled equations of motion for small vibration from twelve to two. A general account of the use of symmetry arguments in the theory of normal modes will be given in chapter 6 and applied to molecular vibrations.

1.2.4 One particle in three dimensions using quantum mechanics—spherical symmetry and degeneracies

In quantum mechanics the energy levels for a particle moving in a spherical potential exhibit degeneracies or, in other words, there is more than one independent wave function with the same energy. The hydrogen atom with the electron moving in the electrostatic field of the proton is such a system. In simple terms the reason for this degeneracy is that in the absence of any preferred direction in space the energy can clearly not depend on the direction of the angular momentum vector. The degeneracy expresses the freedom in the framework of quantum mechanics. If the spherical symmetry is broken, for
example by turning on a magnetic field, then this degeneracy is destroyed and a 'multiplet' of several close-lying energy levels is produced, as in the Zeeman splitting.

The spherical symmetry may also be broken by immersing the atom in an external field which, although not spherically symmetric, has nevertheless some symmetry under specific rotations. In this case the degeneracies are only partially destroyed. Such a phenomenon is observed for an atom in a crystal field and will be analysed in detail in chapter 9.

The degeneracies resulting from spherical symmetry have a simple physical explanation in terms of the orientation of the angular momentum vector, but the occurrence of degeneracies is a characteristic result of any symmetry. This is quickly demonstrated by considering the Schrödinger equation $H\psi = E\psi$, where $H$ is the Hamiltonian operator, $E$ the energy and $\psi$ the wave function. Now introduce a coordinate transformation which transforms $\psi$ into $\psi'$ and $H$ into $H'$ so that, transforming both sides of the Schrödinger equation, we have $H'\psi' = E\psi'$. Here the energy, being a number, is unchanged by the transformation. Suppose now that $H$ is invariant under the transformation so that $H' = H$. Then $H\psi = E\psi'$, which tells us that the wave function $\psi'$ is an eigenfunction of the original Hamiltonian with the same energy as $\psi$. Hence, unless it happens that $\psi'$ is the same function as $\psi$, apart from a multiplicative constant, there will be at least a two-fold degeneracy at energy $E$. In chapter 5 we shall see how the structure of the degenerate multiplets follows from the symmetry alone and is independent of the further details of the Hamiltonian.

1.2.5 One particle in one dimension using quantum mechanics—parity and selection rules

Consider a particle moving in one dimension subject to an even potential $V(x) = V(-x)$ in quantum mechanics. This very simple symmetry leads to the result that the eigenfunctions are either even or odd functions of $x$. The proof of this result is elementary, for if $H\psi(x) = E\psi(x)$ we have also $H\psi(-x) = E\psi(-x)$, as in the example in subsection 1.2.4. Hence, $\psi(x)$ and $\psi(-x)$ both have the same energy so that, assuming the absence of degeneracy, these two functions are physically identical. Thus $\psi(-x) = c\psi(x)$, where $c$ is a constant. But this implies that $\psi(x) = c\psi(-x)$ also so that $\psi(x) = c^2\psi(x)$ which gives $c^2 = 1$ and $c = \pm 1$. Hence, $\psi(x)$ is either even or odd, but cannot be a mixture. This even or odd property of the function is referred to as parity. If there is degeneracy we may not conclude that $\psi(-x) = c\psi(x)$. In this case, however, the linear combinations $(\psi(x) \pm \psi(-x))/\sqrt{2}$, which are even and odd, respectively, may be taken as the pair of degenerate eigenfunctions. (In one dimension it is possible to show that there can be no degeneracy but the above argument may be immediately extended to three dimensions where degeneracy may occur.)

One further consequence of symmetry may be illustrated in this example,
1.2.6 Introduction

namely the concept of a 'selection rule' in quantum mechanics. The transition probability for decay from some initial state $\psi_i$ to a final state $\psi_f$ is proportional to the square of the integral

$$ I = \int_{-\infty}^{\infty} \psi_f^*(x) g(x) \psi_i(x) \, dx $$

where the form of $g(x)$ depends on the particular decay process. Now the integral clearly vanishes if the integrand is odd. Hence if $g(x)$ is an even function of $x$ then the integral is non-zero only if $\psi_i$ and $\psi_f$ are both even or both odd, i.e. the initial and final states have the same 'parity'. On the other hand, if $g(x)$ is odd then the initial and final states must have opposite parity. When $I$ is zero, the probability of the transition taking place is zero—hence the phrase 'selection rule'.

1.2.6 The search for symmetry—elementary particle physics

In describing the theory of symmetry in physics it is natural to explore the consequences of symmetry, but one must always remember that in practice it is the consequences which one observes in the laboratory and one must then ask what is the symmetry which would give rise to them. As with the development of most physical theories it is a two-way process. The experiments suggest possible symmetries and one then explores in detail the consequences of such symmetries, makes predictions and carries out further experiments to test them.

A splendid example of this is provided in elementary particle physics today. The neutron and proton have almost the same mass and so do the $\pi^+$, $\pi^-$ and $\pi^0$ mesons. In fact, all the elementary particles occur in such multiplets. Because of the relativistic connection between mass and energy, the existence of mass multiplets suggests a symmetry in the fundamental Hamiltonian. Since the different members of the multiplet have different charges, the symmetry operators will here involve transformations in the 'charge coordinates' of the particles. The development of this idea leads to the concept of 'isospin' which is of great importance both in the structure of nuclei and in the behaviour of elementary particles and will be described in chapter 10.

In recent years more and more elementary particles have been produced in succeeding generations of particle accelerators as their energy has been increased. It seems that several of the charge multiplets, referred to above, have similar masses and the existence of larger multiplets has been postulated. This, in turn, suggests the existence of a symmetry greater than that described by isospin. It is referred to as $SU_3$ symmetry, a title which will be explained in chapter 11. Unfortunately there is considerable splitting of the $SU_3$-multiplets, suggesting the existence of appreciable symmetry-breaking terms in the Hamiltonian, just as the Zeeman splitting in an atom suggests the breaking of the spherical symmetry by a magnetic field.
1.3 Summary

The examples given above were taken from a wide variety of physical systems but it is the same general theory of symmetry in each case. It is perhaps worth summarising the most important general consequences of symmetry in a system governed by quantum mechanics. They are: (1) conservation laws; (2) degeneracies in energy; (3) the energy eigenfunctions transform 'simply' under the symmetry operations and may be assigned a symmetry 'label' independent of the details of the Hamiltonian; (4) selection rules; (5) relations between matrix elements of observables. However, it must always be remembered that if the symmetry is too simple some of these consequences will not occur.

All of these consequences have featured at one point or another in the foregoing examples except (5). We cannot hope to be very convincing about consequence (5) at this early stage, but it is seen in the Zeeman splitting of atomic levels. The magnitude of the energy shift of different states of any given multiplet is proportional to their angular momentum about the field direction and this is true irrespective of the detailed structure of the wave functions. Thus we have an example in which the matrix elements are simply related, although the absolute value of any one of them would generally be difficult to calculate.

Another example of consequence (5) would be the mass formulae for nuclei and elementary particles. Here, the small mass differences between members of an isospin multiplet are simply related. More generally, the mass differences between members of an SU₃-multiplet are related by a more complicated formula because of the more complicated symmetry. However, the principle is the same as that governing the more familiar Zeeman splitting.

All of the examples mentioned in this introduction will be described in detail later. First, however, we must make ourselves familiar with the appropriate mathematical tools and this will be done in the next three chapters.
2

Groups and Group Properties

The notion of a group is introduced in this chapter and the most important general properties of group elements are deduced. Illustrations are given from a few very simple groups. The detailed properties of specific groups of importance in physical applications will be left until later chapters.

2.1 Definition of a group

Although we shall soon come to some very concrete examples it is worth beginning with the abstract definition of a group which is incredibly simple and yet leads to so many important consequences.

A set $\mathcal{G}$ of elements $G_1, G_2, G_3, \ldots$ is said to form a group if a law of 'multiplication' of the elements is defined which satisfies certain conditions. The result of multiplying two elements $G_a$ and $G_b$ is, naturally, called the 'product' and is written $G_a G_b$. The conditions to be satisfied are the following:

1. The product $G_a G_b$ of any two elements is itself an element in the set, i.e.
   $G_a G_b = G_c$ for some $G_c$ in $\mathcal{G}$  \hspace{1cm} (2.1)

2. In multiplying three elements $G_a, G_b$ and $G_c$ together, it does not matter which product is made first. In other words
   $G_a (G_b G_c) = (G_a G_b) G_c$ \hspace{1cm} (2.2)
where the product inside the brackets is carried out first. This implies that the use of such brackets is unnecessary and we may simply write \( G_s G_a G_b \) for the triple product.

(3) One element of the set, usually denoted by \( E \) and called the identity, must have the properties

\[
E G_s = G_s \quad \text{and} \quad G_s E = G_s
\]

for any \( G_s \) in the set \( \mathcal{G} \).

(4) To each element \( G_s \) in the set there corresponds another element in the set, denoted by \( G_s^{-1} \) and called the 'inverse' of \( G_s \), which has the properties

\[
G_s G_s^{-1} = E \quad \text{and} \quad G_s^{-1} G_s = E
\]

In general it is not permissible to change the order of multiplication of group elements; in other words \( G_s G_a \) is not in general the same element as \( G_a G_s \). A group for which \( G_s G_a = G_a G_s \) for all elements \( G_s \) and \( G_a \) is very much the exception in physical problems and is called an 'Abelian' group. Its elements are said to 'commute'.

Notice that the inverse of a product \( G_s G_a \) is given by

\[
(G_s G_a)^{-1} = G_a^{-1} G_s^{-1}
\]

This is deduced directly from the defining equation

\[
(G_s G_a)^{-1} G_s G_a = E
\]

by multiplying on the right first by \( G_a^{-1} \) and then by \( G_s^{-1} \). A convenient method of recording the multiplication \( G_s G_a = G_a \) of elements of a particular group \( \mathcal{G} \) is to build the multiplication table in which the rows and columns are labelled by the group elements and the result \( G_a \) of the multiplication \( G_s G_a \) is entered at the intersection of the row \( G_s \) and the column \( G_a \). The definitions of a group imply that every group element must appear once and once only in each row and in each column.

We have deliberately not specified the number of elements in the group. In fact the number may be finite, in which case it is denoted by \( g \) and called the 'order' of the group, or it may be infinite. The group is correspondingly called a finite or an infinite group. We shall consider both in this book since both are of importance in physics. For many of the general properties of groups described here and in chapter 4 it will not be necessary to specify whether the group is finite or infinite. In some cases, however, the proofs must be formulated separately for the two possibilities. The finite groups are relatively easy to discuss and for the infinite groups we restrict our attention to 'continuous' groups. This is sufficiently general for the physical problems under discussion and means that the group elements, instead of being distinguished by a discrete label \( a \) or \( b \), are labelled by a set of continuous parameters. Thus, by a small change in a parameter, we may pass continuously from one group element to another.
2.2 Examples of groups

The simplest examples of group elements are ordinary numbers with ordinary multiplication and our first two examples are of this kind.

(1) The two numbers 1 and −1 form a group. The identity is clearly 1. The inverse of the identity is always the identity and the inverse of −1 is itself. These properties are contained in the group multiplication table 2.1.

<table>
<thead>
<tr>
<th>$G_a$</th>
<th>1</th>
<th>−1</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>−1</td>
</tr>
<tr>
<td>−1</td>
<td>−1</td>
<td>1</td>
</tr>
</tbody>
</table>

(2) A slightly larger group of the same kind is the set of numbers 1, −1, $i$ and $−i$ which have the multiplication table 2.2.

<table>
<thead>
<tr>
<th>$G_a$</th>
<th>1</th>
<th>−1</th>
<th>$i$</th>
<th>$−i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1</td>
<td>−1</td>
<td>$i$</td>
<td>$−i$</td>
</tr>
<tr>
<td>−1</td>
<td>−1</td>
<td>1</td>
<td>$−i$</td>
<td>$i$</td>
</tr>
<tr>
<td>$i$</td>
<td>$i$</td>
<td>$−i$</td>
<td>1</td>
<td>−1</td>
</tr>
<tr>
<td>$−i$</td>
<td>$−i$</td>
<td>$i$</td>
<td>−1</td>
<td>1</td>
</tr>
</tbody>
</table>

Both of these groups have the 'cyclic' property which means that all the group elements may be formed by taking powers of a single element. In example (2) the four elements are given by $i^k$, with $k = 0, 1, 2$ and 3. Further powers will clearly reproduce the same cycle. Since 'ordinary' multiplication is used, these two groups must be Abelian, but a little thought will show that every cyclic group must be Abelian.

The behaviour of physical systems under rotations is of considerable importance in the study of symmetry and various sets of rotations form groups. We now move on to some examples of these. The law of multiplication in every case is that if the rotation $R_1$ carries a system from position A to position B and if $R_2$ carries it from B to C, then the product $R_2R_1$ carries it from A to C. Here we shall find our first example of a non-Abelian group, since although $R_2R_1 = R_1R_2$ when the rotations are about the same axis, in general $R_2R_1 \neq R_1R_2$. Rotations do not in general commute.

To illustrate the non-commutative property of rotations let $R_1$ be a rotation through an angle $\pi/2$ about the $z$-axis and $R_2$ a rotation through $\pi$ about the
Groups and Group Properties

2.2

y-axis. (A rotation through a positive angle about a directed axis is defined to be in the sense of a right-handed screw, i.e. clockwise when looking out along the axis.) By following carefully the motion of each of the three axes under the successive operations it is seen that \( R_2 R_1 \) is the same as a rotation through an angle \( \pi \) about the axis \((1, 1, 0)\), while \( R_1 R_2 \) is a rotation through \( \pi \) about the axis \((-1, 1, 0)\). But let us begin with simpler examples!

(3) Let \( E \) be the identity (a rotation through an angle zero) and let \( R \) denote a rotation through an angle \( \pi \) about the z-axis. Then the set \( E, R \) forms a group with multiplication table 2.3. (This group is conventionally called \( C_2 \)).

**Table 2.3**

<table>
<thead>
<tr>
<th>( G_6 )</th>
<th>( G _ _ _ _ )</th>
<th>( R )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E )</td>
<td>( E )</td>
<td>( R )</td>
</tr>
<tr>
<td>( R )</td>
<td>( R )</td>
<td>( E )</td>
</tr>
</tbody>
</table>

(4) Let \( I \) be the inversion, defined to change the direction of any vector. Clearly \( I^2 = E \), the identity, so that the set \( E, I \) forms a group, called \( S_2 \).

(5) The set \( E, R_1, R_2 \) forms a group if \( R_1 \) and \( R_2 \) denote, respectively, rotations through angles \( 2\pi/3 \) and \( 4\pi/3 \) about the z-axis. The multiplication table 2.4 is readily deduced. (This group is called \( C_3 \)).

**Table 2.4**

<table>
<thead>
<tr>
<th>( G_6 )</th>
<th>( E )</th>
<th>( R_1 )</th>
<th>( R_2 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( E )</td>
<td>( E )</td>
<td>( R_1 )</td>
<td>( R_2 )</td>
</tr>
<tr>
<td>( R_1 )</td>
<td>( R_1 )</td>
<td>( R_2 )</td>
<td>( E )</td>
</tr>
<tr>
<td>( R_2 )</td>
<td>( R_2 )</td>
<td>( E )</td>
<td>( R_1 )</td>
</tr>
</tbody>
</table>

(6) The set \( E, R_1, R_2, R_3, R_4, R_5 \) forms a group where \( R_1 \) and \( R_2 \) are rotations through angles \( 2\pi/3 \) and \( 4\pi/3 \) about the z-axis and the remaining elements \( R_3, R_4 \) and \( R_5 \) are rotations through angles \( \pi \) about the three axes in the \( xy \)-plane shown in figure 2.1. (This group is called \( D_3 \).) Geometrically this is the group of rotations of an equilateral triangle which carry it into positions indistinguishable from the initial position. One assumes, in this use of the word 'indistinguishable', that there are no marks or imperfections on the triangle to destroy its symmetry! Such motions of a geometrical figure are called 'proper covering operations', the word 'improper' being used if reflections are also allowed.
2.2 Groups and Group Properties

To visualise the rotations it is nevertheless helpful to imagine the vertices carrying labels 1, 2 and 3 and to follow the movement of these labels. By this method one may build up the multiplication table 2.5. For example

\[ R_1 \begin{array}{c} 1 \\ 2 \\ 3 \end{array} = \begin{array}{c} 3 \\ 1 \\ 2 \end{array} \]

\[ R_4 R_1 \begin{array}{c} 1 \\ 2 \\ 3 \end{array} = R_4 \begin{array}{c} 1 \\ 2 \\ 3 \end{array} = \begin{array}{c} 1 \\ 2 \\ 3 \end{array} = R_3 \begin{array}{c} 1 \\ 2 \\ 3 \end{array} \]

showing that \( R_4 R_1 = R_3 \).

In examples such as this, one may verify that the set forms a group by using the multiplication table. The fact that every entry in the table is one of the set shows that condition (1) of section 2.1 is satisfied. The fact that the identity occurs once, and once only, in every row and column verifies condition (4), while condition (3) is obviously met. The condition (2) is satisfied for all rotations. Alternatively, the very definition of the set to be all proper covering operations of the equilateral triangle ensures that they obey the definitions of a
Groups and Group Properties

Table 2.5

<table>
<thead>
<tr>
<th>G_e</th>
<th>E</th>
<th>R_1</th>
<th>R_2</th>
<th>R_3</th>
<th>R_4</th>
<th>R_5</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>E</td>
<td>R_1</td>
<td>R_2</td>
<td>R_3</td>
<td>R_4</td>
<td>R_5</td>
</tr>
<tr>
<td>R_1</td>
<td>R_1</td>
<td>E</td>
<td>R_2</td>
<td>R_3</td>
<td>R_4</td>
<td>R_5</td>
</tr>
<tr>
<td>R_2</td>
<td>R_2</td>
<td>R_1</td>
<td>E</td>
<td>R_3</td>
<td>R_4</td>
<td>R_5</td>
</tr>
<tr>
<td>R_3</td>
<td>R_3</td>
<td>R_2</td>
<td>R_1</td>
<td>E</td>
<td>R_4</td>
<td>R_5</td>
</tr>
<tr>
<td>R_4</td>
<td>R_4</td>
<td>R_3</td>
<td>R_2</td>
<td>R_1</td>
<td>E</td>
<td>R_5</td>
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<tr>
<td>R_5</td>
<td>R_5</td>
<td>R_4</td>
<td>R_3</td>
<td>R_2</td>
<td>R_1</td>
<td>E</td>
</tr>
</tbody>
</table>

The product of two covering operations is clearly another covering operation, as is the inverse.

(7) The triangle of the previous example is also unchanged by a reflection in the plane of the triangle. It is usual to denote this operation by \( \sigma_h \), imagining that the plane of the triangle is horizontal and using the suffix to refer to the horizontal plane. The inclusion of this new element generates further new elements by taking the products \( R_1 \sigma_h, R_2 \sigma_h, \ldots, R_5 \sigma_h \). Geometrically, one sees that the product \( R_5 \sigma_h \) is just a reflection in the vertical plane containing the \( R_5 \) axis and similarly for \( R_4 \sigma_h \) and \( R_3 \sigma_h \). It is soon verified that the set of 12 elements

\[ E, R_1, R_2, R_3, R_4, R_5, \sigma_h, R_1 \sigma_h, R_2 \sigma_h, \sigma_3, \sigma_4, \sigma_5 \]

where \( \sigma_3 = R_3 \sigma_4 \), etc., form a group which contains \( D_5 \) and is usually denoted by \( D_{10} \). The multiplication table is readily deduced from the table for \( D_5 \) and the property \( \sigma^2 = E \) for a reflection. Notice that although the group \( D_{10} \) contains improper elements (elements which are not rotations) it does not contain the inversion \( I \)—the triangle is clearly not unchanged by the inversion. Elements of the kind \( R_1 \sigma_h \), involving a rotation combined with a reflection in the plane perpendicular to the rotation axis, are called mirror rotations.

(8) The set of all rotations about a single axis form a continuous group, called \( \mathcal{S}_2 \). The group elements are denoted by \( R(a) \), where \( a \) is the angle of rotation and \( 0 \leq a < 2\pi \). The multiplication table would here be infinite, but in fact we may write down a general formula for the multiplication of any two elements. Geometrically we see that

\[ R(a) R(b) = R(a + b) \] (2.6)

with

\[ R(a + 2\pi) = R(a) \]

Hence the elements commute and the inverse is given by

\[ R^{-1}(a) = R(2\pi - a) \] (2.7)

(9) Extending to three dimensions, the set of all rotations about axes through a fixed point will again form a group. It requires three parameters to specify the rotation. One convenient parameterisation is to give two polar