UNIT 5 BASIC NOTIONS OF GROUP THEORY

Structure

5.1 INTRODUCTION

Group theory began as a branch of pure mathematics in the beginning of the nineteenth century. The outstanding French mathematician Evariste Galois (1811-1832) introduced the term "groups" to the specially worked out mathematical theory of symmetry. In mathematics, one generally encounters groups in linear algebra along with other concepts such as ring, field, vector space, inner product space, etc. Physicists soon found uses of group theory in the study of natural systems.

From the point of view of physics, it turned out that group theory could appropriately be applied to study the *symmetry properties of physical systems*. Materials scientists had known that natural crystals exhibit certain definite symmetries. In the middle of the nineteenth century several scientists and mathematicians developed an elegant theory, based on group theory, to enumerate all possible arrangements of atoms in a crystal. We shall discuss some of these concepts in the next unit.

With the development of quantum mechanics in the twentieth century, the applications of group theory to study microscopic physical systems knew no bounds. It was used to study crystals, molecules, atoms, nuclei and so on, with tremendous success. In fact, many physicists enriched group theory during the period from 1930 onwards. These days any serious studies in the field of quantum mechanics, particle physics and solid state physics use the procedures of group theory.

From the point of view of physics, one can say that *group theory is the branch of mathematics used in the study of invariance and symmetry of physical systems*. So in this unit we should begin by studying symmetry in the physical world around us. Then we shall acquaint you with the basic definitions and concepts of group theory.

In the next unit you will learn about some applications of group theory in physics.

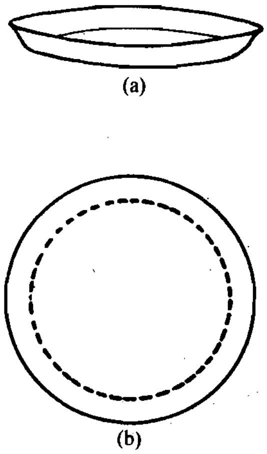
Objectives

After studying this unit you should be able to:

- define a group;
- discuss the **connection** between group theory and symmetry in physical systems; and
- determine the multiplication table, conjugate elements, classes and subgroups of a group.

5.2 SYMMETRY IN REAL SYSTEMS

We encounter symmetry almost everywhere in the world around us – in nature, in arts, in engineering and in science. Imagine for example, the symmetry of a butterfly and a snowflake, the symmetry in paintings, patterns and borders, the symmetry of a bus, a plane and a ship, the symmetry in monuments, the symmetry of atoms in molecules and crystals. Notice that here we have talked of the symmetry of forms, positions and structures. This is the kind of symmetry you can see directly and it can be thought of as *geometrical symmetry*. There is another kind of symmetry of physical phenomena and laws of nature which is called *physical symmetry*. This symmetry is fundamental to nature.



(a)

(b)

Fig.5.1: (a) Side view and (b) top view of a circular plate.

Now that we want to study a theory of symmetry, we would like to know: what is **symmetry**? To answer this question we first consider some concrete examples of classical objects. Suppose that you have before you a round circular plate. If the plate is empty, you have no way of saying which point on the rim of the plate faces you (see Fig. 5.1). Now if you close your eyes and the plate is rotated (or not rotated) and kept in the same position on the table, you have no way of finding out whether the plate has been rotated and, if so, through what angle. So the plate remains unchanged even after being rotated. This is an example of **circular rotational symmetry**.

If the plate is replaced by a completely flat disc, there is no way of saying which side is up and which is down. In addition to the rotational symmetry, this disc also has a **reflection symmetry** about a plane passing through its centre and parallel to the plane of the disc.

Now suppose you are in a huge and extended mango grove which has identical mango trees planted in a very regular pattern (see Fig. 5.2).

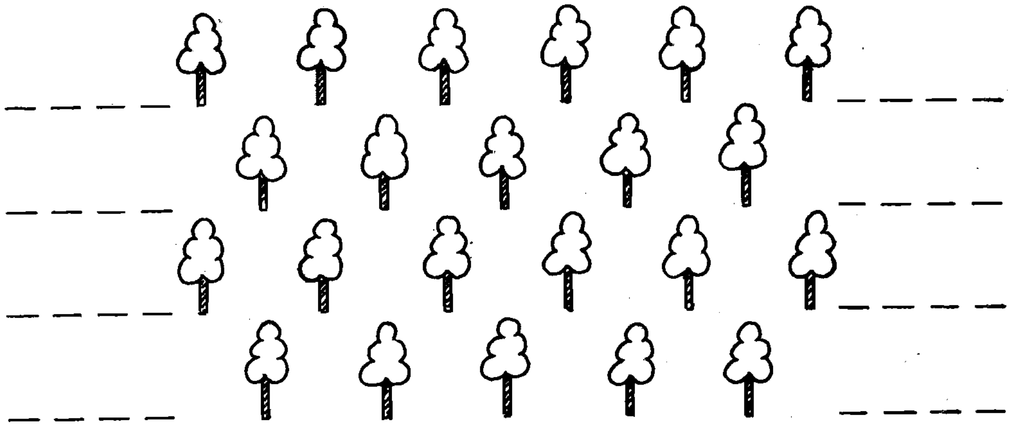


Fig.5.2: A large mango grove with identical trees planted in a regular pattern.

Suppose you are standing at one tree, to begin with and there is no way of distinguishing one tree from the other. Now you are blind-folded, and taken around the grove in a zig-zag path, brought near some tree, and then your eyes are opened. Assuming all ideal conditions, you won't be able to say whether you have come to the same tree or some other tree. What symmetry is exhibited by this system? The symmetry here is called (two-dimensional) *translation symmetry*.

You should notice that in each of these examples, the system remains unchanged (or *invariant*) under a certain transformation – **rotation**, **reflection** or **translation**. This is the defining notion of symmetry:

When an operation performed on a system results in an equivalent system with the same set of properties, the system is said to possess symmetry with respect to that operation.

A similar symmetry prevails in the microscopic world. You will learn about it now.

5.2.1 Symmetry in Microscopic Systems

Let us first examine some examples of geometrical symmetry in microscopic systems. Some common examples are the structural patterns of microscopic systems such as crystals, molecules, atoms, electrons, nuclei etc. Let us consider two simple molecules CO_2 and NH_3, and try to enumerate their symmetries.

You may recall that carbon dioxide is a linear molecule when in equilibrium, with carbon (C) atom at the centre and one oxygen (O) atom on each sides at equal distances (Fig. 5.3a). Now imagine a line AB passing through the **centres of these atoms** and consider a rotation of the molecule about this line through any angle (Fig. 5.3b). Can you distinguish the new state of the molecule from the old? Obviously, you cannot. Similarly, consider a plane perpendicular to the molecular axis passing through the C atom. A reflection at this plane leaves the molecular geometry, including the structure and orientation of the molecule, unchanged. Therefore, these are the symmetry elements of the CO_2 molecule.

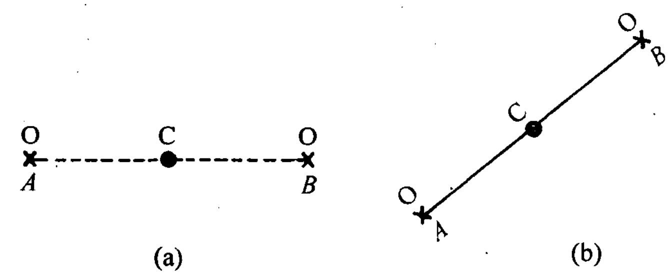


Fig.5.3: The geometrical symmetry of a CO_2 molecule

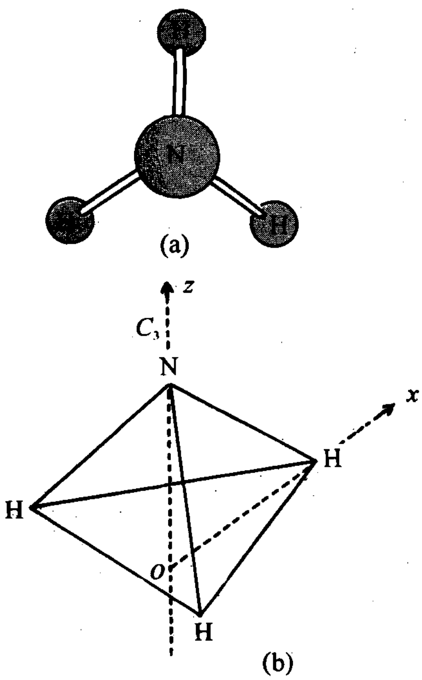


Fig.5.4: The geometrical symmetry of NH_3 molecule

Next, take a look at the ammonia molecule (Fig. 5.4a). In equilibrium, the three H atoms form the corners of an equilateral triangle, with all three H-H bonds of equal length. The N atom lies on the line perpendicular to the HHH plane passing through the centroid of the triangle, on either side of it. It is then clear that this molecule has the following symmetries: (a) A rotation about this line, called the *symmetry axis*, through 120° (Fig. 5.4b); and (b) A reflection in a plane passing through the symmetry axis and the midpoint of any H-H bond.

As yet another example, consider the shape of the charge cloud of an electron in a hydrogen atom. Fig. 5.5 shows the shape of the charge cloud (absolute square of the wave function) in the s and the p_z state. In the s state the charge cloud has a complete spherical symmetry. If we rotate it through any angle about any axis passing through the nucleus, no change can be noticed. In the p_z state, there are two symmetrical lobes along $+z$ and $-z$ directions. Thus it has rotational symmetry about the z-axis and reflection in the x-y plane (normal to the z-axis).

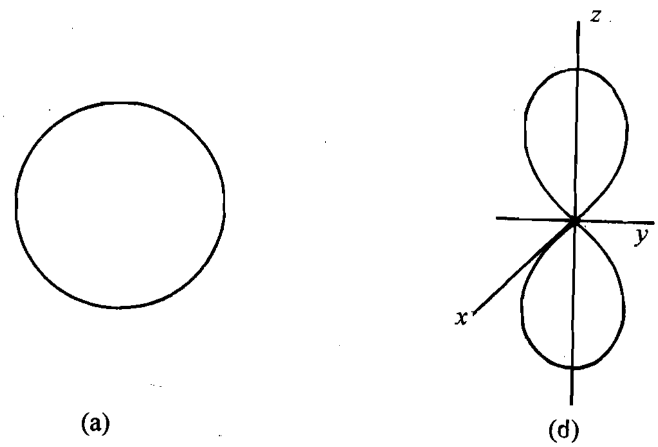


Fig.5.5: The shape of the electron charge cloud in a hydrogen atom in (a) s state and in (b) p_z state.

Incidentally, notice that the CO_2 molecule (Fig. 5.3) and the p_z state electron charge cloud (Fig. 5.5b) have the *same* symmetries – arbitrary rotation about an axis and reflection in a plane normal to that axis.

In this manner, we can say that each system has a specific symmetry. The properties of a macroscopic (bulk) system do not depend much on the shape and symmetry. For example, rectangular, circular, square or octagonal tables may have different symmetries and may differ in their visual and aesthetic appeal, but basically they have the same properties and can be put to the same functional uses. On the other hand, the properties of microscopic systems depend on, and are, in fact, governed by, their symmetries. Let us understand this with the help of an example – the emission of electromagnetic radiations by nuclei, atoms and molecules.

Do you know how a microscopic physical system (such as a molecule, atom, nucleus etc.) exhibits its existence? This is mainly by virtue of the emitted radiation, which is detected by our senses or instruments. For example, the radiation emitted by a molecule may fall in the infrared and visible range, that by an atom in the infrared to X-ray regions, and that by a nucleus in the X-ray and gamma-ray regions of the electromagnetic spectrum. You know that this radiation consists of specific lines of definite frequencies and intensities. **Now the relative intensities of various lines in nuclear, atomic and molecular spectra are decided by the symmetry of the system.**

You know from your study of PHE-11 that every microscopic system is governed by quantum mechanics and has various energy levels. The radiation emitted by the system arises due to transitions of the system from one state to another under the action of an electromagnetic field or some other perturbation. **Whether a system can make a transition between two given states under the action of a perturbation depends on the symmetries of the two states as well as of the perturbation.**

You also know from Unit 10 of PHE-11 that there are certain *selection rules* which tell us whether or not a transition can take place between two states under a perturbation. Thus a system may make a transition between two states under some perturbations but not under others. For example, electric dipole transition is possible between s and p states of an electron in a hydrogen atom but not between s and d or between s and f states (Recall the selection rule $\Delta l = \pm 1$.)

It is not our intention to discuss the selection rules in detail here. We have mentioned these examples merely to indicate the role of symmetry in physics. And, as we have said in the introduction, the study of symmetry is best done through group theory. Suffice it to say that today there is hardly any branch of physics or physical chemistry which does not use group theory. We therefore proceed to discuss some elementary concepts and ideas of group theory. But before that you may like to answer an SAQ based on the ideas presented so far.

SAQ 1

Spend 5 min

Enumerate all the symmetries of (a) a water molecule and (b) an isosceles triangle.

5.3 WHAT IS A GROUP?

So far we have discussed the types of symmetry and their role in physical systems. We have also pointed out that the proper mathematical theory to deal with symmetry is the theory of groups. We now consider a couple of examples of a group which will help you to grasp the concepts given later.

Consider the set $R = \{x : x = \text{a real number}\}$, the set of all real numbers. The elements of R, endowed with *the law of addition*, satisfy four properties:

(a) for any real numbers x and y belonging to R, their sum $(x + y)$ also belongs to R;

(b) for any three elements x, y and z of R, the associative law is satisfied, that is $x + (y + z) = (x + y) + z$;

(c) there exists an element called *zero* (0) in R, such that $x + 0 = 0 + x = x$ for every element $x \in R$;

(d) for every $x \in R$, there exists a unique element y in R such that $x + y = y + x = 0$. Note that this gives us $y = -x$.

Similarly consider another set $U(1) = \{z : |z| = 1\}$, the set of all complex numbers of unit magnitude. The elements of $U(1)$, endowed with the *law of multiplication*, satisfy four properties:

(a) for any two complex numbers x and y of unit magnitude, their product is also a complex number of unit magnitude and hence belongs to $U(1)$;

(b) for any three elements x, y and z of $U(1)$, the associative law is satisfied, that is, $x(yz) = (xy)z$;

(c) there exists an element $1 + 0i$ where $\left(i = \sqrt{-1}\right)$, or just 1 for short, in $U(1)$ such that $x1 = 1x = x$ for every element x of $U(1)$;

(d) for every $x \in U(1)$, there exists a unique element y in $U(1)$ such that $xy = yx = 1$. Note that this allows us to write $y = x^*$, where the asterisk denotes the complex conjugate.

We note that the four properties satisfied by the two sets are similar in nature. In fact, both the sets considered above are examples of a group. We now state the definition of a group.

Definition of a Group

In general, a **group** is defined as a set $G = \{x, y, z, ...\}$ endowed with a *binary law of composition* for its elements such that it satisfies the following four requirements:

(a) **Closure**: For any two elements x and y in the set G, their binary composition (under the chosen law) gives rise to some element which also belongs to G. We say in such a case that the set is *closed* under the binary law of composition. Thus

$$x \circ y \in G, \quad y \circ x \in G \tag{5.1}$$

Here the symbol $\circ$ stands for the binary law of composition.

(b) **Associative Property**: The binary law of composition is associative, that is,

$$x \circ (y \circ z) = (x \circ y) \circ z \qquad \forall x, y \in G \tag{5.2}$$

for any three elements in the set.

(c) **Existence of Identity**: There exists an element in the set G (let us denote it by e or E) whose composition with any other element x of G results in x itself, that is,

$$e \circ x = x \circ e = e \quad \text{for every } x \text{ in } G, \tag{5.3}$$

where e is called the *identity element* under the given law of composition.

(d) **Existence of Inverse**: For any element x in G there exists an element, say y, also in G such that

$$x \circ y = y \circ x = e, \tag{5.4}$$

where e is the identity element defined in (c) above. The elements y and x are then said to be *inverse* of each other under the given law of composition.

If the set G fails to satisfy any of these requirements, it cannot be called a group.

We shall soon consider several examples of groups. But before that it is necessary to clarify a few concepts.

It is not necessary that the law of composition of group elements be commutative. Thus the combination $x \circ y$ may result in an element different from the combination $y \circ x$ (as will happen if x and y are matrices). But if it so happens that $x \circ y = y \circ x$ for any two elements of a group then it is said to be an **abelian group**, otherwise a **non-abelian group**.

The law of associativity described in Eq. (5.2) is a *requirement on the law of combination of two elements*. For example, addition satisfies this requirement because

$$a+(b+c)=(a+b)+c, \tag{5.5a}$$

where a, b, c are any numbers (or matrices). But it is easy to see that subtraction does not satisfy it:

$$a-(b-c)\neq(a-b)-c. \tag{5.5b}$$

Moreover, a set may be a group under one law of composition but not under another.

The number of elements in a group is called its *order*. A group containing a finite number of elements is called a *finite group*; a group containing an infinite number of elements is called an *infinite group*. An infinite group may further be either discrete or continuous; if the number of elements in a group is denumerably infinite (such as the number of all integers), the group is *discrete*; if the number of the elements in a group is nondenumerably infinite (such as the number of all real numbers), the group is *continuous*.

You can understand these ideas better with the help of examples of groups and counter examples.

Examples and Counterexamples

We have already considered two examples of a group right in the beginning of this section. Let us now consider some more examples.

(i) The set containing the four complex numbers $1, i, -1, -i\left(\text{where } i=\sqrt{-1}\right)$ forms a group under multiplication (but not under addition). The multiplication of any two of these numbers results in a number belonging to the same set; for example,

$$(i)(-1)=(-i), \quad (-i)(-i)=-1. \tag{5.6}$$

and so on. You can easily see that the element 1 is the identity because

$$1(i)=i, \quad 1(-1)=(-1), \quad 1(-i)=-i. \tag{5.7}$$

Notice also that

$$(i)(-i)=1, \quad (-1)(-1)=1, \quad (1)(1)=1 \tag{5.8}$$

so that i and $-i$ are inverse of each other, while -1 is its own inverse, and so is 1. Finally, multiplication is associative. This shows that the set under consideration is a group. The order of this group is 4 and it is a finite group.

(ii) We have seen in the beginning of Section 5.3 that the set R of real numbers is a group under addition. Let us examine whether it is a group under multiplication. When two real numbers are multiplied, it results in a real number which belongs to R. So the set R is closed under multiplication. The law of multiplication is associative, as remarked earlier. The number 1 belonging to R is the identity element because it satisfies equations such as $1.x = x$ for any number x belonging to R; see Eq. (5.3). Now let us examine the requirement of inverse. If x belongs to R, we may have another element $1/x$ belonging to R such that $x.(1/x) = 1$; see Eq. (5.4). For example, 5.0 is the inverse of 0.2 because (5) (0.2) = 1, the inverse of 3.542009 is 0.2823263 ..., etc. But can we find an inverse for every element of R? What about the element 0 (zero)? There is no element in R which satisfies (0) (?) = 1. So merely because of the presence of this one element (bad element?), the set R is not a group under multiplication.

Let us now do a trick – *consider the set of all real numbers excluding zero*, and let us examine all four requirements. We now see that closure is satisfied, association is of course satisfied, the identity element (this is 1) exists in the set, and *every* element of the set has an inverse which also belongs to the set. So this set (excluding zero) is a group under multiplication. But then it is not a group under addition!

Thus we have derived a result of great significance: *The set of all real numbers is a continuous group under addition, and the set of all real numbers excluding the element zero is a group under multiplication.*

We will now consider examples of some groups important in theoretical physics.

Example 1: The groups U(N) and SU (N)

The group U (N) for $N \geq 1$ is defined to be the set of all $N \times N$ unitary matrices U with matrix multiplication as the binary law of composition. Let us verify if U (N) is a group. Now we know that $(U_1 U_2)^\dagger = U_2^\dagger U_1^\dagger$ and $(U_1 U_2)^{-1} = U_2^{-1} U_1^{-1}$. So if U_1 and U_2 are unitary $\left(\text{i.e.}, U_1^\dagger U_1 = I_N \text{ and } U_2^\dagger U_2 = I_N\right)$ then so is $U_1 U_2$, since

$$(U_1 U_2)^\dagger U_1 U_2 = U_2^\dagger U_1^\dagger U_1 U_2 = U_2^\dagger I U_2 = U_2^\dagger U_2 = I_N.$$

The associative law is valid for matrix multiplication. Since the unit matrix is a member of U_N, it provides the identity element. Finally, if U is a member of U_N, so is U^{-1} since $U^\dagger = U^{-1}$. Thus U (N) is a group.

The group SU (N) for $N \geq 2$ is defined to be the subset of all $N \times N$ unitary matrices U for which det $U = 1$ with matrix multiplication as the law of composition.

For SU (N), the same considerations apply. In addition if det $U_1 = 1$ and det $U_2 = 1$, then $\det(U_1 U_2) = 1$ since $\det(U_1 U_2) = \det U_1 \det U_2$. Moreover, I_N is a member of SU (N), so it is its identity element. Finally, if U is a member of SU (N), so is U^{-1}. Therefore, SU (N) is a group.

The set of groups SU (N), $N \geq 2$ is particularly important in particle physics. SU (2) is intimately related to angular momentum and isotopic spin. SU (3) is important for the classification of elementary particles.

Now that you have learnt the basic definition of a group, you may like to work out an SAQ to identify whether a set is a group or not.

SAQ 2

Spend 15 min

(a) Show that the set of all matrices of order $m \times n$ is a group under addition of matrices. Is this group abelian?

(b) Does the set of all non-singular square matrices of order n form a group under matrix multiplication?

(c) Show that the set of all non-negative integers {0, 1, 2, …} is not a group under addition. Which requirement(s) does it fail to satisfy?

In the above examples and SAQ, you have learnt two basic laws of composition – addition and multiplication – each referring to numbers and matrices. When the law of composition of a group is addition, the inverse of an element is called the *additive inverse*; when it is multiplication, the inverse is called the *multiplicative inverse*. Thus, if x is a number, $-x$ is its additive inverse and $1/x$ the multiplicative inverse provided $x \neq 0$. If A is a matrix, $-A$ is its additive inverse and A^{-1} the multiplicative inverse provided A is non-singular. Similarly, in the case of a group of numbers, 0 is the additive *identity* and 1 the *multiplicative identity*;

in the case of a group of matrices, the null matrix (of appropriate order) is the additive identity while the unit matrix (of appropriate order) is the multiplicative identity.

So far we have discussed the definition of a group followed by examples of groups whose elements are numbers or matrices. Let us now learn some elementary concepts of group theory relevant from the point of view of physics.

5.4 ELEMENTARY GROUP THEORY

You learnt the role of symmetry in physics in Section 5.2. In Units 1 and 4 of this block, we have discussed transformations of coordinates. A transformation which leaves a physical system invariant is called a **symmetry transformation** of the system. For example, the rotation of a circle through any angle about an axis passing through its centre and perpendicular to the plane of the circle is a symmetry transformation for it. A permutation of two identical atoms in a molecule is a symmetry transformation for the molecule.

Symmetry transformations of a physical system include the following kinds of transformations:

- rotation about an axis
- reflection in a plane
- inversion
- translation
- permutation of identical objects

All symmetry transformations of a system form a group called the **symmetry group** of a system. Let us study this concept in some detail.

5.4.1 Symmetry Group of a System

Let us first show that **the set of all symmetry transformations of a system is a group**. Let us see whether it satisfies the definition of a group:

- First we observe that if we perform two symmetry transformations of the system successively, the system remains invariant. Thus the composition of any two symmetry transformations of the system is again a symmetry transformation of the system. That is, the set considered is closed under the law of successive transformations.
- We can define an identity transformation which leaves the system unchanged; and this obviously belongs to the set.
- Given a symmetry transformation, we see that there exists an inverse transformation which also belongs to the set.
- Finally, the successive transformations of the system obey the associative law.

This proves that the set of symmetry transformations is a group.

To illustrate this concept let us take the example of a square and examine its symmetry group.

Example 2: Symmetry Group of a Square

You should carry out these transformations as an activity for a better understanding. For this, cut out a square from a piece of cardboard. Label the various points of the square as shown in Fig. 5.6: the corners by a, b, c, d; the centres of the edges by e, f, g, h; and the centre of the square by O. Mark points 1, 2, ..., 8 on a piece of paper (they are not to be marked on the square).

What happens when you rotate the square through a right angle about a line perpendicular to the square and passing through O? But for the labelling $a, b, ..., h$, you would not notice any change in the square. Consider all such symmetry transformation of the square (such as rotating or reflecting it, without bending or stretching) which leave the position of the boundaries of the square unchanged but give a distinct labeling of the marked points $a, b, ..., h$. How many symmetry transformations did you arrive at? Do your results agree with ours? Check with Table 5.1.

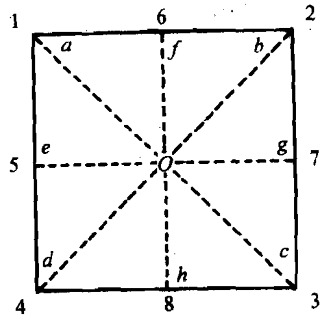


Fig.5.6: The axes and planes of symmetry of a square

Table 5.1: Symmetry transformations of a square

Symbol	Operation	Result
E	The identity	a b d c
C_4	A clockwise rotation through 90° about an axis normal to the square and passing through its centre	d a c b
C_4^2	A clockwise rotation through 180° about the above axis	c d b a
C_4^3	A clockwise rotation through 270° about the same axis	b c a d
m_x	Reflection in the line 5-7	d c a b
m_y	Reflection in the line 6-8	b a c d
σ_u	Reflection in the line 1-3	a d b c
σ_v	Reflection in the line 2-4	c b d a

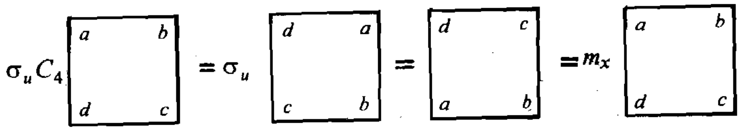
Before continuing further, it would be proper to say a few words about the notation we shall use.

If a clockwise rotation through an angle $2\pi/n$ (n a positive integer) about some axis leaves the system invariant, the axis is known as an *n-fold symmetry axis* of the system and the corresponding operation is denoted by C_n. Its integral powers, which will also be symmetry transformations of the system will be denoted by C_n^k; this represents k successive operations of C_n on the system, or a rotation of $2\pi k/n$ about the axis. A reflection in a plane will be denoted by m or σ with a subscript specifying the plane of reflection. The identity transformation will be denoted by E.

While enumerating all the symmetry transformations of a square listed in Table 5.1, we shall use the shorthand notation 'reflection in a line' to mean 'reflection in a plane perpendicular to the square passing through the line'.

You can see that the operations listed in Table 5.1 exhaust the symmetry transformations of a square, that is, there is no other transformation which leaves the square in the same position and yet gives a distinct labelling for the points $a, b, \ldots, h$. One may think of inversion through the centre O; but it can be readily verified that it is identical to C_4^2.

You can readily verify that the set of eight transformations listed in Table 5.1 is the group of symmetries of a square. For example, consider the operation of C_4 (i.e., clockwise rotation by 90°) followed by that of σ_u on the square. This can be found as follows:



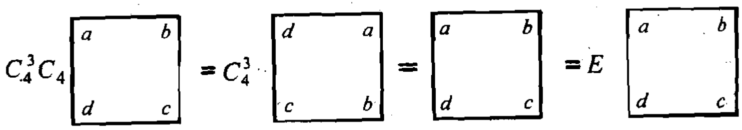
(5.9)

Although, we have operated by the product here on the square, it can be proved that the product $\sigma_u C_4$ operating on *any* system is the same as m_x operating on that system. We state this result (without proof) in the operator notation as

$$\sigma_u C_4 = m_x, \tag{5.10}$$

meaning thereby that the operations of $\sigma_u C_4$ and of m_x on the square or, in fact, on any system, give the same result.

The inverse of an operator is that operator which nullifies the effect of the first one. Thus, consider the successive operation $C_4^3 C_4$ on the square:



(5.11)

The same result would be obtained if we operated by C_4 and C_4^3 in the reverse order. Thus, by (5.4), C_4 is the inverse of C_4^3 and vice versa. In the operator notation, we may write this as

$$(C_4)^{-1} = C_4^3 \quad \text{or} \quad C_4 C_4^3 = C_4^3 C_4 = E. \tag{5.12}$$

Finally, the transformations obey the associative law. Hence the set of the symmetry transformations of a square is a group. This symmetry group of a square of order eight is denoted by C_{4v} in crystallography in the Schoenflies notation.

You should try an SAQ to further understand these ideas.

SAQ 3

Spend 5 min

In the set of symmetry transformations of a square listed in Table 5.1, show that each element has an inverse which is just one of these elements.

When we work with the symmetry group of a physical system, we are often required to find the result of successive transformations of the system, or to find the inverse of an element. Instead of working these out every time, it would be convenient to write all such successive transformations (or 'multiplications') in a table like a ready-reckoner. This is what we are going to do now.

5.4.2 Multiplication Table of a Group

Referring again to the symmetry group of a square of Example 1, let us consider some operations like

$$C_4 m_x = \sigma_u, \quad \sigma_u C_4^3 = m_y, \quad \sigma_u \sigma_v = C_4^2, \text{ and so on.}$$

All such products of the group elements can be represented by a table known as the *group multiplication table*. It is shown in Table 5.2 for the symmetry group of a square, C_{4v}.

Table 5.2: The Multiplication table for the group C_{4v}

Second Operation	First Operation							
	E	C_4	C_4^2	C_4^3	m_x	m_y	σ_u	σ_v
E	E	C_4	C_4^2	C_4^3	m_x	m_y	σ_u	σ_v
C_4^3	C_4^3	E	C_4	C_4^2	σ_v	σ_u	m_x	m_y
C_4^2	C_4^2	C_4^3	E	C_4	m_y	m_x	σ_v	σ_u
C_4	C_4	C_4^2	C_4^3	E	σ_u	σ_v	m_y	m_x
m_x	m_x	σ_v	m_y	σ_u	E	C_4^2	C_4^3	C_4
m_y	m_y	σ_u	m_x	σ_v	C_4^2	E	C_4	C_4^3
σ_u	σ_u	m_x	σ_v	m_y	C_4	C_4^3	E	C_4^2
σ_v	σ_v	m_y	σ_u	m_x	C_4^3	C_4	C_4^2	E

Note that in a successive operation such as ABC ..., the order of operation is *from right to left*. Thus, in the product $C_4 m_x$, m_x is the *first operation* as it acts on the physical system first, and C_4 the *second operation*. The entry for $C_4 m_x$ would therefore be found in Table 5.2 in the column corresponding to m_x and the row corresponding to C_4.

The order of the rows and columns in writing down the multiplication table of a group is immaterial. We have chosen a different ordering for the rows and for the columns; the ordering is such that an element in the first column (second operation) is the inverse of the corresponding element in the first row (first operation). If the multiplication table is written in this way, the principal diagonal contains only the identity element E.

The entire information about a group is contained in its multiplication table.

With the group multiplication table at hand, we can study several interesting features of a group. We shall study a few such concepts now.

5.4.3 Classes, Subgroups, Cyclic Groups and Permutation Groups

Consider a relation such as

$$x^{-1} y x = z, \qquad (5.13)$$

where x, y and z are elements of a group. When such a relation exists between two elements y and z of a group, they are said to be **conjugate elements**. You have encountered a similar transformation for matrices in Sec. 3.2 of Unit 3. It is clear that

$$x z x^{-1} = y. \qquad (5.14)$$

which is a similarity transformation of z by x.

You will not find difficult to discover such relationships among the elements of the group C_{4v}. For example,

$$C_4^{-1} m_x C_4 = m_y, \qquad (5.15)$$

showing that m_x and m_y are conjugate to each other.

You can easily show that if y is conjugate to z and y is also conjugate to p, then z and p are conjugate elements; or y, z and p are all conjugate to each other. Prove this as an exercise before studying further.

We can always split a group into sets such that all the elements of a set are conjugate to each other but no two elements belonging to different sets are conjugate to each other. In fact, such sets of elements are called the **conjugacy classes** or simply the **classes** of a group. The identity element e always constitutes a class by itself in any group, since, for any element x of the group, $x^{-1} e x = e$. The classes of C_{4v} are

$$(E), \ (C_4, C_4^3), \ (C_4^2), \ (m_x, m_y), \ (\sigma_u, \sigma_v) \qquad (5.16)$$

Why don't you prove some of these results?

SAQ 4

Spend 5 min

Verify that (m_x, m_y) is a class of C_{4v}.

Sometimes, a set of elements belonging to a group is itself a group. This gives rise to the concept of a subgroup. A set H is said to be a **subgroup** of a group G if H is itself a group under the same law of composition as that of G and if all the elements of H are also in G.

As an example, consider the four elements (E, C_4, C_4^2, C_4^3) of C_{4v}. You can verify that this set satisfies all the axioms defining a group; hence it is a subgroup of C_{4v}. Some more examples of the subgroups of C_{4v} are (E, C_4^2, m_x, m_y), (E, σ_u), etc.

Every group G has two trivial subgroups – the identity element and the group G itself. A subgroup H of G is called a **proper subgroup** if $H \neq G$, that is, if G has more elements than H.

Another important concept in group theory is that of **cyclic groups**.

If x is an element of a group G, all integral powers of x such as $x^2, x^3, \ldots$, must also be in G. If G is a finite group then there must exist a finite positive integer n such that

$$x^n = e, \qquad (5.17)$$

the identity element. The smallest positive (non-zero) integer n satisfying (5.17) is called the *order of element x*.

The group $(x, x^2, x^3, \ldots, x^n \equiv e)$ has the property that each of its elements is some power of one particular element. Such groups are called *cyclic groups. A group generated by a single element is a cyclic group.*

The group $\{1, i, -1, -i\}$ consisting of 4 elements which we mentioned as an example in Section 5.3 is a cyclic group of order 4 each of whose elements is a power of the element i because $(i)^4 = (-i)^4 = 1$. The group $\{E, C_4, C_4^2, C_4^3\}$, which contains successive rotations of a system through 90° about some axis, is also a cyclic group.

Permutation groups are of considerable importance in the quantum mechanics of identical particles. Consider a system of n identical objects. If we interchange any two or more of these objects, the resulting configuration is indistinguishable from the original one. We can consider each interchange as a transformation of the system and then all such possible transformations form a group under which the system is invariant. Since there are altogether $n!$ permutations on n objects, the group has order $n!$. It is known as the **permutation group** of n objects or the **symmetric group** of degree n and is usually denoted by S_n.

Let us take a specific example of three identical objects. We see that there are six possible permutations which may be denoted as:

$$E = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix}, \; A = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}, \; B = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix},$$

$$C = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}, \; D = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix}, \; F = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix}. \tag{5.18}$$

In quantum mechanics, it is futile to try to label identical particles!

The labels 1, 2 and 3 refer to the positions of the three objects rather than to the objects themselves. The system itself has six possible 'states' which may be denoted by

$$\psi_1 = (1 \;\; 2 \;\; 3), \; \psi_2 = (2 \;\; 3 \;\; 1), \; \psi_3 = (3 \;\; 1 \;\; 2),$$
$$\psi_4 = (2 \;\; 1 \;\; 3), \; \psi_5 = (3 \;\; 2 \;\; 1), \; \psi_6 = (1 \;\; 3 \;\; 2). \tag{5.19}$$

The six operators of Eq. (5.18) then act on any of the above six states and we can interpret their operations as follows. The operation C, for example, on any state ψ_i means that the object in position 1 is to be put in position 2 and the object in position 2 is to be put in position 1, while the object in position 3 is to be left where it is. Thus,

$$C\psi_2 = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix} (2 \;\; 3 \;\; 1) = (3 \;\; 2 \;\; 1) = \psi_5. \tag{5.20}$$

We can readily show that the six permutations of Eq. (5.18) constitute a group. We can easily work out the successive operation of two permutations on a state. Operating on Eq. (5.20) from the left, say, by A, we find

$$A(C\psi_2) = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} (3 \;\; 2 \;\; 1) = (1 \;\; 3 \;\; 2) = \psi_6. \tag{5.21}$$

But we also have

$$D\psi_2 = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} (2 \quad 3 \quad 1) = (1 \quad 3 \quad 2) = \psi_6. \qquad (5.22)$$

Thus, we have

$$AC\,\psi_2 = D\,\psi_2. \qquad (5.23)$$

You can see that if we start from any other state, the result is the same. Thus

$$AC\,\psi_i = D\,\psi_i, \qquad 1 \le i \le 6. \qquad (5.24)$$

Therefore, in the operator notation, we can write

$$AC = D. \qquad (5.25)$$

We leave it as an exercise for you to prove that S_3 is a group.

You may like to know whether you have grasped these concepts. Try the following SAQ.

SAQ 5

Spend 15 min

a) Show that each element in an abelian group is a class by itself.
b) If ω be the imaginary cube root of unity show that the set $\{1, \omega, \omega^2\}$ is a cyclic group of order 3 with respect to multiplication.
c) Show that $\{1, -1\}$ is a subgroup of the multiplicative group $\{1,\ i,\ -1,\ -i\}$.

5.4.4 Abstract Groups and Realisations

What is true about the relationship between any branch of pure mathematics and physics is also true about group theory. The elements of a group may be numbers, matrices, permutations, or coordinate transformations. They can be treated in an abstract manner, by denoting them by algebraic symbols like $x, y, \ldots$, without attaching any meaning to them. Once the rule of binary combination of elements is specified, the combination of any pair of elements can be worked out. Notice that the whole theory of groups is based on the four fundamental axioms (or requirements) listed in Sec. 5.3 and is quite independent of any particular interpretation given to the group elements. This part of the purely mathematical theory is therefore called *abstract group theory*.

When it comes to applying group theory in physics, we must attach a meaning to group elements. This meaning or interpretation depends on the physical system which we wish to study. We may put in a suitable interpretation for the group elements demanded by the physical situation at hand and take out the corresponding results. We can find the symmetry group of any physical system. Every such group is a **realisation** of the abstract concept, and the results emanating from it are applicable in that particular situation. We have already considered some examples and indicated some applications in Section 5.2.

Application of group theory has become extremely essential in studying the properties of crystals, molecules, atoms, nuclei and all such microscopic systems. In fact, the application of group theory to elementary particles in 1964 has even led to the prediction of a new elementary particle along with its properties (such as electric charge, baryon number, strangeness). It was a great triumph of this theory when this elementary particle (known as omega-minus) was soon discovered in the laboratory. We shall consider some applications of group theory in the next unit.

Let us now summarise the contents of this unit.

5.5 SUMMARY

- A set of elements endowed with a binary law of composition satisfying a certain set of four axioms is called a **group**. These four axioms (or hypotheses or requirements) are the **associative law**, **closure**, **existence of identity**, and **existence of inverse**.

- The composition of an element with every other element can be worked out and listed in the form of a table called the **group multiplication table**. The entire information about the group is contained in this table.

- A transformation of a physical system which takes it to a position or orientation indistinguishable from the earlier one is called its **symmetry transformation**.

- All the symmetry transformations of a system, including the identity element (no change), constitute a group known as the **symmetry group of the system.** Particularly in the case of a microscopic system, the properties depend on its symmetry group. A knowledge of the symmetry group helps in understanding these properties.

- As a purely mathematical structure, a group is an **abstract** concept. But for physical systems one can obtain a **realisation** of these abstract concepts in practice by treating symmetry transformations as group elements, revealing many properties of the system.

- A group of elements can be split into subsets such that all the elements are **conjugate** to each other, the similarity transformation being done by some element of the group itself, but no two elements belonging to two different subsets are conjugate to each other. Such subsets are called **classes of the group.**

- A subset of a group whose elements satisfy all the four aximos is called a **subgroup**. Obviously, a subgroup must contain the identity element. A group generated by a single element and containing powers of that element is called a **cyclic group**. The group of order $n!$ formed by the $n!$ permutations on n objects is called the **permutation group**.

- The use of group theory has become very essential in understanding the properties of crystals (electron energy bands, lattice vibrations, etc.), of molecules and atoms, of nucleons and other elementary particles.

5.6 TERMINAL QUESTIONS *Spend* 30 *min*

1. From Table 5.2, find the result of successive products $\sigma_u(m_x C_4^2)$ and $(\sigma_u m_x)C_4^2$. Show that they are same, in accordance with the law of association.

2. Show by operating on a rectangle that $C_4 m_x \mp \sigma_u$.

3. Find the classes of the group $\{1, i, -1, -i\}$ with multiplication as the binary law of composition.

4. Construct the multiplication table of the permutation group S_3.

5.7 SOLUTIONS AND ANSWERS

Self-assessment Questions

1. See Fig. 5.7. Note that both the systems shown in Fig. 5.7 have the same symmetry.

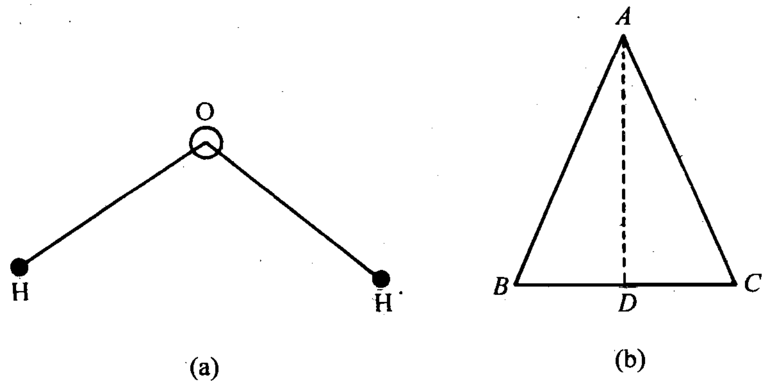


Fig.5.7: (a) The H_2O molecule (with two equal O-H bonds not in the same line); (b) An isosceles triangle with equal sides AB and AC. (Line AD is the bisector of the angle BAC.)

The triangle ABC has these symmetries.

(a) A rotation through 180° about the line AD.

(b) The plane of the triangle is reflection symmetry plane.

(c) Finally, there is reflection symmetry in a plane passing through line AD and normal to the plane of the triangle.

2. a) We note that the addition of two matrices of order $m \times n$ is also a matrix of the same order. Matrix addition is associative, that is, if A, B, C are any three matrices of order $m \times n$, then $A + (B + C) = (A + B) + C$. The null matrix O (with all elements zero) is the identity element because $A + O = A$. Finally, $A + (-A) = O$, so that $-A$ is the 'inverse' of A. Thus the set is a group. The group is abelian because for any two matrices, $A + B = B + A$.

   b) The multiplication of two square matrices of the same order gives a square matrix of the same order. Matrix multiplication is associative. The unit matrix I of order $n \times n$ is the identity element. Finally, by definition, a nonsingular matrix A has an inverse denoted by A^{-1} such that $AA^{-1} = I$. The group is non-abelian because for two arbitrary matrices, $A\,B \neq B\,A$.

   c) The set is closed under addition. The associative law is satisfied. The identity element is 0 which exists in the set. But none of the elements other than 0 possess an 'inverse' within the given set. (For example, the 'inverse' of 6 under addition is -6, but it does not belong to the set.)

3. By the method illustrated in Eq. (5.11), you can see that, while C_4 and C_4^3 are inverse of each other, each of the remaining six elements is its own inverse. For example, $(E)^{-1} = E, (m_x)^{-1} = m_x$, etc.

4. We perform similarity transformations of m_x with respect to all the elements of C_{4v}. We find the following result:

$$(E)^{-1} m_x E = E m_x = m_x, \qquad (C_4)^{-1} m_x C_4 = C_4^3 \sigma_v = m_y,$$

$$\left(C_4^2\right)^{-1} m_x C_4^2 = C_4^2 m_y = m_x, \quad \left(C_4^3\right)^{-1} m_x C_4^3 = C_4 \sigma_u = m_y,$$

$$(m_x)^{-1} m_x m_x = m_x E = m_x, \quad \left(m_y\right)^{-1} m_x m_y = m_y C_4^2 = m_x,$$

$$(\sigma_u)^{-1} m_x \sigma_u = \sigma_u C_4^2 = m_y, \quad (\sigma_v)^{-1} m_x \sigma_v = \sigma_v C_4 = m_y.$$

In these eight similarity transformations, we find that we get m_x four times and m_y four times. No other element is conjugate to m_x. Thus (m_x, m_y) forms a class of the group C_{4v}.

5. a) Any two elements A, B in an abelian group satisfy the condition

$$AB = BA$$

Multiplying from the left by B^{-1}, we get

$$B^{-1}AB = B^{-1}BA = A$$

implying that A forms a class on its own.

b) Let us prepare the group multiplication table:

	1	ω	ω^2
1	1	ω	ω^2
ω	ω	ω^2	$\omega^3 = 1$
ω^2	ω^2	$\omega^3 = 1$	$\omega^4 = \omega$

From the table we see that

(i) the closure property is satisfied since the relation $x\,y \in G \;\forall\; x, y$ holds for 1, ω and ω^2.

(ii) Multiplication is associative.

(iii) Identity element is 1.

(iv) The inverse of 1, ω, ω^2 is 1, ω^2, ω, respectively.

Hence the set is a group with respect to multiplication. It is a cyclic group of order 3 since $\omega^3 = 1$.

c) $\{1, -1\}$ is a subgroup of $\{1, i, -1, -i\}$ as it has elements from the larger group. It satisfies the four group axioms of closure $(1 \times -1 = -1)$, associativity, having an identity element (1); and a multiplicative inverse: 1 for 1 and −1 for −1.

Terminal Questions

1. We find from Table 5.2, that

$$m_x C_4^2 = m_y, \quad \sigma_u m_x = C_4.$$

Then again from the same table, we find that

$$\sigma_u\left(m_x C_4^2\right) = \sigma_u m_y = C_4^3;$$

$$(\sigma_u m_x) C_4^2 = C_4 C_4^2 = C_4^3.$$

Thus they are the same and satisfy the law of associativity.

2. We have remarked in the text following Eq. (5.9) that operator equations are valid irrespective of the system on which they operate. This question illustrates this concept. Thus we see that

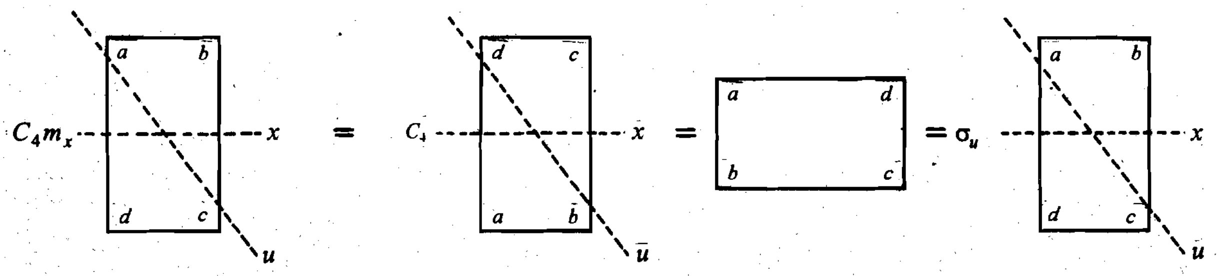


Fig.5.8

Thus Fig. 5.8 shows that $C_4 m_x = \sigma_u$. Notice that neither C_4 nor σ_u is a symmetry transformation for the rectangle. But the operator equation remains valid.

3. We perform similarity transformations of each element with respect to every other element in the group. For example, the similarity transformation of i with respect to other elements gives

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

Thus the element i in the given group is conjugate to itself and not to any other element. Therefore it forms a class by itself. For the other elements, we find:

$$(i)^{-1} 1(i) = 1, \quad (-1)^{-1} 1(-1) = 1, \quad (-i)^{-1} 1(-i) = 1;$$

$$(1)^{-1}(-1)(1) = -1, \quad (i)^{-1}(-1)(i) = -1, \quad (-i)^{-1}(-1)(-i) = -1;$$

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

Thus each of the four elements in the group is a class by itself.

4. Multiplication table of S_3:

Second Operation	First Operation					
	E	B	A	C	D	F
E	E	A	B	C	D	F
A	A	E	B	D	F	C
B	B	A	E	F	C	D
C	C	D	F	E	B	A
D	D	F	C	A	E	B
F	F	C	D	B	A	E

The calculations are as follows:

$$AA(\psi_1) = AA(1 \quad 2 \quad 3) = A(2 \quad 3 \quad 1) = (3 \quad 1 \quad 2) = \psi_3 = B\psi_1$$

$$AB(\psi_1) = A(3 \quad 1 \quad 2) = (1 \quad 2 \quad 3) = E\psi_1$$

$$AD(\psi_1) = A(3 \quad 2 \quad 1) = (1 \quad 3 \quad 2) \equiv \psi_6 \equiv F\psi_1$$

$$AF(\psi_1) = A(1 \quad 3 \quad 2) = (2 \quad 1 \quad 3) \equiv C\psi_1$$

$$BA(\psi_1) = B(2 \quad 3 \quad 1) = (1 \quad 2 \quad 3) \equiv E\psi_1$$

$$BB(\psi_1) = B(3 \quad 1 \quad 2) = (2 \quad 3 \quad 1) = A\psi_1$$

$$BC\psi_1 = B(2 \quad 1 \quad 3) = (1 \quad 3 \quad 2) = F\psi_1$$

$$BD\psi_1 = B(3 \quad 2 \quad 1) = (2 \quad 1 \quad 3) = C\psi_1$$

$$BF\psi_1 = B(1 \quad 3 \quad 2) = (3 \quad 2 \quad 1) = D\psi_1$$

$$CB\psi_1 = C(3 \quad 1 \quad 2) = (3 \quad 2 \quad 1) = D\psi_1$$

$$CA\psi_1 = C(2 \quad 3 \quad 1) = (1 \quad 3 \quad 2) = F\psi_1$$

$$CC\psi_1 = C(2 \quad 1 \quad 3) = (1 \quad 2 \quad 3) = E\psi_1$$

$$CD\psi_1 = C(3 \quad 2 \quad 1) = (3 \quad 1 \quad 2) = B\psi_1$$

$$CF\psi_1 = C(1 \quad 3 \quad 2) = (2 \quad 3 \quad 1) = A\psi_1$$

$$DB\psi_1 = D(3 \quad 1 \quad 2) = (1 \quad 3 \quad 2) = F\psi_1$$

$$DA\psi_1 = D(2 \quad 3 \quad 1) = (2 \quad 1 \quad 3) = C\psi_1$$

$$DC\psi_1 = D(2 \quad 1 \quad 3) = (2 \quad 3 \quad 1) = A\psi_1$$

$$DD\psi_1 = D(3 \quad 2 \quad 1) = (1 \quad 2 \quad 3) = E\psi_1$$

$$DF\psi_1 = D(1 \quad 3 \quad 2) = (3 \quad 1 \quad 2) = B\psi_1$$

$$FB\psi_1 = F(3 \quad 1 \quad 2) = (2 \quad 1 \quad 3) = C\psi_1$$

$$FA\psi_1 = F(2 \quad 3 \quad 1) = (3 \quad 2 \quad 1) = D\psi_1$$

$$FC\psi_1 = F(2 \quad 1 \quad 3) = (3 \quad 1 \quad 2) = B\psi_1$$

$$FD\psi_1 = F(3 \quad 2 \quad 1) = (2 \quad 3 \quad 1) = A\psi_1$$

$$FF\psi_1 = F(1 \quad 3 \quad 2) = (1 \quad 2 \quad 3) = E\psi_1$$