CHAPTER 17

GROUP THEORY

Disciplined judgment, about what is neat and symmetrical and elegant, has time and time again proved an excellent guide to how nature works.

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17.1 INTRODUCTION TO GROUP THEORY

Symmetry has long been important in the study of physical systems. Connections between the geometric symmetry of crystalline systems and their x-ray diffraction spectra were found to be crucial to the interpretation of the diffraction patterns and the extraction therefrom of information locating the atoms in the crystal. The geometric symmetries of molecules determine which vibrational modes will be active in absorbing or emitting radiation; the symmetries of periodic systems have implications as to their energy bands, their ability to conduct electricity, and even their superconductivity. The invariance of physical laws with respect to position or orientation (i.e., the symmetry of space) gives rise to **conservation laws** for linear and angular momentum. Sometimes the implications of symmetry invariance are far more complicated or sophisticated than might at first be supposed; the invariance of the forces predicted by electromagnetic theory when measurements are made in observation frames moving uniformly at different speeds (**inertial frames**) was an important clue leading Einstein to the discovery of special relativity. With the advent of quantum mechanics, considerations of angular momentum and spin introduced new symmetry concepts into physics. These ideas have since catalyzed the modern development of particle theory.

Central to all these symmetry notions is the fact that complete sets of symmetry operations form what in mathematics are known as groups. The elements of a group may be finite in number, in which case the group is then termed **finite** or **discrete**, as for example the symmetry operations shown for the object depicted in Fig. 17.2. But alternatively, the

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symmetry operations may be infinite in number and described by continuously variable parameter(s); such groups are termed **continuous**. An example of a continuous group is the set of possible rotational displacements of a circular object about its axis (in which case the parameter is the rotation angle).

Definition of a Group

A group G is defined as a set of objects or operations (e.g., rotations or other transformations), called the elements of G, that may be combined, by a procedure to be called **multiplication** and denoted by *, to form a well-defined **product**, subject to the following four conditions:

1. If a and b are any two elements of G, then the product $a * b$ is also an element of G; more formally, $a * b$ associates an element of G with the ordered pair (a, b) of elements of G. In other words, G is **closed** under multiplication of its own elements.
2. This multiplication is associative: $(a * b) * c = a * (b * c)$.
3. There is a unique identity element[1] I in G, such that $I * a = a * I = a$ for every element a in G.
4. Each element a of G has an inverse, denoted a^{-1}, such that $a * a^{-1} = a^{-1} * a = I$.

The above simple rules have a number of direct consequences, including the following:

- It can be shown that the inverse of any element a is unique: If a^{-1} and $\hat{a}^{-1}$ are both inverses of a, then $\hat{a}^{-1} = \hat{a}^{-1} * (a * a^{-1}) = (\hat{a}^{-1} * a) * a^{-1} = a^{-1}$.
- The products $g * a$, where a is fixed and g ranges over all elements of the group, consist (in some order) of all the elements of the group. If g and g' produce the same element, then $g * a = g' * a$. Multiplying on the right by a^{-1}, we get $(g * a) * a^{-1} = (g' * a) * a^{-1}$, which reduces to $g = g'$.

Here are some useful conventions and further definitions:

- The * for multiplication is tedious to write; when no ambiguity will result it is customary to drop it, and instead of $a * b$ we write ab.
- When a and b are operations, and ab is to be applied to an object appearing to their right, b is deemed to act first, with a then applied to the result of operation with b.
- If a discrete group possesses n elements (including I), its **order** is n; a continuous group of order n has elements that are defined by n parameters.
- If $ab = ba$ for all a, b of G, the multiplication is **commutative**, and the group is called **abelian**.
- If a group possesses an element a such that the sequence I, a, $a^2 (= aa)$, a^3, $\cdots$ includes all elements of the group, it is termed **cyclic**. If a group is cyclic, it must also be abelian. However, not all abelian groups are cyclic.

[1] Following E. Wigner, the identity element of a group is often labeled E, from the German **Einheit**, that is, unit; some other authors just write 1.

- Two groups $\{I, a, b, \cdots\}$ and $\{I', a', b', \cdots\}$ are **isomorphic** if their elements can be put into one-to-one correspondence such that for all a and b, $ab = c \Longleftrightarrow a'b' = c'$. If the correspondence is many-to-one, the groups are **homomorphic**.
- If a subset G' of G is closed under the multiplication defined for G, it is also a group and called a **subgroup** of G. The identity I of G always forms a subgroup of G.

Examples of Groups

Example 17.1.1 D_3, Symmetry of an Equilateral Triangle

The symmetry operations of an equilateral triangle form a finite group with six elements; our triangle can be placed either side up, and with any vertex in the top position. The six operations that convert the initial orientation into symmetry equivalents are I (the identity operation that makes no orientation change), C_3, an operation which rotates the triangle counterclockwise by 1/3 of a revolution, C_3^2 (two successive C_3 operations), C_2, rotation by 1/2 a revolution (for this group the rotation is about an axis in the plane of the triangle), and C_2' and C_2'' (180° rotations about additional axes in the plane of the triangle). Figure 17.1 is a schematic diagram indicating these symmetry operations, and Fig. 17.2 shows their result, with the vertices of the triangle numbered to show the effect of each operation. The multiplication table for the group is shown in Table 17.1, where the product ab (which describes the result of first applying operation b, and then operation a) is

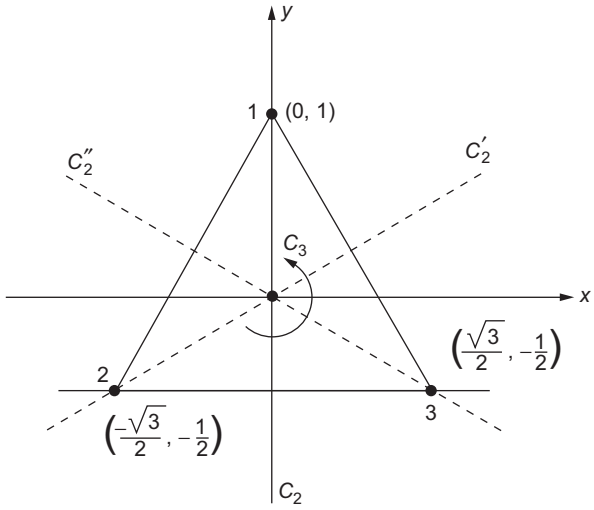

FIGURE 17.1 Diagram identifying symmetry operations of an equilateral triangle. I is the identity operation (the diagram as shown here). C_3 and C_3^2 are counterclockwise rotations, by, respectively, 120° and 240°; C_2, C_2', C_2'' are operations that turn the triangle over by rotation about the indicated axes.

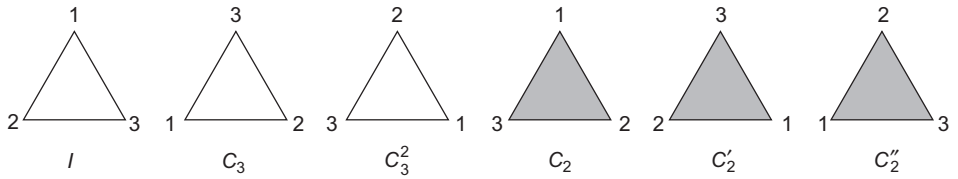

FIGURE 17.2 Result of applying the symmetry operations identified in Fig. 17.1 to an equilateral triangle. One side of the triangle is shaded to make it obvious when that side is up.

Table 17.1 Multiplication Table for Group D_3

	I	C_3	C_3^2	C_2	C_2'	C_2''
I	I	C_3	C_3^2	C_2	C_2'	C_2''
C_3	C_3	C_3^2	I	C_2''	C_2	C_2'
C_3^2	C_3^2	I	C_3	C_2'	C_2''	C_2
C_2	C_2	C_2'	C_2''	I	C_3	C_3^2
C_2'	C_2'	C_2''	C_2	C_3^2	I	C_3
C_2''	C_2''	C_2	C_2'	C_3	C_3^2	I

Operations are pictured in Fig. 17.2. The table entry for row a and column b is the product element ab. For example, $C_2C_3 = C_2'$.

the group element listed in row a and column b of the table. This group has several names, of which one is D_3 ("D" for **dihedral**, referring to a 180° rotation axis lying in a plane perpendicular to the main symmetry axis). From the multiplication table or by examination of the symmetry operations themselves, we can see that the inverse of I is I, the inverse of C_3 is C_3^2 (so the inverse of C_3^2 is C_3), and each C_2 is its own inverse. This group is not abelian; $C_3C_2 \neq C_2C_3$ ($C_3C_2 = C_2''$, while $C_2C_3 = C_2'$). ■

Example 17.1.2 ROTATION OF A CIRCULAR DISK

The rotations of a circular disk about its symmetry axis form a continuous group of order 1 whose elements consist of rotations through angles φ. The group elements $\mathsf{R}(\varphi)$ are infinite in number, with φ any angle in the range $(0, 2\pi)$. The identity element is clearly $\mathsf{R}(0)$; the inverse of $\mathsf{R}(\varphi)$ is $\mathsf{R}(2\pi - \varphi)$. The multiplication rule for this group is $\mathsf{R}(\varphi)\mathsf{R}(\theta) = \mathsf{R}(\varphi + \theta)$ (reduced to a value between 0 and 2π), so $\mathsf{R}(\varphi)\mathsf{R}(\theta) = \mathsf{R}(\theta)\mathsf{R}(\varphi)$, and this group is abelian. It will be useful to figure out what happens to a point on the disk that before the rotation was at (x, y). The rotation is by an angle φ about the z axis, clockwise, looking down from positive z, a choice made to be consistent with the counterclockwise rotations of the coordinate axes used elsewhere in this book. The final location of this point, (x', y'),

is given by the matrix equation

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}. \tag{17.1}$$

■

Example 17.1.3 AN ABSTRACT GROUP

Groups do not need to represent geometric operations. Consider a set of four quantities (elements) I, A, B, C, with our knowledge about them only that when any two are multiplied, the result is an element of the set. The multiplication table of this four-element set is shown in Table 17.2. These elements form a group, because each has an inverse (itself), there is an identity element (I), and the set is closed under multiplication.

Table 17.2 Multiplication Table for the Vierergruppe

	I	A	B	C
I	I	A	B	C
A	A	I	C	B
B	B	C	I	A
C	C	B	A	I

The table entry for row a and column b is the product element ab.

■

Example 17.1.4 ISOMORPHISM AND HOMOMORPHISM: C_4 GROUP

The symmetry operations of a square that cannot be turned over form a four-membered group sometimes called C_4 whose elements can be named I, C_4 (90° rotation), C_2 (180° rotation), C_4' (270° rotation). The four complex numbers 1, i, -1, $-i$ also form a group when the group operation is ordinary multiplication. These groups are isomorphic, and can be put into correspondence in two different ways:

$$I \leftrightarrow 1,\ \ C_4 \leftrightarrow i,\ \ C_2 \leftrightarrow -1,\ \ C_4' \leftrightarrow -i \quad \text{or} \quad I \leftrightarrow 1,\ \ C_4 \leftrightarrow -i,\ \ C_2 \leftrightarrow -1,\ \ C_4' \leftrightarrow i.$$

This group is also cyclic, as $C_4^2 = C_2$, $C_4^3 = C_4'$, or equivalently $i^2 = -1$, $i^3 = -i$.

The group C_4 has a two-to-one correspondence with the ordinary multiplicative group containing only 1 and -1: I and $C_2 \leftrightarrow 1$, while C_4 and $C_4' \leftrightarrow -1$. This is a homomorphism. A more trivial homomorphism, possessed by all groups, is obtained when every element is assigned to correspond to the identity. ■

Exercises

17.1.1 The **Vierergruppe** (German: four-membered group) is a group different from the C_4 group introduced in Example 17.1.4. The Vierergruppe has the multiplication table shown in Table 17.2. Determine whether this group is cyclic and whether it is abelian.

17.1.2 (a) Show that the permutations of n distinct objects satisfy the group postulates.

(b) Construct the multiplication table for the permutations of three objects, giving each permutation a name of some sort. (Suggestion: Use I for the permutation that leaves the order unchanged.)

(c) Show that this permutation group (named S_3) is isomorphic with D_3 and identify corresponding operations. Is your identification unique?

17.1.3 **Rearrangement theorem:** Given a group of distinct elements $(I, a, b, \ldots, n)$, show that the set of products $(aI, a^2, ab, ac, \ldots, an)$ reproduces all the group elements in a new order.

17.1.4 A group G has a subgroup H with elements h_i. Let x be a fixed element of the original group G and **not** a member of H. The transform

$$xh_i x^{-1}, \quad i = 1, 2, \ldots$$

generates a **conjugate subgroup** xHx^{-1}. Show that this conjugate subgroup satisfies each of the four group postulates and therefore is a group.

17.1.5 (a) A particular group is abelian. A second group is created by replacing g_i by g_i^{-1} for each element in the original group. Show that the two groups are isomorphic.

Note. This means showing that if $ab = c$, then $a^{-1}b^{-1} = c^{-1}$.

(b) Continuing part (a), show that the second group is also abelian.

17.1.6 Consider a cubic crystal consisting of identical atoms at $\mathbf{r} = (la, ma, na)$, with l, m, and n taking on all integral values.

(a) Show that each Cartesian axis is a fourfold symmetry axis.

(b) The cubic **point group** will consist of all operations (rotations, reflections, inversion) that leave the simple cubic crystal invariant and that do not move the atom at $l = m = n = 0$. From a consideration of the permutation of the positive and negative coordinate axes, predict how many elements this cubic group will contain.

17.1.7 A plane is covered with regular hexagons, as shown in Fig. 17.3.

(a) Determine the rotational symmetry of an axis perpendicular to the plane through the common vertex of three hexagons (A). That is, if the axis has n-fold symmetry, show (with careful explanation) what n is.

(b) Repeat part (a) for an axis perpendicular to the plane through the geometric center of one hexagon (B).

(c) Find all the different kinds of axes within the plane of hexagons about which a 180° rotation is a symmetry element (this corresponds to turning the plane over by rotation about that axis).

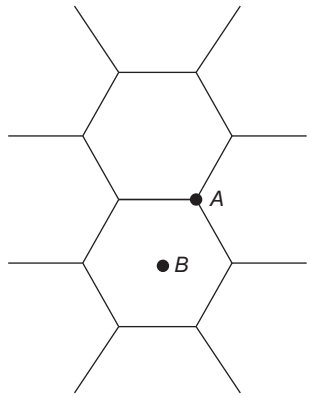

FIGURE 17.3 Plane covered by hexagons.

17.2 REPRESENTATION OF GROUPS

All discrete groups and the continuous groups we study here can be represented by square matrices. By this we mean that to each element of the group we can associate a matrix, and that if $\mathsf{U}(a)$ is the matrix associated with a and $\mathsf{U}(b)$ the matrix associated with b, then the matrix product $\mathsf{U}(a)\mathsf{U}(b)$ will be the matrix associated with ab. In other words, the matrices have the same multiplication table as the group. We call these matrices U because they can be chosen to be unitary. It is not necessary that U have a dimension equal to the order of the group.

Sometimes we need to identify representations with a label. For specific representations we can use their generally adopted names; when we need a generic label, we will use K or K'. Thus, we can refer to representation K, consisting of matrices $\mathsf{U}^K(a)$.

Example 17.2.1 A UNITARY REPRESENTATION

Here is a unitary representation of the group D_3 illustrated in Fig. 17.2:

$$\mathsf{U}(I) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad \mathsf{U}(C_3) = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix},$$

$$\mathsf{U}(C_3^2) = \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix}, \qquad \mathsf{U}(C_2) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\mathsf{U}(C_2') = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} \end{pmatrix}, \qquad \mathsf{U}(C_2'') = \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & \frac{1}{2} \end{pmatrix}. \tag{17.2}$$

Several features of this representation are apparent:

- The unit operation is represented by a unit matrix.
- The inverse of an operation is represented by the inverse of its matrix.

We can check that the U form a representation: From the multiplication table, we have $C_2 C_3 = C_2'$. Now we evaluate

$$\mathsf{U}(C_2)\mathsf{U}(C_3) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ -\frac{1}{2}\sqrt{3} & -\frac{1}{2} \end{pmatrix} = \begin{pmatrix} -\frac{1}{2} & \frac{1}{2}\sqrt{3} \\ \frac{1}{2}\sqrt{3} & \frac{1}{2} \end{pmatrix},$$

which is indeed $\mathsf{U}(C_2')$. The reader can easily verify that other products of group elements correspond to the products of the representation matrices. Matrix multiplication is in general not commutative, and gives results that are consistent with the lack of commutativity of the group operations.

The 2×2 representation shown above is **faithful**, meaning that each group element corresponds to a different matrix. In other words, our 2×2 representation is isomorphic with the original group. Not all representations are faithful; consider the relatively trivial representation in which every group element is represented by the 1×1 matrix (1). Every group will possess this representation. A somewhat less trivial, but still unfaithful, representation of D_3 is one in which

$$\mathsf{U}(I) = \mathsf{U}(C_3) = \mathsf{U}(C_3^2) = 1, \quad \mathsf{U}(C_2) = \mathsf{U}(C_2') = \mathsf{U}(C_2'') = -1. \tag{17.3}$$

This representation distinguishes elements according to whether they involve turning the triangle over. Not all groups will possess this 1×1 representation; if we had not permitted the triangle to be turned over, this representation would have been excluded. These unfaithful representations are homomorphic with the original group. ■

An important feature of a representation of a group G is that its essential features are invariant if we make the same unitary transformation on the matrices representing all the group elements. To see this, consider what happens when we replace each $\mathsf{U}(g)$ by $\mathsf{V}\mathsf{U}(g)\mathsf{V}^{-1}$. Then the product $\mathsf{U}(g)\mathsf{U}(g')$, which is some $\mathsf{U}(g'')$, becomes $(\mathsf{V}\mathsf{U}(g)\mathsf{V}^{-1})(\mathsf{V}\mathsf{U}(g')\mathsf{V}^{-1}) = \mathsf{V}\mathsf{U}(g)\mathsf{U}(g')\mathsf{V}^{-1} = \mathsf{V}\mathsf{U}(g'')\mathsf{V}^{-1}$, so the transformed matrices still form a representation of G. Representations that can be transformed into each other by application of a unitary transformation are termed **equivalent**.

The possibility of unitary transformation also enables us to consider whether a representation of G is **reducible**. An **irreducible** representation of G is defined as one that cannot be broken into a **direct sum** of representations of smaller dimension by application of the same unitary transformation to all members of the representation. What we mean by a direct sum of representations is that each matrix will be block diagonal (all with the same sequence of blocks). Since different blocks will not mix under matrix multiplication, corresponding blocks of the representation members will themselves define representations (see Fig. 17.4). If a representation named K is a direct sum of smaller representations K_1 and K_2, that fact can be indicated by the notation

$$K = K_1 \oplus K_2.$$

It is not always obvious whether a representation is reducible. We will shortly encounter theorems that provide (for discrete groups) ways of determining what irreducible representations are present in a representation that may be reducible. Moreover, if a group is **abelian**, then the fact that all its elements commute means that the matrices representing them can all be diagonalized simultaneously. From that fact we can conclude that all irreducible representations of abelian groups are 1×1.

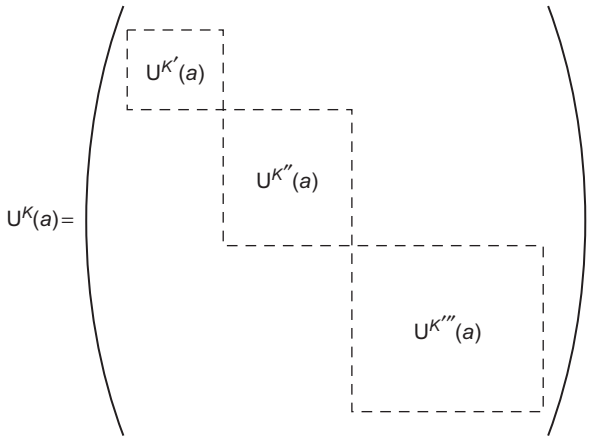

FIGURE 17.4 A member of a reducible representation in direct-sum form. All members will have the same block structure, so individual blocks define representations of smaller dimension.

It is important to understand that **reducibility** implies the **existence** of a unitary transformation that brings all members of a representation to the same block-diagonal form; a reducible representation may not exhibit the block-diagonal form if it has not been subjected to a suitable unitary transformation. Here is an example illustrating that point.

Example 17.2.2 A REDUCIBLE REPRESENTATION

Here is a reducible representation for our equilateral triangle:

$$\mathsf{U}(I)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\quad \mathsf{U}(C_3)=\begin{pmatrix}0&1&0\\0&0&1\\1&0&0\end{pmatrix},\quad \mathsf{U}(C_3^2)=\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix},$$

$$\mathsf{U}(C_2)=\begin{pmatrix}0&0&1\\0&1&0\\1&0&0\end{pmatrix},\quad \mathsf{U}(C_2')=\begin{pmatrix}1&0&0\\0&0&1\\0&1&0\end{pmatrix},\quad \mathsf{U}(C_2'')=\begin{pmatrix}0&1&0\\1&0&0\\0&0&1\end{pmatrix}. \tag{17.4}$$

Note that some of these matrices are not in any direct-sum form. To show that the representation of Eq. (17.4) is reducible, we transform all the U to $\mathsf{U}'=\mathsf{V}\mathsf{U}\mathsf{V}^{-1}$, using

$$\mathsf{V}=\begin{pmatrix}1/\sqrt{3}&1/\sqrt{3}&1/\sqrt{3}\\1/\sqrt{6}&-\sqrt{2/3}&1/\sqrt{6}\\1/\sqrt{2}&0&-1/\sqrt{2}\end{pmatrix},$$

which brings us to

$$\mathsf{U}'(I)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&1\end{pmatrix},\qquad \mathsf{U}'(C_3)=\begin{pmatrix}1&0&0\\0&-\frac{1}{2}&\frac{1}{2}\sqrt{3}\\0&-\frac{1}{2}\sqrt{3}&-\frac{1}{2}\end{pmatrix},$$

$$\mathsf{U}'(C_3^2)=\begin{pmatrix}1&0&0\\0&-\frac{1}{2}&-\frac{1}{2}\sqrt{3}\\0&\frac{1}{2}\sqrt{3}&-\frac{1}{2}\end{pmatrix},\quad \mathsf{U}'(C_2)=\begin{pmatrix}1&0&0\\0&1&0\\0&0&-1\end{pmatrix},$$

$$\mathsf{U}'(C_2')=\begin{pmatrix}1&0&0\\0&-\frac{1}{2}&\frac{1}{2}\sqrt{3}\\0&\frac{1}{2}\sqrt{3}&\frac{1}{2}\end{pmatrix},\qquad \mathsf{U}'(C_2'')=\begin{pmatrix}1&0&0\\0&-\frac{1}{2}&-\frac{1}{2}\sqrt{3}\\0&-\frac{1}{2}\sqrt{3}&\frac{1}{2}\end{pmatrix}. \tag{17.5}$$

All the matrices of this representation are block diagonal, and are direct sums that consist of an upper 1×1 block that is the trivial representation, all of whose elements are (1), and a lower 2×2 block that is exactly the 2×2 representation illustrated in Eq. (17.2). There exists no unitary transformation that will simultaneously reduce the 2×2 blocks of all members of the representation to direct sums of 1×1 blocks, so we have reduced the representation of Eq. (17.4) to its irreducible components.[2] ■

Example 17.2.3 Representations of a Continuous Group

Example 17.1.2 presented a continuous group of order 1 whose elements are rotations $R(\varphi)$ about the symmetry axis of a circular disk. These rotations were taken to be **defined** by the matrix equation presented as Eq. (17.1). The 2×2 matrix in that equation can also be viewed as a representation of $R(\varphi)$:

$$\mathsf{U}(\varphi)=\begin{pmatrix}\cos\varphi&\sin\varphi\\-\sin\varphi&\cos\varphi\end{pmatrix}.$$

Because this group is abelian (two successive rotations yield the same result if applied in either order), we know that this representation is reducible. If we apply the unitary transformation

$$\mathsf{U}'(\varphi)=\mathsf{V}\mathsf{U}(\varphi)\mathsf{V}^{-1},\qquad \text{with}\qquad \mathsf{V}=\begin{pmatrix}1/\sqrt{2}&-i/\sqrt{2}\\1/\sqrt{2}&i/\sqrt{2}\end{pmatrix},$$

the result is

$$\mathsf{U}'(\varphi)=\begin{pmatrix}\cos\varphi+i\sin\varphi&0\\0&\cos\varphi-i\sin\varphi\end{pmatrix}=\begin{pmatrix}e^{i\varphi}&0\\0&e^{-i\varphi}\end{pmatrix}. \tag{17.6}$$

[2] We know this because some of these 2×2 matrices do not commute with each other and therefore cannot be diagonalized simultaneously.

Equation (17.6) applies to every element of our rotation group after transforming with V, and we see that every rotation now has a diagonal representation. In other words, $\mathsf{U}(\varphi)$ has been transformed into a direct sum of two one-dimensional (1-D) representations, $\mathsf{U}' = \mathsf{U}_1 \oplus \mathsf{U}_{(-1)}$, with $\mathsf{U}_1(\varphi) = e^{i\varphi}$ and $\mathsf{U}_{(-1)}(\varphi) = e^{-i\varphi}$. In fact, these are only two of an infinite number of irreducible representations, all of dimension 1:

$$\mathsf{U}_n(\varphi) = e^{in\varphi},$$

where n can have any positive or negative integer value, including zero. The reason n is limited to integer values is to assure that $\mathsf{U}(2\pi) = \mathsf{U}(0)$. Note that only the n values ± 1 lead to faithful representations. ■

Exercises

17.2.1 For any representation K of a group, and for any group element a, show that

$$\left[\mathsf{U}^K(a)\right]^{-1} = \mathsf{U}^K(a^{-1}).$$

17.2.2 Show that these four matrices form a representation of the Vierergruppe, whose multiplication table is in Table 17.2.

$$\mathsf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \mathsf{A} = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathsf{B} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \mathsf{C} = \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}.$$

17.2.3 Show that the matrices $\mathsf{1}$, A, B, and C of Exercise 17.2.2 are reducible. Reduce them.

Note. This means transforming B and C to diagonal form (by the same unitary transformation).

17.2.4 (a) Once you have a matrix representation of any group, a 1-D representation can be obtained by taking the determinants of the matrices. Show that the multiplicative relations are preserved in this determinant representation.

(b) Use determinants to obtain a 1-D representation of D_3 from the 2×2 representation in Eq. (17.2).

17.2.5 Show that the cyclic group of n objects, C_n, may be represented by r^m, $m = 0, 1, 2, \ldots, n-1$. Here r is a generator given by

$$r = \exp(2\pi i s/n).$$

The parameter s takes on the values $s = 1, 2, 3, \ldots, n$, with each value of s yielding a different 1-D (irreducible) representation of C_n.

17.2.6 Develop the irreducible 2×2 matrix representation of the group of rotations (including those that turn it over) that transform a square into itself. Give the group multiplication table.

Note. This group has the name D_4 (see Fig. 17.5).

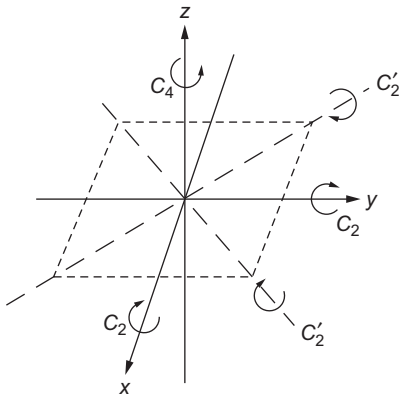

FIGURE 17.5 D_4 symmetry group.

17.3 SYMMETRY AND PHYSICS

Representations of groups provide a key connection between group theory and the symmetry properties of physical systems. Our discussion will be directed mainly at quantum systems, but much of it will also apply to systems that can be described using classical physics.

Consider a quantum system whose Hamiltonian H possesses certain geometric symmetries. If we write $H = T + V$, the symmetries will be those of the potential energy V, since the kinetic energy operator T is invariant with respect to rotations and displacements of the coordinate axes. A concrete example that illustrates the concept would be the determination of the wave function of an electron in the presence of nuclei in some fixed configuration possessing symmetry, such as the equilibrium locations of the nuclei in a symmetric molecule.

The symmetry of H corresponds to a requirement that H be invariant with respect to the application of any element of its symmetry group. Letting R denote such a symmetry element, the invariance of H means that if φ is a solution of the Schrödinger equation with energy E, then $R\varphi$ must also be a solution with the same energy eigenvalue:

$$H(R\varphi) = E(R\varphi).$$

By successively applying the elements of our symmetry group to φ, we can generate a set of eigenfunctions, all with the same eigenvalue. If φ happened to have the full symmetry of H, this set would contain only one member and the situation would be easy to understand. But if φ had less symmetry,[3] our eigenfunction set would have more than one member, with its maximum possible size being the number of elements in our symmetry group. When the eigenfunction set has more than one member, the eigenfunctions do not individually have the complete symmetry of the Hamiltonian, but they form a closed set that permits the partial symmetry to be expressed in all symmetry-equivalent ways. For example, the hydrogenic eigenfunctions known as p states form a three-membered set;

[3] This is possible; an example is a hydrogen-atom p state.

none has the full spherical symmetry of the hydrogen atom Hamiltonian, but linear combinations of the three p states can describe a p orbital at an arbitrary orientation (obvious because a vector in an arbitrary direction can be written as a linear combination of vectors in the coordinate directions).

So let's assume that, starting from some chosen φ, we have found a full set of symmetry-related eigenfunctions, have eliminated from them any linear dependence, and have formed an orthonormal eigenfunction set, denoted φ_i, $i = 1 \ldots N$.

Because of the way in which the φ_i were constructed, they will transform linearly among themselves if we apply to them any operation R from our symmetry group, so we may write

$$R\varphi_i = \sum_j U_{ji}(R)\varphi_j. \tag{17.7}$$

If we apply two symmetry operations (R followed by S), the transformation rule for the result will be

$$SR\varphi_i = \sum_{jk} U_{kj}(S)\, U_{ji}(R)\varphi_k. \tag{17.8}$$

Equations (17.7) and (17.8) show that the transformation for the group element SR is the matrix product of those for S and R, so the matrices $\mathsf{U}(S)$ and $\mathsf{U}(R)$ have properties that make them members of a representation of our symmetry group. What is new here is that we have identified U as a representation **associated with the basis** $\{\varphi_i\}$.

At this point we do not know whether the representation formed from our $\{\varphi_i\}$ basis is reducible; its reducibility depends on the quantum system under study and the particular choice made for the initial function φ. If our U are reducible, let's assume we now apply a transformation that will convert them into the direct-sum form. The transformation to obtain the direct-sum separation corresponds to a division of the basis into smaller sets of functions that transform only among themselves. Our overall conclusion from the above analysis is:

> *If a Hamiltonian H is fully symmetric under the operations of a symmetry group, all its eigenfunctions can be classified into sets, with each set forming a* **basis** *for an irreducible representation of the symmetry group. The members of a symmetry-related set of eigenfunctions will be degenerate and are referred to as a* **multiplet**. *Ordinarily different multiplets will correspond to different eigenvalues; any degeneracy between eigenfunctions of different irreducible representations arises from sources other than the symmetry under study.*

Because the eigenfunctions of a Hamiltonian possessing geometric symmetry can be identified with irreducible representations of its symmetry group, it is natural to use **approximate** eigenfunctions with similar symmetry restrictions.

Example 17.3.1 AN EVEN HAMILTONIAN

Consider a Hamiltonian $H(x)$, which is **even** in x, meaning that $H(-x) = H(x)$, but has no other symmetry. Letting $\boldsymbol{\sigma}$ stand for the reflection operator $x \to -x$ ($\boldsymbol{\sigma}$ is the usual

notation for a reflection operation), our symmetry group, called C_s, consists only of the two operations I and $\boldsymbol{\sigma}$, and its multiplication table is

$$I\,I = \boldsymbol{\sigma}\,\boldsymbol{\sigma} = I, \quad I\boldsymbol{\sigma} = \boldsymbol{\sigma}\,I = \boldsymbol{\sigma}.$$

This group is abelian, and has two irreducible representations of dimension 1: one (A_1) that is completely symmetric, $U(I) = U(\boldsymbol{\sigma}) = 1$, and one ($A_2$) with sign alternation, $U(I) = 1$, $U(\boldsymbol{\sigma}) = -1$. The eigenfunctions of H will therefore be even or odd, and there is no inherent symmetry requirement that even and odd states be degenerate with each other.

If we start with a function $\varphi(x)$ that is even, we will have $I\varphi = \boldsymbol{\sigma}\varphi = \varphi$, so our basis will consist only of φ, and $U(I) = U(\boldsymbol{\sigma}) = 1$, indicating that the representation constructed using this basis will be the fully symmetric A_1.

On the other hand, if our starting function $\varphi(x)$ was odd, then $I\varphi = \varphi$ but $\boldsymbol{\sigma}\varphi = -\varphi$; again our basis will consist only of $\varphi(x)$, but now the representation constructed from it will consist of $U(I) = 1$, $U(\boldsymbol{\sigma}) = -1$, and will be the alternating-sign representation A_2.

But if we start with a function $\varphi(x)$ that is neither even nor odd, then $I\varphi(x) = \varphi(x)$, but $\boldsymbol{\sigma}\varphi(x) = \varphi(-x)$. Our assumption that $\varphi(x)$ is neither even nor odd means that $\varphi(x)$ and $\varphi(-x)$ are linearly independent, so our basis will consist of two members (and therefore be of dimension 2). Since the symmetry group has only A_1 and A_2 as irreducible representations, the representation built from our two-membered basis will be reducible, and will reduce to $A_1 \oplus A_2$. The basis will separate into the two members $\varphi(x) + \varphi(-x)$ (a 1-D A_1 basis) and $\varphi(x) - \varphi(-x)$ (an A_2 basis).

Given a problem with an even Hamiltonian, one may use the above-identified symmetry analysis to seach for solutions that are restricted to have either even or odd symmetry. This strategy may greatly simplify the process of finding solutions. The notion can be extended to problems with different or greater degrees of symmetry. ■

It is important to note that all geometric symmetry groups (other than the trivial group, which has only the element I) will possess representations other than A_1, which means that they will have bases of less symmetry than the original group. In Example 17.3.1, our Hamiltonian was even, but could have eigenfunctions that are either even (A_1) or odd (A_2). A Hamiltonian with D_3 symmetry (which we have already seen has irreducible representations of dimensions 1 and 2) can have A_1 eigenfunctions of the full three-dimensional (3-D) symmetry or A_2 eigenfunctions with alternating-sign symmetry. It can also have sets of two degenerate eigenfunctions corresponding to the representation in Eq. (17.2), where (as indicated by the 2×2 matrices) the symmetry operations can convert either of the basis members into linear combinations of both. The irreducibility means that there exists no single function built from this two-member basis that will remain the same (except for a possible sign or phase factor) under all the group operations. The existence of an irreducible basis with more than one member is a consequence of the fact that the symmetry group is not abelian.

Although the elements of a symmetry group may not all commute with each other, they all commute with a Hamiltonian (or other operator) having the full group symmetry. To show this, note that for any eigenfunction ψ and any group element R,

$$H\psi = E\psi \longrightarrow H(R\psi) = E(R\psi) = R(E\psi) = RH\psi \longrightarrow HR = RH.$$

The last step follows because the previous steps are valid for all members of a complete set of eigenfunctions ψ.

Sometimes, especially for continuous groups, we will know in advance how to construct bases for irreducible representations. For example, the spherical harmonics of a given l value form a basis for representation of the 3-D rotation group. From Chapter 16, we know that these spherical harmonics form a closed set under rotation, but only if the set includes all m values. This information, together with the orthonormality of the Y_l^m, tells us that Y_l^m, $m = -l, \ldots, l$ is an orthonormal basis of dimension $2l+1$ for an irreducible representation of the 3-D rotation group, which is named $\mathsf{SO}(3)$. In contrast to the situation for discrete groups, continuous groups (even of low order) may possess an infinite number of finite-dimensional irreducible representations.

An experienced investigator can often find bases for irreducible representations by inspection or educated insight. However, if simple methods for finding a basis prove insufficient, general methods can be used to construct basis functions if the matrices defining the relevant irreducible representation are available. Details of the process can be found in the works by Falicov, Hamermesh, and Tinkham (see Additional Readings).

Example 17.3.2 QUANTUM MECHANICS, TRIANGULAR SYMMETRY

Let's consider a Hamiltonian that has the D_3 symmetry of an equilateral triangle that can be turned over, and our problem is such that its solution can be approximated as a wave function that is distributed over orbitals centered at the three vertices $\mathbf{R}_i$ of the triangle, of the form $\psi(\mathbf{r}) = a_1\varphi(r_1) + a_2\varphi(r_2) + a_3\varphi(r_3)$, where r_i is the distance $|\mathbf{r} - \mathbf{R}_i|$, and φ is a spherically symmetric orbital. The function

$$\psi_0 = \varphi(r_1) + \varphi(r_2) + \varphi(r_3)$$

is a basis for the trivial (A_1) representation of the D_3 group. But because we have three orbitals, there will be two other linear combinations of them that are linearly independent of ψ_0, and one way to choose them is

$$\psi_1 = \frac{1}{\sqrt{2}}\big[\varphi(r_1) - \varphi(r_3)\big], \quad \psi_2 = \frac{1}{\sqrt{6}}\big[-\varphi(r_1) + 2\varphi(r_2) - \varphi(r_3)\big].$$

Neither of these functions (nor any linear combination of them) has enough symmetry to be either A_1 or A_2 basis functions, and they therefore must (together) form a basis for a 2×2 irreducible representation of the D_3 symmetry group that is called E. Knowing that this would be the case, we chose these functions in a way that makes them orthogonal and at a consistent normalization, and they are in fact a basis for the irreducible representation given in Eq. (17.2).

We can check this by applying group operations to ψ_1 and ψ_2, verifying that the result corresponds to the appropriate column of the matrix for the operation. We make one such check here: Applying C_3 to ψ_1, we get $C_3\psi_1 = [\varphi(r_3) - \varphi(r_2)]/\sqrt{2}$, while the first column of $\mathsf{U}(C_3)$ in Eq. (17.2) yields

$$C_3\psi_1 = -\frac{1}{2}\,\psi_1 - \frac{\sqrt{3}}{2}\,\psi_2 = -\frac{1}{2}\left(\frac{\varphi(r_1) - \varphi(r_3)}{\sqrt{2}}\right) - \frac{\sqrt{3}}{2}\left(\frac{-\varphi(r_1) + 2\varphi(r_2) - \varphi(r_3)}{\sqrt{6}}\right).$$

The reader can verify that these two expressions for $C_3\psi_1$ are equal, and can make further checks if desired.

One might think that because of the triangular symmetry there would be an irreducible representation of dimension 3. But mathematics is not that simple; all D_3 representations of dimension 3 are reducible! ■

The symmetries required of solutions to Schrödinger equations have implications beyond their role in causing or explaining degeneracy. The dominant interaction between an electromagnetic field and a molecule can occur only if the molecule has an electric dipole moment, and the presence of a dipole moment depends on the symmetry of the electronic wave function. Another context in which symmetry is important is in the evaluation of the expectation values of quantum operators. These expectation values will vanish unless the integrals that define them have integrands with a fully symmetric part. In addition, it is worth mentioning that many quantum calculations are simplified by limiting them to contributions that do not vanish by reason of symmetry. All these issues can be framed in terms of the irreducible representations for which our wave functions are bases.

In the next sections, we develop some key results of group representation theory, first for discrete groups because the analysis is simpler, and then (in less detail) for continuous groups that have become important in particle theory and relativity.

Exercises

17.3.1 Consider a quantum mechanics problem with D_3 symmetry, with the threefold symmetry axis taken as the z direction, and with orbitals $\varphi(\mathbf{r} - \mathbf{R}_j)$ located at the vertices of an equilateral triangle. This is the same system geometry as in Example 17.3.2, but in the present problem φ will no longer be chosen to have spherical symmetry.

Given that $\varphi(\mathbf{r}) = (z/r)f(r)$ (so φ has the symmetry of a p orbital oriented along the symmetry axis), construct linear combinations of the φ that are bases for irreducible representations of D_3, for each basis indicating its representation.

17.4 DISCRETE GROUPS

Classes

It has been found useful to divide the elements of a finite group G into sets called **classes**. Starting from a group element a_1, one can apply similarity transformations of the form ga_1g^{-1}, where g can be any member of G. If we let a_1 be transformed in this way, using all the elements g of G, the result will be a set of elements that we can denote $a_1, \ldots, a_k$, where k may or may not be larger than 1. Certainly this set will include a_1 itself, as that result is obtained when $g = I$ and also when $g = a_1$ or $g = a_1^{-1}$. The set of elements obtained in this way is called a **class** of G, and can be identified by specifying one of its members. If we choose $a_1 = I$, we find that I is in a class all by itself; often classes will have larger numbers of members.

A class will have the same members no matter which of its elements is assigned the role of a_1. This is clear, since if $a_i = ga_1g^{-1}$ then also $a_1 = g^{-1}a_ig$, showing that we can get a_1 from any other element of the class, and therefrom all the elements reachable from a_1.

Example 17.4.1 CLASSES OF THE TRIANGULAR GROUP D_3

As observed already in general, one class of D_3 will consist solely of I. The class including C_3 contains also C_3^2 (the result of $C_2C_3C_2^{-1}$). Finally, C_2, C_2', and C_2'' constitute a third class. ■

Classes are important because:

- For a given representation (whether or not reducible), all matrices of the same class will have the same value of their trace—obvious because $\text{trace}(gag^{-1}) = \text{trace}(ag^{-1}g) = \text{trace}(a)$. In the group theory world, the trace is also known as the **character**, customarily identified with the symbol Γ.
- It can be shown that the number of inequivalent irreducible representations of a finite group is equal to its number of classes. (For proof and fuller discussion, see Additional Readings at the end of this chapter.)

It can be shown (again, see Additional Readings) that the set of characters for all elements and irreducible representations of a finite group defines an orthogonal finite-dimensional vector space. Writing $\Gamma^K(g)$ as the character of group element g in irreducible representation K, we have the key relations, for a group of order n:

$$n_g \sum_K \Gamma^K(g)\Gamma^K(g') = n\,\delta_{gg'}, \quad \sum_g \Gamma^K(g)\Gamma^{K'}(g) = n\,\delta_{KK'}. \tag{17.9}$$

Here n_g is the number of elements in the class containing g. These relations enable any reducible representation to be decomposed into a direct sum of irreducible representations, and can also be of aid in finding the characters of irreducible representations if they were not already known.

Another theorem of great importance in the theory of finite groups, sometimes called the **dimensionality theorem**, is that the sum of the squares of the dimensions n_K of the inequivalent irreducible representations is equal to the order, n, of the group:

$$\sum_K n_K^2 = n. \tag{17.10}$$

This theorem, together with the theorem that the number of irreducible K equals the number of classes, imposes stringent limits on the number and size of the irreducible representations of a group. These two requirements are often enough to determine completely the inventory of irreducible representations.

Since the finite groups of interest in physics have been well studied, the most frequent use of these orthogonality relations is to extract from a basis that may be reducible (i.e., a basis for a possibly reducible representation) the irreducible bases that may be included therein. This task is usually carried out with a table of irreducible representations at hand.

Example 17.4.2 ORTHOGONALITY RELATIONS, GROUP D_3

The usual scheme for tabulating discrete group characters is called a **character table**; that for our triangle group D_3 is shown in Table 17.3. The rows of the table are labeled with

Table 17.3 Character Table for Group D_3

	I	$2C_3$	$3C_2$
A_1	1	1	1
A_2	1	1	–1
E	2	–1	0
Ψ	3	0	1

Each row corresponds to an irreducible representation, and each column corresponds to a class. The table entry is the character for each element of that irreducible representation and class. The row below the boxed table (labeled Ψ) is not part of the table but is used in connection with Example 17.4.4.

the usual names assigned the irreducible representations: The labels A and B (the latter not used for this group) are reserved for 1×1 representations. Representations of dimension 2 are normally assigned a label E, and those of dimension 3 (also not occurring here) are called T. Each column of the character table is labeled with a typical member of the class, preceded by a number indicating the number of group elements in the class. This number is omitted if the class contains only one element.

Because the representation of group element I is a unit matrix, the characters (traces) in column I directly indicate the dimensions of the representations. We see that A_1 is a 1×1 representation, so each A_1 matrix contains a single number equal to the character shown, meaning that A_1 is the trivial totally symmetric representation. We see that A_2 is also 1×1, but the three group elements for which the triangle was turned over are now represented by -1. Finally, representation E is seen to be 2×2, and is the representation we found long ago in Eq. (17.2).

Checking the first orthogonality relation for $g = g' = I$, for which $n_g = 1$, we have $1(1^2 + 1^2 + 2^2) = 6$, as expected. For $g = I$, $g' = C_3$, we have $1[1(1) + 1(1) + 2(-1)] = 0$, and for $g = g' = C_3$, we note that $n_g = 2$ and we have $2[1^2 + 1^2 + (-1)^2] = 6$. The reader can check other cases of this orthogonality relation.

Moving to the second orthogonality relation, we take $K = K' = E$, finding $1(2^2) + 2(-1)^2 + 3(0^2) = 6$; the 1, 2, and 3 multiplying individual terms allow for the fact that the sum is over all **elements**, not just over **classes**. Other cases follow similarly. ■

Example 17.4.3 COUNTING IRREDUCIBLE REPRESENTATIONS

We consider two cases, first the group C_4, which was the subject of Example 17.1.4. This group is cyclic, with elements I, a, a^2, a^3; those are all the elements, because $a^4 = I$. As already indicated, a faithful representation of this group consists of 1, i, -1, $-i$, with the group operation being ordinary multiplication. Another realization of C_4 is an object that is symmetric under 90° rotation about a single axis. This group is abelian, as $a^p a^q = a^q a^p$. Then $gag^{-1} = a$ for any group elements a and g, so each element is in a class by itself. So we have four classes, and hence four irreducible representations. We also have, from the

dimension theorem,

$$\sum_{K=1}^{4} n_K^2 = 4.$$

The only way to satisfy this equation is to have four irreducible representations, each of dimension 1. This result should have been expected, since C_4 is abelian. Our irreducible representations can be built from the four following choices of $\mathsf{U}(a)$: $1, i, -1, -i$, leading to the following character table.

	I	a	a^2	a^3
A_1	1	1	1	1
A_2	1	i	-1	$-i$
A_3	1	-1	1	-1
A_4	1	$-i$	-1	i

Our second case is D_3, which has six elements and the three classes identified in Example 17.4.1. This means that it has three irreducible representations with dimensions whose squares add to six. The only set of dimensions satisfying this requirements is 1, 1, and 2. ■

Example 17.4.2 can be generalized to deal with reducible representations; any representation whose characters do not match any row of the character table must be reducible (unless just wrong!). If we were to transform a reducible representation to direct-sum form, it would then be obvious that its trace will be the sum of the traces of its blocks, and that property will hold even if we do not know how to make the block-diagonalizing transformation. In group-theory lingo we would say that the characters of a reducible representation will be the sum of the characters of the irreducible representations it contains. Note that if a given irreducible representation occurs more than once, its characters must be added a corresponding number of times.

Now suppose that we have a reducible representation Ψ of a group of order n. Even if we do not yet know its decomposition into irreducible components, we can write its characters for group elements g in the form

$$\Gamma^{\Psi}(g) = \sum_K c_K \Gamma^K(g), \tag{17.11}$$

where c_K is the number of times irreducible representation K is contained in Ψ. If we multiply both sides of this equation by $\Gamma^{K'}(g)$ and sum over g, the orthogonality kicks in, and

$$\sum_g \Gamma^{K'}(g)\Gamma^{\Psi}(g) = \sum_g \sum_K c_K \Gamma^{K'}(g)\Gamma^K(g) = n c_{K'}. \tag{17.12}$$

Evaluating the left-hand side of Eq. (17.12), we easily solve for $c_{K'}$. We can repeat this sequence of steps with different K' until all the irreducible representations in Ψ have been found.

Example 17.4.4 DECOMPOSING A REDUCIBLE REPRESENTATION

Suppose we start from the following set of three basis functions for the triangular group D_3[4]:

$$\psi_1 = x^2, \quad \psi_2 = y^2, \quad \psi_3 = \sqrt{2}\,xy, \tag{17.13}$$

where x, y, z are Cartesian coordinates with origin at the center of the triangle, and the axes are in the directions shown in Fig. 17.1. Since $C_3\,x = -\frac{1}{2}\,x + \frac{1}{2}\sqrt{3}\,y$, $C_3\,y = -\frac{1}{2}\sqrt{3}\,x - \frac{1}{2}\,y$, we can (somewhat tediously) determine that

$$C_3\,x^2 = \frac{1}{4}\,x^2 + \frac{3}{4}\,y^2 - \sqrt{\frac{3}{8}}(\sqrt{2}\,xy),$$

$$C_3\,y^2 = \frac{3}{4}\,x^2 + \frac{1}{4}\,y^2 + \sqrt{\frac{3}{8}}(\sqrt{2}\,xy),$$

$$C_3\,(\sqrt{2}\,xy) = \sqrt{\frac{3}{8}}\,x^2 - \sqrt{\frac{3}{8}}\,y^2 - \frac{1}{2}(\sqrt{2}\,xy),$$

so in the ψ basis,

$$\mathsf{U}^{\Psi}(C_3) = \begin{pmatrix} \frac{1}{4} & \frac{3}{4} & \sqrt{\frac{3}{8}} \\ \frac{3}{4} & \frac{1}{4} & -\sqrt{\frac{3}{8}} \\ -\sqrt{\frac{3}{8}} & \sqrt{\frac{3}{8}} & -\frac{1}{2} \end{pmatrix}. \tag{17.14}$$

Similar analysis can be used to obtain the matrix of C_2, which is easier because the operation involved is just $x \longrightarrow -x$, with y remaining unchanged. We get

$$\mathsf{U}^{\Psi}(C_2) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{17.15}$$

The representation of I is, of course, just the 3×3 unit matrix. Since the only data we need right now are the traces of one representative of each class, we are ready to proceed, and we see that

$$\Gamma^{\Psi}(I) = 3, \quad \Gamma^{\Psi}(C_3) = 0, \quad \Gamma^{\Psi}(C_2) = 1.$$

We are labeling the characters with superscript Ψ as a reminder that the representation is that associated with the ψ_i. These characters have been appended below their respective columns in Table 17.3.

Now we use the fact that the Ψ representation must decompose into

$$\Psi = c_1 A_1 \oplus c_2 A_2 \oplus c_3 E, \tag{17.16}$$

[4]These basis functions have been chosen in a way that makes the reducible representation unitary. The factor $\sqrt{2}$ in ψ_3 is needed to make all the ψ_i at the same scale.

and we find the c_i by applying Eq. (17.12). Using the data in Table 17.3, and taking K' to be in turn A_1, A_2, and E,

$$A_1 : (1)(3) + 2(1)(0) + 3(1)(1) = 6 = 6c_1, \text{ so } c_1 = 1,$$
$$A_2 : (1)(3) + 2(1)(0) + 3(-1)1) = 0 = 6c_2, \text{ so } c_2 = 0,$$
$$E : (2)(3) + 2(-1)(0) + 3(0)(1) = 6 = 6c_3, \text{ so } c_3 = 1.$$

Thus, $\Psi = A_1 \oplus E$. We can check our work by summing the A_1 and E entries from the character table. As they must, they add to give the entries for Ψ. ■

For some purposes it is insufficient just to know which irreducible representations are included in a reducible basis for a group G. We may also need to know how to transform the basis so that each basis member will be associated with a specific irreducible representation of G. Sometimes it is easy to see how to do this. For the above example, the basis function for A_1 must have the full group symmetry, while the E basis functions must be orthogonal to the A_1 basis. These considerations lead us to

$$A_1 : \varphi = \psi_1 + \psi_2 = x^2 + y^2, \tag{17.17}$$
$$E : \varphi_1 = \psi_1 - \psi_2 = x^2 - y^2, \quad \varphi_2 = \sqrt{2}\,\psi_3 = 2xy. \tag{17.18}$$

However, if finding the irreducible basis functions by inspection proves difficult, there are formulas that can be used to find them. See Additional Readings.

Other Discrete Groups

Most of the examples we have used have been for one group, D_3, in which we have considered symmetry operations that involve rotations about axes through the center of the system. Groups keeping a central point fixed are called **point groups**, and they arise, among other places, when studying phenomena that depend on the geometric symmetries of molecules. Some point groups have additional symmetries associated with inversion or reflection. It is possible for a point group to have a single n-fold axis for any positive integer n (meaning that a symmetry element is a rotation through an angle $2\pi/n$). However, the number of point groups having multiple symmetry axes with $n \geq 3$ is very limited; they correspond to the Platonic regular polyhedra, and therefore can only be tetrahedral, cubic/octahedral, and dodecahedral/icosahedral.

Other discrete groups arise when we consider permutational symmetry; the **symmetric group** is important in many-body physics and is the subject of a separate section of this chapter.

Exercises

17.4.1 The Vierergruppe has the multiplication table shown in Table 17.2.

(a) Divide its elements into classes.

(b) Using the class information, determine for the Vierergruppe its number of inequivalent irreducible representations and their dimensions.

(c) Construct a character table for the Vierergruppe.

17.4.2 The group D_3 may be discussed as a **permutation** group of three objects. Operation C_3, for instance, moves vertex 1 to the position formerly occupied by vertex 2; likewise vertex 2 moves to the original position of vertex 3 and vertex 3 moves to the original position of vertex 1. So this shuffling could be described as the permutation of (1,2,3) to (2,3,1). Using now letters a, b, c to avoid notational confusion, this permutation $(abc) \to (bca)$ corresponds to the matrix equation

$$C_3 \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} b \\ c \\ a \end{pmatrix},$$

thereby identifying a 3×3 representation of the operation C_3.

(a) Develop analogous 3×3 representations for the other elements of D_3.

(b) Reduce your 3×3 representation to the direct sum of a 1×1 and a 2×2 representation. *Note:* This 3×3 representation must be reducible or Eq. (17.10) would be violated.

17.4.3 The group named D_4 has a fourfold axis of symmetry, and twofold axes in four directions perpendicular to the fourfold axis. See Fig. 17.5. D_4 has the following classes (the numbers preceding the class descriptors indicate the number of elements in the class): $I, 2C_4, C_2, 2C_2', 2C_2''$. The twofold axes marked with primes are in the plane of fourfold symmetry.

(a) Find the number and dimensions of the irreducible representations.

(b) Given that all the characters of the representations of dimension 1 are ± 1 and that $C_2 = C_4^2$, use the orthogonality conditions to construct a complete character table for D_4.

17.4.4 The eight functions $\pm x^3$, $\pm x^2 y$, $\pm x y^2$, $\pm y^3$ form a reducible basis for D_4, with C_4 a 90° counterclockwise rotation in the xy plane, $C_2 = C_4^2$, $C_2' = (x \to -x, y \to y)$, $C_2'' = (x \to y, y \to x)$, and the remaining members of D_4 are additional members of the classes containing the above operations. Find the characters of the reducible representation for which these functions form a basis, and find the direct sum of irreducible representations of which it consists.

17.4.5 The group C_{4v} has a fourfold symmetry axis in the z direction, reflection symmetries (σ_v) about the xz and yz planes, and additional reflection symmetries (σ_d, d = dihedral) about planes that contain the z axis but are 45° from the x and y axes. See Fig. 17.6. The character table for C_{4v} follows.

	I	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
B_1	1	−1	1	1	−1
B_2	1	−1	1	−1	1
E	2	0	−2	0	0

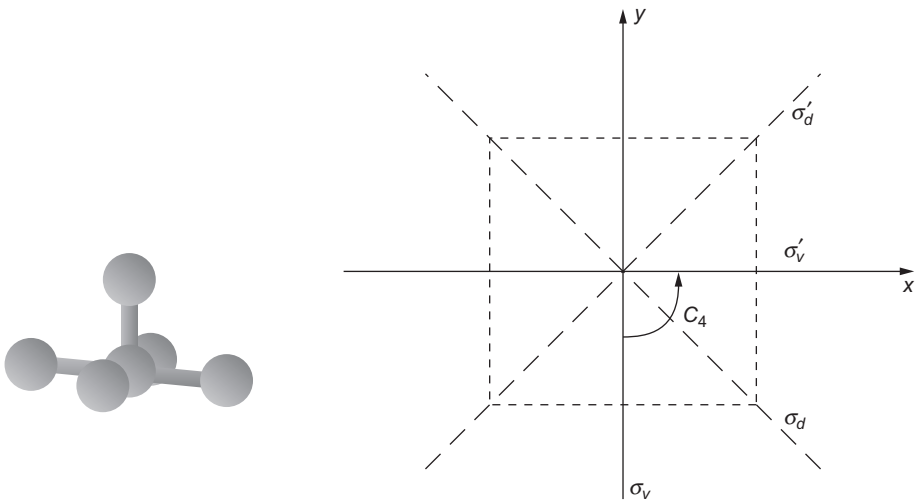

FIGURE 17.6 C_{4v} symmetry group. At left, a molecule with this symmetry. At right, a diagram identifying the reflection planes, which are perpendicular to the plane of the diagram.

(a) Construct the matrix representing one member of each class of C_{4v} using as a basis a p_z orbital at each of the points $(x, y) = (a, 0), (0, a), (-a, 0), (0, -a)$, and therefrom extract the characters of the reducible representation for which these p_z orbitals form a basis. A p_z orbital has functional form $(z/r)f(r)$.

(b) Determine the irreducible representations contained in our reducible p_z representation.

(c) Form those linear combinations of our p_z functions that are bases for each of the irreducible representations found in part (a).

17.4.6 Using the notation and geometry of Exercise 17.4.5, repeat that exercise for the eight-member basis consisting of a p_x and a p_y orbital at each of the points $(x, y) = (a, 0), (0, a), (-a, 0), (0, -a)$.

17.5 DIRECT PRODUCTS

Many multiparticle quantum-mechanical systems are described using wave functions that are products of individual-particle states. This approach is that of an independent-particle model, which at a higher degree of approximation can include interparticle interactions. The single-particle states can then be chosen to reflect the symmetry of the system, meaning that each one-particle state will be a basis member of some irreducible representation of the system's symmetry group. This idea is obvious, for example, in atomic structure, where we encounter notations such as $1s^2 2s^2 2p^3$ (the ground-state electron configuration of the N atom).

When a multiparticle system with symmetry group G is subjected to one of its symmetry operations, each single-particle factor in its wave function transforms according to its individual irreducible representation of G, so the overall wave function may contain products of arbitrary components of each particle's representation. Thus, the multiparticle basis consists of all the products that can be formed by taking one member of each single-particle basis. This is what is termed a **direct product**. This multiparticle basis will also constitute a representation of G. The notation

$$K = K_1 \otimes K_2$$

indicates that the representation K of G is the direct product of the representations K_1 and K_2. This means also that the representation matrix $\mathsf{U}^K(a)$ of any element a of G can be formed as the direct product (see Eq. 2.55) of the matrices $\mathsf{U}^{K_1}(a)$ and $\mathsf{U}^{K_2}(a)$.

The representation of a group G formed as a direct product of two (or more) of its irreducible representations may or may not be irreducible. For finite groups, a useful theorem is that the characters for a direct product of representations are, for each class, the product of the individual characters for that class. Once the characters for the direct product have been constructed, the methods of the previous section can be used to find the irreducible components of the product states.

Example 17.5.1 EVEN-ODD SYMMETRY

Sometimes the analysis of a direct product is simple. Consider a system of n independent particles subject to a potential whose only symmetry element (other than I) is inversion (denoted $\boldsymbol{i}$) through the origin of the coordinate system, so $V(-\mathbf{r}) = V(\mathbf{r})$. In this case, G (conventionally named C_i) has the two elements I and $\boldsymbol{i}$, with the following character table.

	I	$\boldsymbol{i}$
A_g	1	1
A_u	1	-1

Individual particles with A_1 wave functions, which remain unchanged under inversion, are conventionally labeled g (from the German word **gerade**). Particles with A_2 wave functions, which change sign on inversion, are labeled u, for **ungerade**. In fact, the usual notation for the character table of the C_i group writes A_g and A_u in place of A_1 and A_2, thereby conveying more information about the symmetries of the corresponding basis functions.

Now suppose that this system is in a state with j of the particles in u states and $n - j$ of the particles in g states. Intuitively, we know that if j is an odd number, the overall wave function will change sign on inversion, but will not change sign if j is even. Formally, we examine the direct product representation K:

$$K = u(1) \otimes u(2) \otimes \cdots \otimes u(j) \otimes g(j+1) \otimes \cdots \otimes g(n).$$

Using the theorem that the characters of representation K can be obtained by multiplying those of its constituent factors, we find $\Gamma^K(I) = 1$, $\Gamma^K(i) = (-1)^j$. Irrespective of the value of j, K will be irreducible: It is A_g if j is even, and A_u if j is odd. ■

Example 17.5.2 TWO QUANTUM PARTICLES IN D_3 SYMMETRY

This case is not as simple. Suppose both particles are in states of E symmetry, a situation spectroscopists would identify with the notation e^2; they use lower-case symbols to identify individual-particle states, reserving capital letters for the overall symmetry designation. For definiteness, let's further suppose[5] that each particle has a wave function of the form found in Eq. (17.18), so particle i will have the two-member basis

$$\varphi_a(i) = \left(x_i^2 - y_i^2\right), \quad \varphi_b(i) = 2x_i y_i,$$

and the product basis will therefore have the four members

$$\begin{aligned} \Phi_{aa} &= \varphi_a(1)\varphi_a(2), \quad \Phi_{ab} = \varphi_a(1)\varphi_b(2), \\ \Phi_{ba} &= \varphi_b(1)\varphi_a(2), \quad \Phi_{bb} = \varphi_b(1)\varphi_b(2). \end{aligned} \tag{17.19}$$

The matters at issue are (1) to find the overall symmetries this system can exhibit, and (2) to identify the basis functions for each symmetry.

Consulting Table 17.3, we compute the products for $e \otimes e$:

	I	$2C_3$	$3C_2$
$e \otimes e$:	4	1	0.

Since this representation has dimension 4 while the largest irreducible representation has dimension 2, it must be reducible. Applying the technique of Example 17.4.4, we can find that it decomposes into $e \otimes e = A_1 \oplus A_2 \oplus E$, a result that is easily checked by adding entries in the D_3 character table.

A set of basis functions corresponding to the decomposition into irreducible representations are

$$\psi^{A_1} = (x_1^2 - y_1^2)(x_2^2 - y_2^2) + 4x_1y_1x_2y_2, \tag{17.20}$$

$$\psi^{A_2} = 2\left[(x_1^2 - y_1^2)x_2y_2 - x_1y_1(x_2^2 - y_2^2)\right], \tag{17.21}$$

$$\begin{aligned} \psi_1^E &= (x_1^2 - y_1^2)(x_2^2 - y_2^2) - 4x_1x_1y_1x_2y_2, \\ \psi_2^E &= 2\left[(x_1^2 - y_1^2)x_2y_2 + x_1y_1(x_2^2 - y_2^2)\right]. \end{aligned} \tag{17.22}$$

Finding these could be challenging; verifying them is less so. ■

For continuous groups, it is usually simpler to decompose direct-product representations in other ways. For example, in Chapter 16 we used ladder operators to identify overall

[5] An actual problem will have a wave function that, in addition to the functional dependence shown here, will have a completely symmetric additional factor that is not relevant for the present group-theoretic discussion.

Table 17.4 Character Table, Group C_{4v}

	I	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
B_1	1	−1	1	1	−1
B_2	1	−1	1	−1	1
E	2	0	−2	0	0

angular-momentum states (irreducible representations) formed from products of individual angular momenta. The resulting multiplets correspond to the irreducible representations, and the angular momentum functions that we found are their bases.

Exercises

17.5.1 The group C_{4v} has eight elements, corresponding to the rotational and reflection symmetries of a square that **cannot** be turned over. See Fig. 17.6. Symmetry rotations about the z axis are denoted C_4, C_2, C_4'. Reflections relative to the xz and yz planes are named $\boldsymbol{\sigma}_v$ and $\boldsymbol{\sigma}_v'$; those at 45° relative to the xz and yz planes are called $\boldsymbol{\sigma}_d$ and $\boldsymbol{\sigma}_d'$ (d indicates "dihedral"). The character table for C_{4v} is in Table 17.4.

(a) Find the direct sum of irreducible representations of C_{4v} corresponding to the direct product $E \otimes E$.

(b) A basis for E (in the context of Fig. 17.5) consists of the two functions $\varphi_1 = x$, $\varphi_2 = y$. Apply a few of the group operations to this basis and verify the entries for E in the character table.

(c) Assume now that we have two sets of variables, x_1, y_1 and x_2, y_2, and we form the direct-product basis x_1x_2, x_1y_2, y_1x_2, y_1y_2. Determine how the direct-product basis functions can be combined to form bases for each of the irreducible representations in the direct sum corresponding to $E \otimes E$.

17.6 SYMMETRIC GROUP

The **symmetric group** $\mathbf{S}_n$ is the group of permutations of n distinguishable objects, and is therefore of order $n!$. To see this, note that to make a permutation, we may choose the first object in n different ways, then the second in $n-1$ ways, etc., until we reach the nth object, which can be chosen in only one way. The total number of possible permutations is therefore $n(n-1)\dots(1) = n!$. This group is important in the physics of identical-particle systems, whose wave functions must be either symmetric with respect to particle interchanges (particles with this symmetry are called **bosons**), or antisymmetric under pairwise particle interchanges (these particles are called **fermions**). This means that an n-boson wave function $\Psi_B(1, 2, \dots, n)$ must satisfy

$$P\Psi_B(1, \dots, n) = \Psi_B(1, \dots, n), \tag{17.23}$$

where P is any permutation of the particle numbers. From a group-theoretical viewpoint this means that Ψ_B is a sole basis function for the trivial A_1 representation of $\mathbf{S}_n$: 1×1, with all members of the representation equal to (1). Many-fermion wave functions $\Psi_F(1, \ldots, n)$ satisfy

$$P\Psi_F(1, \ldots, n) = \epsilon_P \Psi_F(1, \ldots, n), \tag{17.24}$$

where ϵ_P is the n-particle Levi-Civita symbol with an index string corresponding to P; in simple language this means $\epsilon_P = 1$ if P is an **even** permutation of the particle numbers (one requiring an even number of pairwise interchanges), and $\epsilon_P = -1$ if P is **odd**. This means that Ψ_F is the sole basis function for the 1×1 totally antisymmetric representation of $\mathbf{S}_n$ with members (ϵ_P), which we will call A_2.

Since the representations needed for either bosons or fermions are simple and of dimension 1×1, it might seem that sophisticated group-theoretic considerations would be unnecessary. But that is an oversimplification, because many-fermion systems (and some boson systems) consist of direct products of spatial and spin functions, and the spin functions may form a basis of $\mathbf{S}_n$ of dimension larger than one.

Example 17.6.1 TWO AND THREE IDENTICAL FERMIONS

In elementary quantum mechanics, the ground state of a two-fermion system such as the two electrons of the He atom can be treated using a simple wave function of the form

$$\Psi_F = \Big(f(1)g(2) + g(1)f(2)\Big)\Big(\alpha(1)\beta(2) - \beta(1)\alpha(2)\Big).$$

Here f and g are single-particle spatial functions, and α, β describe single-particle spin states. We continue, using a streamlined notation in which the particle numbers are suppressed, understanding that they always occur in ascending numerical order, so Ψ_F will henceforth be written $(fg + gf)(\alpha\beta - \beta\alpha)$. It is obvious that Ψ_F has the fermion (anti)symmetry; we note that it is an A_2 basis function, which is the product of a symmetric A_1 spatial function and an antisymmetric A_2 spin function. The physics of this problem demands that the overall ground-state wave function Ψ_F contain spin function $\alpha\beta - \beta\alpha$ because it is a two-particle spin eigenstate. The two-particle example shows that the A_2 overall representation was obtained as $A_1 \otimes A_2$.

For three particles, things are different. To treat the ground state of the Li atom, we cannot form a completely antisymmetric spin function using only the two single-particle spin functions α and β. The actual spin functions relevant for the ground state form a 2×2 representation of $\mathbf{S}_n$, which we will call E:

$$\theta_1 = \frac{1}{\sqrt{6}}(2\alpha\alpha\beta - \alpha\beta\alpha - \beta\alpha\alpha), \quad \theta_2 = \frac{1}{\sqrt{2}}(\beta\alpha\alpha - \alpha\beta\alpha). \tag{17.25}$$

Since permutations mix θ_1 and θ_2, the overall wave function for this three-particle system must be of the form

$$\Psi_F = \chi_1\theta_1 + \chi_2\theta_2,$$

where χ_1 and χ_2 are three-body spatial functions such that Ψ_F has the required A_2 symmetry. If the χ_i are built from spatial orbitals f, g, and h, one possible set of χ_i are

$$\begin{aligned}\chi_1 &= \frac{1}{2}(ghf - hfg - hgf + fhg),\\ \chi_2 &= \frac{1}{\sqrt{3}}\left(fgh + gfh - \frac{1}{2}ghf - \frac{1}{2}hfg - \frac{1}{2}hgf - \frac{1}{2}fhg\right),\end{aligned} \tag{17.26}$$

a result that it is difficult to find by trial and error. Since the spin functions, and therefore also the spatial functions, become more complicated as the system size increases, the value of a group-theoretic description clearly becomes more urgent. ■

We consider now, from a formal viewpoint, only the many-fermion case. As illustrated in Example 17.6.1, we deal with space-spin functions in which the spin function has, for reasons we will not discuss here, been chosen to be built from an irreducible representation K of the symmetric group, whose member for permutation P is a unitary matrix designated $\mathsf{U}^K(P)$, and whose basis is a set of spin functions θ_i, $i = 1, \ldots, n_K$, where n_K is the dimension of the spin representation. This means that

$$P\,\theta_i = \sum_{j=1}^{n_K} U_{ji}^K(P)\theta_j. \tag{17.27}$$

We shall now show that an antisymmetric overall space-spin function can result if we form

$$\Psi_F = \sum_{i=1}^{n_K} \chi_i\,\theta_i, \tag{17.28}$$

where the χ_i are basis functions for a representation K', of the same dimension as K, meaning that

$$P\,\chi_i = \sum_{k=1}^{n_K} U_{ki}^{K'}(P)\chi_k. \tag{17.29}$$

The representation K' is assumed to have members that satisfy

$$\mathsf{U}^{K'}(P) = \epsilon_P \mathsf{U}^K(P)^*. \tag{17.30}$$

The representation K' must exist, since it is (apart from a complex conjugate) the direct product of representations K and A_2. Because A_2 only imparts sign changes to various U^K, the representation K' will be irreducible because representation K is. The representation K' is termed **dual** to representation K.

To verify that the assumed form of Ψ_F has the required A_2 symmetry, we take it, as given in Eq. (17.28), and apply to it an arbitrary permutation P:

$$P\,\Psi_F = \sum_{i=1}^{n_K} (P\chi_i)\,(P\theta_i) = \sum_i \left(\sum_k U_{ki}^{K'}(P)\chi_k\right)\left(\sum_j U_{ji}^{K}(P)\theta_j\right)$$

$$= \sum_{jk}\left(\sum_i U_{ki}^{K'}(P)U_{ji}^{K}(P)\right)\chi_k\,\theta_j$$

$$= \sum_{jk}\left(\sum_i \epsilon_P U_{ki}^{K}(P)^* U_{ji}^{K}(P)\right)\chi_k\,\theta_j. \tag{17.31}$$

The steps taken in the processing of Eq. (17.31) are substitutions of Eqs. (17.27) and (17.29) for $P\chi_i$ and $P\theta_i$, followed by a conversion from $\mathsf{U}^{K'}$ to U^{K} through the use of Eq. (17.30). We complete our analysis by recognizing that because $\mathbf{U}$ is unitary, $U_{ki}(P)^* = (\mathsf{U}^{-1})_{ik}(P)$, so

$$\sum_i \epsilon_P U_{ki}^{K}(P)^* U_{ji}^{K}(P) = \epsilon_P \delta_{jk},$$

leading to the final result

$$P\Psi_F = \sum_{jk} \epsilon_P\,\delta_{jk}\chi_k\,\theta_j = \epsilon_P \sum_k \chi_k\,\theta_k = \epsilon_P \Psi_F. \tag{17.32}$$

Equation (17.32) shows that the overall wave function Ψ_F has the required fermion antisymmetry.

Our only remaining problem is to construct spatial functions χ_k, which are bases for representation K'. We state without proof (see Additional Readings) that this can be accomplished using the formula

$$\chi_i^{\,j} = \sum_P U_{ij}^{K'}(P)^* P\chi_0, \tag{17.33}$$

where χ_0 is a single spatial function whose permutations will be used to construct the χ_i. The index j identifies an entire set of χ_i; if χ_0 has no permutational symmetry, we can create sets of χ_i in $n_{K'}$ different ways, each corresponding to a different value of j.

Example 17.6.2 CONSTRUCTION OF MANY-BODY SPATIAL FUNCTIONS

We consider a three-electron problem in which the spin states are given by Eq. (17.25). We need the representation of $\mathbf{S}_3$ for which these θ_i are a basis. We are fortunate to already have this representation, as $\mathbf{S}_3$ is isomorphic (in 1–1 correspondence) with D_3, so we can use the set of 2×2 representation matrices given in Eq. (17.2), if we make the identification $C_2 \leftrightarrow P(12)$, $C_2' \leftrightarrow P(13)$, $C_2'' \leftrightarrow P(23)$, where $P(ij)$ denotes the permutation that interchanges the ith and jth items in the ordered list to which the permutation is applied. The permutation $P(123 \to 312)$ corresponds to C_3, and $P(123 \to 231)$ corresponds to C_3^2.

We now apply Eq. (17.33); an easy way to do this is to start by generating the matrix T that results from keeping all i and j. In the present case, that means forming the matrix sum

$$\mathsf{T} = \mathsf{U}(I)\chi_0 - \mathsf{U}(C_2)P(12)\chi_0 - \mathsf{U}(C_2')P(13)\chi_0 - \mathsf{U}(C_2'')P(23)\chi_0$$
$$+ \mathsf{U}(C_3)P(123 \to 312)\chi_0 + \mathsf{U}(C_3^2)P(123 \to 231)\chi_0.$$

The minus signs for the $\mathsf{U}(C_2)$ terms arise from the ϵ_P which is needed to convert U^K into $\mathsf{U}^{K'}$.

Taking χ_0 as the product $f(1)g(2)h(3)$, hereafter written fgh, and inserting numerical values for the U, we reach

$$\mathsf{T} = \begin{pmatrix} fgh - gfh - \frac{1}{2}(ghf & \frac{1}{2}\sqrt{3}(ghf - hfg \\ +hfg - hgf - fhg) & -hgf + fhg) \\ \frac{1}{2}\sqrt{3}(-ghf + hfg & fgh + gfh - \frac{1}{2}(ghf \\ -hgf + fhg) & +hfg + hgf + fhg) \end{pmatrix}. \tag{17.34}$$

Each column of Eq. (17.34) defines a set of χ_i, in a form that is not guaranteed to be normalized. From the second column, dividing through by $\sqrt{3}$ for normalization, we obtain the χ_i that were listed as a possible wave function in Example 17.6.1 at Eq. (17.26). The first column of Eq. (17.34) shows that there is a second possibility for an antisymmetric wave function built from the spatial product fgh, namely one that can be written

$$\Psi_F' = \chi_1'\theta_1 + \chi_2'\theta_2,$$

with the normalized spatial functions

$$\chi_1' = \frac{1}{\sqrt{3}}\left(fgh - gfh - \frac{1}{2}ghf - \frac{1}{2}hfg + \frac{1}{2}hgf + \frac{1}{2}fhg\right),$$
$$\chi_2' = \frac{1}{2}(-ghf + hfg - hgf + fhg).$$

■

Exercises

17.6.1 (a) The objects $(abcd)$ are permuted to $(dacb)$. Write out a 4×4 matrix representation of this one permutation.

Hint: Compare with Exercise 17.4.2.

(b) Is the permutation $(abdc) \to (dacb)$ odd or even?

(c) Is this permutation a possible member of the D_4 group, which was the subject of Exercise 17.4.3? Why or why not?

17.6.2 (a) The permutation group of four objects, S_4, has $4! = 24$ elements. Treating the four elements of the cyclic group, C_4, as permutations, set up a 4×4 matrix representation of C_4. Note that C_4 is a subgroup of P_4.

(b) How do you know that this 4×4 matrix representation of C_4 **must** be reducible?

17.6.3 The permutation group of four objects, S_4, has five classes.

(a) Determine the number of elements in each class of S_4 and identify one element of each class as a product of cycles.

(b) Two of the irreducible representations of S_4 are of dimension 1 (and are usually denoted A_1 and A_2). Noting that permutations can be classified as even or odd, find the characters of A_1 and A_2.

Hint. Set up a character table and fill in the A_1 and A_2 lines.

(c) One irreducible representation of S_4 (usually denoted E) is of dimension 2. Determine the dimensions of all the irreducible representations of S_4 other than A_1, A_2, and E.

(d) Complete the character table of S_4.

Hint. Only the even permutations have nonzero characters in the E representation.

17.7 CONTINUOUS GROUPS

Several continuous groups whose importance in physics was recognized long ago correspond to rotational symmetry in two- or three-dimensional space. Here the group elements are the rotations, the angles of which can vary continuously and thereby assume an infinite number of values. For rotations, the group multiplication rule corresponds to the application of successive rotations, which we have seen can be described by matrix multiplication. Rotations clearly form a group since they contain an identity element (no rotation), successive rotations are equivalent to a single rotation, and every rotation has an inverse (its reverse).

Rotations in two-dimensional (2-D) space can be described by 2×2 orthogonal matrices with determinant $+1$; the group consisting of these rotations is named $\mathsf{SO}(2)$ (SO stands for "special orthogonal"). If we also include reflections, so that the determinant can be ± 1, the group is named $\mathsf{O}(2)$. Since a 2-D rotation is completely specified by a single angle, $\mathsf{SO}(2)$ is a one-parameter group. A matrix representation of $\mathsf{SO}(2)$ was introduced in Eq. (17.1); the group parameter is the rotation angle φ.

Rotations in 3-D space are described by 3×3 orthogonal matrices. The resulting groups are designated $\mathsf{O}(3)$ and $\mathsf{SO}(3)$; for $\mathsf{SO}(3)$, three angles (e.g., the Euler angles) are group parameters. Generalizing to $n \times n$ matrices, the groups are named $\mathsf{O}(n)$ and $\mathsf{SO}(n)$; the number of parameters needed to specify fully an $n \times n$ real orthogonal matrix is $n(n-1)/2$, and that is the number of independent parameters (generalizations of the Euler angles) needed in $\mathsf{SO}(n)$. If we further generalize to unitary matrices, we have the groups $\mathsf{SU}(n)$ and $\mathsf{U}(n)$. Proof that these sets of unitary matrices form groups is left as an exercise.

Let's introduce some nomenclature. The $n \times n$ matrices referred to above can be thought of as the defining, or **fundamental**, representations of the groups involved. The **order** of a continuous group is defined as the number of independent parameters needed to specify its fundamental representation, so the order of $\mathsf{SO}(\mathrm{n})$ is the previously stated $n(n-1)/2$; the order of the group $\mathsf{SU}(n)$ is $n^2 - 1$.

In addition to their use for the treatment of rotational symmetry, continuous groups are also relevant to the classification of elementary (and not so elementary) particles. It has been experimentally observed that regularities in the masses and charges of sets of particles

can be explained if their wave functions are identified as basis members of an irreducible representation of an appropriate group. Note that now the group does not describe rotations in ordinary space, but refers to a more abstract space relevant to an understanding of the physics involved. The earliest example of this idea was **electron spin**; spin wave functions are objects in an abstract SU(2) space, together with rules to unravel their observational properties. A further abstraction began with the notion that the proton and neutron might form a basis for an abstract SU(2) representation, and has since blossomed with the introduction of SU(3) and other continuous groups into particle physics. A brief survey of these ideas is presented in our specific discussion of SU(3).

Lie Groups and Their Generators

It is extremely useful to manage groups such as SO(n) or SU(n) in ways that do not explicitly involve an infinite number of elements; a formalism for doing so was devised by the Norwegian mathematician Sophus Lie. Groups for which Lie's analysis is applicable, called Lie groups, have elements that depend continuously on parameters that vary over closed intervals (meaning that the parameter set includes the limit of any converging sequence of parameters). The groups SO(n) and SU(n) are Lie groups.

Lie's essential idea was to describe a group in terms of its **generators**, a minimal set of quantities that could be used in a specific way (multiplied by parameters) to produce any element of the group. Our starting point is, for each parameter φ controlling a group operation, to introduce a generator S with the property that when φ is infinitesimal (and therefore written $\delta\varphi$) the group element with parameter $\delta\varphi$ (which must be close to the identity element of the group) can be represented by

$$\mathsf{U}(\delta\varphi) = \mathbf{1} + i\,\delta\varphi\,\mathsf{S}. \tag{17.35}$$

The factor i in Eq. (17.35) could have been included in S but it is more convenient not to do so. Group operations corresponding to larger values of φ can now be generated from repeated operation (N times) by φ/N, where φ/N is small. We therefore identify U(φ) as the limit

$$\mathsf{U}(\varphi) = \lim_{N\to\infty}\left(1 + \frac{i\,\varphi\,\mathsf{S}}{N}\right)^N;$$

This large-N limit defines the exponential, so we have the general result

$$\mathsf{U}(\varphi) = \exp(i\varphi\,\mathsf{S}). \tag{17.36}$$

Given any representation U of our continuous group, we can find the generator S corresponding to the parameter φ for that representation by differentiation of Eq. (17.36), evaluated at the identity element of our group. In particular,

$$-i\left[\frac{d\mathsf{U}(\varphi)}{d\varphi}\right]_{\varphi=0} = \mathsf{S}, \tag{17.37}$$

revealing that the entire behavior of a representation U can be deduced from its behavior in an infinitesimal parameter-space neighborhood of the identity operation. However, to obtain complete knowledge of the structure of a Lie group we need to study the behavior

of its generators for a representation that is **faithful**; for that purpose it is desirable to use the fundamental representation.

Example 17.7.1 SO(2) Generator

SO(2) involves rotational symmetry about a single axis, and its operations are counterclockwise rotations of the coordinate axes through angles φ. Working with the 2×2 fundamental representation of SO(2), an infinitesimal rotation $\delta\varphi$ causes (to first order) $(x', y') = (x + y\,\delta\varphi, y - x\,\delta\varphi)$, or

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} 1 & \delta\varphi \\ -\delta\varphi & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \left[\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \delta\varphi \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \right] \begin{pmatrix} x \\ y \end{pmatrix} = \mathbf{1} + i\,\delta\varphi \mathsf{S},$$

with

$$i\mathsf{S} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \text{or} \quad \mathsf{S} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \boldsymbol{\sigma}_2, \tag{17.38}$$

where $\boldsymbol{\sigma}_2$ is a Pauli matrix. A general rotation is then represented by Eq. (17.36) as

$$\mathsf{U}(\varphi) = e^{i\varphi\mathsf{S}} = \mathbf{1}_2 \cos\varphi + i\boldsymbol{\sigma}_2 \sin\varphi = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix}, \tag{17.39}$$

where we have evaluated the exponential of the matrix in Eq. (17.39) using the Euler identity, Eq. (2.80). This equation can be recognized as the transformation law for a 2-D coordinate rotation, Eq. (3.23), verifying that the generator formalism works as expected.

If we had started from the final expression for $\mathsf{U}(\varphi)$ given in Eq. (17.39), we could have generated S from it by applying the differentiation formula, Eq. (17.37). ■

The generator form, Eq. (17.36), has some nice features:

1. For the groups SO(n) and SU(n), any U will be unitary (remember, "orthogonal" is a special case of "unitary"). This means that

$$\mathsf{U}^{-1} = \exp(-i\varphi\mathsf{S}) = U^\dagger = \exp(-i\varphi\mathsf{S}^\dagger), \tag{17.40}$$

   so $\mathsf{S} = \mathsf{S}^\dagger$, showing that S is Hermitian. That is the proximate reason for inclusion of i in the defining equation for S.
2. Because for both SO(n) and SU(n), $\det(\mathsf{U}) = 1$, we also have, invoking the trace formula, Eq. (2.84),

$$\det(\mathsf{U}) = \exp\big(\operatorname{trace}(\ln \mathsf{U})\big) = \exp\big(i\varphi \operatorname{trace}(\mathsf{S})\big) = 1. \tag{17.41}$$

   This condition is satisfied for general φ only if $\operatorname{trace}(\mathsf{S}) = 0$. So S is not only Hermitian, but traceless.
3. It can be shown (but is not proved here) that the number of independent generators of a Lie group is equal to the order of the group.

One of Lie's key observations was that by focusing on infinitesimal group elements, various properties of the generators could be deduced. We have already seen that if the form of U in terms of its parameters is known, the generators S can be obtained by differentiation of Eq. (17.36) in the limit corresponding to the identity group element.

Second, relations between the generators can be developed, as follows: Let us consider two operations $\mathsf{U}_j(\epsilon_j)$ and $\mathsf{U}_k(\epsilon_k)$ of a group G, that respectively correspond to the generators S_j and S_k. The values of ϵ_j and ϵ_k are assumed small, so the resulting U_j and U_k differ, but only slightly, from the identity element. Expanding the exponentials and keeping terms through second order in ϵ,

$$\mathsf{U}_j = \exp(i\epsilon_j \mathsf{S}_j) = 1 + i\epsilon_j \mathsf{S}_j - \frac{1}{2}\epsilon_j^2 \mathsf{S}_j^2 + \cdots,$$

$$\mathsf{U}_k = \exp(i\epsilon_k \mathsf{S}_k) = 1 + i\epsilon_k \mathsf{S}_k - \frac{1}{2}\epsilon_k^2 \mathsf{S}_k^2 + \cdots,$$

we evaluate the leading term (in ϵ) of the matrix product $\mathsf{U}_k^{-1}\mathsf{U}_j^{-1}\mathsf{U}_k\mathsf{U}_j$. The linear terms all cancel, as do several of the quadratic terms. The remaining quadratic terms can be grouped so as to reach the result

$$\begin{aligned}\mathsf{U}_k^{-1}\mathsf{U}_j^{-1}\mathsf{U}_k\mathsf{U}_j &= 1 + \epsilon_j\epsilon_k[\mathsf{S}_j, \mathsf{S}_k] + \cdots \\ &= 1 + i\epsilon_j\epsilon_k \sum_l f_{jkl}\mathsf{S}_l + \cdots. \end{aligned} \tag{17.42}$$

The last line of Eq. (17.42) reflects the fact that the left-hand side of the equation must correspond to some group element, and that element must, to first order in the generators, be of the form shown. Note that the premultipliers $i\epsilon_j\epsilon_k$ are not a form restriction, as their presence simply changes the value of f_{jkl}.

Comparing the two lines of Eq. (17.42), we obtain the important **closure** relation among the generators of the group G:

$$[\mathsf{S}_j, \mathsf{S}_k] = i \sum_l f_{jkl}\mathsf{S}_l. \tag{17.43}$$

The coefficients f_{jkl} are called the **structure constants** of G. It can be shown that f_{jkl} is antisymmetric with respect to index permutations, so $f_{jkl} = f_{klj} = f_{ljk} = -f_{kjl} = -f_{lkj} = -f_{jlkj}$. The structure constants provide a representation-independent characterization of a Lie group, but as already mentioned, to determine them we will need to work with a faithful representation, such as the group's fundamental representation. We will shortly do so for the groups we study in detail.

As is obvious from the foregoing analysis, Lie group generators will not in general commute. In 3-D, rotations about different axes do not commute, and therefore their generators cannot commute either. An additional indicator for group classification is the maximum number of independent generators that all mutually commute. This number is called the **rank** of the group; it is significant because the generators can be subjected to unitary transformations without changing the ultimate group structure, and the mutually commuting generators can therefore be brought simultaneously to diagonal form. Once this is done, the basis members of the generator set can be labeled using the diagonal elements (the

eigenvalues) of the commuting generators. The values of the labels (and the physical phenomena related thereto) depend on the representation in use.

For the orthogonal groups $\mathsf{SO}(n)$ and unitary groups $\mathsf{SU}(n)$ the commutation relations, Eq. (17.43), can be developed along the lines of angular momentum, leading to generalized ladder operators (and selection rules) in conjunction with the mutually commuting operators. For these central aspects of (the so-called classical) Lie groups we refer to the work by Greiner and Mueller (see Additional Readings).

Summarizing, the rank of a group indicates the number of indices needed to label the basis. In applications to quantum mechanics, these indices are often referred to as quantum numbers. For example, in $\mathsf{SO}(3)$, which is of rank 1, the index is usually taken to be M_L, usually identified physically as the z component of an angular momentum; when $\mathsf{SU}(2)$, also of rank 1, is used for the description of electron spin, the index is usually called M_S. The possible values of M_L or M_S depend on the representation, and we saw in Chapter 16 that the values range, in unit steps, between $+L$ and $-L$ (or $+S$ and $-S$), so that diagrams identifying these basis members can be plotted on a line. In contrast, we will see that $\mathsf{SU}(3)$ is of rank 2, so its basis members are labeled with two quantum numbers. Diagrams identifying the label assignments will in that case need to be 2-D.

It is also possible to label entire representations. One way to label them is to use the eigenvalues of operators that commute with all the generators of the group; such operators are called **Casimir operators**; the number of independent Casimir operators is equal to the rank of the group. $\mathsf{SO}(3)$ has therefore one Casimir operator; it is the operator usually known in angular-momentum applications as L^2 or J^2.

Groups $\mathsf{SO}(2)$ and $\mathsf{SO}(3)$

$\mathsf{SO}(2)$ and $\mathsf{SO}(3)$ are rotation groups; $\mathsf{SO}(2)$ corresponds to rotational symmetry about one axis, which we will take to be the z axis when the symmetry is for a 3-D system. $\mathsf{SO}(2)$ will therefore have only one generator, that already found in Eq. (17.38):

$$\mathsf{S}_z = \boldsymbol{\sigma}_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \tag{17.44}$$

To use S_z as one of the generators of $\mathsf{SO}(3)$, we extend to a 3×3 basis, calling the generator S_3, obtaining

$$\mathsf{S}_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \tag{17.45}$$

$\mathsf{SO}(3)$ has two other generators, S_1 and S_2. To obtain S_1, the generator corresponding to

$$\mathsf{U}_x(\psi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\psi & \sin\psi \\ 0 & -\sin\psi & \cos\psi \end{pmatrix}, \tag{17.46}$$

we apply Eq. (17.37):

$$\mathsf{S}_1 = -i\left[\frac{dR_x(\phi)}{d\psi}\right]_{\psi=0} = -i\begin{pmatrix} 0 & 0 & 0 \\ 0 & -\sin\psi & \cos\psi \\ 0 & -\cos\psi & -\sin\psi \end{pmatrix}_{\psi=0} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}. \tag{17.47}$$

In a similar fashion, starting from

$$\mathsf{U}_y(\theta) = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix}, \tag{17.48}$$

we find

$$\mathsf{S}_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}. \tag{17.49}$$

Summarizing, the structure of $\mathsf{SO}(2)$ is trivial, as it has only a single generator, and has order 1 and rank 1. However, the structure of $\mathsf{SO}(3)$ is not entirely trivial. Because no two of S_1, S_2, and S_3 commute, $\mathsf{SO}(3)$ will have order 3, but rank 1. By matrix multiplication, we may compute its structure constants. It is easily verified that

$$[\mathsf{S}_j, \mathsf{S}_k] = i\epsilon_{jkl}\mathsf{S}_l, \tag{17.50}$$

where ϵ_{jkl} is a Levi-Civita symbol. Thus, the Levi-Civita symbols are the structure constants for $\mathsf{SO}(3)$. Note also that the S_j obey the angular momentum commutation rules. In fact, these are the same matrices that were called K_i in Eq. (16.86) in Chapter 16, and they were identified there as matrices describing the components of angular momentum in a basis consisting of x, y, and z. This observation can be generalized to reach the conclusion that for any representation of $\mathsf{SO}(3)$, the generators can be taken to be the angular momentum components L_j $(j = 1, 2, 3)$ as expressed in any basis for that representation.

Example 17.7.2 GENERATORS DEPEND ON BASIS

To show that the generators indeed have a form that depends on the choice of basis, consider a basis for $\mathsf{SO}(3)$ proportional to the spherical harmonics for $l = 1$ with standard phases,

$$\psi_1 = -\frac{1}{\sqrt{2}}(x + iy), \quad \psi_2 = z, \quad \psi_3 = \frac{1}{\sqrt{2}}(x - iy). \tag{17.51}$$

We now apply $L_x = -i[y\partial/\partial z - z\partial/\partial y]$ to the basis members, getting the result $L_x\psi_1 = z/\sqrt{2} = \psi_2/\sqrt{2}$, $L_x\psi_2 = -iy = (\psi_1 + \psi_3)/\sqrt{2}$, $L_x\psi_3 = z/\sqrt{2} = \psi_2/\sqrt{2}$, meaning that the matrix representation of L_x, and therefore of a generator we will call S_x, is

$$\mathsf{S}_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}. \tag{17.52}$$

Applying L_y and L_z to the spherical harmonic basis, we obtain generators S_y and S_z:

$$\mathsf{S}_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \mathsf{S}_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \tag{17.53}$$

These generators, though different from those given in Eqs. (17.45), (17.47), and (17.49), are equivalent to them in the sense that they define the same irreducible representation of SO_3. ■

Group SU(2) and SU(2)–SO(3) Homomorphism

A complete set of generators for the fundamental representation of $\mathsf{SU}(2)$ must span the space of traceless 2×2 Hermitian matrices; since there is only one off-diagonal element above the diagonal that can have an arbitrary complex value, it can, if nonzero, be assigned in two linearly independent ways (such as 1 and $-i$). The below-diagonal element is then completely determined by Hermiticity. There is only one independent way to assign the diagonal elements, as there are two and they must be real and sum to zero. Thus, a simple set of matrices satisfying the necessary conditions consists of the three Pauli matrices $\boldsymbol{\sigma}_j$, $j = 1, 2, 3$. Noting also that there would be advantages to having the generators scaled so that they would satisfy the angular momentum commutation relations, we choose the definition

$$\mathsf{S}_j = \frac{1}{2}\boldsymbol{\sigma}_j, \quad j = 1, 2, 3. \tag{17.54}$$

Then, based on our many previous encounters or by performing the matrix multiplications, we can confirm

$$[\mathsf{S}_j, \mathsf{S}_k] = i\epsilon_{jkl}\mathsf{S}_l. \tag{17.55}$$

In addition, for rotation parameters denoted as α_j in connection with generators S_j, we have, calling the corresponding $\mathsf{SU}(2)$ members U_j,

$$\mathsf{U}_j(\alpha_j) = \exp(i\alpha_j\boldsymbol{\sigma}_j/2), \quad j = 1, 2, 3. \tag{17.56}$$

Invoking the Euler identity, Eq. (2.80), we can rewrite Eq. (17.56) as

$$\mathsf{U}_j(\alpha_j) = 1_2 \cos\left(\frac{\alpha_j}{2}\right) + i\boldsymbol{\sigma}_j \sin\left(\frac{\alpha_j}{2}\right). \tag{17.57}$$

The group $\mathsf{SU}(2)$ was first recognized as relevant for physics when it was observed that spin states of the electron form a basis for its fundamental representation. We already know, from Chapter 16, that orbital angular momentum multiplets come in sets with odd numbers of members ($2L + 1$, with L integral). But we also observed that abstract quantities that obey the angular momentum commutation rules with half-integer L values come in multiplets with even numbers of members. The multiplet with two members is the fundamental basis for the group $\mathsf{SU}(2)$. These basis functions are conventionally written $|\uparrow\rangle$ and $|\downarrow\rangle$, (or just α and β), and in matrix notation are

$$|\uparrow\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\downarrow\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{17.58}$$

Since the structure constants for SU(2) show that its generators satisfy the angular momentum commutation rules, we may conclude that all angular momentum multiplets define representations of SU(2); in Chapter 16 we found that the multiplets of odd dimension ($2L+1$ with L integral) can be chosen to be the spherical harmonics of angular momentum L and are therefore also a basis for a representation of SO(3). Angular momentum multiplets of even dimension do not have a 3-D spatial representation and cannot correspond to a representation of SO(3). They are the more abstract quantities we call spinors, have half-integer angular-momentum quantum numbers, and are bases only for representations of SU(2).

Further understanding of the situation can be obtained by applying $\mathsf{U}_x(\varphi)$, a synonym for $\mathsf{U}_1(\varphi)$, to the spin function $|\uparrow\rangle$. Taking $\varphi=\pi$, this corresponds to a 180° rotation about the x axis, which we might expect would convert $|\uparrow\rangle$ into $|\downarrow\rangle$. Applying Eq. (17.57), which for the current case assumes the form $\mathsf{U}_x = i\boldsymbol{\sigma}_1$, we have

$$\mathsf{U}_x|\uparrow\rangle = i\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = i\begin{pmatrix}0\\1\end{pmatrix} = i|\downarrow\rangle\,. \tag{17.59}$$

So far, so good. But let's now try a similar rotation with $\varphi=2\pi$. We then have $\mathsf{U}_x=-1_2$, meaning that a complete 360° rotation does not restore $|\uparrow\rangle$, but gives instead $-|\uparrow\rangle$, namely the expected state, but with a change of sign. To recover $|\uparrow\rangle$ with its original (+) sign would require a rotation $\varphi=4\pi$, i.e., two revolutions. Each rotation between $\varphi=2\pi$ and $\varphi=4\pi$ is, with opposite sign, equivalent to one in the $(0,2\pi)$ range.

We now see the essential difference between SU(2) and SO(3): The angular range of the rotation parameters in SU(2) is twice that in SO(3), so each SO(3) element is generated twice in each dimension (with different signs) in SU(2). Thus the correspondence between the two groups is not one-to-one (an isomorphism), but is two-to-one, a homomorphism. The existence of this homomorphism is not important for irreducible representations of odd dimension (corresponding to integer L or, in more general contexts, J), since then $\mathsf{U}(2\pi)=\mathsf{U}(0)$ and the range $(2\pi,4\pi)$ simply duplicates $(0,2\pi)$. But the homomorphism remains important for even-dimension representations of SU(2), which correspond to half-integer J and are not representations of SO(3). However, the fact that all representations of SO(3) are also representations of SU(2) means that we can form within SU(2) direct products that include representations of both even and odd dimension. This observation validates our analysis of states with both orbital and spin angular momentum.

In summary, we observe that half-integer angular momentum basis functions, which in earlier discussion we have already labeled as **spinors**, not only are objects that cannot be represented as functions in ordinary 3-D space, but are also objects whose rotational properties are unusual in that their angular periodicity is 4π, not the value 2π that would ordinarily be expected. They are thus somewhat abstract quantities whose relevance to physics rests on their ability to explain the "spin" properties of electrons and other fermions.

Group SU(3)

Starting in the 1930s, physicists began to give considerable attention to the symmetries of **baryons**, particles that, as the prefix "bary" implies, are heavy in comparison to electrons, and that interact subject to a force called the **strong interaction**. The earliest conjecture,

by Heisenberg, was to the effect that the approximate charge independence of the nuclear forces involving protons and neutrons suggested that they could be viewed as different quantum states of the same particle (called the **nucleon**), with the nucleon having a symmetry appropriate to the existence of a doublet of states. The nucleon was postulated to have the same symmetry as electron spin, namely that of the continuous group SU(2). Although the nucleon symmetry has nothing to do with spin, it is referred to as **isospin**, with the isospin symmetry described by the matrices $\boldsymbol{\tau}_i$, $i = 1, 2, 3$ (equal to the corresponding Pauli spin matrices $\boldsymbol{\sigma}_i$), and the isospin states can be classified by the eigenvalue of τ_3 (designated I_3), with $I_3 = +1/2$ corresponding to the proton, $I_3 = -1/2$ corresponding to the neutron.

By the early 1960s, a large number of additional baryons with strong interactions had been identified, of which eight (proton, neutron, and six others) were rather similar in mass. The masses of the baryons discussed in this section are listed in Table 17.5.

In 1961, Gell-Mann, and independently Ne'eman, suggested that these eight baryons might be symmetry-related, and proposed that they be identified with an irreducible representation of the group SU(3), with the relatively small mass differences attributed to forces weaker than the strong interaction and with different symmetry. The states describing these eight particles would be a basis for the generators of an SU_3 representation of dimension 8. Subsequently, it was proposed that all eight of these particles were actually formed from combinations of three smaller, and presumably more fundamental, particles called **quarks**, and the three types of quarks initially postulated, given the names **up** (u), **down** (d), and **strange** (s), were ultimately identified as forming a basis for the generators of SU(3). This original insight then led to the identification of a set of mesons involved with strong interaction as species consisting of one quark and one antiquark, thereby also corresponding to basis members of representations of SU(3).

The situation described in the preceding paragraph can be more fully understood by proceeding to a somewhat detailed discussion of the group SU(3). This group is defined by its generators, of which there are eight. The maximum number that commute with each other is two, so the group is of order $3^2 - 1 = 8$ and rank 2. The simplest useful way to specify the

Table 17.5 Baryon Octet

	Mass	Y	I_3	
Ξ :	Ξ^-	1321.32	-1	$-\frac{1}{2}$
	Ξ^0	1314.9	-1	$+\frac{1}{2}$
Σ :	Σ^-	1197.43	0	-1
	Σ^0	1192.55	0	0
	Σ^+	1189.37	0	$+1$
Λ :	Λ	1115.63	0	0
N :	n	939.566	1	$-\frac{1}{2}$
	p	938.272	1	$+\frac{1}{2}$

Masses are given as rest-mass energies, in MeV (1 MeV = 10^6 eV).

generators is to write them as 3×3 matrices in the SU(3) fundamental representation. Like other continuous groups, SU(3) has an infinite number of other irreducible representations of various sizes, but the key properties of the generators (specifically, their commutation rules) will be the same as those of the fundamental representation. We accordingly write the eight SU(3) generators in terms of zero-trace Hermitian matrices $\boldsymbol{\lambda}_1$ through $\boldsymbol{\lambda}_8$, with

$$\mathsf{S}_i = \frac{1}{2}\boldsymbol{\lambda}_i, \tag{17.60}$$

where the $\boldsymbol{\lambda}_i$, known as the **Gell-Mann matrices**, are

$$\begin{aligned}
\boldsymbol{\lambda}_1 &= \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \qquad \boldsymbol{\lambda}_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \\
\boldsymbol{\lambda}_3 &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{\lambda}_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \\
\boldsymbol{\lambda}_5 &= \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix}, \quad \boldsymbol{\lambda}_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \\
\boldsymbol{\lambda}_7 &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \boldsymbol{\lambda}_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.
\end{aligned} \tag{17.61}$$

In our use of SU(3), we will associate the rows and columns of this representation (in order) to the quarks u, d, and s. Note that $\boldsymbol{\lambda}_1$, $\boldsymbol{\lambda}_2$, and $\boldsymbol{\lambda}_3$ are block diagonal with the upper block being the SU(2) isospin matrices, signaling the presence of an SU(2) subgroup with generators $\boldsymbol{\lambda}_1/2$, $\boldsymbol{\lambda}_2/2$, and $\boldsymbol{\lambda}_3/2$. If we combine $\boldsymbol{\lambda}_3$ and $\boldsymbol{\lambda}_8$ so as to choose the generators in different ways, we can replace $\boldsymbol{\lambda}_3$ with one of the following:

$$\boldsymbol{\lambda}_3' = \sqrt{3}\,\boldsymbol{\lambda}_8 - \boldsymbol{\lambda}_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{17.62}$$

$$\boldsymbol{\lambda}_3'' = \sqrt{3}\,\boldsymbol{\lambda}_8 + \boldsymbol{\lambda}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{17.63}$$

indicating the existence of another SU(2) subgroup with generators $\mathsf{S}_1' = \boldsymbol{\lambda}_6/2$, $\mathsf{S}_2' = \boldsymbol{\lambda}_7/2$, $\mathsf{S}_3' = \boldsymbol{\lambda}_3'/2$, and a third SU(2) subgroup, with generators $\mathsf{S}_1'' = \boldsymbol{\lambda}_4/2$, $\mathsf{S}_2'' = \boldsymbol{\lambda}_5/2$, $\mathsf{S}_3'' = \boldsymbol{\lambda}_3''/2$. These observations support the notion that isospin multiplets can exist within an SU(3) basis.

Because SU(3) is of rank 2, the members of its representations can be labeled according to the eigenvalues of two commuting generators, in contrast to the single label, S_z or I_z, that we employed to label SU(2) members. It is customary to use for this purpose the two generators ($\boldsymbol{\lambda}_3$ and $\boldsymbol{\lambda}_8$) already in diagonal form. Continuing with the notation introduced for the nucleon, the eigenvalue of the SU(3) generator S_3 is identified as I_3, while S_8 is used to construct the identifier Y (known as **hypercharge**), defined as the eigenvalue of $2\mathsf{S}_8/\sqrt{3}$. An oft-used alternative to Y is the **strangeness** $S \equiv Y - 1$.

Example 17.7.3 QUANTUM NUMBERS OF QUARKS

From

$$\mathsf{S}_3 = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

we can read out the quark I_3 values $+\frac{1}{2}$ for u, $-\frac{1}{2}$ for d, and 0 for s. From

$$2\mathsf{S}_8/\sqrt{3} = \boldsymbol{\lambda}_8/\sqrt{3} = \frac{1}{3}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix},$$

we find the Y values $\frac{1}{3}$ for u and d, and $-\frac{2}{3}$ for s. ■

From the definitions of the S_i in Eq. (17.60), one can readily carry out the matrix operations needed to establish their commutation rules. Note that even though the commutation rules will be obtained by examining the specific representation introduced in Eq. (17.60), they apply to all representations of the SU(3) generators.

We will use the commutation rules in a ladder-operator approach to the analysis of the symmetry properties of the three-quark multiplets. It is helpful to systematize the work by temporarily renaming S_1, S_2 as I_1, I_2; S_6, S_7 as U_1, U_2; and S_4, S_5 as V_1, V_2. Then we introduce

$$\begin{aligned} \mathsf{I}_+ &= \mathsf{I}_1 + i\mathsf{I}_2, \qquad \mathsf{I}_- = \mathsf{I}_1 - i\mathsf{I}_2, \\ \mathsf{U}_+ &= \mathsf{U}_1 + i\mathsf{U}_2, \quad \mathsf{U}_- = \mathsf{U}_1 - i\mathsf{U}_2, \\ \mathsf{V}_+ &= \mathsf{V}_1 + i\mathsf{V}_2, \quad \mathsf{V}_- = \mathsf{V}_1 - i\mathsf{V}_2, \end{aligned} \tag{17.64}$$

and write some relevant commutators as

$$\begin{aligned} &[\mathsf{S}_3, \mathsf{I}_\pm] = \pm\mathsf{I}_\pm, \quad [\mathsf{S}_3, \mathsf{U}_\pm] = \mp\frac{1}{2}\mathsf{U}_\pm, \qquad [\mathsf{S}_3, \mathsf{V}_\pm] = \pm\frac{1}{2}\mathsf{V}_\pm, \\ &[\mathsf{S}_8, \mathsf{I}_\pm] = 0, \qquad [\mathsf{S}_8, \mathsf{U}_\pm] = \pm\frac{1}{2}\sqrt{3}\,\mathsf{U}_\pm, \quad [\mathsf{S}_8, \mathsf{V}_\pm] = \pm\frac{1}{2}\sqrt{3}\,\mathsf{V}_\pm. \end{aligned} \tag{17.65}$$

Using the logic of ladder operators (described in detail for applications to angular momentum operators in Section 16.1), the above commutators can be used to show that, starting from a basis function $\psi(I_3, Y)$, we can apply $\mathsf{I}_\pm$, $\mathsf{U}_\pm$, or $\mathsf{V}_\pm$ to obtain basis functions with other label sets. For example,

$$[\mathsf{S}_8, \mathsf{U}_+]\psi(I_3, Y) = \mathsf{S}_8\mathsf{U}_+\psi(I_3, Y) - \mathsf{U}_+\mathsf{S}_8\psi(I_3, Y) = \frac{1}{2}\sqrt{3}\,\mathsf{U}_+\psi(I_3, Y).$$

Replacing $\mathsf{S}_8\psi(I_3, Y)$ by $\frac{1}{2}\sqrt{3}\,Y\psi(I_3, Y)$, this equation can be rearranged to

$$\mathsf{S}_8\Big(\mathsf{U}_+\psi(I_3, Y)\Big) = \frac{1}{2}\sqrt{3}\,(Y+1)\Big(\mathsf{U}_+\psi(I_3, Y)\Big),$$

which shows that if it does not vanish, $\mathsf{U}_+\psi(I_3, Y)$ is an eigenvector of S_8 with an eigenvalue corresponding to an increase of one unit in Y. Similarly, from the relation $[\mathsf{S}_3, \mathsf{U}_+]\psi(I_3, Y) = -\frac{1}{2}\mathsf{U}_+\psi(I_3, Y)$, we find that $\mathsf{U}_+\psi(I_3, Y)$, if nonvanishing, is an

eigenvector of S_3 with an eigenvalue less by 1/2 than that of $\psi(I_3, Y)$. These observations correspond to the equation $\mathsf{U}_+\psi(I_3, Y) = C\psi(I_3 - \frac{1}{2}, Y + 1)$. This and other ladder identities are summarized in the following equations:

$$\begin{aligned} \mathsf{I}_\pm\psi(I_3, Y) &= C_I\ \psi(I_3 \pm 1, Y), \\ \mathsf{U}_\pm\psi(I_3, Y) &= C_U\ \psi(I_3 \mp \frac{1}{2}, Y \pm 1), \\ \mathsf{V}_\pm\psi(I_3, Y) &= C_V\ \psi(I_3 \pm \frac{1}{2}, Y \pm 1). \end{aligned} \tag{17.66}$$

The constants C will depend on the representation under study and on the values of I_3 and Y; if the result of an operation according to any of these equations leads to an (I_3, Y) set that is not part of the representation's basis, the C associated with that equation will vanish and the ladder construction will terminate.

It is important to stress that the operators in Eq. (17.66) only move **within** the representation under study, so if we start with a basis member of an irreducible representation, all the functions we will be able to reach will also be members of the same representation.

Example 17.7.4 QUARK LADDERS

As a preliminary to our study of baryon and meson symmetries, let's see how the ladder operators work, with the quarks, symbolically $\psi(I_3, Y)$, represented by

$$u = \psi\left(\frac{1}{2}, \frac{1}{3}\right) = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad d = \psi\left(-\frac{1}{2}, \frac{1}{3}\right) = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad s = \psi\left(0, -\frac{2}{3}\right) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

As explained in Example 17.7.3, the values of I_3 and Y are obtained from the diagonal elements (the eigenvalues) of S_3 and S_8. The 3×3 matrices representing the ladder operators in this example are

$$\begin{aligned} \mathsf{I}_+ &= \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathsf{U}_+ = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathsf{V}_+ = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}, \\ \mathsf{I}_- &= \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad \mathsf{U}_- = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \quad \mathsf{V}_- = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \end{aligned} \tag{17.67}$$

By straightforward matrix multiplication, we find $\mathsf{I}_-u = d$, $\mathsf{I}_+d = u$, $\mathsf{U}_-d = s$, $\mathsf{U}_+s = d$, $\mathsf{V}_-u = s$, $\mathsf{V}_+s = u$; all other operations yield vanishing results. These relationships can be represented in the 2-D graph shown as Fig. 17.7 with Y in the vertical direction and I_3 horizontal. The arrows in the graph are labeled to indicate the results of application of the ladder operators. ■

Continuing now to the baryons, we consider representations appropriate to three quarks, which we can form as the direct product of three single-quark representations. Using the notation **3** as shorthand for the fundamental representation (which is of dimension 3), the

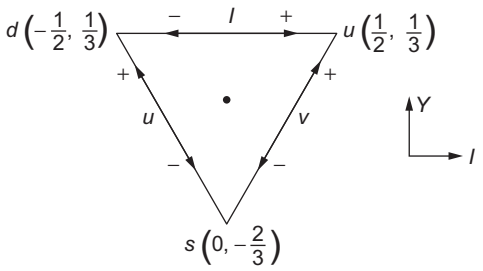

FIGURE 17.7 Conversions between u, d, and s quarks by application of ladder operators $I_\pm$, $U_\pm$, and $V_\pm$. The coordinates of each particle are its (I, Y).

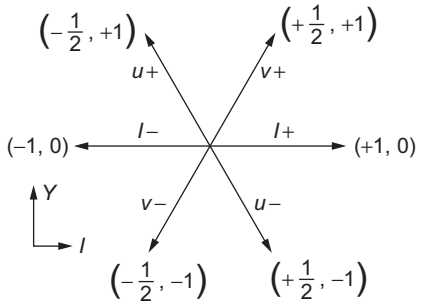

FIGURE 17.8 Root diagram of SU(3). Each operator is labeled by the changes it causes: $(\Delta I, \Delta Y)$.

direct product we need is $\mathbf{3}\otimes\mathbf{3}\otimes\mathbf{3}$. This direct product is a reducible representation, which decomposes into the direct sum

$$\mathbf{3}\otimes\mathbf{3}\otimes\mathbf{3} = \mathbf{10}\oplus\mathbf{8}\oplus\mathbf{8}\oplus\mathbf{1}, \tag{17.68}$$

where **10**, **8**, and **1** refer to irreducible representations of the indicated dimensions.

A standard way to decompose product representations such as we have here uses diagrams known as Young tableaux. Because development of the rules for construction and use of Young tableaux would take us beyond the scope of this text, we pursue here an alternate route that uses the ladder operators of Eq. (17.66). Use of the ladder operators also has the advantage that it yields explicit expressions for the I_3, Y eigenfunctions. Since the direction in which ladder operators connect states in an I_3, Y diagram is general, we can draw a picture that summarizes their properties. Such a picture is called a **root diagram**; that for SU(3) is shown in Fig. 17.8.

Example 17.7.5 GENERATORS FOR DIRECT PRODUCTS

If we apply an operation R depending on a parameter φ to a product of basis functions for different particles, each function will transform according to its representation, which we

presently assume to be the fundamental representation:

$$\begin{aligned} R\Big(\psi_i(1)\psi_j(2)\Big) &= \Big(\mathsf{U}(R)\psi_i(1)\Big)\Big(\mathsf{U}(R)\psi_j(2)\Big) \\ &= \Big(e^{i\varphi\mathsf{S}(1)}\psi_i(1)\Big)\Big(e^{i\varphi\mathsf{S}(2)}\psi_j(2)\Big) \\ &= e^{i\varphi[\mathsf{S}(1)+\mathsf{S}(2)]}\psi_i(1)\psi_j(2), \end{aligned}$$

where the notation is supposed to indicate that $\mathsf{S}(1)$ acts only on particle 1 and $\mathsf{S}(2)$ acts only on particle 2 (this can be arranged by an appropriate definition of the direct-product matrices and the operators to which they correspond). The important point here is that because generators appear in an exponent, a **product** of single-particle operations can be obtained using a **sum** of single-particle generators. This observation is a generalization of our earlier writing of resultant multiparticle angular momenta as sums of individual contributions, and enables us to write, for three-quark products, expressions such as

$$\mathsf{I}_\pm = \mathsf{I}_\pm(1) + \mathsf{I}_\pm(2) + \mathsf{I}_\pm(3);$$

so, for example (dropping the proportionality constant C_I),

$$\mathsf{I}_- u(1)u(2)u(3) = d(1)u(2)u(3) + u(1)d(2)u(3) + u(1)u(2)d(3).$$

Suppressing the explicit particle numbers, this can be shortened to $\mathsf{I}_- uuu = duu + udu + uud$. Corresponding results apply to all the other ladder operators and to all three-quark products, and to the application of the diagonal generators, such as

$$\begin{aligned} \mathsf{S}_3\, u(1)u(2)u(3) &= \Big(\mathsf{S}_3(1)u(1)\Big)u(2)u(3) + u(1)\Big(\mathsf{S}_3(2)u(2)\Big)u(3) \\ &\quad + u(1)u(2)\Big(\mathsf{S}_3(3)u(3)\Big) = \frac{3}{2}\,u(1)u(2)u(3), \end{aligned}$$

or $\mathsf{S}_3\, uuu = \frac{3}{2}\,uuu$, equivalent to assigning $I_3 = \frac{3}{2}$ to uuu. Similar analysis can yield results such as $I_3 = \frac{1}{2}$ for uud, or $(2\mathsf{S}_8/\sqrt{3})dss = -dss$, showing that dss has $Y = -1$. ■

We are now ready to return to the verification of Eq. (17.68).

Example 17.7.6 Decomposition of Baryon Multiplets

There are 27 three-quark products, which, using the analysis of Example 17.7.5, have the (I_3, Y) values shown here.

$\left(+\frac{3}{2}, 1\right)$	uuu	$(0, 0)$	$uds, dus, usd, dsu, sud, sdu$
$\left(+\frac{1}{2}, 1\right)$	uud, udu, duu	$(-1, 0)$	dds, dsd, sdd
$\left(-\frac{1}{2}, 1\right)$	udd, dud, ddu	$\left(+\frac{1}{2}, -1\right)$	uss, sus, ssu
$\left(-\frac{3}{2}, 1\right)$	ddd	$\left(-\frac{1}{2}, -1\right)$	dss, sds, ssd
$(+1, 0)$	uus, usu, suu	$(0, -2)$	sss

We can find the irreducible representations in our direct product in a relatively mechanical way. We start by placing the 27 quark products at their coordinate positions in an I_3, Y diagram. We note that the point $(\frac{3}{2}, 1)$ is occupied by only one product, uuu, so it must, by itself, be a member of some irreducible representation of SU_3. Starting there, we may take steps in any of the directions indicated in the root diagram, providing there is a function at each point to which we move. Since all we are doing is identifying possible states, we need not make any sophisticated computations as we proceed. Since uuu is completely symmetric under permutations, the basis function at each point will be a symmetric sum of the products at each point reached. When we have reached all the points, we will have identified a total of 10 basis functions, all members of the same irreducible representation, the one we called **10**. This set of 10 basis functions is called a **decuplet**. The graph for these basis functions, called a **weight diagram**, is shown in Fig. 17.9.

At the points where there was more than one quark product, there will be products left over after accounting for **10**; if we want to be quantitative, they will be linear combinations that are orthogonal to the symmetric forms used in **10**. Continuing with either of the two leftover functions at $(\frac{1}{2}, 1)$, we may construct another set of basis functions from the leftovers; these sets will contain eight members, with the weight diagram shown in Fig. 17.10. (There are only seven points still occupied in the diagram, but the one at (0,0) yields two different functions when approached from different directions; the function obtained when (0,0) is reached horizontally can, via a subgroup analysis, be related to the members of its representation at $(\pm 1, 0)$. These points are elaborated in Exercise 17.7.4.) After accounting for these two **octets**, corresponding to representations **8**, there will be one completely antisymmetric function left at (0,0); it is a basis for **1**. ■

Both the representations **8** and **10** are relevant for particle physics. The rationalization of the similar-mass baryon octet was based on assignment of those particles to members of **8**, with the small mass differences associated with the breaking of the strong-interaction symmetry by a weaker force which retained some of the $\mathsf{SU}(2)$ subgroup symmetries, and by the (weaker still) electromagnetic forces that also broke the $\mathsf{SU}(2)$ symmetries. The identification of the octet members with the basis functions of **8** is included in Fig. 17.10, and the energetics of the overall situation is indicated schematically in Fig. 17.11.

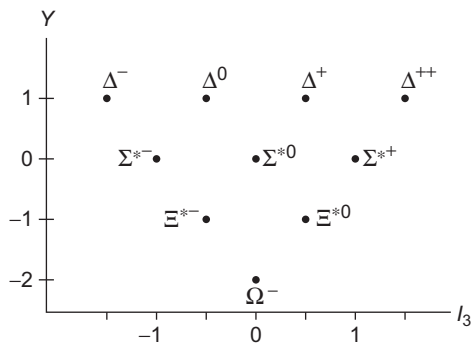

FIGURE 17.9 Weight diagram, baryon decuplet. The symbols at the various points are the names of particles assigned to the basis.

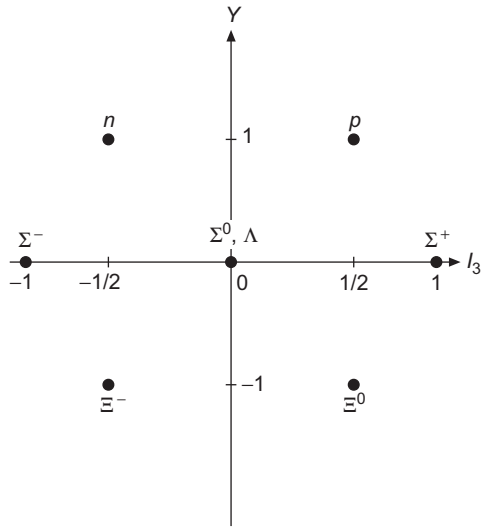

FIGURE 17.10 Weight diagram, baryon octet.

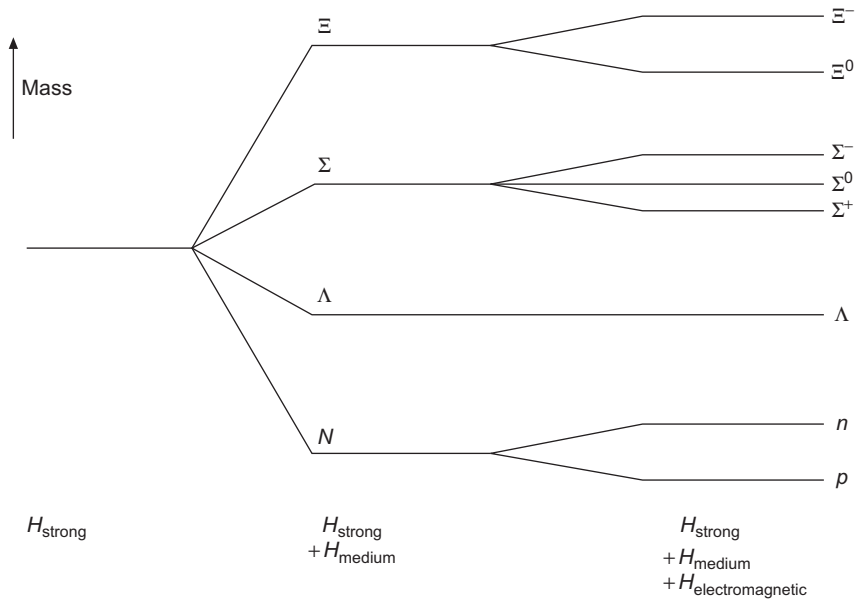

FIGURE 17.11 Baryon mass splitting.

The representation **10** provides an explanation for the set of 10 excited-state baryons whose weight diagram is shown in Fig. 17.9. When Gell-Mann fitted the then existent data to the decuplet representation, the Ω^- particle had not yet been discovered, and its prediction and subsequent detection provided a strong indication of the relevance of SU(3)

to physics. Yet another instance of the importance of SU(3) is provided by the existence of a meson octet (displaced by one unit in Y relative to the primary baryon octet).

Finally, we caution the reader that the foregoing discussion is by no means complete. It does not take full account of fermion antisymmetry requirements, the consideration of which led to the SU(3)-color gauge theory of the strong interaction called quantum chromodynamics (QCD). QCD also, at a minimum, involves the group SU(3). We have also left much unsaid about subgroup decompositions of the overall symmetry group, qualitatively alluded to in the discussion supporting Fig. 17.9.

To keep group theory and its very real value in proper perspective, we should emphasize that group theory identifies and formalizes symmetries. It classifies (and sometimes predicts) particles. But apart from saying, e.g., that one part of the Hamiltonian has SU(2) symmetry and another part has SU(3) symmetry, group theory says nothing about the particle interaction. Likewise, a spherically symmetric Hamiltonian has (in ordinary space) SO(3) symmetry, but this fact tells us nothing about the radial dependence of either the potential or the wave function.

Exercises

17.7.1 Determine three SU(2) subgroups of SU(3).

17.7.2 Prove that the matrices U(n) (unitary matrices of order n) form a group, and that SU(n) (those with determinant unity) form a subgroup of U(n).

17.7.3 Using Eq. (17.56) for the matrix elements of SU(2) corresponding to rotations about the coordinate axes, find the matrix corresponding to a rotation defined by Euler angles (α, β, γ). The Euler angles are defined in Section 3.4.

17.7.4 For a product of three quarks, the member of SU(3) representation **10** with $(I_3, Y) = (+\frac{3}{2}, 1)$ is uuu.

(a) Apply operators in the root diagram for SU(3), Fig. 17.8, to obtain all the remaining members of the decuplet comprising the representation **10**.

(b) The two representations **8** can be chosen to have for $I_3 = \frac{1}{2}$, $Y = 1$ the respective members $\psi_1\left(\frac{1}{2}, 1\right) = (ud - du)u$ and $\psi_2\left(\frac{1}{2}, 1\right) = 2uud - udu - duu$. Briefly explain why this choice is possible.

(c) Using the operators in the root diagram and the above $\psi_1\left(\frac{1}{2}, 1\right)$, find expressions for $\psi_1\left(-\frac{1}{2}, 1\right)$, $\psi_1(-1, 0)$, $\psi_1(1, 0)$, $\psi_1\left(-\frac{1}{2}, -1\right)$, and $\psi_1\left(\frac{1}{2}, -1\right)$.

(d) Taking each of the six ψ_1 functions you now have, apply an operator that will convert it into $\psi_1(0, 0)$. Show that you obtain exactly two linearly independent $\psi_1(0, 0)$, thereby justifying the claim that the ψ_1 are an octet at the points shown in Fig. 17.10.

(e) Show that the octet built starting from $\psi_2(\frac{1}{2}, 1)$ is linearly independent from that built from ψ_1.

(f) Find the wave function $\psi(0, 0)$ that is linearly independent of all the $\psi(0, 0)$ functions found in parts (a)–(e). It is the sole member of the representation **1**.

17.8 LORENTZ GROUP

It has long been accepted that the laws of physics should be **covariant**, meaning that they should have forms that are (1) independent of the origin of the coordinates used to describe them (leading from an isolated system to the law of conservation of linear momentum); (2) independent of the orientation of our coordinates (leading to a conservation law for angular momentum); and (3) independent of the zero from which time is measured. Most of our experience suggests that velocities should add like ordinary vectors; for example, a person walking toward the front of a moving train would, as viewed by a stationary observer, have a net velocity equal to the sum of that of the train and the walker's velocity relative to the train. This rule for velocity addition is identified as **Galilean**, and is correct in the limit of small velocities. However, it is now known that transformations between coordinate systems with a constant nonzero relative velocity must lead to a non-intuitive velocity addition law that causes the velocity of light to be the same as measured by observers in all coordinate systems (reference frames). As Einstein showed in 1905, the necessary velocity addition law could be obtained if coordinate-system changes were described by **Lorentz transformations**. Einstein's theory, now known as **special relativity** (its extension to curved space-time to describe gravitation is called **general relativity**), also helped to complete an understanding of the way in which electric and magnetic phenomena become interconverted when charges at rest in one coordinate system are viewed as moving in another.

The transformations that are consistent with the symmetry of space-time form a group known as the **inhomogeneous Lorentz group** or the **Poincaré group**. The Poincaré group consists of space and time displacements and all Lorentz transformations; here we shall only discuss the Lorentz transformations, which by themselves form the **Lorentz group**, sometimes for clarity referred to as the **homogeneous Lorentz group**.

Homogeneous Lorentz Group

Lorentz transformations can be likened to rotations that affect both the spatial and the time coordinates. An ordinary spatial rotation about the origin, in which $(x_1, x_2) \to (x_1', x_2')$, has the property that the length of the associated vector is unchanged by the rotation, so that $x_1^2 + x_2^2 = x_1'^2 + x_2'^2$. But we now consider transformations involving a spatial coordinate (let's choose z) and a time coordinate t, but with $z^2 - c^2t^2 = z'^2 - c^2t'^2$, so that the velocity of light, c, computed for travel from the origin $(0, 0)$ to (z, t) will be the same as that for travel from the origin to (z', t'). We are therefore abandoning the notion that the time variable is universal, assuming instead that it changes together with changes in the spatial variable(s) in a way that keeps the velocity of light constant. We also see that it is natural to rescale the t coordinate to $x_0 = ct$, so that the invariant of the transformation becomes $z^2 - x_0^2$.

Let's now examine a situation in which the coordinate system is moving in the $+z$ direction at an infinitesimal velocity $c\,\delta\rho$ (so that a Galilean transformation applies to z):

$$z' = z - c(\delta\rho)t = z - (\delta\rho)x_0.$$

But we assume that t also changes, to

$$t' = t - a(\delta\rho)z, \quad \text{or} \quad x_0' = x_0 - ac(\delta\rho)z,$$

with a chosen to keep $z^2 - x_0^2$ constant to first order in $\delta\rho$. The value of a that satisfies this requirement is $a = +1/c$, so our infinitesimal Lorentz transformation is

$$\begin{pmatrix} x_0' \\ z' \end{pmatrix} = \begin{pmatrix} 1 & -\delta\rho \\ -\delta\rho & 1 \end{pmatrix} \begin{pmatrix} x_0 \\ z \end{pmatrix} = \left[\mathbf{1}_2 - \delta\rho \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \right] \begin{pmatrix} x_0 \\ z \end{pmatrix}.$$

To identify this equation in terms of a generator, we note that

$$-\delta\rho \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = i(\delta\rho)\,\mathsf{S}, \quad \text{or} \quad \mathsf{S} = i \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = i\boldsymbol{\sigma}_1, \tag{17.69}$$

where $\boldsymbol{\sigma}_1$ is a Pauli matrix. Extending now to a finite velocity just as we did for ordinary rotations in the passage from Eq. (17.35) to Eq. (17.36), we have an expression that is similar to Eq. (17.39), except that we now have $\boldsymbol{\sigma}_1$ instead of $\boldsymbol{\sigma}_2$, while in place of φ we now have $i\rho$. The result is

$$\begin{aligned} U(\rho) &= \exp(i\rho[i\boldsymbol{\sigma}_1]) = \cos(i\rho) + i\boldsymbol{\sigma}_1 \sin(i\rho) = \cosh(\rho) - \boldsymbol{\sigma}_1 \sinh(\rho) \\ &= \begin{pmatrix} \cosh\rho & -\sinh\rho \\ -\sinh\rho & \cosh\rho \end{pmatrix}. \end{aligned} \tag{17.70}$$

While $\delta\rho$ was an infinitesimal velocity (in units of c), it does not follow that ρ, the result of repeated $\delta\rho$ transformations, is proportional to the resultant velocity in the final transformed coordinates. However, from the equation $z' = z\cosh\rho - x_0\sinh\rho$, we identify the resultant velocity as $v = c\sinh\rho/\cosh\rho = c\tanh\rho$.

Summarizing, and introducing the symbols usually used in relativistic mechanics, we identify

$$\beta \equiv \frac{v}{c}, \quad \tanh\rho = \beta, \quad \cosh\rho = \frac{1}{\sqrt{1-\beta^2}} \equiv \gamma, \quad \sinh\rho = \beta\gamma. \tag{17.71}$$

The range of ρ (sometimes called the **rapidity**) is unlimited, but $\tanh\rho < 1$, thereby showing that c is an upper limit to v (which cannot be reached for finite ρ).

A Lorentz transformation that does not also involve a spatial rotation is known as a **boost** or a **pure Lorentz transformation**. Successive boosts can be analyzed using the group property of the Lorentz transformations: A boost of rapidity ρ followed by another, of rapidity ρ', both in the z direction, must have transformation matrix

$$\begin{aligned} U(\rho')U(\rho) &= \begin{pmatrix} \cosh\rho' & -\sinh\rho' \\ -\sinh\rho' & \cosh\rho' \end{pmatrix} \begin{pmatrix} \cosh\rho & -\sinh\rho \\ -\sinh\rho & \cosh\rho \end{pmatrix} \\ &= \begin{pmatrix} \cosh\rho'\cosh\rho + \sinh\rho'\sinh\rho & -\cosh\rho'\sinh\rho - \sinh\rho'\cosh\rho \\ \sinh\rho'\cosh\rho - \cosh\rho'\sinh\rho & \sinh\rho'\sinh\rho + \cosh\rho'\cosh\rho \end{pmatrix} \\ &= \begin{pmatrix} \cosh(\rho+\rho') & -\sinh(\rho+\rho') \\ -\sinh(\rho+\rho') & \cosh(\rho+\rho') \end{pmatrix} = U(\rho+\rho'), \end{aligned}$$

showing that the rapidity (not the velocity) is the additive parameter for successive boosts in the same direction. The result we have just obtained is obvious if we write it in the generator notation; it is

$$U(\rho')U(\rho) = \exp(-\rho'\boldsymbol{\sigma}_1)\exp(-\rho\boldsymbol{\sigma}_1) = \exp(-(\rho'+\rho)\boldsymbol{\sigma}_1) = U(\rho'+\rho). \tag{17.72}$$

Because of the group property, successive boosts in different spatial directions must yield a resultant Lorentz transformation, but the result is not equivalent to any single boost, and corresponds to a boost plus a spatial rotation. This rotation is the origin of the Thomas precession that arises in the treatment of spin-orbit coupling terms in atomic and nuclear physics. A good discussion of the Thomas precession frequency is in the work by Goldstein (Additional Readings).

Example 17.8.1 ADDITION OF COLLINEAR VELOCITIES

Let's now apply Eq. (17.72) to two successive boosts in the z direction, identifying each by its individual velocity (v' for the first boost, v'' for the second), or equivalently $\beta' = v'/c$, $\beta'' = v''/c$. The corresponding rapidities will be denoted ρ' and ρ'', so

$$\tanh\rho' = \beta' = \frac{v'}{c}, \quad \tanh\rho'' = \beta'' = \frac{v''}{c}.$$

The resultant of the two successive boosts will have rapidity $\rho = \rho' + \rho''$, and will therefore be associated with a resultant velocity v satisfying $\tanh(\rho'+\rho'') = v/c = \beta$. From the summation formula for the hyperbolic tangent, we have

$$\frac{v}{c} = \beta = \tanh(\rho'+\rho'') = \frac{\tanh\rho' + \tanh\rho''}{1+\tanh\rho'\tanh\rho''} = \frac{\dfrac{v'}{c}+\dfrac{v''}{c}}{1+\dfrac{v'v''}{c^2}} = \frac{\beta'+\beta''}{1+\beta'\beta''}. \tag{17.73}$$

Equation (17.73) shows that when v' and v'' are both small compared to c, the velocity addition is approximately Galilean, becoming exactly Galilean in the small-velocity limit. But as the individual velocities increase, their resultant decreases relative to their arithmetic sum, and never exceeds c. This behavior is to be expected, since (for real arguments) the hyperbolic tangent cannot exceed unity. ■

Minkowski Space

If we make the definition $x_4 = ict$, the formulas we have just obtained, and many others as well, can be written in a systematic form that does not have minus signs explicitly present for the time coordinate. Then Lorentz transformations act like rotations in a space with basis (x_1, x_2, x_3, x_4), and the conserved quantity is $x_1^2 + x_2^2 + x_3^2 + x_4^2$. This approach is appealing and is widely used.

An alternative way to proceed, which has the disadvantage of being a bit more cumbersome, but with the advantage of providing a framework suitable for the extension to general relativity, is to use real coordinates (as was done in the preceding subsection), but to handle the difference in behavior of the spatial and time coordinates by introducing a suitably defined metric tensor. One possibility (for basis $x_0 = ct$, x_1, x_2, x_3), where x_i

($i = 1, 2, 3$) are Cartesian spatial coordinates, is to use the **Minkowski** metric tensor, first introduced in Example 4.5.2,

$$(g^{\mu\nu}) = (g_{\mu\nu}) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \tag{17.74}$$

where it is understood that Greek indices run over the four-index set 0 to 3, and that displacements are rendered as scalar products of the form $x^\mu g_{\mu\nu} x'^\nu$ or $x_\mu g^{\mu\nu} x'_\nu$, where the repeated indices are understood to be summed (the Einstein summation convention). Note that because all the analysis in this section is in Cartesian coordinates, the distinction between contravariant and covariant indices is limited to the insertion of minus signs in some elements of products that involve the metric tensor.

As was pointed out in Example 4.6.2, this metric tensor sometimes appears with the signs of all its diagonal elements reversed. Either choice of signs is valid and yields proper results for problems of physics if used consistently, but trouble can arise if material from inconsistent sources is combined. The cited example also indicates how Maxwell's equations can be written in a manifestly covariant form.

Note that the transformation matrices S and U must be mixed tensors, since they convert a vector (whether covariant or contravariant) into another vector of the same variance status. Since for a pure boost these matrices are symmetric, either index can be deemed to be covariant (the other then being contravariant).

Exercises

17.8.1 Show that in $3 + 1$ dimensions (this means three spatial dimension plus time), a boost in the xy plane at an angle θ from the x direction has, in coordinates (x_0, x_1, x_2, x_3), the generator

$$\mathsf{S} = i \begin{pmatrix} 0 & \cos\theta & \sin\theta & 0 \\ \cos\theta & 0 & 0 & 0 \\ \sin\theta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

17.8.2 (a) Show that the generator in Exercise 17.8.1 produces a Lorentz transformation matrix for rapidity ρ given by

$$U(\rho;\theta) = \begin{pmatrix} \cosh\rho & -\cos\theta\sinh\rho & -\sin\theta\sinh\rho & 0 \\ -\cos\theta\sinh\rho & \sin^2\theta + \cos^2\theta\cosh\rho & \cos\theta\sin\theta(\cosh\rho - 1) & 0 \\ -\sin\theta\sinh\rho & \cos\theta\sin\theta(\cosh\rho - 1) & \cos^2\theta + \sin^2\theta\cosh\rho & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

Note. This transformation matrix is symmetric. All single boosts (in any spatial direction) have symmetric transformation matrices.

(b) Verify that the transformation matrix of part (a) is consistent with (1) rotating the spatial coordinates to align the boost direction with a coordinate axis, (2) performing a boost in the direction of that axis using Eq. (17.70), and (3) rotating back to the original coordinate system.

17.8.3 Obtain the Lorentz transformation matrix for a boost of finite amount ρ' in the x direction followed by a finite boost ρ'' in the y direction. Show that there are no values of ρ and θ that can bring this transformation to the form given in Exercise 17.8.2.

17.9 LORENTZ COVARIANCE OF MAXWELL'S EQUATIONS

We start our discussion of Lorentz covariance by recalling how the magnetic and electric fields **B** and **E** depend on the vector and scalar potentials **A** and φ:

$$\begin{aligned} \mathbf{B} &= \nabla \times \mathbf{A}, \\ \mathbf{E} &= -\frac{\partial \mathbf{A}}{\partial t} - \nabla \varphi. \end{aligned} \tag{17.75}$$

Restricting consideration to situations where ε and μ have their free-space values ε_0 and μ_0 (with $\varepsilon_0 \mu_0 = 1/c^2$), it can be shown that **A** and φ form a four-vector whose components $\mathcal{A}^\mu$ (in contravariant form) are

$$\begin{aligned} \mathcal{A}^i &= c\varepsilon_0 A_i, \quad i = 1, 2, 3, \\ \mathcal{A}^0 &= \varepsilon_0 \varphi. \end{aligned} \tag{17.76}$$

We now form the tensor $F^{\mu\lambda}$ with elements

$$F^{\mu\lambda} = \frac{\partial \mathcal{A}^\lambda}{\partial x_\mu} - \frac{\partial \mathcal{A}^\mu}{\partial x_\lambda}, \tag{17.77}$$

which we evaluate (consistently with our choice of Minkowski metric) using

$$\frac{\partial}{\partial x_0} = \frac{\partial}{c\partial t}, \quad \frac{\partial}{\partial x_1} = -\frac{\partial}{\partial x}, \quad \frac{\partial}{\partial x_2} = -\frac{\partial}{\partial y}, \quad \frac{\partial}{\partial x_3} = -\frac{\partial}{\partial z}. \tag{17.78}$$

The resulting form for $F^{\mu\lambda}$, known as the **electromagnetic field tensor**, is

$$F^{\mu\lambda} = \varepsilon_0 \begin{pmatrix} 0 & -E_x & -E_y & -E_z \\ E_x & 0 & -cB_z & cB_y \\ E_y & cB_z & 0 & -cB_x \\ E_z & -cB_y & cB_x & 0 \end{pmatrix}. \tag{17.79}$$

The quantity $F^{\mu\lambda}$ is, as its name implies, a second-order tensor that must have the transformation properties associated with the Lorentz group. We know this to be the case because we constructed $F^{\mu\lambda}$ as a linear combination of terms, each of which was the derivative of a four-vector; differentiation of a vector (in a Cartesian system) generates a second-order tensor.

An interesting aside to the above analysis is provided by the discussion of Maxwell's equations in the language of differential forms. In Example 4.6.2 we showed that the differential form

$$F = -E_x\, dt \wedge dx - E_y\, dt \wedge dy - E_z\, dt \wedge dz + B_x\, dy \wedge dz + B_y\, dz \wedge dx + B_z\, dx \wedge dy$$

was a starting point from which Maxwell's equations could be derived; we now observe that the individual terms of this differential form correspond to the elements of the tensor under discussion here.

Lorentz Transformation of E and B

Returning to the main matter of present concern, we now apply a Lorentz transformation to $F^{\mu\lambda}$. For simplicity we take a pure boost in the z direction, which will have matrix elements similar to those of Eq. (17.70); using the notations introduced in Eq. (17.71), our transformation matrix can be written

$$\mathsf{U} = \begin{pmatrix} \gamma & 0 & 0 & -\beta\gamma \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\beta\gamma & 0 & 0 & \gamma \end{pmatrix}. \tag{17.80}$$

Noting that we must apply our Lorentz transformation to both indices of $F^{\mu\lambda}$, and keeping in mind that U is symmetric and, as pointed out in Section 17.8, a mixed tensor, we can write

$$\mathsf{F}' = \mathsf{U}\mathsf{F}\mathsf{U}, \tag{17.81}$$

where F and F' are both contravariant matrices. If we now compare the individual elements of F' with those of F, we obtain formulas for the components of $\mathbf{E}'$ and $\mathbf{B}'$ in terms of the components of $\mathbf{E}$ and $\mathbf{B}$. For the transformation at issue here, the results are (where v is the velocity of the transformed coordinate system, in the z direction, relative to the original coordinates):

$$\begin{aligned} E'_x &= \gamma\left(E_x - \beta c B_y\right) = \gamma\left(E_x - v B_y\right), \\ E'_y &= \gamma\left(E_y + \beta c B_x\right) = \gamma\left(E_y + v B_x\right), \\ E'_z &= E_z, \end{aligned} \tag{17.82}$$

$$\begin{aligned} B'_x &= \gamma\left(B_x + \frac{\beta}{c} E_y\right) = \gamma\left(B_x + \frac{v}{c^2} E_y\right), \\ B'_y &= \gamma\left(B_y - \frac{\beta}{c} E_x\right) = \gamma\left(B_y - \frac{v}{c^2} E_x\right), \\ B'_z &= B_z. \end{aligned} \tag{17.83}$$

We can generalize the above to a boost $\mathbf{v}$ in an arbitrary direction:

$$\begin{aligned} \mathbf{E}' &= \gamma(\mathbf{E} + \mathbf{v} \times \mathbf{B}) + (1-\gamma)\mathbf{E}_v, \\ \mathbf{B}' &= \gamma\left(B - \frac{\mathbf{v} \times \mathbf{E}}{c^2}\right) + (1-\gamma)\mathbf{B}_v, \end{aligned} \tag{17.84}$$

where $\mathbf{E}_v = (\mathbf{E}\cdot\hat{\mathbf{v}})\hat{\mathbf{v}}$ and $\mathbf{B}_v = (\mathbf{B}\cdot\hat{\mathbf{v}})\hat{\mathbf{v}}$ are the projections of $\mathbf{E}$ and $\mathbf{B}$ in the direction of $\mathbf{v}$. In the limit $v \ll c$, these equations reduce to

$$\begin{aligned}\mathbf{E}' &= \mathbf{E} + \mathbf{v}\times\mathbf{B},\\ \mathbf{B}' &= \mathbf{B} - \frac{\mathbf{v}\times\mathbf{E}}{c^2}.\end{aligned} \tag{17.85}$$

Note that the coordinate transformation changes the velocity with which charges move and therefore changes the magnetic force. It is now clear that the Lorentz transformation explains how the total force (electric plus magnetic) can be independent of the **reference frame** (i.e., the relative velocities of the coordinate systems). In fact, the need to make the total electromagnetic force independent of the reference frame was first noted by Lorentz and Poincaré. This was where Lorentz transformations were first recognized as relevant for physics, and that may have provided Einstein with a clue as he developed his formulation of special relativity.

Example 17.9.1 TRANSFORMATION TO BRING CHARGE TO REST

Consider a charge q moving at a velocity $\mathbf{v}$, with $v \ll c$. By giving the coordinate system a boost $\mathbf{v}$, we transform to a frame in which the charge is at rest and experiences only an electric force $q\mathbf{E}'$. But since the total force is independent of the reference frame, it is also given, according to Eq. (17.86), as

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v}\times\mathbf{B}), \tag{17.86}$$

which is just the classical Lorentz force. ■

The ability to write Maxwell's equations in a tensor form that gives the experimentally observed results under Lorentz transformation is an important achievement because it guarantees that the formulation is consistent with special relativity. This is one of the reasons that modern theories of quantum electrodynamics and elementary particles are often written in this **manifestly covariant** form. Conversely, the insistence on such a tensor form has been a useful guide in the construction of these theories.

We close with the following general observations:

> *The Lorentz group is the symmetry group of electrodynamics, of the electroweak gauge theory, and of the strong interactions described by quantum chromodynamics. It appears necessary that mechanics in general have the symmetry of the Lorentz group, and that requirement corresponds to the general applicability of special relativity. With respect to electrodynamics, the Lorentz symmetry explains the fact that the velocity of light is the same in all inertial frames, and it explains how electric and magnetic forces are interrelated and yield physical results that are frame-independent. While a detailed study of relativistic mechanics is beyond the scope of this book, the extension to special relativity of Newton's equations of motion is straightforward and leads to a variety of results, some of which challenge human intuition.*

Exercises

17.9.1 Apply the Lorentz transformation of Eq. (17.80) to $F^{\mu\lambda}$ as given in Eq. (17.79). Verify that the result is a matrix F' whose elements confirm the results given in Eqs. (17.82) and (17.83).

17.9.2 Confirm that the generalization of Eqs. (17.82) and (17.83) to a boost corresponding to an arbitrary velocity $\mathbf{v}$ is properly given by Eq. (17.84).

17.10 Space Groups

Perfect crystals exhibit translational symmetry, meaning that they can be considered as a space-filling array of parallelepipeds stacked end-to-end and side-to-side, with each containing an identical set of identically placed atoms. A single parallelepiped is referred to as the **unit cell** of the crystal; a unit cell can be specified by giving the vectors that define its edges. Calling these vectors $\mathbf{h}_1$, $\mathbf{h}_2$, $\mathbf{h}_3$, equivalent points in any two unit cells are separated from each other by vectors

$$\mathbf{b} = n_1\mathbf{h}_1 + n_2\mathbf{h}_2 + n_3\mathbf{h}_3,$$

where n_1, n_2, n_3 can be any integers (positive, negative, or zero). The set of these equivalent points is called the **Bravais lattice** of the crystal.

A Bravais lattice will have a symmetry that depends on the angles and relative lengths of the lattice vectors; in three dimensions there are 14 different symmetries possible for Bravais lattices. There are 32 3-D point groups that are symmetry-compatible with at least one Bravais lattice; these are called **crystallographic point groups** to distinguish them from the infinite number of point groups that can exist in the absence of any compatibility requirement.

Example 17.10.1 Tiling a Floor

To understand the notion of crystallographic point group, consider what would happen (in two dimensions) if we try to tile a floor with identical tiles in the shape of a regular polygon. We will have success with squares and triangles, and even with hexagons. These work because an integer number of tiles can be placed so that they have vertices at the same point. A triangle has an internal angle of 60°, so six of them can meet at a point; similarly, four squares can meet at a point, as can three hexagons (internal angle 120°). But we cannot tile with regular pentagons (internal angle 108°) or any regular polygon with more than six sides. ■

Combining Bravais lattices and compatible point groups, there is a total of 230 different groups in 3-D that exhibit translational symmetry and some sort of point-group symmetry. These 230 groups are called **space groups**. Their study and use in crystallography (e.g., to determine the detailed structure of a crystal from its x-ray scattering) is the topic of several of the larger books in the Additional Readings.

Systems with periodicity in only one or two dimensions also exist in nature; some linear polymers are 1-D periodic systems; surface systems and single-layer arrays such as **graphene** (a macroscopic hexagonal array of carbon atoms) exhibit periodicity in two

dimensions. There is even a kind of translational symmetry that involves elements that form helical structures. The recognition of this type of symmetry in crystallographic studies of DNA was the key contribution leading to the discovery that DNA existed as a double helix.

Additional Readings

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