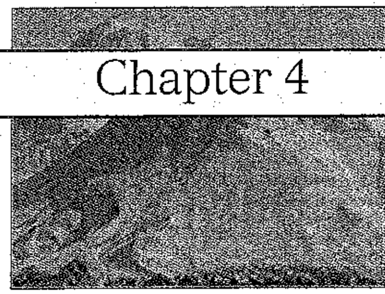

Chapter 4

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.
>
> —Murray Gell-Mann

4.1 Introduction to Group Theory

In classical mechanics the **symmetry** of a physical system leads to **conservation laws**. Conservation of angular momentum (**L**) is a direct consequence of rotational symmetry, which means **invariance** of some physical observables (such as $\mathbf{L}^2$) or geometrical quantities (such as length of a vector or distance between points) under spatial rotations. In the first third of this century, Wigner and others realized that invariance was a key concept in understanding the new quantum phenomena and in developing appropriate theories. For example, Noether's theorem establishes a conserved current from an invariance of the Lagrangian of a field theory. Thus, in quantum mechanics the concept of angular momentum and spin has become even more central. Its generalizations, **isospin** in nuclear physics and the **flavor symmetry** in particle physics, are indispensable tools in building and solving theories. Generalizations of the concept of **gauge invariance** of classical electrodynamics to the isospin symmetry lead to the electroweak gauge theory.

In each case the set of these symmetry operations forms a group, a mathematical concept we shall soon define. Group theory is the mathematical tool to treat invariants and symmetries. It brings unification and formalization of principles such as spatial reflections, or parity, angular momentum, and geometry that are widely used by physicists.

In geometry the fundamental role of group theory was recognized more than a century ago by mathematicians (e.g., Felix Klein's Erlanger Programm). In Euclidean geometry the distance between two points, the scalar product of two vectors or metric, does not change under rotations or translations. These symmetries are characteristic of this geometry. In special relativity the metric, or scalar product of four-vectors, differs from that of Euclidean geometry in that it is no longer positive definite and is invariant under Lorentz transformations.

For a crystal, the symmetry group contains only a finite number of rotations at discrete values of angles or reflections. The theory of such **discrete** or **finite** groups, developed originally as a branch of pure mathematics, is now a useful tool for the development of crystallography and condensed matter physics. When the rotations depend on continuously varying angles (e.g., the Euler angles of Section 3.3) the rotation groups have an infinite number of elements. Such continuous (or **Lie**)[1] **groups** are the topic of this chapter.

Definition of Group

A group G may be defined as a set of objects or, in physics usually, symmetry operations (such as rotations or Lorentz transformations), called the elements g of G, that may be combined or "multiplied" to form a well-defined product in G that satisfies the following conditions:

1. If a and b are any two elements of G, then the product ab is also an element of G. In terms of symmetry operations, b is applied to the physical system before a in the product, and the product ab is equivalent to a single symmetry operation in G. Multiplication associates (or maps) an element ab of G with the pair (a, b) of elements of G; this property is known as **closure** under multiplication.
2. This multiplication is **associative,** $(ab)c = a(bc)$.
3. There is a **unit or identity** element[2] 1 in G such that $1a = a1 = a$ for every element a in G.
4. G must contain an **inverse or reciprocal** of every element a of G, labeled a^{-1} such that $aa^{-1} = a^{-1}a = 1$.

Note that the unit is unique, as is the inverse. The inverse of 1 is 1 because $1a = a1 = a$ for $a = 1$ yields $1 \cdot 1 = 1$. If a second unit $1'$ existed we would have $11' = 1'1 = 1'$ and $1'1 = 11' = 1$. Comparing we see that $1' = 1$. Similarly, if a second inverse a'^{-1} existed we would have $a^{-1}a = aa^{-1} = 1 = aa'^{-1}$. Multiplying by a^{-1}, we get $a^{-1} = a'^{-1}$.

[1]After the Norwegian mathematician Sophus Lie.
[2]Following E. Wigner, the unit element of a group is often labeled E, from the German **Einheit** (i.e., unit) or just 1 or I for identity.

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EXAMPLE 4.1.1

Coordinate Rotation An example of a group is the set of counterclockwise coordinate rotations

$$|\mathbf{x}'\rangle = \begin{pmatrix} x' \\ y' \end{pmatrix} \equiv \mathsf{R}(\varphi)\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} \tag{4.1}$$

through an angle φ of the xy-coordinate system to a new orientation (see Fig. 2.20). The product of two rotations is defined by rotating first by the angle φ_2 and then by φ_1. According to Eqs. (3.36) and (3.37), the product of the orthogonal 2×2 matrices, $\mathsf{R}(\varphi_1)\mathsf{R}(\varphi_2)$, describes the product of two rotations

$$\begin{aligned} &\begin{pmatrix} \cos\varphi_1 & \sin\varphi_1 \\ -\sin\varphi_1 & \cos\varphi_1 \end{pmatrix}\begin{pmatrix} \cos\varphi_2 & \sin\varphi_2 \\ -\sin\varphi_2 & \cos\varphi_2 \end{pmatrix} \\ &\quad = \begin{pmatrix} \cos(\varphi_1+\varphi_2) & \sin(\varphi_1+\varphi_2) \\ -\sin(\varphi_1+\varphi_2) & \cos(\varphi_1+\varphi_2) \end{pmatrix}, \end{aligned} \tag{4.2}$$

using the addition formulas for the trigonometric functions. The product is clearly a rotation represented by the orthogonal matrix with angle $\varphi_1 + \varphi_2$. The product is the associative matrix multiplication. It is **commutative** or **Abelian** because the order in which these rotations are performed does not matter. The inverse of the rotation with angle φ is that with angle $-\varphi$. The unit corresponds to the angle $\varphi = 0$. The group's name is SO(2), which stands for **special orthogonal rotations in two dimensions**, where special means the 2×2 rotation matrices have determinant $+1$, and the angle φ varies continuously from 0 to 2π, so that the group has infinitely many elements. The angle is the **group parameter.** ■

A **subgroup** G' of a group G is a group consisting of elements of G so that the product of any of its elements is again in the subgroup G'; that is, G' is **closed** under the multiplication of G. For example, the unit 1 of G always forms a subgroup of G, and the unity with angle $\varphi = 0$ and the rotation with $\varphi = \pi$ about some axis form a finite subgroup of the group of rotations about that axis.

If $gg'g^{-1}$ is an element of G' for any g of G and g' of G', then G' is called an **invariant subgroup** of G. If the group elements are matrices, then the element $gg'g^{-1}$ corresponds to a similarity transformation [see Eq. (3.108)] of g' in G' by an element g of G (discussed in Chapter 3). Of course, the unit 1 of G always forms an invariant subgroup of G because $g1g^{-1} = 1$. When an element g of G lies outside the subgroup G', then $gg'g^{-1}$ may also lie outside G'. Let us illustrate this by three-dimensional rotations.

EXAMPLE 4.1.2

Similarity Transformation Rotations of the coordinates through a finite angle φ counterclockwise about the z-axis in three-dimensional space are described as

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = \mathsf{R}_z(\varphi)\begin{pmatrix} x \\ y \\ z \end{pmatrix} \equiv \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ -\sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix}, \tag{4.3}$$

which form a group by a generalization of Eq. (4.2) to our special 3×3 matrices that keep their special form on multiplication. Moreover, the order of the rotations in a product does not matter, just like in Eq. (4.2), so that the group is Abelian. A general rotation about the x-axis is given by the matrix

$$\mathsf{R}_x(\varphi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & \sin\varphi \\ 0 & -\sin\varphi & \cos\varphi \end{pmatrix}.$$

Now consider a rotation R_x by 90° about the x-axis. Its matrix is

$$\mathsf{R}_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix},$$

and its inverse is

$$\mathsf{R}_x^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix},$$

corresponding to the angle $-90°$. This can be checked by multiplying them: $\mathsf{R}_x\mathsf{R}_x^{-1} = 1$. Then

$$\mathsf{R}_x\mathsf{R}_z(\varphi)\mathsf{R}_x^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\varphi & \sin\varphi \\ 0 & -\sin\varphi & \cos\varphi \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$= \begin{pmatrix} \cos\varphi & 0 & -\sin\varphi \\ 0 & 1 & 0 \\ \sin\varphi & 0 & \cos\varphi \end{pmatrix},$$

which is a rotation by $-\varphi$ about the y-axis and no longer a rotation about the z-axis so that this element lies outside the subgroup of rotations about the z-axis, and this subgroup is not an invariant subgroup. The set of these elements for all φ form a group called **conjugate** to the group of rotations about the z-axis. ■

Orthogonal $n \times n$ matrices form the group $\mathrm{O}(n)$, and they form $\mathrm{SO}(n)$ if their determinants are $+1$ (S stands for "special" and O for "orthogonal"), with elements denoted by O_i. Because $\tilde{\mathsf{O}}_i = \mathsf{O}_i^{-1}$ (see Section 3.3 for orthogonal 3×3 matrices that preserve the lengths of vectors and distances between points in three-dimensional Euclidean space), we see that the product

$$\widetilde{\mathsf{O}_1\mathsf{O}_2} = \tilde{\mathsf{O}}_2\tilde{\mathsf{O}}_1 = \mathsf{O}_2^{-1}\mathsf{O}_1^{-1} = (\mathsf{O}_1\mathsf{O}_2)^{-1}$$

is also an orthogonal matrix in $\mathrm{O}(n)$ or $\mathrm{SO}(n)$. The inverse is the transpose (orthogonal) matrix. The unit of the group is 1_n. A real orthogonal $n \times n$ matrix has $n(n-1)/2$ independent parameters. For $n = 2$, there is only one parameter: one angle in Eq. (4.1). For $n = 3$, there are three independent parameters: for example, the three Euler angles of Section 3.3, and SO(3) is related to rotations in three dimensions, just as SO(2) is in two dimensions. Because $O(n)$ contains orthogonal transformations with determinant -1, this group includes reflections of coordinates or parity inversions. Likewise, unitary $n \times n$ matrices form the group $U(n)$, and they form $SU(n)$ if their determinants are $+1$. Because $U_i^\dagger = U_i^{-1}$ (see Section 3.4 for unitary matrices, which preserve the norm of vectors with complex components and distances between points in n-dimensional complex space), we see that

$$(U_1U_2)^\dagger = U_2^\dagger U_1^\dagger = U_2^{-1}U_1^{-1} = (U_1U_2)^{-1}$$

so that the product is unitary and an element of $U(n)$ or $SU(n)$. Each unitary matrix obviously has an inverse, which again is unitary. Orthogonal matrices are unitary matrices that are real so that $SO(n)$ forms a subgroup of $SU(n)$, as does $O(n)$ of $U(n)$.

EXAMPLE 4.1.3

Simple Unitary Groups The phase factors $e^{i\theta}$, with real angle θ, of quantum mechanical wave functions form a group under multiplication of complex numbers because the phase angles add on multiplying $e^{i\theta_1}e^{i\theta_2} = e^{i(\theta_1+\theta_2)}$. Moreover, $(e^{i\theta})^\dagger = e^{-i\theta}$ and $e^{i\theta}e^{-i\theta} = 1$ show unitarity and inverse, and $\theta = 0$ gives the unit. This group (of unitary 1×1 matrices) has one continuous real parameter and is therefore called U(1). The two elements ± 1 form a finite (unitary) subgroup, and the four elements ± 1, $\pm i$ form another subgroup.

A finite unitary group of 2×2 matrices is defined by the two-dimensional unit matrix and one of the three Pauli matrices, σ_i, using matrix multiplication. Because $\sigma_i^2 = 1_2$, the inverse $\sigma_i^{-1} = \sigma_i$ and $1_2^{-1} = 1_2$. ■

When a potential has spherical symmetry we choose polar coordinates, and the associated group of transformations is a rotation group. For problems with spin (or other internal properties such as isospin or flavor), unitary groups play a similar role. Therefore, in the following we discuss only the rotation groups $SO(n)$ and the unitary group SU(2) among the classical Lie groups.

Biographical Data

Lie, Sophus. Lie, who was born in 1842 in Nordfjordeid, Norway, and died in 1899 in Kristiana (now Oslo), started his analysis of continuous groups of transformations in Paris and continued it throughout his life.

Wigner, Eugen Paul. Wigner, who was born in 1902 in Budapest, Hungary, and died in 1995 in Princeton, New Jersey, studied in Berlin, moved to the United States in the 1930s, and received the Nobel prize in 1963 for his contributions to nuclear theory and applications of fundamental principles of symmetry, such as the charge independence of nuclear forces. He developed the unitary representations of the Lorentz group.

4.2 Generators of Continuous Groups

A characteristic of continuous groups known as Lie groups is that the elements are functions of parameters having derivatives of arbitrary orders such as $\cos\varphi$ and $\sin\varphi$ in Eq. (4.1). This unlimited differentiability of the functions allows us to develop the concept of generator and reduce the study of the whole group to a study of the group elements in the neighborhood of the identity element.

Lie's essential idea was to study elements R in a group G that are infinitesimally close to the unity of G. Let us consider the SO(2) group as a simple example. The 2×2 rotation matrices in Eq. (4.1) can be written in exponential form using the Euler identity [Eq. (3.183)] as

$$\mathsf{R}(\varphi) = \begin{pmatrix} \cos\varphi & \sin\varphi \\ -\sin\varphi & \cos\varphi \end{pmatrix} = 1_2\cos\varphi + i\sigma_2\sin\varphi = \exp(i\sigma_2\varphi). \tag{4.9}$$

From the exponential form it is obvious that multiplication of these matrices is equivalent to addition of the arguments

$$\mathsf{R}(\varphi_2)\mathsf{R}(\varphi_1) = \exp(i\sigma_2\varphi_2)\exp(i\sigma_2\varphi_1) = \exp(i\sigma_2(\varphi_1+\varphi_2)) = \mathsf{R}(\varphi_1+\varphi_2).$$

Of course, the rotations close to 1 have small angle $\varphi \approx 0$.

This suggests that we look for an exponential representation

$$\mathsf{R} = \exp(i\varepsilon\mathsf{S}), \quad \varepsilon \to 0, \tag{4.10}$$

for group elements R in G close to the unity 1. The operators S of the infinitesimal transformations $i\varepsilon\mathsf{S}$ are called generators of G. Therefore, σ_2 in Eq. (4.9) is the generator of rotations about the z-axis. Thus, for SO(2) as defined by Eq. (4.1) there is only one linearly independent generator, σ_2. In SO(3) there is a generator for rotations about each axis. These generators form a linear space because multiplication of the elements R of the group translates into addition of generators S; its dimension is defined as the **order** of G. Therefore, the order of SO(2) is 1, and it is 3 for SO(3). One can also show that the commutator of two generators is again a generator

$$[S_j, S_k] = i\sum_l c^l_{jk} S_l,$$

where the c's are defined as the **structure constants** of the group. The vector space of generators can be endowed with a multiplication by defining the commutator as the product of two generators. This way the vector space of generators becomes an algebra, the so-called **Lie algebra**.

Because R does not change the volume—that is, $\det(\mathsf{R}) = 1$—we use Eq. (3.184) to see that

$$\det(\mathsf{R}) = \exp(\mathrm{trace}(\ln\mathsf{R})) = \exp(i\varepsilon\,\mathrm{trace}(\mathsf{S})) = 1,$$

which implies that **generators are traceless**:

$$\mathrm{tr}(\mathsf{S}) = 0. \tag{4.11}$$

This is the case for the rotation groups SO(n) and unitary groups SU(n).

If R of G in Eq. (4.10) is unitary, then $S^\dagger = S$ is Hermitian, which is also the case for SO(n) and SU(n). Hence the i in Eq. (4.10).

Returning to Eq. (4.5), we now emphasize the most important result from group theory. The inverse of R is just $\mathsf{R}^{-1} = \exp(-i\varepsilon\mathsf{S})$. We expand H_R according to the Baker–Hausdorff formula [Eq. (3.185)]; taking the Hamiltonian H and S to be operators or matrices we see that

$$H = H_R = \exp(i\varepsilon\mathsf{S})H\exp(-i\varepsilon\mathsf{S}) = H + i\varepsilon[\mathsf{S}, H] - \frac{1}{2}\varepsilon^2[\mathsf{S}[\mathsf{S}, H]] + \cdots. \quad (4.12)$$

We subtract H from Eq. (4.12), divide by ε, and let $\varepsilon \to 0$. Then Eq. (4.12) implies that for any rotation close to 1 in G the commutator

$$[\mathsf{S}, H] = 0. \quad (4.13)$$

We see that S **is a constant of the motion: A symmetry of the system has led to a conservation law**. If S and H are Hermitian matrices, Eq. (4.13) states that S and H can be simultaneously diagonalized; that is, the eigenvalues of S are constants of the motion. If S and H are differential operators like the Hamiltonian and orbital angular momentum $\mathbf{L}^2$, L_z in quantum mechanics, then Eq. (4.13) states that S and H have common eigenfunctions, and that the degenerate eigenvalues of H can be distinguished by the eigenvalues of the generators S. These eigenfunctions and eigenvalues, s, are solutions of separate differential equations, $\mathsf{S}\psi_s = s\psi_s$, so that group theory (i.e., symmetries) leads to a separation of variables for a partial differential equation that is invariant under the transformations of the group. For examples, see the separation of variables method for partial differential equations in Section 8.9 and special functions in Chapter 11. This is by far the most important application of group theory in quantum mechanics.

In the following sections, we study orthogonal and unitary groups as examples to understand better the general concepts of this section.

√ Rotation Groups SO(2) and SO(3)

For SO(2) as defined by Eq. (4.1) there is only one linearly independent generator, σ_2, and the order of SO(2) is 1. We get σ_2 from Eq. (4.9) by differentiation at the unity of SO(2) (i.e., $\varphi = 0$),

$$-i\frac{d\mathsf{R}(\varphi)}{d\varphi}\bigg|_{\varphi=0} = -i\begin{pmatrix} -\sin\varphi & \cos\varphi \\ -\cos\varphi & -\sin\varphi \end{pmatrix}\bigg|_{\varphi=0} = -i\begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} = \sigma_2. \quad (4.14)$$

For the rotations $\mathsf{R}_z(\varphi)$ about the z-axis described by 3×3 matrices in Eq. (4.3), the generator is given by

$$-i\frac{d\mathsf{R}_z(\varphi)}{d\varphi}\bigg|_{\varphi=0} = \mathsf{S}_z = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (4.15)$$

Here, σ_2 is recognized in the upper left-hand corner of S_z. The rotation $\mathsf{R}_z(\delta\varphi)$ through an infinitesimal angle $\delta\varphi$ may then be expanded near the unity ($\varphi = 0$) as

$$\mathsf{R}_z(\delta\varphi) = 1_3 + i\delta\varphi\mathsf{S}_z, \tag{4.16}$$

with terms of order $(\delta\varphi)^2$ and higher omitted. A finite rotation $\mathsf{R}(\varphi)$ may be compounded of successive infinitesimal rotations

$$\mathsf{R}_z(\delta\varphi_1 + \delta\varphi_2) = (1_3 + i\delta\varphi_1\mathsf{S}_z)(1_3 + i\delta\varphi_2\mathsf{S}_z). \tag{4.17}$$

Let $\delta\varphi = \varphi/N$ for N rotations, with $N \to \infty$. Then,

$$\mathsf{R}_z(\varphi) = \lim_{N\to\infty}[\mathsf{R}_z(\varphi/N)]^N = \lim_{N\to\infty}[1_3 + (i\varphi/N)\mathsf{S}_z]^N = \exp(i\varphi\mathsf{S}_z), \tag{4.18}$$

which is another way of getting Eq. (4.10). This form identifies S_z as the generator of the group R_z, an Abelian subgroup of SO(3), the group of rotations in three dimensions with determinant +1. Each 3×3 matrix $\mathsf{R}_z(\varphi)$ is orthogonal (hence unitary), and trace$(\mathsf{S}_z) = 0$ in accordance with Eq. (4.11).

By differentiation of the coordinate rotations

$$\mathsf{R}_x(\psi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\psi & \sin\psi \\ 0 & -\sin\psi & \cos\psi \end{pmatrix}, \quad \mathsf{R}_y(\theta) = \begin{pmatrix} \cos\theta & 0 & -\sin\theta \\ 0 & 1 & 0 \\ \sin\theta & 0 & \cos\theta \end{pmatrix}, \tag{4.19}$$

we get the generators

$$\mathsf{S}_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad \mathsf{S}_y = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \tag{4.20}$$

of $\mathsf{R}_x(\mathsf{R}_y)$, the subgroup of rotations about the x- (y-)axis.

Rotation of Functions and Orbital Angular Momentum

In the foregoing discussion the group elements are matrices that rotate the coordinates. Any physical system being described is held fixed. Now let us hold the coordinates fixed and rotate a function $\psi(x, y, z)$ relative to our fixed coordinates. With R to rotate the coordinates,

$$\mathbf{x}' = \mathsf{R}\mathbf{x}, \tag{4.21}$$

we define R on ψ by

$$\mathsf{R}\psi(x, y, z) = \psi'(x, y, z) \equiv \psi(\mathbf{x}'). \tag{4.22}$$

In words, R operates on the function ψ, creating a **new function** ψ' that is numerically equal to $\psi(\mathbf{x}')$, where $\mathbf{x}'$ are the coordinates rotated by R. If R rotates the coordinates counterclockwise, the effect of R is to rotate the pattern of the function ψ counterclockwise, as shown in Fig. 2.20.

Returning to Eqs. (4.3), (4.15), and (4.20) consider an infinitesimal rotation again, $\varphi \to \delta\varphi$. Then, using R_z [Eq. (4.3)], we obtain

$$\mathsf{R}_z(\delta\varphi)\psi(x, y, z) = \psi(x + y\delta\varphi, y - x\delta\varphi, z). \tag{4.23}$$

The right side may be expanded to first order in $\delta\varphi$ to give

$$\begin{aligned}\mathsf{R}_z(\delta\varphi)\psi(x, y, z) &= \psi(x, y, z) - \delta\varphi\{x\partial\psi/\partial y - y\partial\psi/\partial x\} + O(\delta\varphi)^2 \\ &= (1 - i\delta\varphi L_z)\psi(x, y, z),\end{aligned} \tag{4.24}$$

where the differential expression in curly brackets is the orbital angular momentum iL_z (Exercise 1.7.12). This shows how the orbital angular momentum operator arises as a generator. Since a rotation of first φ and then $\delta\varphi$ about the z-axis is given by

$$\mathsf{R}_z(\varphi + \delta\varphi)\psi = \mathsf{R}_z(\delta\varphi)\mathsf{R}_z(\varphi)\psi = (1 - i\delta\varphi L_z)\mathsf{R}_z(\varphi)\psi, \tag{4.25}$$

we have (as an operator equation)

$$\frac{d\mathsf{R}_z}{d\varphi} = \lim_{\delta\varphi\to 0}\frac{\mathsf{R}_z(\varphi + \delta\varphi) - \mathsf{R}_z(\varphi)}{\delta\varphi} = -iL_z\mathsf{R}_z(\varphi). \tag{4.26}$$

In this form, Eq. (4.26) integrates immediately to

$$\mathsf{R}_z(\varphi) = \exp(-i\varphi L_z). \tag{4.27}$$

Note that $\mathsf{R}_z(\varphi)$ rotates functions (counterclockwise) relative to fixed coordinates [so Eqs. (4.27) and (4.10) are similar but not the same] and that L_z is the z-component of the orbital angular momentum $\mathbf{L}$. The constant of integration is fixed by the boundary condition $\mathsf{R}_z(0) = 1$.

If we recognize that the operator

$$L_z = (x, y, z)\mathsf{S}_z\begin{pmatrix}\partial/\partial x \\ \partial/\partial y \\ \partial/\partial z\end{pmatrix}, \tag{4.28}$$

it becomes clear why L_x, L_y, and L_z satisfy the same commutation relation

$$[L_i, L_j] = i\varepsilon_{ijk}L_k \tag{4.29}$$

as S_x, S_y, and S_z and yield the structure constants ε_{ijk} of SO(3).

√

Special Unitary Group SU(2)

Since unitary 2×2 matrices transform complex two-dimensional vectors preserving their norm, they represent the most general transformations of (a basis in the Hilbert space of) spin $\frac{1}{2}$ wave functions in nonrelativistic quantum mechanics. The basis states of this system are conventionally chosen to be

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

corresponding to spin $\frac{1}{2}$ up and down states, respectively. We can show that the **special unitary** group SU(2) of such unitary 2×2 matrices with determinant

+1 has the three Pauli matrices σ_i as generators. Therefore, we expect SU(2) to be of order 3 and to depend on three real continuous parameters ξ, η, ζ, which are often called the **Cayley–Klein** parameters and are essentially the SU(2) analog of Euler angles. We start with the observation that orthogonal 2×2 matrices [Eq. (4.1)] are real unitary matrices, so they form a subgroup of SU(2). We also see that

$$\begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix}$$

is unitary for real angle α with determinant +1. Therefore, these simple and manifestly unitary matrices form another subgroup of SU(2) from which we can obtain all elements of SU(2)—that is, the general 2×2 unitary matrix of determinant +1. For a two-component spin $\frac{1}{2}$ wave function of quantum mechanics, this diagonal unitary matrix corresponds to multiplication of the spin-up wave function with a phase factor $e^{i\alpha}$ and the spin-down component with the inverse phase factor. Using the real angle η instead of φ for the rotation matrix and then multiplying by the diagonal unitary matrices, we construct a 2×2 unitary matrix that depends on three parameters and is clearly a more general element of SU(2):

$$\begin{aligned}
&\begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix}\begin{pmatrix} \cos\eta & \sin\eta \\ -\sin\eta & \cos\eta \end{pmatrix}\begin{pmatrix} e^{i\beta} & 0 \\ 0 & e^{-i\beta} \end{pmatrix} \\
&= \begin{pmatrix} e^{i\alpha}\cos\eta & e^{i\alpha}\sin\eta \\ -e^{-i\alpha}\sin\eta & e^{-i\alpha}\cos\eta \end{pmatrix}\begin{pmatrix} e^{i\beta} & 0 \\ 0 & e^{-i\beta} \end{pmatrix} \\
&= \begin{pmatrix} e^{i(\alpha+\beta)}\cos\eta & e^{i(\alpha-\beta)}\sin\eta \\ -e^{-i(\alpha-\beta)}\sin\eta & e^{-i(\alpha+\beta)}\cos\eta \end{pmatrix}.
\end{aligned}$$

Defining $\alpha + \beta \equiv \xi$, $\alpha - \beta \equiv \zeta$, we have in fact constructed the general element of SU(2):

$$\mathsf{U}_2(\xi, \eta, \zeta) = \begin{pmatrix} e^{i\xi}\cos\eta & e^{i\zeta}\sin\eta \\ -e^{-i\zeta}\sin\eta & e^{-i\xi}\cos\eta \end{pmatrix} = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}, \tag{4.30}$$

where $|a|^2 + |b|^2 = 1$. It is easy to check that the determinant $\det(\mathsf{U}_2) = 1$ by the product theorem of Section 3.2 and that $\mathsf{U}_2^\dagger \mathsf{U}_2 = 1 = \mathsf{U}_2 \mathsf{U}_2^\dagger$ holds provided ξ, η, ζ are real numbers.

To get the generators, we differentiate

$$-i\frac{\partial \mathsf{U}_2}{\partial \xi}\bigg|_{\xi=0,\eta=0} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma_3, \tag{4.31a}$$

$$-i\frac{\partial \mathsf{U}_2}{\partial \eta}\bigg|_{\eta=0,\zeta=0} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} = \sigma_2. \tag{4.31b}$$

To avoid a factor $1/\sin\eta$ for $\eta \to 0$ upon differentiating with respect to ζ, we use instead the right-hand side of Eq. (4.30) for U_2 for pure imaginary $b = i\beta$

with $\beta \to 0$. Differentiating such a U_2, we get the third generator

$$-i\frac{\partial}{\partial\beta}\begin{pmatrix}\sqrt{1-\beta^2} & i\beta \\ i\beta & \sqrt{1-\beta^2}\end{pmatrix}\Bigg|_{\beta=0} = -i\begin{pmatrix}\frac{-\beta}{\sqrt{1-\beta^2}} & i \\ i & \frac{-\beta}{\sqrt{1-\beta^2}}\end{pmatrix}\Bigg|_{\beta=0} = \begin{pmatrix}0 & 1 \\ 1 & 0\end{pmatrix} = \sigma_1. \tag{4.31c}$$

Being generators, these Pauli matrices are all traceless and Hermitian. A correspondence with the physical world is obtained if we scale the SU(2) generators so that they yield the angular momentum commutators. With the Pauli matrices as generators, the elements U_1, U_2, U_3 of SU(2) may be generated by

$$\mathsf{U}_1 = \exp(-i\alpha\sigma_1/2), \quad \mathsf{U}_2 = \exp(-i\beta\sigma_2/2), \quad \mathsf{U}_3 = \exp(-i\gamma\sigma_3/2). \tag{4.32}$$

The three parameters are real, and we interpret them as angles. The extra scale factor $1/2$ is present in the exponents because $\mathsf{S}_i = \sigma_i/2$ satisfy the same commutation relations,[4]

$$[\mathsf{S}_i, \mathsf{S}_j] = i\varepsilon_{ijk}\mathsf{S}_k, \tag{4.33}$$

as the orbital angular momentum in Eq. (4.29).

Using the angular momentum matrix S_3, we have as the corresponding rotation operator $\mathsf{R}_z(\varphi) = \exp(i\varphi\sigma_3/2)$ in two-dimensional (complex wave function) space, analogous to Eq. (4.3) that gives the operator for rotating the Cartesian coordinates in the three-space.

For rotating the two-component vector wave function (spinor) or a spin $\frac{1}{2}$ particle relative to fixed coordinates, the rotation operator is $\mathsf{R}_z(\varphi) = \exp(-i\varphi\sigma_3/2)$ according to Eq. (4.27).

Using in Eq. (4.32) the Euler identity [Eq. (3.183)] we obtain

$$\mathsf{U}_j = \cos(\alpha/2) - i\sigma_j\sin(\alpha/2), \tag{4.34}$$

etc. Here, the parameter α appears as an angle, the coefficient of an angular momentum matrix–like φ in Eq. (4.27). With this identification of the exponentials, the general form of the SU(2) matrix (for rotating functions rather than coordinates) may be written as

$$\mathsf{U}(\alpha, \beta, \gamma) = \exp(-i\gamma\sigma_3/2)\exp(-i\beta\sigma_2/2)\exp(-i\alpha\sigma_3/2), \tag{4.35}$$

where the SU(2) Euler angles α, β, γ differ from the α, β, γ used in the definition of the Cayley–Klein parameters ξ, η, ζ by a factor of $1/2$. Further discussion of the relation between SO(3) and orbital angular momentum appears in Sections 4.3 and 11.7.

SUMMARY

The orbital angular momentum operators are the generators of the rotation group SO(3) and (1/2) the Pauli spin matrices are those for SU(2), the symmetry group of the Schrödinger equation for a spin $\frac{1}{2}$ particle such as the electron. Generators obey commutation relations characteristic of the group.

[4] The structure constants (ε_{ijk}) lead to the SU(2) representations of dimension $2J+1$ for generators of dimension $2J+1$, $J = 0, 1/2, 1, \ldots$. The **integral** J cases also lead to the representations of SO(3).

EXERCISES

4.2.1 (i) Show that the Pauli matrices are the generators of SU(2) without using the parameterization of the general unitary 2×2 matrix in Eq. (4.30).
Hint. Exploit the general properties of generators.

4.2.2 Prove that the general form of a 2×2 unitary, unimodular matrix is

$$\mathsf{U} = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix},$$

with $a^*a + b^*b = 1$. Based on this result, derive the parameterization of Eq. (4.30).

4.2.3 A **translation** operator $T(a)$ converts $\psi(x)$ to $\psi(x+a)$,

$$T(a)\psi(x) = \psi(x+a).$$

In terms of the (quantum mechanical) linear momentum operator $p_x = -id/dx$, show that $T(a) = \exp(iap_x)$ (i.e., p_x is the generator of translations).
Hint. Expand $\psi(x+a)$ as a Taylor series.

4.2.4 Consider the general SU(2) element Eq. (4.30) to be built up of three Euler rotations: (i) a rotation of $a/2$ about the z-axis, (ii) a rotation of $b/2$ about the new x-axis, and (iii) a rotation of $c/2$ about the new z-axis. (All rotations are counterclockwise.) Using the Pauli σ generators, show that these rotation angles are determined by

$$\begin{aligned} a &= \xi - \zeta + \pi/2 = \alpha + \pi/2 \\ b &= 2\eta \qquad\quad\; = \beta \\ c &= \xi + \zeta - \pi/2 = \gamma - \pi/2. \end{aligned}$$

Note. The angles a and b here are not the a and b of Eq. (4.30).

4.2.5 We know that any 2×2 matrix A can be expanded as $\mathsf{A} = a_0 \cdot 1 + \mathbf{a} \cdot \boldsymbol{\sigma}$, where 1 is the two-dimensional unit matrix. Determine a_0 and $\mathbf{a}$ for the general SU(2) matrix in Eq. (4.30).

4.2.6 Rotate a nonrelativistic wave function $\tilde{\psi} = (\psi_\uparrow, \psi_\downarrow)$ of spin $\frac{1}{2}$ about the z-axis by a small angle $d\theta$. Find the corresponding generator.

4.3 Orbital Angular Momentum

The classical concept of angular momentum $\mathbf{L}_{\text{class}} = \mathbf{r} \times \mathbf{p}$ is presented in Section 1.3 to introduce the cross product. Following the usual Schrödinger representation of quantum mechanics, the classical linear momentum $\mathbf{p}$ is replaced by the operator $-i\boldsymbol{\nabla}$. The quantum mechanical orbital angular