Chapter 3

Representations of Groups

How can it be that mathematics, being after all a product of human thought which is independent of experience, is so admirably appropriate to the objects of reality?
—Albert Einstein

The structure of abstract groups developed in Chapter 2 forms the basis for the application of group theory to physical problems. Typically in such applications, the group elements correspond to symmetry operations which are carried out on spatial coordinates. When these operations are represented as linear transformations with respect to a coordinate system, the resulting matrices, together with the usual rule for matrix multiplication, form a group that is equivalent to the group of symmetry operations in a sense to be made precise later in this chapter. In essence, these matrices form what is called a *representation* of the symmetry group with each element corresponding to a particular matrix.

For applications to quantum mechanics, as we have seen in Section 1.2, the symmetry operations are performed on the Hamiltonian, whose invariance properties determine the symmetry group. The wavefunctions, which do not all share the symmetry of the Hamiltonian, will be seen to determine the representations of the symmetry group in the sense described above. These representations will, in turn, provide a classification scheme for the eigenfunctions of the Hamiltonian, in analogous fashion to the identification of even and odd eigenfunctions in Section 1.2. The strength of the group-theoretic formalism that we will develop is that this procedure can be carried out in a systematic fashion for a Hamiltonian having any symmetry without undue computational effort.

In this chapter, we will set out the basic definitions that enable us to construct a mathematical definition of what we mean by a representation and discuss the basic types of representation. In the next chapter we will develop a number of remarkable properties of representations that lie at the heart of applications of discrete group theory to quantum mechanics.

3.1 Homomorphisms and Isomorphisms

Consider two finite groups G and G' with elements $\{e, a, b, \ldots\}$ and $\{e', a', b', \ldots\}$ and which need not be of the same order. Suppose there is a mapping ϕ between the elements of G and G' which preserves their composition rules, i.e., if $a' = \phi(a)$ and $b' = \phi(b)$, then

$$\phi(ab) = \phi(a)\phi(b) = a'b'$$

If the order of the two groups is the same, then this mapping is said to be an **isomorphism** and the two groups are **isomorphic** to one another. This is denoted by $G \approx G'$. If the order of the two groups is *not* the same, then the mapping is a **homomorphism** and the two groups are said to be **homomorphic**. Thus, an isomorphism is a one-to-one correspondence between two groups, while a homomorphism is a many-to-one correspondence. An isomorphism preserves the structure of the original group, but a homomorphism causes some of the structure of the original group to be lost. Both properties are reflected in the behavior of multiplication tables under these mappings. Homomorphisms and isomorphisms are not limited to finite groups nor even to groups with discrete elements.

Example 3.1. We saw in Sec. 2.2 that S_3 is isomorphic to the planar symmetry operations of an equilateral triangle, since there is a one-to-one correspondence between the elements of the two groups and they have the same multiplication table. On the other hand, consider the correspondence between the elements of S_3 and the elements of the quotient group of S_3 discussed in Examples 2.9 and 2.11):

$$\{e, d, f\} \mapsto \{\mathcal{E}\}, \qquad \{a, b, c\} \mapsto \{\mathcal{A}\} \tag{3.1}$$

i.e. the mapping ϕ is defined by

$$\begin{array}{lll} \phi(e) = \mathcal{E} & \phi(d) = \mathcal{E} & \phi(f) = \mathcal{E} \\ \phi(a) = \mathcal{A} & \phi(b) = \mathcal{A} & \phi(c) = \mathcal{A} \end{array} \tag{3.2}$$

This is a *homomorphism* because three elements of S_3 correspond to a single element of the quotient group. To see that this mapping preserves multiplication, we rearrange the multiplication table of S_3 (Example 2.2) as follows:

	e	d	f	a	b	c
e	e	d	f	a	b	c
d	d	f	e	c	a	b
f	f	e	d	b	c	a
a	a	b	c	e	d	f
b	b	c	a	f	e	d
c	c	a	b	d	f	e

$\mapsto$

	$\mathcal{E}$	$\mathcal{A}$
$\mathcal{E}$	$\mathcal{E}$	$\mathcal{A}$
$\mathcal{A}$	$\mathcal{A}$	$\mathcal{E}$

where the mapping of the multiplication table onto the elements $\{\mathcal{E}, \mathcal{A}\}$ is precisely that of a two-element group (cf. Example 2.9). This homomorphism clearly causes some of the structure of the original group to be lost. For example, S_3 is non-Abelian group, but the two-element group is Abelian.∎

3.2 Representations

A **representation** of dimension n of an abstract group G is a homomorphism or isomorphism between the elements of G and the group of nonsingular $n \times n$ matrices (i.e. $n \times n$ matrices with non-zero determinant) with complex entries and with ordinary matrix multiplication as the composition law (Example 2.4). An isomorphic representation

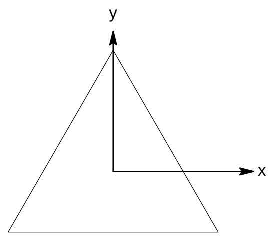

Figure 3.1: The coordinate system used to generate a two-dimensional representation of the symmetry group of the equilateral triangle. The origin of the coordinate system coincides with the geometric center of the triangle.

is called a **faithful** representation and a homomorphic representation is called an **unfaithful** representation.

According to this definition, if elements a and b of G are assigned matrices $D(a)$ and $D(b)$, then $D(a)D(b) = D(ab)$. The nonsingular nature of the matrices is required because inverses must be contained in the set (Example 2.4). Representations can also be comprised of numbers; the dimensionality of such representations is unity.

Example 3.2. Consider the following matrix representation of S_3 based on the correspondence with planar symmetry operations of an equilateral triangle:

$$
\begin{aligned}
&e = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad a = \tfrac{1}{2}\begin{pmatrix} 1 & -\sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}, \quad b = \tfrac{1}{2}\begin{pmatrix} 1 & \sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix} \\
&c = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad d = \tfrac{1}{2}\begin{pmatrix} -1 & -\sqrt{3} \\ \sqrt{3} & -1 \end{pmatrix}, \quad f = \tfrac{1}{2}\begin{pmatrix} -1 & \sqrt{3} \\ -\sqrt{3} & -1 \end{pmatrix}
\end{aligned}
\tag{3.3}
$$

These matrices were generated by regarding each of the symmetry operations as a linear transformation in the coordinate system shown in Fig. 3.1. Matrices a, b, and c correspond to reflections, so their determinant is -1, while matrices d and f correspond to rotations, so their determinant is 1. These matrices form a faithful representation of S_3.

Consider now the following mapping between the elements of S_3 and the set $\{1, -1\}$:

$$\{e, f\} \mapsto \{1\}, \qquad \{a, b, c\} \mapsto \{-1\} \tag{3.4}$$

This is essentially a mapping between the elements of S_3 and the determinant of their matrix representation discussed above. Thus, the identity matrix e and the rotations d and f have determinants of 1, while the reflections a, b, and c have determinants of -1. The physical interpretation of this homomorphism is therefore as a mapping from the individual elements of S_3 to their parity, i.e., whether they change the orientation of the coordinate system (-1) or not (1).[1] Since the determinant provides less information about a transformation than its matrix representation, it is clear that some information about the group structure of S_3 is not preserved by this homomorphism.

Finally, we note that the mapping of *all* elements to unity,

$$\{e, a, b, c, d, f\} \mapsto 1$$

is a representation of any group, though clearly an unfaithful one. This is called the **identical representation**. In the present case, the identical representation corresponds to a mapping from the group element to the absolute value of the determinant. Since all of the transformations preserve the lengths of vectors, any product of these transformations does so as well. ∎

Representations of groups are important in quantum mechanics for several reasons. First, the eigenfunctions of a Hamiltonian will transform under the symmetry operations of that Hamiltonian according to a particular representation of that group. Second, quantum mechanical operators are often written in terms of their matrix elements, so it is convenient to write symmetry operations in the same kind of matrix representation. Moreover, the evaluation of these matrix elements may sometimes be simplified by identifying the appropriate selection rules

[1] In terms of the operations of S_3, even parity corresponds to an even number of pairwise interchanges, while odd parity corresponds to an odd number of such interchanges.

(Section 1.2). Finally, the algebra of matrices is generally simpler to carry out than abstract symmetry operations. Thus, in the next section, we discuss some of the important properties of matrix representations of groups.

3.3 Reducible and Irreducible Representations

The definition of a representation provides for considerable flexibility in constructing matrix representations, which is manifested in several ways, but also indicates that representations are not unique. We consider some examples.

Given a matrix representation

$$\Big\{D(e), D(a), D(b), \ldots\Big\}$$

of an abstract group with elements $\{e, a, b, \ldots\}$, we can obtain a new set of matrices which also form a representation by performing a transformation known variously as a **similarity**, **equivalence**, or **canonical** transformation (cf. Sec. 2.6):

$$\Big\{BD(e)B^{-1}, BD(a)B^{-1}, BD(b)B^{-1}, \ldots\Big\} \tag{3.5}$$

Such transformations arise quite naturally, for example, in carrying out a change of basis for a set of matrices. Thus, suppose one begins with the matrix equation $\boldsymbol{b} = A\boldsymbol{a}$ relating two vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ through a transformation A. If we now wish to express this equation in another basis which is obtained from the original basis by applying a transformation B, we can write

$$B\boldsymbol{b} = BA\boldsymbol{a} = BAB^{-1}B\boldsymbol{a}$$

so in the new basis, our original equation becomes

$$\boldsymbol{b}' = A'\boldsymbol{a}'$$

where $\boldsymbol{b}' = B\boldsymbol{b}$, $\boldsymbol{a}' = B\boldsymbol{a}$, and $A' = BAB^{-1}$. A similarity transformation can therefore be interpreted as a sequence of transformations involving first a transformation to the original basis (B^{-1}), then performing the transformation A, and finally transforming back to the new basis (B). Referring back to the discussion in Section 2.6 on conjugacy classes, we see that group elements in the same conjugacy class represent the same type of transformation (e.g., reflection or rotation) which can be transformed into one another by particular symmetry operations.

Suppose we have representations of dimensions m and n. We can construct a representation of dimension $m+n$ by forming block-diagonal matrices:

$$\left\{\begin{bmatrix} D(e) & 0 \\ 0 & D'(e) \end{bmatrix}, \begin{bmatrix} D(a) & 0 \\ 0 & D'(a) \end{bmatrix}, \begin{bmatrix} D(b) & 0 \\ 0 & D'(b) \end{bmatrix}, \ldots\right\} \tag{3.6}$$

where $\{D(e), D(a), D(b), \ldots\}$ is an n-dimensional representation and $\{D'(e), D'(a), D'(b), \ldots\}$ an m-dimensional representation of the group G, and the symbol 0 is an $n \times m$ or an $m \times n$ zero matrix, as required by its position in the supermatrix. Each of the $m+n$-dimensional matrices formed in this manner is called a **direct sum** of the n- and m-dimensional component matrices. The direct sum is denoted by "$\oplus$" to distinguish it from the ordinary addition of two matrices. Thus, we can write the representation in (3.6) as

$$\left\{D(e) \oplus D'(e), D(a) \oplus D'(a), D(b) \oplus D'(b), \cdots\right\}$$

The two representations that form this direct sum can be either distinct or identical and, of course, the block-diagonal form can be continued indefinitely simply by incorporating additional representations in diagonal blocks. However, in all such constructions, we are not actually generating anything intrinsically new; we are simply reproducing the properties of known representations. Thus, although representations are a convenient way of associating matrices with group elements, the freedom we have in constructing representations, exemplified in (3.5) and (3.6), does not readily demonstrate that these matrices embody any intrinsic characteristics of the group they represent. Accordingly, we now describe a way of classifying equivalent representations and then introduce a refinement of our definition of a representation.

To overcome the problem of nonuniqueness posed by representations that are related by similarity transformations we consider the sum of the diagonal elements of an $n \times n$ matrix A, called the **trace** of A and by "tr":

$$\mathrm{tr}(A) = \sum_{i=1}^{n} A_{ii}$$

The utility of the trace stems from its *invariance* under similarity transformations, i.e.,

$$\mathrm{tr}(A) = \mathrm{tr}(BAB^{-1})$$

The importance of this invariance, the proof of which is discussed in Problem Set 4, is that, although there is an infinite variety of representations related by similarity transformations, each such representation has the same set of traces associated with each of its elements.

But working with the trace alone does not alleviate the nonuniqueness of representations posed by (3.6). To address this issue, we introduce the concept of an *irreducible* representation. Representations such as those in (3.6) are termed *reducible* because they are the direct sum of two (or more) representations. We could, of course, perform a similarity transformation to obtain a representation that is not in block form, but the representation so obtained is still deemed to be reducible because it was obtained from matrices which originally were in block form. Based on these considerations, we define reducible and irreducible representations as follows:

Definition. If the *same* similarity transformation brings all of the matrices of a representation into the same block form (by which we mean matrices of the same dimension in the same positions), then this representation is said to be **reducible**. Otherwise, the representation is said to be **irreducible**.

Thus, irreducible representations cannot be expressed in terms of representations of lower dimensionality. One-dimensional representations are, by definition, always irreducible. Determining the irreducible representations of groups is one of the central issues to be covered in the following chapters.

Example 3.4. All of the representations of S_3 discussed in Example 3.2 are *irreducible*. This is clear for the identical representation and for the representation in (3.4), since they are composed of numbers. But we can use these representations to construct the following manifestly *reducible* representation of S_3:

$$e = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad a = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad b = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$c = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad d = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad f = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

The representation in (3.3) is *irreducible*. There is no similarity transformation that will bring all of the matrices into block-diagonal form which, for the case here, means simple diagonalization. The easiest way to see this is from the point of view of the commutability of two matrices. If two matrices can be brought into diagonal form by the same similarity transformation, then they commute. As diagonal matrices, they certainly commute, so they must also commute in their original form. But a glance at the multiplication table for these matrices (recall that they are a *faithful* representation of S_3) in Example 2.2 shows that they do not all commute. Hence, they cannot all be simultaneously diagonalized, so this representation is *irreducible*. ∎

3.4 Unitary Representations

Representations of groups are useful because of orthogonality theorems which we will prove in the next chapter. As background to that discussion, we will prove in this section an important result about the unitarity of representations. But we first review some general properties of matrices.

We begin by considering the transformation of an $n \times n$ matrix A with entries A_{ij}, $i, j = 1, 2, \ldots, n$, under the action of various operations. The *complex conjugate* of A, denoted by A^*, has entries which are the complex conjugates of the corresponding entries of A:

$$(A^*)_{ij} = (A_{ij})^* \tag{3.7}$$

The *transpose* of A, denoted by $A^{\rm t}$, has its rows and columns interchanged with respect to those of A:

$$(A^{\rm t})_{ij} = A_{ji} \tag{3.8}$$

When applied to vectors, the transpose transforms a row vector into a column vector and *vice versa*. The transpose of a product of matrices $A, B, C, \ldots$ is

$$(ABC\cdots)^{\rm t} = \cdots C^{\rm t} B^{\rm t} A^{\rm t} \tag{3.9}$$

i.e., the order of matrix multiplication is *reversed*. This can be proven easily from the definition (3.8). Finally, the *adjoint* or **Hermitian conjugate** of A, denoted by $A^\dagger$, is the transposed conjugate of A, i.e.

$$(A^\dagger)_{ij} = (A_{ji})^* \tag{3.10}$$

In common with the transpose, the application of the Hermitian conjugate to a product of matrices $A, B, C, \ldots$ can be expressed as a product of Hermitian conjugates of the individual matrices, but with the order reversed:

$$(ABC\cdots)^\dagger = \cdots C^\dagger B^\dagger A^\dagger \tag{3.11}$$

3.4.1 Hermitian and Orthogonal Matrices

A matrix A is **Hermitian** if

$$A^\dagger = A \tag{3.12}$$

Hermitian matrices and Hermitian operators are familiar from quantum mechanics, where their properties of having real eigenvalues and orthogonal eigenvectors are of fundamental importance. A matrix A is **orthogonal** if its transpose is its inverse:

$$A^{\rm t} A = A A^{\rm t} = I \tag{3.13}$$

where I is the $n \times n$ unit matrix. In terms of matrix components, this condition reads

$$\sum_{k=1}^{n} a_{ki} a_{kj} = \sum_{k=1}^{n} a_{ik} a_{jk} = \delta_{ij} \tag{3.14}$$

where

$$\delta_{ij} = \begin{cases} 0, & \text{if } i \neq j; \\ 1, & \text{if } i = j \end{cases} \tag{3.15}$$

is the **Kronecker delta**. Thus, the rows of an orthogonal matrix are mutually orthogonal, as are the columns. The consequences of the orthogonality of a transformation matrix can be seen by examining the effect of applying an orthogonal matrix A to two n-dimensional vectors $\boldsymbol{u}$ and $\boldsymbol{v}$, yielding vectors $\boldsymbol{u}'$ and $\boldsymbol{v}'$:

$$\boldsymbol{u}' = A\boldsymbol{u}, \qquad \boldsymbol{v}' = A\boldsymbol{v}$$

We now take the scalar, or 'dot,' product between $\boldsymbol{u}'$ and $\boldsymbol{v}'$:

$$(\boldsymbol{u}', \boldsymbol{v}') = (\boldsymbol{u}')^{\mathrm{t}} \boldsymbol{v}' = (A\boldsymbol{u})^{\mathrm{t}} A\boldsymbol{v} = \boldsymbol{u}^{\mathrm{t}} A^{\mathrm{t}} A\boldsymbol{v} = \boldsymbol{u}^{\mathrm{t}} \boldsymbol{v} = (\boldsymbol{u}, \boldsymbol{v}) \tag{3.16}$$

where we have used (3.11) and the fact that A is orthogonal. This shows that the relative orientations and the lengths of vectors are preserved by orthogonal transformations. Such transformations are either rigid rotations, which preserve the "handedness" (i.e., left or right) of a coordinate system, and are called **proper** rotations, or reflections, which reverse the "handedness" of a coordinate system, and are called **improper** "rotations."

3.4.2 Unitary Matrices

A third type of matrix, called **unitary**, has the property that

$$A^{\dagger} A = A A^{\dagger} = I \tag{3.17}$$

By writing this condition in terms of matrix components,

$$\sum_{k=1}^{n} a_{ki}^{*} a_{kj} = \sum_{k=1}^{n} a_{ik} a_{jk}^{*} = \delta_{ij} \tag{3.18}$$

we see that, in common with orthogonal matrices, the rows and columns of a unitary matrix are orthogonal, but with respect to a different scalar product. For two vectors $\boldsymbol{u}$ and $\boldsymbol{v}$, this scalar product is defined as

$$(\boldsymbol{u}, \boldsymbol{v}) = \boldsymbol{u}^\dagger \boldsymbol{v} \tag{3.19}$$

This generalizes the familiar dot product to complex vectors in n dimensions. We can now show, by proceeding as above, that unitary transformations leave the scalar product invariant:

$$(\boldsymbol{u}', \boldsymbol{v}') = (\boldsymbol{u}')^\dagger \boldsymbol{v}' = (A\boldsymbol{u})^\dagger A\boldsymbol{v} = \boldsymbol{u}^\dagger A^\dagger A\boldsymbol{v} = \boldsymbol{u}^\dagger \boldsymbol{v} = (\boldsymbol{u}, \boldsymbol{v}) \tag{3.20}$$

The property of unitarity, when applied to operators, is of immense importance in quantum mechanics because it enables changes of bases to be performed while preserving the orthogonality of bases and, thus, the overlap between wavefunctions. In this sense, unitary matrices are associated with proper and improper "rotations," in analogy with orthogonal matrices.

3.4.3 Diagonalization of Hermitian Matrices*

Let H be an $n \times n$ Hermitian matrix. The eigenvalue equation for this matrix is

$$H\boldsymbol{a} = \lambda \boldsymbol{a} \tag{3.21}$$

By writing this equation as

$$(H - \lambda I)\boldsymbol{a} = 0 \tag{3.22}$$

the eigenvalue equation in (3.21) has nontrivial solutions for $\boldsymbol{a}$ if and only if the determinant of the matrix of coefficients in (3.22) vanishes:

$$\det(H - \lambda I) = 0 \tag{3.23}$$

The expansion of the determinant leads to an nth-order polynomial in λ whose solution yields the n (not necessarily distinct) eigenvalues of H: $\lambda_1, \lambda_2, \ldots, \lambda_n$.

We now show that the eigenvectors of H which correspond to *distinct* eigenvalues are orthogonal. Consider the eigenvalue equations for two eigenvectors $\boldsymbol{a}$ and $\boldsymbol{b}$ corresponding to distinct eigenvalues λ and μ, respectively:

$$H\boldsymbol{a} = \lambda\boldsymbol{a} \tag{3.24}$$

$$H\boldsymbol{b} = \mu\boldsymbol{b} \tag{3.25}$$

We now take the scalar product between $\boldsymbol{b}$ and (3.24) and that between (3.25) and $\boldsymbol{a}$:

$$\boldsymbol{b}^\dagger(H\boldsymbol{a}) = \lambda\boldsymbol{b}^\dagger\boldsymbol{a} \tag{3.26}$$

$$(\boldsymbol{b}^\dagger H^\dagger)\boldsymbol{a} = \mu\boldsymbol{b}^\dagger\boldsymbol{a} \tag{3.27}$$

Subtracting (3.27) from (3.26), and using the fact that H is Hermitian yields

$$(\lambda - \mu)\boldsymbol{b}^\dagger\boldsymbol{a} = \boldsymbol{b}^\dagger H\boldsymbol{a} - \boldsymbol{b}^\dagger H^\dagger\boldsymbol{a} = 0 \tag{3.28}$$

which, since $\lambda \neq \mu$, implies that $\boldsymbol{b}^\dagger\boldsymbol{a} = 0$, i.e., that $\boldsymbol{a}$ and $\boldsymbol{b}$ are orthogonal. If λ and μ are not distinct, we must use a Gram–Schmidt procedure to explicitly construct an orthogonal set of eigenvectors associated with the degenerate eigenvalue. Thus, the eigenvectors of a Hermitian matrix can always be chosen to form an orthogonal set.

Consider the matrix U whose columns are the eigenvectors of H:

$$U = (\boldsymbol{a}_1, \boldsymbol{a}_2, \ldots, \boldsymbol{a}_n)$$

We can then write (3.21) in a form that subsumes *all* the eigenvectors of H as follows:

$$HU = UD \tag{3.29}$$

where D is the diagonal matrix whose entries are the eigenvalues of H:

$$D = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_d \end{pmatrix}$$

Since the rows of U are composed of the (orthogonal) eigenvectors of H, it has the property that (cf. 3.18)

$$U^\dagger U = UU^\dagger = I$$

i.e., $U^{-1} = U^\dagger$, so U is *unitary.* Hence, we can rewrite (3.29) as

$$U^{-1}HU = U^\dagger HU = D$$

We have proven the following theorem:

Theorem 3.1. Any Hermitian matrix can be diagonalized by an appropriate unitary transformation.

This theorem will be used in the next section to prove an important result concerning the existence of unitary group representations.

3.4.4 Transformation to Unitary Representations

We have seen in Section 3.3 that there is considerable flexibility in constructing group representations. In this section, we take a first step in restricting this freedom by showing that any representation can be expressed entirely in terms of unitary matrices. Quite apart from the convenient properties of unitary matrices discussed in Section 3.4.2, this theorem allows to think of group representations as proper and improper complex "rotations."

Theorem 3.2. Every representation can be brought into unitary form by a similarity transformation.

Proof. Let $\{A_1, A_2, \ldots, A_{|G|}\}$ be a d-dimensional representation of a group G, i.e., the A_α are a set of $|G|$ $d \times d$ matrices with nonvanishing determinants. From these matrices we form a matrix H given by the sum

$$H = \sum_{\alpha=1}^{|G|} A_\alpha A_\alpha^\dagger$$

This matrix is Hermitian because, using the property (3.11),

$$H^\dagger = \sum_\alpha (A_\alpha A_\alpha^\dagger)^\dagger = \sum_\alpha A_\alpha A_\alpha^\dagger = H$$

According to Theorem 3.1, any Hermitian matrix can be diagonalized by some unitary transformation U. Denoting the diagonalized form of H by D, we have $D = U^\dagger H U$, which enables us to write D as

$$D = \sum_\alpha U^\dagger A_\alpha A_\alpha^\dagger U = \sum_\alpha (U^\dagger A_\alpha U)(U^\dagger A_\alpha^\dagger U) = \sum_\alpha (U^\dagger A_\alpha U)(U^\dagger A_\alpha U)^\dagger$$

By introducing the notation $\tilde{A}_\alpha = U^\dagger A_\alpha U$, we can write the last equation in a more concise form as

$$D = \sum_\alpha \tilde{A}_\alpha \tilde{A}_\alpha^\dagger \tag{3.30}$$

The diagonal elements of D are real, because

$$\begin{aligned} D_{kk} &= \sum_\alpha \sum_j (\tilde{A}_\alpha)_{kj} (\tilde{A}^\dagger{}_\alpha)_{jk} \\ &= \sum_\alpha \sum_j (\tilde{A}_\alpha)_{kj} (\tilde{A}_\alpha)^*_{kj} \\ &= \sum_\alpha \sum_j \left| (\tilde{A}_\alpha)_{kj} \right|^2 \end{aligned}$$

for $k = 1, 2, \ldots, d$, and positive, because the summation over j includes a diagonal element of the identity, which is a $d \times d$ unit matrix, and hence is equal to unity. Thus, the diagonal matrix $D^{1/2}$,

$$D^{1/2} = \begin{pmatrix} D_{11}^{1/2} & 0 & \cdots & 0 \\ 0 & D_{22}^{1/2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & D_{dd}^{1/2} \end{pmatrix}$$

and $D^{-1/2}$, which is given by an analogous expression, both have positive entries.

We now form the matrices

$$B_\alpha = D^{-1/2}\tilde{A}_\alpha D^{1/2}$$

from which we obtain the corresponding Hermitian conjugates:

$$B_\alpha^\dagger = (D^{-1/2}\tilde{A}_\alpha D^{1/2})^\dagger = D^{1/2}\tilde{A}^\dagger{}_\alpha D^{-1/2}$$

We will now demonstrate that the B_α are unitary by first showing that the product $B_\alpha B_\alpha^\dagger$ is equal to the identity matrix. The product $B_\alpha B_\alpha^\dagger$ is given by

$$\begin{aligned} B_\alpha B_\alpha^\dagger &= \Big(D^{-1/2}\tilde{A}_\alpha D^{1/2}\Big)\Big(D^{1/2}\tilde{A}^\dagger{}_\alpha D^{-1/2}\Big) \\ &= D^{-1/2}\tilde{A}_\alpha D\tilde{A}^\dagger{}_\alpha D^{-1/2} \end{aligned}$$

The definition of D in (3.30) and the associativity of matrix multiplication allow us to write this expression as

$$\begin{aligned} B_\alpha B_\alpha^\dagger &= D^{-1/2}\sum_j \tilde{A}_\alpha\tilde{A}_\beta\tilde{A}^\dagger{}_\beta\tilde{A}^\dagger{}_\alpha D^{-1/2} \\ &= D^{-1/2}\sum_j (\tilde{A}_\alpha\tilde{A}_\beta)(\tilde{A}_\alpha\tilde{A}_\beta)^\dagger D^{-1/2} \end{aligned}$$

Since the A_α are a representation of G, then so are the $\tilde{A}_\alpha$ (Problem 3, Problem Set 4). Hence, the product $\tilde{A}_\alpha\tilde{A}_\beta$ is another matrix $\tilde{A}_\gamma$ in this representation. Moreover, according to the Rearrangement Theorem, the sum over all β means that the set of $\tilde{A}_\gamma$ obtained from these products contains the matrix corresponding to each group element once and only once. Thus,

$$B_\alpha B_\alpha^\dagger = D^{-1/2}\underbrace{\sum_\gamma \tilde{A}_\gamma\tilde{A}_\gamma^\dagger}_{D} D^{-1/2} = I$$

where I is the $d \times d$ unit matrix. This result can also be used to show that $B_\alpha^\dagger B_\alpha = I$. Thus, the B_α, which are obtained from the original representation by a similarity transformation,

$$B_\alpha = D^{-1/2}U^{-1}A_\alpha U D^{1/2} = (UD^{1/2})^{-1}A_\alpha(UD^{1/2})$$

form a *unitary* representation of G. Hence, without any loss of generality, we may always assume that a representation is unitary. ▮

3.5 Summary

The main concepts introduced in this chapter are faithful and unfaithful representations, based on isomorphic and homomorphic mappings, respectively, reducible and irreducible representations, and the fact that we may confine ourselves to unitary representations of groups. In the next chapter we will focus on irreducible representations, both faithful and unfaithful, since these cannot be decomposed into representations of lower dimension and are, therefore, "intrinsic" to a symmetry group, since *all* reducible representations will be shown to be composed of direct sums of irreducible representations. Irreducible representations occupy a special place in group theory because they can be classified for a given symmetry group solely according to their traces and dimension.