2 ABSTRACT GROUP THEORY

2-1 Definitions and Nomenclature

By a group we mean a set of *elements* $A, B, C, \ldots$ such that a form of *group multiplication* may be defined which associates a third element with any ordered pair. This multiplication must satisfy the requirements:

1. The product of any two elements is in the set; i.e., the set is *closed* under group multiplication.

2. The *associative law* holds; for example, $A(BC) = (AB)C$.

3. There is a *unit element* E such that $EA = AE = A$.

4. There is in the group an inverse A^{-1} to each element A such that $AA^{-1} = A^{-1}A = E$.

For the present we shall restrict our attention primarily to *finite groups*. These contain a finite number h of group elements, where h is said to be the

order of the group. If group multiplication is commutative, so that $AB = BA$ for all A and B, the group is said to be *Abelian*.

2-2 Illustrative Examples

An example of an Abelian group of infinite order is the set of all positive and negative integers including zero. In this case, ordinary addition serves as the group-multiplication operation, zero serves as the unit element, and $-n$ is the inverse of n. Clearly the set is closed, and the associative law is obeyed.

An example of a non-Abelian group of infinite order is the set of all $n \times n$ matrices with nonvanishing determinants. Here the group-multiplication operation is matrix multiplication, and the unit element is the $n \times n$ unit matrix. The inverse matrix of each matrix may be constructed by the usual methods,[1] since the matrices are required to have nonvanishing determinants.

A physically important example of a finite group is the set of covering operations of a symmetrical object. By a covering operation, we mean a rotation, reflection, or inversion which would bring the object into a form indistinguishable from the original one. For example, all rotations about the center are covering operations of a sphere. In such a group the product AB means the operation obtained by first performing B, then A. The unit operation is no operation at all, or perhaps a rotation through 2π. The inverse of each operation is physically apparent. For example, the inverse of a rotation is a rotation through the same angle in the reverse sense about the same axis.

As a complete example, which we shall often use for illustrative purposes, consider the non-Abelian group of order 6 specified by the following *group-multiplication table:*

	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D

The meaning of this table is that each entry is the product of the element labeling the row times the element labeling the column. For example, $AB = D \neq BA$. This table results, for example, if we take our elements to be the following six matrices, and if ordinary matrix multiplication is

[1] See Appendix A and references cited there.

used as the group-multiplication operation:

$$E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad B = \begin{pmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$$

$$C = \begin{pmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \qquad D = \begin{pmatrix} \frac{-1}{2} & \frac{\sqrt{3}}{2} \\ \frac{-\sqrt{3}}{2} & \frac{-1}{2} \end{pmatrix} \qquad F = \begin{pmatrix} \frac{-1}{2} & \frac{-\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{-1}{2} \end{pmatrix}$$

Verification of the table is left as a simple exercise.

The very same multiplication table could be obtained by considering the group elements $A, \ldots, F$ to represent the proper covering operations of

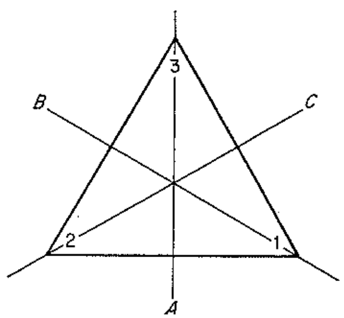

Fig. 2-1. *Symmetry axes of equilateral triangle.*

an equilateral triangle as indicated in Fig. 2-1. The elements A, B, and C are rotations by π about the axes shown. Element D is a clockwise rotation by $2\pi/3$ in the plane of the triangle, and F is a counterclockwise rotation through the same angle. The numbering of the corners destroys the symmetry so that the position of the triangle can be followed through successive operations. If we make the convention that we consider the rotation axes to be kept fixed in space (not rotated with the object), it is easy to verify that the multiplication table given above describes this group as well.

Two groups obeying the same multiplication table are said to be *isomorphic*.

2-3 Rearrangement Theorem

In the multiplication table in the example above, each column or row contains each element once and only once. This rule is true in general and is

called the *rearrangement theorem*. Stated more formally, in the sequence

$$EA_k, A_2A_k, A_3A_k, \ldots, A_hA_k,$$

each group element A_i appears exactly once (in the form A_rA_k). The elements are merely rearranged by multiplying each by A_k.

PROOF: For any A_i and A_k, there exists an element $A_r = A_iA_k^{-1}$ in the group since the group contains inverses and is closed. Since $A_rA_k = A_i$ for this particular A_r, A_i must appear in the sequence at least once. But there are h elements in the group and h terms in the sequence. Hence there is no opportunity for any element to make more than a single appearance.

2-4 Cyclic Groups

For any group element X, one can form the sequence

$$X, X^2, X^3, \ldots, X^{n-1}, X^n = E$$

This is called the *period* of X, since the sequence would simply repeat this period over and over if it were extended. (Eventually we must find repetition, since the group is assumed to be finite.) The integer n is called the *order* of X, and this period clearly forms a group as it stands, although it need not exhaust all the elements of the group with which we started. Hence it may be said to form a *cyclic group* of order n. If it is indeed only part of a larger group, it is referred to as a cyclic *subgroup*.[1] We note that all cyclic groups must be Abelian.

In our standard example of the triangle, the period of D is D, $D^2 = F$, $D^3 = DF = E$. Thus D is of order 3, and D, F, E form a cyclic subgroup of our entire group of order 6.

2-5 Subgroups and Cosets

Let $\mathscr{S} = E, S_2, S_3, \ldots, S_g$ be a *subgroup* of order g of a larger group $\mathscr{G}$ of order h. We then call the set of g elements $EX, S_2X, S_3X, \ldots, S_gX$ a *right coset* $\mathscr{S}X$ if X is not in $\mathscr{S}$. (If X were in $\mathscr{S}$, $\mathscr{S}X$ would simply be the subgroup $\mathscr{S}$ itself, by the rearrangement theorem.) Similarly, we define the set $X\mathscr{S}$ as being a *left coset*. These cosets cannot be subgroups, since they cannot include the identity element. In fact, a coset $\mathscr{S}X$ contains *no* elements in common with the subgroup $\mathscr{S}$.

The proof of this statement is easily given by assuming, on the contrary, that for some element S_k we have $S_kX = S_l$, a member of $\mathscr{S}$. Then $X = S_k^{-1}S_l$, which is in the subgroup, and $\mathscr{S}X$ is not a coset at all, but just $\mathscr{S}$ itself.

[1] Although the concept is introduced here in connection with cyclic groups, subgroups need not be cyclic. Any subset of elements within a group which in itself forms a group is called a subgroup of the larger group.

Next we note that two right (or left) cosets of subgroup $\mathscr{S}$ in $\mathscr{G}$ either are identical or have no elements in common.

PROOF: Consider two cosets $\mathscr{S}X$ and $\mathscr{S}Y$. Assume that there exists a common element $S_kX = S_lY$. Then $XY^{-1} = S_k^{-1}S_l$, which is in $\mathscr{S}$. Therefore $\mathscr{S}XY^{-1} = \mathscr{S}$, by the rearrangement theorem. Postmultiplying both sides by Y leads to $\mathscr{S}X = \mathscr{S}Y$. Thus the two cosets are completely identical if a single common element exists.

If we combine the results of the preceding paragraphs, we can prove the following theorem: *The order g of a subgroup must be an integral divisor of the order h of the entire group.* That is, $h/g = l$, where the integer l is called the *index* of the subgroup $\mathscr{S}$ in $\mathscr{G}$.

PROOF: Each of the h elements of $\mathscr{G}$ must appear either in $\mathscr{S}$ or in a coset $\mathscr{S}X$, for some X. Thus each element must appear in one of the sets $\mathscr{S}, \mathscr{S}X_2, \mathscr{S}X_3, \ldots, \mathscr{S}X_l$, where we have listed all the *distinct* cosets of $\mathscr{S}$ together with $\mathscr{S}$ itself. But we have shown that there are no elements common to any of these collections of g elements. Hence it must be possible to divide the total number of elements h into an integral number of sets of g each, and consequently $h = l \times g$.

As an example, consider the subgroup $\mathscr{S} = A, E$ of our illustrative group of order 6. The right cosets with B and D are identical, namely, $\mathscr{S}B = \mathscr{S}D = B, D$. Also $\mathscr{S}C = \mathscr{S}F = C, F$. We note that, as proved in general, these cosets contain no common elements unless entirely identical and they contain no elements in common with $\mathscr{S}$. Also, the order (2) of the subgroup *is* an integral divisor of the order (6) of the group. To generalize, the order of *any* cyclic subgroup formed by the period of some group element must be a divisor of the order of the group.

2-6 Example Groups of Finite Order

1. *Groups of order* 1. The only example is the group consisting solely of the identity element E.

2. *Groups of order* 2. Again there is only one possibility, the group $(A, A^2 = E)$. This is an Abelian group, and in physical applications A might represent reflection, inversion, or an interchange of two identical particles.

3. *Groups of order* 3. In this case, if we start with two elements A and E, it must be that $A^2 = B \neq E$. Otherwise, if A^2 were to equal E, then (A, E) would form a subgroup of order 2 in a group of order 3, which would violate our theorem. Thus the only possibility is the cyclic group $(A, A^2 = B, A^3 = E)$.

4. *Groups of order* 4. With order 4 we begin to have more than one possible distinct group-multiplication table of given order. The two possibilities here are (1) the cyclic group $(A, A^2, A^3, A^4 = E)$ and (2) the

so-called *Vierergruppe* (A, B, C, E) whose multiplication table is:

	E	A	B	C
E	E	A	B	C
A	A	E	C	B
B	B	C	E	A
C	C	B	A	E

Both these groups are Abelian, and in both cases we can pick out subgroups of order 2, as allowed by our theorem. A physical example of the cyclic group of order 4 is provided by the four fold rotations about an axis. On the other hand, the *Vierergruppe* is the rotational-symmetry group of a rectangular solid, if A, B, C are taken to be the rotations by π about the three orthogonal symmetry axes.

5. *Groups of prime order.* These must all be cyclic Abelian groups. Otherwise the period of some element would have to appear as a subgroup whose order was a divisor of a prime number. This general result allows us to note at once that there can be only single groups of order 1, 2, 3, 5, 7, 11, 13, etc.

6. *Permutation groups (of factorial order).* One group of order $n!$ can always be set up based on all the permutations of n distinguishable things. (Of course, others, such as a cyclic group, can also be found.) A permutation can be specified by a symbol such as

$$\begin{pmatrix} 1 & 2 & 3 & \cdots & n \\ \alpha_1 & \alpha_2 & \alpha_3 & \cdots & \alpha_n \end{pmatrix}$$

where $\alpha_1, \alpha_2, \ldots, \alpha_n = 1, 2, \ldots, n$, except for order. The permutation described by this symbol is one in which the item in position i is shifted to the position indicated in the lower line. Successive permutations form the group-multiplication operation. As an example, our standard example group of order 6 can be viewed as the permutation group of the three numbered corners of the triangle. The permutations may be expressed in the above notation as

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

$$C = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} \qquad D = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix} \qquad F = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}$$

For example, operator A interchanges corners 1 and 2, whereas D replaces 1 by 3, 2 by 1, and 3 by 2, corresponding to a clockwise rotation by $2\pi/3$.

Applying B followed by A leads to

$$AB = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}\begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix} = D$$

which is consistent with the group-multiplication table worked out previously.

Because of the identity of like particles, permutation of them leaves the Hamiltonian invariant. Accordingly, the permutation group plays an important role in quantum theory.

2-7 Conjugate Elements and Class Structure

An element B is said to be *conjugate* to A if

$$B = XAX^{-1} \quad \text{or} \quad A = X^{-1}BX$$

where X is some member of the group. Clearly this is a reciprocal property of the pair of elements. Further, if B and C are both conjugate to A, they are conjugate to each other.

PROOF: Assume that

$$B = XAX^{-1} \quad \text{and} \quad C = YAY^{-1}$$

Then
$$A = Y^{-1}CY$$

and
$$B = XY^{-1}CYX^{-1} = (XY^{-1})C(XY^{-1})^{-1}$$
$$= ZCZ^{-1}$$

[In this proof we have used the fact that the inverse of the product of two group elements is the product of the inverses of the elements in inverse order. This is clearly true, since $(RS)(S^{-1}R^{-1}) = R(SS^{-1})R^{-1} = RR^{-1} = E$.]

The properties of conjugate elements given above allow us to collect all mutually conjugate elements into what is called a *class* of elements. The class including A_i is found by forming all products of the form

$$EA_iE^{-1} = A_i,\ A_2A_iA_2^{-1}, \ldots, A_hA_iA_h^{-1}$$

Of course, some elements may be found several times by this procedure. By proceeding in this way, we can divide all the elements of the group among the various distinct classes. Luckily, we may usually avoid this rather tedious method by using physical-symmetry considerations, as shown below. For example, in the group of covering operations of an equilateral triangle, the two rotations by $2\pi/3$ form a class, the three rotations by π form a class, and, as always, *the identity element is in a class by itself.* The latter follows, since $AEA^{-1} = AA^{-1} = E$ for all A. Note that E is the *only class* which is also a *subgroup*, since all other classes must lack the identity element.

In Abelian groups, each element is in a class by itself, since $XAX^{-1} = AXX^{-1} = AE = A$.

If the group elements are represented by matrices, the traces of all elements in a class must be the same. This follows, since in this case the operation of conjugation becomes that of making a similarity transformation, which leaves the trace invariant.[1]

Physical interpretation of class structure. In physical applications the group elements can often be considered to be symmetry operations which are the covering operations of a symmetrical object. In this case, the operation $B = X^{-1}AX$ is the net operation obtained by first rotating the object to some equivalent position by X, next carrying out the operation A, and then undoing the initial rotation by X^{-1}. Thus B must be an operation of the same physical sort as A, such as a rotation through the same angle, but performed about some different (but physically equivalent) axis which is related to the axis of A by the group operation X^{-1}. This is the significance of operators being in the same class.

As a concrete example, consider the covering operations of the equilateral triangle indicated in Fig. 2-1. If we consider the conjugation of A with D, we have $D^{-1}AD = C$. To follow this through in detail, D rotates the triangle clockwise by $2\pi/3$ so that vertex 2 instead of 3 lies on axis A; next the rotation by π about the A axis interchanges 1 and 3; finally $D^{-1} = F$ rotates the triangle back $2\pi/3$ counterclockwise. This sequence leaves precisely the result of a single rotation by π about axis C, which is an axis equivalent to A but rotated $2\pi/3$ counterclockwise by the symmetry operator D^{-1}.

2-8 Normal Divisors and Factor Groups

If a subgroup $\mathscr{S}$ of a larger group $\mathscr{G}$ consists entirely of complete classes, it is called an *invariant subgroup*, or *normal divisor*. By consisting of complete classes, we mean that, if an element A is in $\mathscr{S}$, then all elements $X^{-1}AX$ are in $\mathscr{S}$, even when X runs over elements of $\mathscr{G}$ which are not in $\mathscr{S}$. Such a subgroup is called invariant because by the rearrangement theorem it is unchanged (except for order) by conjugation with any element of $\mathscr{G}$.

To allow a compact discussion, we introduce the notion of a *complex* such as $\mathscr{K} = (K_1, K_2, \ldots, K_n)$, which is a collection of group elements disregarding order. Such a complex can be multiplied by a single element or by another complex. For example,

$$\mathscr{K}X = (K_1X, K_2X, \ldots, K_nX)$$

and
$$\mathscr{K}\mathscr{R} = (K_1R_1, K_1R_2, \ldots, K_1R_m, \ldots, K_nR_m)$$

[1] See Appendix A.

Elements are considered to be included only once, regardless of how often they are generated.

We can now state our argument concisely by treating sets of elements as complexes. First, a subgroup is defined by the property of closure, that is, $\mathscr{S}\mathscr{S} = \mathscr{S}$. Second, if $\mathscr{S}$ is an *invariant* subgroup, then $X^{-1}\mathscr{S}X = \mathscr{S}$, for all X in the group $\mathscr{G}$. From this it follows that $\mathscr{S}X = X\mathscr{S}$, or, in words, the left and right cosets of an invariant subgroup are identical.

In Sec. 2-5 we have shown that there are a finite number $(l-1)$ of distinct cosets for any subgroup $\mathscr{S}$. We may denote each of these as a complex, and if $\mathscr{S}$ is an invariant subgroup, we have, for example, $\mathscr{K}_i = \mathscr{S}K_i = K_i\mathscr{S}$. Note that $\mathscr{S}K_i = \mathscr{S}K_j$ if K_i and K_j are group elements in the same coset, since we are not concerned with the order in which the elements of the complex appear. Together with the subgroup $\mathscr{S}$, this set of $(l-1)$ distinct complexes can themselves be regarded as the elements of a smaller group (of order $l = h/g$) on a higher level of abstraction. This new group is called the *factor group* of $\mathscr{G}$ with respect to the *normal divisor* (or invariant subgroup) $\mathscr{S}$. In this factor group, $\mathscr{S}$ forms the unit element. We can see this by considering

$$\mathscr{S}\mathscr{K}_i = \mathscr{S}(\mathscr{S}K_i) = (\mathscr{S}\mathscr{S})K_i = \mathscr{S}K_i = \mathscr{K}_i$$

Group multiplication works out as shown in the following example,

$$\mathscr{K}_i\mathscr{K}_j = (\mathscr{S}K_i)(\mathscr{S}K_j) = K_i\mathscr{S}\mathscr{S}K_j = K_i\mathscr{S}K_j = \mathscr{S}(K_iK_j) = (\mathscr{K}_i\mathscr{K}_j)$$

where the last expression refers to the complex which is the coset associated with the product K_iK_j. The concept of factor groups and normal divisors will prove useful in analyzing the structure of groups.

Isomorphy and homomorphy. We have already introduced the concept of isomorphy by noting that two groups having the same multiplication table are called isomorphic. This means that there is a one-to-one correspondence between the elements $A, B, \ldots$ of one group and those $A', B', \ldots$ of the other, such that $AB = C$ implies $A'B' = C'$, and vice versa.

Two groups are said to be *homomorphic* if there exists a correspondence between the elements of the two groups of the sort $A \leftrightarrow A_1', A_2', \ldots$. By this we mean that, if $AB = C$, then the product of any A_i' with any B_j' will be a member of the set C_k'. In general, a homomorphism is a many-to-one correspondence, as indicated here. It specializes to an isomorphism if the correspondence is one-to-one. For example, the group containing the single element E is homomorphic to any other group, since, in view of the fact that each group element is represented by E, group multiplication reduces simply to $EE = E$. A much less trivial example is provided by the homomorphic relation between any group and one of its factor groups (if it has one). The invariant subgroup $\mathscr{S}$ corresponds to all the members of $\mathscr{S}$, and the cosets $\mathscr{K}_i = \mathscr{S}K_i$ correspond to all members of the coset (including K_i and all other group elements having the same coset, which are just the members of $\mathscr{K}_i$). Thus, if $\mathscr{S}$ is of order g, there is a g-to-one correspondence between the original group elements and the elements of the factor group.

2-9 Class Multiplication

In this section we consider a different form of multiplication of collections of group elements in which we do keep track of the number of times an element appears. That is, $\mathscr{R} = \mathscr{K}$ implies that each element appears as often in $\mathscr{R}$ as in $\mathscr{K}$. In this notation

$$X^{-1}\mathscr{C}X = \mathscr{C} \tag{2-1}$$

where $\mathscr{C}$ is any complete *class* of the group and X is any element of the group. (Proof: Each element produced on the left must appear on the right because they are all conjugate to elements in $\mathscr{C}$ and hence are in $\mathscr{C}$ by the definition of a class. But each element on the left is different, because of the uniqueness of group multiplication, as is each on the right. These two statements are consistent only if the two sides of the equation are equal.)

The converse of this theorem is also true: any collection $\mathscr{C}$ obeying (2-1) for all X in the group is comprised wholly of complete classes. (Proof: First subtract all complete classes from both sides and denote any remainder by $\mathscr{R}$. Now consider any element R_i of $\mathscr{R}$ on the left in $X^{-1}\mathscr{R}X = \mathscr{R}$. Since this is assumed true for all X, $\mathscr{R}$ must by definition include the complete class of R. Thus $\mathscr{C}$ must be composed of complete classes.)

If we now apply the theorem (2-1) to the product of two classes, we have

$$\begin{aligned}\mathscr{C}_i\mathscr{C}_j &= X^{-1}\mathscr{C}_iXX^{-1}\mathscr{C}_jX \\ &= X^{-1}(\mathscr{C}_i\mathscr{C}_j)X\end{aligned}$$

for all X. Then, upon applying the converse theorem, it follows that $\mathscr{C}_i\mathscr{C}_j$ consists of complete classes. This may be expressed formally by writing

$$\mathscr{C}_i\mathscr{C}_j = \sum_k c_{ijk}\mathscr{C}_k \tag{2-2}$$

where c_{ijk} is the integer telling how often the complete class $\mathscr{C}_k$ appears in the product $\mathscr{C}_i\mathscr{C}_j$.

An an example, in the symmetry group of the triangle whose class structure we noted earlier, let $\mathscr{C}_i = E$; $\mathscr{C}_2 = A, B, C$; and $\mathscr{C}_3 = D, F$. Then $\mathscr{C}_1\mathscr{C}_2 = \mathscr{C}_2$; $\mathscr{C}_1\mathscr{C}_3 = \mathscr{C}_3$; $\mathscr{C}_2\mathscr{C}_2 = 3\mathscr{C}_1 + 3\mathscr{C}_3$; $\mathscr{C}_2\mathscr{C}_3 = 2\mathscr{C}_2$.

EXERCISES

2-1 Consider the symmetry group of the proper covering operations of a square (D_4). This consists of eight elements:

E = the identity

A, B, C, D = 180° rotations about the corresponding labeled axes in Fig. 2-2 which are considered fixed in *space*, not on the body

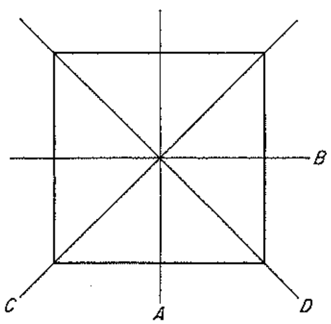

Fig. 2-2. *Symmetry axes of square.*

F, G, H = clockwise rotations in plane of the paper by $\pi/2$, π, and $3\pi/2$, respectively

(*a*) From the geometry, work out the multiplication table of the group; take advantage of the rearrangement theorem to check your result.

(*b*) From the nature of the operations, divide the group elements into classes. If in doubt, check by using the multiplication table [from (*a*)] and the definition of conjugate elements.

(*c*) Write down all the subgroups of the complete group. Note that the orders of the subgroups must be divisors of 8. Which of these subgroups are invariant subgroups (normal divisors)?

(*d*) Work out the cosets of the normal divisors.

(*e*) Work out the group-multiplication tables of the factor groups corresponding to the nontrivial normal divisors of the group.

(*f*) Determine the coefficients c_{ijk} appearing in all class multiplication products.

2-2 List the symmetries of a general rectangle. Work out the multiplication table, and divide the elements into classes.

2-3 Use the multiplication table for the symmetry group of the triangle to verify in several cases the rule for the inverse of a product.

2-4 Consider the group of order $(p - 1)$ obtained by taking as group elements the integers $1, 2, \ldots, (p - 1)$ and as group multiplication ordinary multiplication modulo p, where p is a prime number. (Modulo p means that $m + np$ is considered to be equal to m, where m and n are any integers.)

(*a*) Show that this is a group, and work out the multiplication table when $p = 7$.

(*b*) Prove in general that $A^{p-1} = E$, for all elements A of the group. In this way you have proved Fermat's number-theoretical theorem that $n^p = n(\text{mod}\, p)$, where n is an integer and p is a prime.

(*c*) Check the theorem for $p = 7$ and $n = 2, 3, 5$.

2-5 Prove that all elements in the same class have the same order when used to generate a cyclic group.

2-6 Show that there is a homomorphism between the cyclic groups of order 4 and 2.

2-7 Prove that a group is Abelian if, and only if, the correspondence of each element to its inverse forms an isomorphism.

2-8 Prove that $c_{ijk} = c_{jik}$ in Eq. (2-2). In other words, prove that $\mathscr{C}_i\mathscr{C}_j = \mathscr{C}_j\mathscr{C}_i$, even if the group is not Abelian.

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3 THEORY OF GROUP REPRESENTATIONS

3-1 Definitions

By a *representation* of an abstract group we mean in general any group composed of concrete mathematical entities which is homomorphic to the original group. However, we shall restrict our attention to representation by square matrices, with matrix multiplication as the group multiplication operation. That is, we associate a matrix $\mathbf{\Gamma}(A)$ with each group element A in such a way that

$$\mathbf{\Gamma}(A)\mathbf{\Gamma}(B) = \mathbf{\Gamma}(AB)$$

These matrices then satisfy the group-multiplication table and in every way "represent" the abstract group elements. Clearly this is possible only if $\mathbf{\Gamma}(E) = \mathbf{E}$, the unit matrix. The number of rows and columns in the matrix is called the *dimensionality* of the representation.

If each matrix is different, then the two groups are isomorphic rather than merely homomorphic and the representation is said to be *true*, or *faithful*. On the other hand, if several elements correspond to a single matrix, one can easily see that all elements corresponding to the unit matrix form an invariant subgroup of the full group. Similarly, the elements corresponding to each of the other matrices of the representation form the distinct cosets of the invariant subgroup, and the matrices form a true representation of the factor group of this invariant subgroup.

Obviously the 2×2 matrices introduced in Sec. 2-2 form a true matrix representation of our standard example group of order 6. Another representation of the same group can be obtained by taking the determinant of each matrix, because of the fact that

$$|\mathbf{\Gamma}(A)| \cdot |\mathbf{\Gamma}(B)| = |\mathbf{\Gamma}(A)\mathbf{\Gamma}(B)| = |\mathbf{\Gamma}(AB)|$$

This operation reduces the matrices to ordinary numbers, namely, ± 1, giving a one-dimensional representation. This representation is no longer true, since there are only two distinct "matrices," whereas there are six group elements. A still simpler one-dimensional representation is obtained by representing each element by $+1$. This corresponds to the rather trivial homomorphism which can be set up by associating the unit element with all members of the original group, and it is often called the *identical representation*. We shall soon be able to prove that these three form the only possible, essentially different representations of the example group. After we establish the close connection between these matrix representations and quantum-mechanical eigenfunctions, it will become clear that such unconditional statements of group theory will have great practical value.

In discussing the various possible matrix representations of a group, it is important to note that a similarity transformation leaves matrix equations unchanged. That is, if we define $\mathbf{\Gamma}'(A) = \mathbf{S}^{-1}\mathbf{\Gamma}(A)\mathbf{S}$, then

$$\begin{aligned}\mathbf{\Gamma}'(A)\mathbf{\Gamma}'(B) &= [\mathbf{S}^{-1}\mathbf{\Gamma}(A)\mathbf{S}][\mathbf{S}^{-1}\mathbf{\Gamma}(B)\mathbf{S}] = \mathbf{S}^{-1}\mathbf{\Gamma}(A)\mathbf{\Gamma}(B)\mathbf{S} \\ &= \mathbf{S}^{-1}\mathbf{\Gamma}(AB)\mathbf{S} = \mathbf{\Gamma}'(AB)\end{aligned}$$

and the transformed matrices $\mathbf{\Gamma}'$ form a representation if the $\mathbf{\Gamma}$ matrices do. However, the infinity of representations related to each other in this way for various matrices $\mathbf{S}$ differ only in that they are stated with respect to different coordinate axes of some sort, and hence all are considered to be *equivalent*.

Reducible and irreducible representations. Clearly one can take two (or more) representations and construct from them a new representation by combining the matrices into larger matrices. For a typical element, we could form

$$\mathbf{\Gamma}(A) = \begin{pmatrix} \mathbf{\Gamma}^{(1)}(A) & \mathbf{0} \\ \mathbf{0} & \mathbf{\Gamma}^{(2)}(A) \end{pmatrix}$$

where $\mathbf{\Gamma}^{(1)}(A)$ and $\mathbf{\Gamma}^{(2)}(A)$ are the matrices representing element A in the original representations and $\mathbf{\Gamma}(A)$ represents A in the new larger representation. However, such an artificially enlarged matrix representation is said to be *reducible*. This reducibility might be concealed by applying a similarity transformation which scrambles rows and columns, leaving an equivalent representation which is *not* in block form. Thus our real criterion for reducibility is that it be possible to reduce the matrices representing *all* the elements of the group to block form (with the same block structure) by the *same* similarity transformation. If this *cannot* be done, a representation is said to be *irreducible*, meaning that it cannot be expressed in terms of representations of lower dimensionality. It is customary to indicate the structure of reducible representations by giving the irreducible representations which form the blocks after reduction to block form. In our example, we would write $\Gamma = \Gamma^{(1)} + \Gamma^{(2)}$; more generally, $\Gamma = \Sigma\, a_i \Gamma^{(i)}$, where the a_i are integers telling how often $\Gamma^{(i)}$ appears in Γ. (Observe that this notation does *not* refer to matrix addition.) In many quantum-mechanical applications each irreducible representation will display the transformation properties of a set of degenerate eigenfunctions. Hence, as we shall see, the number of irreducible representations may give the number of distinct energy levels, a very useful piece of information.

3-2 Proof of the Orthogonality Theorem

We commence this section by proving several lemmas leading up to the orthogonality theorem which is central to the development of the theory of group representations. The method of proof given here follows closely that in Wigner's classic book.[1] A review of the various properties of matrices which are used here may be found in Appendix A.

LEMMA: Any representation by matrices with nonvanishing determinants is equivalent through a similarity transformation to a representation by *unitary* matrices.

PROOF: For simplicity in notation let the matrix representing the element A_i be written $\mathbf{A}_i$. We can then construct a Hermitian matrix $\mathbf{H}$ by

$$\mathbf{H} = \sum_{i=1}^{h} \mathbf{A}_i \mathbf{A}_i^{\dagger} \tag{3-1}$$

since each term is already Hermitian. (In our notation a matrix is Hermitian if $\mathbf{H}^{\dagger} = \mathbf{H}$, or $H_{ji}^{*} = H_{ij}$.) But it is well known[2] that any Hermitian matrix can be diagonalized by the unitary transformation made up from

[1] E. P. Wigner, "Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren," Friedr. Vieweg & Sohn, Brunswick, Germany, 1931; revised and translated edition, Academic Press Inc., New York, 1959.

[2] See Appendix A.

the orthonormal eigenvectors found by solving the associated secular equation. Thus we can write

$$\begin{aligned}\mathbf{d} = \mathbf{U}^{-1}\mathbf{H}\mathbf{U} &= \sum_i \mathbf{U}^{-1}\mathbf{A}_i\mathbf{A}_i^{\dagger}\mathbf{U} \\ &= \sum_i \mathbf{U}^{-1}\mathbf{A}_i\mathbf{U}\mathbf{U}^{-1}\mathbf{A}_i^{\dagger}\mathbf{U} = \sum_i \mathbf{A}_i'\mathbf{A}_i'^{\dagger}\end{aligned} \tag{3-2}$$

where the primed matrices differ from the original ones by the unitary transformation $\mathbf{U}$. Consideration of a typical element shows that not only is $\mathbf{d}$ diagonal but it has only real positive diagonal elements. This enables us to form other real positive diagonal matrices for $\mathbf{d}^{\frac{1}{2}}$ and $\mathbf{d}^{-\frac{1}{2}}$ by simply taking the appropriate power of the elements of $\mathbf{d}$. Taking advantage of the commutation of diagonal matrices, we can then write (3-2) as

$$\mathbf{E} = \mathbf{d}^{-\frac{1}{2}} \sum_i \mathbf{A}_i'\mathbf{A}_i'^{\dagger}\, \mathbf{d}^{-\frac{1}{2}}$$

where $\mathbf{E}$ is the unit matrix. We can also define a new set of doubly transformed matrices by $\mathbf{A}_j'' = \mathbf{d}^{-\frac{1}{2}}\mathbf{A}_j'\mathbf{d}^{\frac{1}{2}}$. We conclude the proof by showing that these matrices $\mathbf{A}_j''$ are unitary.

To do this, consider

$$\begin{aligned}\mathbf{A}_j''\mathbf{A}_j''^{\dagger} &= \mathbf{d}^{-\frac{1}{2}}\mathbf{A}_j'\mathbf{d}^{\frac{1}{2}}[\mathbf{d}^{-\frac{1}{2}}\sum_i \mathbf{A}_i'\mathbf{A}_i'^{\dagger}\mathbf{d}^{-\frac{1}{2}}]\mathbf{d}^{\frac{1}{2}}\mathbf{A}_j'^{\dagger}\mathbf{d}^{-\frac{1}{2}} \\ &= \mathbf{d}^{-\frac{1}{2}}\sum_i \mathbf{A}_j'\mathbf{A}_i'\mathbf{A}_i'^{\dagger}\mathbf{A}_j'^{\dagger}\mathbf{d}^{-\frac{1}{2}} \\ &= \mathbf{d}^{-\frac{1}{2}}\sum_i \mathbf{A}_j'\mathbf{A}_i'(\mathbf{A}_j'\mathbf{A}_i')^{\dagger}\mathbf{d}^{-\frac{1}{2}} \\ &= \mathbf{d}^{-\frac{1}{2}}\sum_k \mathbf{A}_k'\mathbf{A}_k'^{\dagger}\mathbf{d}^{-\frac{1}{2}} = \mathbf{E}\end{aligned}$$

In making the change to the sum on k we have used the rearrangement theorem. Since we have shown that $\mathbf{A}_j''\mathbf{A}_j''^{\dagger} = \mathbf{E}$, we have shown that $\mathbf{A}_j''$ is unitary. Hence we can always construct a unitary representation from any given one by forming

$$\mathbf{A}_j'' = \mathbf{d}^{-\frac{1}{2}}\mathbf{U}^{-1}\mathbf{A}_j\mathbf{U}\mathbf{d}^{\frac{1}{2}} \tag{3-3}$$

where $\mathbf{U}$ and $\mathbf{d}$ have been defined above in (3-2).

SCHUR'S LEMMA: Any matrix which commutes with all matrices of an irreducible representation must be a constant matrix (i.e., a multiple of $\mathbf{E}$). Thus, if a nonconstant commuting matrix exists, the representation is reducible, whereas if none exists, the representation is irreducible.

PROOF: On the basis of our first lemma, we can restrict our attention to unitary representations. Let $\mathbf{M}$ be a matrix which commutes with all matrices of the representation. Then

$$\mathbf{A}_i\mathbf{M} = \mathbf{M}\mathbf{A}_i \qquad i = 1, 2, \ldots, h$$

and taking the adjoint of both sides,

$$\mathbf{M}^{\dagger}\mathbf{A}_i^{\dagger} = \mathbf{A}_i^{\dagger}\mathbf{M}^{\dagger}$$

Pre- and postmultiplying the second of these by $\mathbf{A}_i$ leads to

$$\mathbf{A}_i\mathbf{M}^\dagger = \mathbf{M}^\dagger\mathbf{A}_i$$

Thus, if $\mathbf{M}$ commutes, $\mathbf{M}^\dagger$ also commutes. From this, it follows that the two Hermitian matrices $\mathbf{H}_1 = \mathbf{M} + \mathbf{M}^\dagger$ and $\mathbf{H}_2 = i(\mathbf{M} - \mathbf{M}^\dagger)$ also commute with all $\mathbf{A}_i$. If we can now show that a commuting Hermitian matrix is a constant, then it follows that $\mathbf{M} = \mathbf{H}_1 - i\mathbf{H}_2$ is also a constant.

Confining our attention to Hermitian commuting matrices, we can always reduce them to diagonal form by a unitary transformation: $\mathbf{d} = \mathbf{U}^{-1}\mathbf{M}\mathbf{U}$. If we define a transformed $\mathbf{A}_i' = \mathbf{U}^{-1}\mathbf{A}_i\mathbf{U}$, then

$$\mathbf{A}_i'\mathbf{d} = \mathbf{d}\mathbf{A}_i'$$

by the invariance of matrix equations under unitary transformations. We now must show that $\mathbf{d}$ is not only diagonal but also constant. To do this, consider the $\mu\nu$ element of the matrix, namely,

$$(A_i')_{\mu\nu}d_{\nu\nu} = d_{\mu\mu}(A_i')_{\mu\nu}$$

or

$$(A_i')_{\mu\nu}(d_{\nu\nu} - d_{\mu\mu}) = 0 \qquad i = 1, 2, \ldots, h$$

Now, if $d_{\nu\nu} \neq d_{\mu\mu}$, so that the matrix is not constant, then $(A_i')_{\mu\nu}$ must be zero for all A_i' and our transformation U has brought A_i to block form, showing that the representation was in fact reducible. On the other hand, if we assume the representation was irreducible, then it follows that $d_{\nu\nu} = d_{\mu\mu}$ and any commuting matrix must be a constant.

LEMMA: If we are given two irreducible representations of the same group $\mathbf{\Gamma}^{(1)}(A_i)$ and $\mathbf{\Gamma}^{(2)}(A_i)$ of dimensionality l_1 and l_2, and if a rectangular matrix $\mathbf{M}$ exists such that

$$\mathbf{M}\mathbf{\Gamma}^{(1)}(A_i) = \mathbf{\Gamma}^{(2)}(A_i)\mathbf{M} \qquad i = 1, 2, \ldots, h \tag{3-4}$$

then (1) if $l_1 \neq l_2$, $\mathbf{M} = \mathbf{0}$, or (2) if $l_1 = l_2$, $\mathbf{M} = \mathbf{0}$, or else $|\mathbf{M}| \neq 0$. In the latter case, $\mathbf{M}$ has an inverse, $\mathbf{M}\mathbf{\Gamma}^{(1)}(A_i)\mathbf{M}^{-1} = \mathbf{\Gamma}^{(2)}(A_i)$, and the two representations are equivalent.

PROOF: As shown in the first lemma, we may confine our attention to unitary representations. Also, we may assume $l_1 \leqq l_2$ without loss of generality. Then, taking the adjoint of (3-4), we have

$$\mathbf{\Gamma}^{(1)}(A_i)^\dagger\mathbf{M}^\dagger = \mathbf{M}^\dagger\mathbf{\Gamma}^{(2)}(A_i)^\dagger$$

or

$$\mathbf{\Gamma}^{(1)}(A_i^{-1})\mathbf{M}^\dagger = \mathbf{M}^\dagger\mathbf{\Gamma}^{(2)}(A_i^{-1}) \tag{3-5}$$

by the unitary property which implies $\mathbf{\Gamma}^{(1)}(A_i)^\dagger = \mathbf{\Gamma}^{(1)}(A_i)^{-1} = \mathbf{\Gamma}^{(1)}(A_i^{-1})$. If we now premultiply both sides of (3-5) by $\mathbf{M}$ and use the fact that (3-4) holds for A_i^{-1} as well as A_i, since it holds for all group elements, we find

$$\mathbf{\Gamma}^{(2)}(A_i^{-1})\mathbf{M}\mathbf{M}^\dagger = \mathbf{M}\mathbf{M}^\dagger\mathbf{\Gamma}^{(2)}(A_i^{-1}) \tag{3-6}$$

Thus the matrix $\mathbf{M}\mathbf{M}^\dagger$ commutes with all the matrices of the representation and hence must be a multiple of the unit matrix, by Schur's lemma. That is,

$$\mathbf{M}\mathbf{M}^\dagger = c\mathbf{E} \tag{3-7}$$

Consider first the case when $l_1 = l_2$, so that $\mathbf{M}$ is a square matrix. Taking the determinant of (3-7) then yields $|\mathbf{M}|^2 = c^{l_1}$. Now, if $c \neq 0$, $|\mathbf{M}| \neq 0$, $\mathbf{M}$ has an inverse and the two representations are equivalent. On the other hand, if $c = 0$, then $\mathbf{M}\mathbf{M}^\dagger = \mathbf{0}$. In terms of components, this means that $\sum_\lambda M_{\mu\lambda}M_{\lambda\nu}{}^\dagger = \sum_\lambda M_{\mu\lambda}M_{\nu\lambda}{}^* = 0$, for all μ and ν. Taking in particular $\mu = \nu$, we have $\sum_\lambda |\mathbf{M}_{\mu\lambda}|^2 = 0$, which is possible only if all $M_{\mu\lambda} = 0$, or in other words, if $\mathbf{M} = \mathbf{0}$.

Now consider the case when $l_1 < l_2$, so that $\mathbf{M}$ has l_1 columns and l_2 rows. We can fill $\mathbf{M}$ out to a square $l_2 \times l_2$ matrix $\mathbf{N}$ by inserting $(l_2 - l_1)$ columns of zeros. Inspection then shows that $\mathbf{N}\mathbf{N}^\dagger \equiv \mathbf{M}\mathbf{M}^\dagger$. Since $\mathbf{N}$ clearly has zero determinant, so does $\mathbf{N}\mathbf{N}^\dagger$ and hence $\mathbf{M}\mathbf{M}^\dagger$. But by (3-7) $\mathbf{M}\mathbf{M}^\dagger$ is a constant matrix, which we now see has $c = 0$, since the determinant vanishes. From this it follows that $\mathbf{M} = \mathbf{0}$. This completes the full proof of our lemma.

The great orthogonality theorem. If we consider all the *inequivalent, irreducible, unitary* representations of a group, then

$$\sum_R \Gamma^{(i)}(R)^*_{\mu\nu}\Gamma^{(j)}(R)_{\alpha\beta} = \frac{h}{l_i}\,\delta_{ij}\delta_{\mu\alpha}\delta_{\nu\beta} \tag{3-8}$$

where in the summation R runs over all group elements $E, A_2, \ldots, A_h$ and l_i is the dimensionality of $\Gamma^{(i)}$.

PROOF: We first consider the case of two inequivalent representations $\mathbf{\Gamma}^{(1)}$ and $\mathbf{\Gamma}^{(2)}$. Then we may construct a matrix $\mathbf{M}$ satisfying our third lemma by forming

$$\mathbf{M} = \sum_R \mathbf{\Gamma}^{(2)}(R)\mathbf{X}\mathbf{\Gamma}^{(1)}(R^{-1})$$

where $\mathbf{X}$ is a completely arbitrary matrix having l_1 columns and l_2 rows. To show that this $\mathbf{M}$ satisfies (3-4), take

$$\begin{aligned}
\mathbf{\Gamma}^{(2)}(S)\mathbf{M} &= \sum_R \mathbf{\Gamma}^{(2)}(S)\mathbf{\Gamma}^{(2)}(R)\mathbf{X}\mathbf{\Gamma}^{(1)}(R^{-1}) \\
&= \sum_R \mathbf{\Gamma}^{(2)}(S)\mathbf{\Gamma}^{(2)}(R)\mathbf{X}\mathbf{\Gamma}^{(1)}(R^{-1})\mathbf{\Gamma}^{(1)}(S^{-1})\mathbf{\Gamma}^{(1)}(S) \\
&= \sum_R \mathbf{\Gamma}^{(2)}(SR)\mathbf{X}\mathbf{\Gamma}^{(1)}(R^{-1}S^{-1})\mathbf{\Gamma}^{(1)}(S) \\
&= [\sum_R \mathbf{\Gamma}^{(2)}(SR)\mathbf{X}\mathbf{\Gamma}^{(1)}(SR)^{-1}]\mathbf{\Gamma}^{(1)}(S) \\
&= [\sum_R \mathbf{\Gamma}^{(2)}(R)\mathbf{X}\mathbf{\Gamma}^{(1)}(R^{-1})]\mathbf{\Gamma}^{(1)}(S)
\end{aligned}$$

by the rearrangement theorem; so finally

$$\mathbf{\Gamma}^{(2)}(S)\mathbf{M} = \mathbf{M}\mathbf{\Gamma}^{(1)}(S)$$

Therefore, our lemma shows that $\mathbf{M} = \mathbf{0}$. But then

$$M_{\alpha\mu} = 0 = \sum_R \sum_{\kappa\lambda} \Gamma^{(2)}(R)_{\alpha\kappa} X_{\kappa\lambda} \Gamma^{(1)}(R^{-1})_{\lambda\mu}$$

Since $\mathbf{X}$ is arbitrary, we may set all $X_{\kappa\lambda} = 0$ except $X_{\beta\nu} = 1$. Then

$$\sum_R \Gamma^{(2)}(R)_{\alpha\beta} \Gamma^{(1)}(R^{-1})_{\nu\mu} = 0 \tag{3-9}$$

Using the unitary property of $\mathbf{\Gamma}^{(1)}$, we have the equivalent form

$$\sum_R \Gamma^{(1)}(R)^*_{\mu\nu} \Gamma^{(2)}(R)_{\alpha\beta} = 0 \tag{3-9a}$$

which completes the proof of the δ_{ij} factor in (3-8).

Next we consider the case when $i = j = 1$, say. In analogy with the previous paragraph, we may construct a matrix $\mathbf{M}$ which commutes with all matrices of the representation by forming

$$\mathbf{M} = \sum_R \mathbf{\Gamma}^{(1)}(R)\mathbf{X}\mathbf{\Gamma}^{(1)}(R^{-1})$$

Then by Schur's lemma $\mathbf{M} = c\mathbf{E}$. Thus, taking the $\mu\mu'$ element,

$$\sum_{\kappa,\lambda} \sum_R \Gamma^{(1)}(R)_{\mu\kappa} X_{\kappa\lambda} \Gamma^{(1)}(R^{-1})_{\lambda\mu'} = c\delta_{\mu\mu'}$$

Choosing $X_{\kappa\lambda} = 0$ except $X_{\nu\nu'} = 1$ reduces this to

$$\sum_R \Gamma^{(1)}(R)_{\mu\nu} \Gamma^{(1)}(R^{-1})_{\nu'\mu'} = c_{\nu\nu'}\delta_{\mu\mu'} \tag{3-10}$$

We have put subscripts on the constant c to indicate the particular choice of $\mathbf{X}$. Now, choose $\mu' = \mu$, and sum on μ. This yields, on interchanging the order of the factors,

$$\sum_R \sum_\mu \Gamma^{(1)}(R^{-1})_{\nu'\mu} \Gamma^{(1)}(R)_{\mu\nu} = c_{\nu\nu'} \sum_\mu \delta_{\mu\mu}$$

or

$$\sum_R \Gamma^{(1)}(R^{-1}R)_{\nu'\nu} = l_1 c_{\nu\nu'}$$

since μ runs over the l_1 rows of the $\Gamma^{(1)}$ representation. We may reduce the left member further by noting that

$$\sum_R \Gamma^{(1)}(R^{-1}R)_{\nu'\nu} = \sum_R \Gamma^{(1)}(E)_{\nu'\nu} = h\Gamma^{(1)}(E)_{\nu'\nu} = h\delta_{\nu'\nu}$$

Therefore $c_{\nu\nu'} = h\delta_{\nu'\nu}/l_1$. Substituting back into (3-10), we have

$$\sum_R \Gamma^{(1)}(R)_{\mu\nu} \Gamma^{(1)}(R^{-1})_{\nu'\mu'} = \frac{h}{l_1}\, \delta_{\mu'\mu}\delta_{\nu'\nu} \tag{3-11}$$

By using the unitary property of $\mathbf{\Gamma}^{(1)}$, this becomes

$$\sum_R \Gamma^{(1)}(R)^*_{\mu'\nu'} \Gamma^{(1)}(R)_{\mu\nu} = \frac{h}{l_1}\, \delta_{\mu'\mu}\delta_{\nu'\nu} \tag{3-11a}$$

Combining (3-9a) and (3-11a), we have proved the general theorem (3-8). Moreover, (3-9) and (3-11) provide a generalization of (3-8) for nonunitary representations.

Geometric interpretation. To appreciate the significance of this result, it is helpful to interpret it as stating the orthogonality of a set of vectors in "group-element space." This is an h-dimensional vector space in which the axes or components are labeled by the various group elements $R = E, A_2, \ldots, A_h$. The vectors themselves are labeled by three indices—the representation index i and the subscripts $\mu\nu$, indicating row and column within the representation matrix. The theorem then states that all these vectors are mutually orthogonal in this h-dimensional space.

From this result we may readily draw an extremely important conclusion. If we count up the number of these orthogonal vectors, we find $\sum_i l_i^2$, where i runs over all the distinct irreducible representations, since there are l_i^2 entries in a matrix of dimensionality l_i. But clearly the maximum number of orthogonal vectors in an h-dimensional vector space is just h. Thus it follows that $\sum_i l_i^2 \leq h$. In fact we shall soon prove that the equality always holds. This gives us the dimensionality theorem

$$\sum_i l_i^2 = h \tag{3-12}$$

which is essential for working out the irreducible representations of any group. For example, in our example group of order 6, we have $h = 6$, and we have already found three irreducible representations—one of dimensionality 2 and two of dimensionality 1. Since $2^2 + 1^2 + 1^2 = 6$, this simple theorem tells us that it is impossible for any other distinct irreducible representations to exist.

3-3 The Character of a Representation

Because all matrix representations related to each other through unitary transformations are equivalent, it is clear that there is a large degree of arbitrariness in the actual forms of the matrices. This makes it worthwhile to seek a way of characterizing any given representation which is invariant under such transformations. This immediately suggests using the traces of the matrices, since these are invariant. Accordingly, we define the *character* of the jth representation as being the set of h numbers $\chi^{(j)}(E)$, $\chi^{(j)}(A_2), \ldots, \chi^{(j)}(A_h)$, where

$$\chi^{(j)}(R) = \mathrm{Tr}\, \mathbf{\Gamma}^{(j)}(R) = \sum_{\mu=1}^{l_j} \Gamma^{(j)}(R)_{\mu\mu} \tag{3-13}$$

Since the matrix representations of all elements in the same class are related by similarity transformations (by definition of conjugate group elements), the invariance of traces shows that all elements in the same class have the same character. This enables us to specify the character of any given representation by simply giving the trace of one matrix from each class of group elements. We denote this by $\chi^{(i)}(\mathscr{C}_k)$ for the kth class.

We can profitably apply the orthogonality theorem to the character in the following way. If we set $\nu = \mu$ and $\beta = \alpha$ in Eq. (3-8), we have

$$\sum_R \Gamma^{(i)}(R)^*_{\mu\mu}\Gamma^{(j)}(R)_{\alpha\alpha} = \frac{h}{l_i}\delta_{ij}\delta_{\mu\alpha}$$

Now summing over μ and α and use of (3-13) yields

$$\begin{aligned}\sum_R \chi^{(i)}(R)^*\chi^{(j)}(R) &= \frac{h}{l_i}\delta_{ij}\sum_{\mu\alpha}\delta_{\mu\alpha}\\ &= h\delta_{ij}\end{aligned} \tag{3-14}$$

Thus, the characters form a set of orthogonal vectors in group-element space. Collecting the group elements according to classes, within which the $\chi^{(j)}(R)$ are the same, we can rewrite (3-14) as

$$\sum_k \chi^{(i)}(\mathscr{C}_k)^*\chi^{(j)}(\mathscr{C}_k)N_k = h\delta_{ij} \qquad \blacktriangleright \text{(3-15)}$$

where N_k is the number of elements in the class $\mathscr{C}_k$ and the sum now runs over *classes*.

Written in the form (3-15), our result shows that the characters of the various irreducible representations also form an orthogonal vector system in the vector space where axes are labeled by classes $\mathscr{C}_k$ rather than group elements R. Since the number of mutually orthogonal vectors in a space cannot exceed its dimensionality, it follows that the number of irreducible representations cannot exceed the number of classes. In fact it can be shown that they are always equal. Thus,

$$\text{Number of irreducible representations} = \text{number of classes} \qquad \blacktriangleright \text{(3-16)}$$

This rule, together with (3-12), enables us to work out the number and dimensionality of the irreducible representations from the numbers of group elements and classes. Thus these numerological results are of great importance in applications. Applying them to our example group of order 6, we recall that there are three classes: $\mathscr{C}_1 = E$; $\mathscr{C}_2 = A, B, C$; and $\mathscr{C}_3 = D, F$. By (3-16), this implies that there are just three irreducible representations. Then, since $2^2 + 1^2 + 1^2 = 6$ is the only solution of (3-12) for the case in which the sum of three squares must equal 6, we conclude that there must be one two-dimensional and two one-dimensional

irreducible representations. Of course we already had noted these results for this case, but the method is very effective in more difficult examples where the representations are by no means obvious.

Character tables. It is convenient to display the characters of the various representations in a *character table* for any given group. The columns are labeled by the various classes, preceded by the number N_k of elements in the class. The rows are labeled by the irreducible representations, and the entries in the table are the $\chi^{(i)}(\mathscr{C}_k)$. Thus in our example group we have the table

	$\mathscr{C}_1$	$3\mathscr{C}_2$	$2\mathscr{C}_3$
$\Gamma^{(1)}$	1	1	1
$\Gamma^{(2)}$	1	−1	1
$\Gamma^{(3)}$	2	0	−1

as may be verified by using the explicit representations noted in Sec. 3-1. Note that the rows of the table are orthogonal if we use the N_k weighting factors as prescribed by (3-15). We also note that the columns form orthogonal vectors. This is not an accident, and we now proceed to prove it to be true in general.

Second orthogonality relation for characters. Since the number of classes equals the number of irreducible representations, we may form a square matrix $\mathbf{Q}$ which has the same form as the character table, namely,

$$\mathbf{Q} = \begin{pmatrix} \chi^{(1)}(\mathscr{C}_1) & \chi^{(1)}(\mathscr{C}_2) & \cdots \\ \chi^{(2)}(\mathscr{C}_1) & \chi^{(2)}(\mathscr{C}_2) & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix}$$

Now consider the related matrix $\mathbf{Q}'$ defined by

$$\mathbf{Q}' = \begin{pmatrix} \dfrac{\chi^{(1)}(\mathscr{C}_1)^*N_1}{h} & \dfrac{\chi^{(2)}(\mathscr{C}_1)^*N_1}{h} & \cdots \\ \dfrac{\chi^{(1)}(\mathscr{C}_2)^*N_2}{h} & \dfrac{\chi^{(2)}(\mathscr{C}_2)^*N_2}{h} & \cdots \\ \cdots & \cdots & \cdots \end{pmatrix}$$

Then a typical element of the product is

$$(\mathbf{QQ}')_{ij} = \sum_k \frac{\chi^{(i)}(\mathscr{C}_k)\chi^{(j)}(\mathscr{C}_k)^*N_k}{h} = \delta_{ij}$$

by the first orthogonality relation for characters, (3-15). Thus $\mathbf{Q}' = \mathbf{Q}^{-1}$. But any matrix commutes with its inverse. Therefore, we also must have

$(\mathbf{Q}'\mathbf{Q})_{ij} = \delta_{ij}$. Carrying out the multiplication in the reverse order leads directly to our result,

$$\sum_i \chi^{(i)}(\mathscr{C}_k)^*\chi^{(i)}(\mathscr{C}_l) = \frac{h}{N_k}\,\delta_{kl} \qquad \blacktriangleright \text{(3-17)}$$

Since (3-17) is actually a direct consequence of (3-15), it contains no fundamentally new information. However, as we shall see directly, it is often a convenient aid in setting up character tables by inspection.

3-4 Construction of Character Tables

Although the character table gives much less information about a group than would a complete set of matrices for the irreducible representations, it does give enough information for many purposes. Thus it is highly desirable to be able to obtain the character table of a group directly, without first working out explicit representation matrices. In fact, in the simple cases of most interest it is possible to work out the table by inspection with the aid of a few simple rules based on the results of the previous sections. These rules are collected here for convenience.

1. The *number* of irreducible representations equals the number of classes of group elements. The latter is easily found by considering the nature of the operations or, more mechanically, by computing conjugate elements with the aid of the group-multiplication table.

2. The *dimensionalities* l_i of the irreducible representations are then determined by the fact that $\sum_i l_i^2 = h$. In most cases this has a unique solution. Since the identity element must be represented by a unit matrix, the trace of a matrix of the identity class is simply l_i. This determines the first column of the table, $\chi^{(i)}(E) = l_i$. Also, since we always have the one-dimensional representation (referred to as *totally symmetric*, *identical*, or *invariant*) in which each group element is represented by unity, we can always fill in the first row by $\chi^{(1)}(\mathscr{C}_k) = 1$.

3. The rows of the table must be orthogonal and normalized to h, with weighting factor N_k, the number of elements in $\mathscr{C}_k$. That is,

$$\sum_k \chi^{(i)}(\mathscr{C}_k)^*\chi^{(j)}(\mathscr{C}_k)N_k = h\delta_{ij} \qquad \text{(3-15)}$$

4. The columns of the table must be orthogonal vectors normalized to h/N_k. That is,

$$\sum_i \chi^{(i)}(C_k)^*\chi^{(i)}(\mathscr{C}_l) = \frac{h}{N_k}\,\delta_{kl} \qquad \text{(3-17)}$$

5. Elements within the ith row are related by

$$N_j\chi^{(i)}(\mathscr{C}_j)N_k\chi^{(i)}(\mathscr{C}_k) = l_i\sum_l c_{jkl}N_l\chi^{(i)}(\mathscr{C}_l) \qquad \text{(3-18)}$$

where the c_{jkl} are the constants defined by the expression governing class multiplication $\mathscr{C}_j\mathscr{C}_k = \sum_l c_{jkl}\mathscr{C}_l$. These constants may be determined given the group-multiplication table, as explained in Sec. 2-9.

PROOF: Recall that any class satisfies $X^{-1}\mathscr{C}_kX = \mathscr{C}_k$, or, equivalently, $\mathscr{C}_kX = X\mathscr{C}_k$, for all X. Now consider this equation in terms of a matrix representation. If we introduce the matrix $\mathscr{C}_k$, which is the sum of the matrices of all the elements in the class $\mathscr{C}_k$, then it follows that $\mathscr{C}_k\mathbf{X} = \mathbf{X}\mathscr{C}_k$, because matrix multiplication by $\mathbf{X}$ is linear and matrix addition is commutative. But if this is so, Schur's lemma states that $\mathscr{C}_k$ must be a constant matrix, say, $\eta_k\mathbf{E}$. In this case, one readily sees that the matrix form of the equation defining the c_{jkl} reduces to $\eta_j\eta_k = \sum_l c_{jkl}\eta_l$. We now evaluate η_k by taking the trace of $\mathscr{C}_k$ in two ways and comparing, namely,

$$\mathrm{Tr}\,\mathscr{C}_k = \mathrm{Tr}\,\eta_k\mathbf{E} = \eta_k l_i$$

and

$$\mathrm{Tr}\,\mathscr{C}_k = \mathrm{Tr}\sum_{\mu=1}^{N_k}\mathbf{A}_\mu = N_k\chi^{(i)}(\mathscr{C}_k)$$

Thus

$$\eta_k = \frac{N_k\chi^{(i)}(\mathscr{C}_k)}{l_i}$$

and rule 5 follows directly.

The first three rules usually suffice to work out a character table, but the last two often facilitate the process of inspection. For example, by use of these rules the complete character table for the group of the equilateral triangle, as given above, could be quickly found without any knowledge of the explicit matrices at all. The first row and column are fixed by rule 2, and the four integers to complete the table so as to satisfy rules 3 and 4 are readily picked out. In case the characters should be nonintegral, as may occur in various instances, the procedure is less simple. However, if a set of integers satisfying the rules can be found, one may normally take it to be the proper character table.

3-5 Decomposition of Reducible Representations

Clearly the character of a reducible representation Γ is the sum of the characters of the component irreducible representations $\Gamma^{(j)}$. This can be seen by supposing that the representation has been brought into block form by a suitable similarity transformation. In that case, the trace of the large matrix is simply the sum of the traces of the submatrices in the blocks along the diagonal. Thus we can write

$$\chi(R) = \sum_j a_j\chi^{(j)}(R) \qquad \text{(3-19)}$$

where χ is the character of Γ and a_j is the number of times $\Gamma^{(j)}$ appears in Γ. Since the $\chi^{(j)}(R)$ form an orthogonal vector system, the expansion coefficients a_i can be determined as usual by taking the scalar product with $\chi^{(i)}(R)$. Thus, using (3-14),

$$\sum_R \chi(R)\chi^{(i)}(R)^* = \sum_R \sum_j a_j \chi^{(j)}(R)\chi^{(i)}(R)^* = ha_i$$

and therefore

$$a_j = h^{-1} \sum_R \chi^{(j)}(R)^*\chi(R) = h^{-1} \sum_k N_k \chi^{(j)}(\mathscr{C}_k)^*\chi(\mathscr{C}_k) \quad \blacktriangleright \text{(3-20)}$$

We conclude that the number of times the various irreducible representations appear in a given reducible representation is uniquely determined by the character of the reducible representation, assuming that the character table of the group is known. We shall find this result central to the enumeration of residual degeneracies when a representation is rendered reducible by decreasing the size of the symmetry group.

The regular representation. Given the multiplication table of a group, we can always form a reducible representation called the *regular representation* as follows: Write down the multiplication table, rearranging rows so that they correspond to the *inverses* of the elements labeling the columns. In this way one naturally obtains only the identity element E along the principal diagonal. The matrix of the regular representation for the group element R is then obtained by replacing R by unity and all other elements by zero in the resulting table. For our example group, the rearranged multiplication table and a typical matrix of $\Gamma^{(\text{reg})}$ are shown below:

.	E	A	B	C	D	F
E^{-1}	E	A	B	C	D	F
A^{-1}	A	E	D	F	B	C
B^{-1}	B	F	E	D	C	A
C^{-1}	C	D	F	E	A	B
D^{-1}	F	B	C	A	E	D
F^{-1}	D	C	A	B	F	E

$$\mathbf{\Gamma}^{(\text{reg})}(A) = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}$$

Evidently, in general $\chi^{(\text{reg})}(E) = h$, and $\chi^{(\text{reg})}(R) = 0$ for $R \neq E$, since by construction only $\Gamma^{(\text{reg})}(E)$ has nonzero elements on the diagonal, and it has unity h times.

Before proceeding, we should confirm that the matrices defined above do in fact form a representation. That is, we must show that

$$\mathbf{\Gamma}^{(\text{reg})}(BC) = \mathbf{\Gamma}^{(\text{reg})}(B)\mathbf{\Gamma}^{(\text{reg})}(C)$$

or in component form

$$\Gamma^{(\text{reg})}(BC)_{A_k^{-1}A_i} = \sum_{A_j} \Gamma^{(\text{reg})}(B)_{A_k^{-1}A_j}\Gamma^{(\text{reg})}(C)_{A_j^{-1}A_i}$$

where the subscripts label the rows and columns in the rearranged multiplication table. By construction, we know that

$$\Gamma^{(\text{reg})}(B)_{A_k^{-1}A_j} = \begin{cases} 1 & \text{if } A_k^{-1}A_j = B \\ 0 & \text{otherwise} \end{cases}$$

and a similar relation holds for $\mathbf{\Gamma}^{(\text{reg})}(C)$. Thus the indicated sum over A_j will vanish unless for some A_j both $\Gamma^{(\text{reg})}(B)_{A_k^{-1}A_j}$ and $\Gamma^{(\text{reg})}(C)_{A_j^{-1}A_i}$ are simultaneously nonzero. This will occur if, and only if,

$$BC = (A_k^{-1}A_j)(A_j^{-1}A_i) = A_k^{-1}A_i,$$

in which case the sum equals unity. But this coincides with the definition of the left member $\Gamma^{(\text{reg})}(BC)_{A_k^{-1}A_i}$. Hence the matrices defined above do form a representation.

CELEBRATED THEOREM: This theorem states that the regular representation contains each irreducible representation a number of times equal to the dimensionality of the irreducible representation.

PROOF: We apply our formula (3-20) for the decomposition of representations. Thus a_j, the number of times $\Gamma^{(j)}$ appears in $\Gamma^{(\text{reg})}$, is given by

$$\begin{aligned} a_j &= h^{-1} \sum_R \chi^{(j)}(R)^*\chi^{(\text{reg})}(R) \\ &= h^{-1}\chi^{(j)}(E)h \\ &= l_j \end{aligned}$$

We now use this theorem to prove that the equality sign in (3-12) must in fact hold. By construction, the dimensionality of the regular representation is equal to h, the order of the group. But it also must equal the sum of the dimensionalities of all the irreducible representations of which it is composed. By the celebrated theorem, the latter is $\sum_j l_j \times l_j = \sum_j l_j^2$. Therefore,

$$\sum_j l_j^2 = h$$

This result removes the possible inequality sign left in our earlier argument based simply on the number of possible orthogonal vectors in a space of given dimension.

3-6 Application of Representation Theory in Quantum Mechanics

Transformation operators. Let us now depart from our formal development of the theory of group representations to examine the relation of this theory to quantum mechanics, which provides our reason for presenting the theory in the first place. In the applications which we shall consider, the group of interest is the group of symmetry operators which leave the

Hamiltonian of the problem invariant. Each such operator can be specified by giving a real orthogonal transformation of coordinates $\mathbf{R}$ such that the new coordinates $\mathbf{x}'$ are related to the original ones $\mathbf{x}$ by

$$\mathbf{x}' = \mathbf{R}\mathbf{x} \tag{3-21}$$

or in terms of components

$$x_i' = \sum_j R_{ij} x_j$$

Depending on the particular form of $\mathbf{R}$, it may represent a rotation of coordinates, a reflection, an inversion, or any combination of these. In all these cases, $\mathbf{R}$ is a real orthogonal matrix, and hence $\mathbf{R}^{-1} = \mathbf{R}^{\dagger} = \tilde{\mathbf{R}}$, where $\tilde{\mathbf{R}}$ is the transpose of $\mathbf{R}$. Thus we can write the inverse transformation as

$$x_i = \sum_j R^{-1}{}_{ij} x_j' = \sum_j R_{ji} x_j'$$

As discussed earlier, such a set of matrices $\mathbf{R}$ form a group under matrix multiplication. Although the present discussion will be given in the language of such orthogonal transformations, the results are readily carried over when the symmetry operations include, e.g., permutation of the coordinates of identical particles and translation of coordinates.

For our purposes, we now introduce a new group isomorphic to this group of coordinate transformations, in which the group elements are transformation operators which operate on *functions* rather than *coordinates*. We denote the operator which corresponds to $\mathbf{R}$ by P_R and follow Wigner's convention in defining P_R by requiring that the following be satisfied identically in $\mathbf{x}$:

$$P_R f(\mathbf{R}\mathbf{x}) = f(\mathbf{x})$$

Equivalently,

$$P_R f(\mathbf{x}) = f(\mathbf{R}^{-1}\mathbf{x}) \tag{3-22}$$

That is, P_R changes the functional form of $f(\mathbf{x})$ in such a way as to compensate for the change of variable $\mathbf{R}$.

As an example, let $\mathbf{R}$ be the transformation to X', Y', Z' axes rotated by 90° about the X axis. Then $x' = x$, $y' = z$, $z' = -y$, and the matrices concerned are

$$\mathbf{R} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{pmatrix} \qquad \mathbf{R}^{-1} = \tilde{\mathbf{R}} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

Thus

$$\mathbf{R}^{-1}\mathbf{x} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x \\ -z \\ y \end{pmatrix}$$

and from our definition above

$$P_R f(x, y, z) = P_R f(\mathbf{x}) = f(\mathbf{R}^{-1}\mathbf{x}) = f(x, -z, y)$$

For example, if we let this P_R operate on the three orthogonal p-like functions for an atom with nucleus at the origin, we obtain

$$P_R\{x\varphi(r)\} = x\varphi(r)$$
$$P_R\{y\varphi(r)\} = -z\varphi(r)$$
$$P_R\{z\varphi(r)\} = y\varphi(r)$$

since $r = (x^2 + y^2 + z^2)^{\frac{1}{2}}$ is invariant under such a rotation. We note that the contours of these functions are rotated clockwise with respect to the axes, whereas the axes are rotated counterclockwise. These two rotations compensate, as required by the definition of P_R, and one can consider the operation from either point of view. However, we shall emphasize the viewpoint in which the transformation operator P_R rotates the contours of the function, so that we minimize the chance of confusion with several sets of coordinate axes.

Before proceeding, let us verify that the group of operators P_R is in fact isomorphic to the group of coordinate transformations $\mathbf{R}$. To see this, we need to show that

$$P_S P_R = P_{SR}$$

where S and R are two transformations. We consider the successive operations in detail. First,

$$P_R f(\mathbf{x}) = f(\mathbf{R}^{-1}\mathbf{x}) = g(\mathbf{x})$$

where $g(\mathbf{x})$ is the new function which incorporates the effect of $\mathbf{R}^{-1}$ into the functional form. [In our example above, if $f(\mathbf{x}) = y\varphi(r)$, then $g(\mathbf{x}) = -z\varphi(r)$.] Now we apply the second operator P_S, obtaining

$$P_S[P_R f(\mathbf{x})] = P_S g(\mathbf{x}) = g(\mathbf{S}^{-1}\mathbf{x}) = f[\mathbf{R}^{-1}(\mathbf{S}^{-1}\mathbf{x})]$$
$$= f[(\mathbf{S}\mathbf{R})^{-1}\mathbf{x}] = P_{SR} f(\mathbf{x})$$

Thus the transformation P_{SR} arising from the product SR is the product of the transformation P_S and P_R applied in the proper order.

The group of the Schrödinger equation. Now let us consider that special group of operators P_R which commute with the Hamiltonian operator H for any given problem. These will be the operators arising from transformations which leave the Hamiltonian invariant. For example, if the potential energy in an atom depends only on the distance from the nucleus and is independent of the angular coordinates, then any rotation or reflection leaves the potential unchanged. To illustrate precisely what we mean by this, consider a simple Coulomb potential $V = -e^2/r = -e^2/(x^2 + y^2 + z^2)^{\frac{1}{2}}$. Now, under the example transformation treated above, this becomes $V = -e^2/[x^2 + (-z)^2 + y^2]^{\frac{1}{2}}$, which is in fact the same as the expression with which we began. A similar argument could be applied to the kinetic energy operator $-(\hbar^2/2m)(\partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2)$. Clearly, if an operator leaves H invariant, it is immaterial whether it appears to the left or right of it, that is, $P_R H\psi = HP_R\psi$, and the two operators commute. The set of all such operators which commute with H are said to form *the group of the Schrödinger equation.* They certainly do form a group because inverse coordinate transformations exist and because the product of two operators which leave H invariant will also leave it invariant since the product simply indicates that the two operate in succession. In the alternate language, the product of two operators which commute with H will also commute with H.

If we apply one of these commuting transformation operators to the Schrödinger equation, we have

$$P_R H\psi_n = P_R E_n \psi_n$$

or

$$HP_R\psi_n = E_n P_R \psi_n$$

since P_R commutes with H and of course with the eigenvalue E_n. From this result we conclude that any function $P_R\psi_n$ obtained by operating on an eigenfunction ψ_n by a symmetry operator from the group of the Schrödinger equation will also be an eigenfunction having the same energy as the original one. Thus, given any eigenfunction, we can generate other eigenfunctions degenerate with it by application of all the symmetry operators which commute with H. If this procedure yields *all* the degenerate functions, the degeneracy is said to be *normal.* For example, given one atomic p function, we can generate the other two degenerate with it by making rotations of coordinates, which commute with the atomic Hamiltonian because of its spherical symmetry. (Depending on the particular choice of p functions, it may be necessary to use linear combinations of rotated functions, but this is a trivial extension.) Any degenerate functions which cannot be obtained in this way are said to comprise an *accidental degeneracy*, meaning one with no obvious origin in symmetry. A classical example is the degeneracy in the hydrogen atom of states of different angular momentum l but the same principal quantum number n, for example, of $2s$ and $2p$ functions. Deeper study usually shows either that the degeneracy is not exact or else that a hidden symmetry in the Hamiltonian can be found which "explains" the degeneracy. In the example of hydrogen, Fock[1] has shown that the degeneracy can be considered to arise from a four-dimensional rotational symmetry of the Hamiltonian in momentum space.

Representations. Let us assume that the eigenvalue E_n is l_n-fold degenerate (excluding any accidental degeneracies). Then we may choose a set of l_n orthonormal eigenfunctions belonging to E_n. By our result above, operation with any commuting P_R on any one of the l_n functions produces

[1] V. Fock, *Z. Physik*, **98**, 145 (1935).

another function having the same energy, which accordingly must be expressible as a linear combination of this complete set of degenerate functions. In the language of algebra, the l_n degenerate functions form basis vectors in an l_n-dimensional vector space. This space is a subspace of the entire Hilbert space of eigenfunctions of H, a subspace invariant under all the operations of the group of the Schrödinger equation. Thus, the effect of each of these transformation operators on any function in this subspace can be represented by a matrix which can be worked out by considering the effect of the operator on each of the basis functions in turn. These matrices $\mathbf{\Gamma}$ are defined formally by

$$P_R\psi_\nu^{(n)} = \sum_{\kappa=1}^{l_n} \psi_\kappa^{(n)}\Gamma^{(n)}(R)_{\kappa\nu} \tag{3-23}$$

where the sum runs over the l_n degenerate eigenfunctions $\psi_\kappa^{(n)}$ having the same energy E_n as $\psi_\nu^{(n)}$. These l_n-dimensional matrices then form an l_n-dimensional representation of the group of the Schrödinger equation. Such a representation can be based on each set of degenerate eigenfunctions. These representations are irreducible since (excluding accidental degeneracies) there is always an operator in the group which transforms each function into any other degenerate with it. Thus no smaller matrices could express the most general transformation. To prove that the matrices defined in (3-23) actually form a representation of the group, we consider two successive operations. For simplicity we suppress the index n, which denotes the particular representation.

$$\begin{aligned} P_{SR}\psi_\nu &= P_S P_R \psi_\nu = P_S \sum_\kappa \psi_\kappa \Gamma(R)_{\kappa\nu} \\ &= \sum_\kappa (P_S\psi_\kappa)\Gamma(R)_{\kappa\nu} = \sum_{\kappa,\lambda} \psi_\lambda \Gamma(S)_{\lambda\kappa}\Gamma(R)_{\kappa\nu} \\ &= \sum_\lambda \psi_\lambda [\mathbf{\Gamma}(S)\mathbf{\Gamma}(R)]_{\lambda\nu} \end{aligned}$$

But by definition of $\mathbf{\Gamma}(SR)$,

$$P_{SR}\psi_\nu = \sum_\lambda \psi_\lambda \Gamma(SR)_{\lambda\nu}$$

Therefore

$$\mathbf{\Gamma}(SR) = \mathbf{\Gamma}(S)\mathbf{\Gamma}(R)$$

and the matrices do in fact form a representation of the group. Thus we conclude that *the set of l_n degenerate eigenfunctions $\psi_\nu^{(n)}$ of energy E_n form basis functions for an l_n-dimensional irreducible representation $\Gamma^{(n)}$ of the group of the Schrödinger equation.* One can readily show that the representation is *unitary* if one chooses an orthonormal set of basis functions.

PROOF: If we denote the Hermitian scalar product of ψ and φ by $(\psi, \varphi) = \int \psi^*\varphi\, d\tau$, and if we assume the basis functions ψ_κ to be orthonormal, then

$$\delta_{\kappa\nu} = (\psi_\kappa, \psi_\nu) = (P_R\psi_\kappa, P_R\psi_\nu)$$

since in the second form the integral may be considered simply to be carried out in a rotated coordinate system. Using the definition of the representation matrices, we find

$$\begin{aligned}
\delta_{\kappa\nu} &= \Big(\sum_\lambda \psi_\lambda \Gamma(R)_{\lambda\kappa}, \sum_\mu \psi_\mu \Gamma(R)_{\mu\nu}\Big) \\
&= \sum_{\lambda,\mu} (\psi_\lambda, \psi_\mu) \Gamma(R)^*_{\lambda\kappa} \Gamma(R)_{\mu\nu} \\
&= \sum_\lambda \Gamma(R)^*_{\lambda\kappa} \Gamma(R)_{\lambda\nu} = \sum_\lambda \Gamma(R)^\dagger_{\kappa\lambda} \Gamma(R)_{\lambda\nu} \\
&= [\mathbf{\Gamma}(R)^\dagger \mathbf{\Gamma}(R)]_{\kappa\nu}
\end{aligned}$$

Thus $\mathbf{\Gamma}(R)^\dagger \mathbf{\Gamma}(R) = \mathbf{E}$, and the matrix representation is unitary.

Group theory and quantum numbers. Finally, let us consider the effect of choosing a different set of linearly independent basis functions ψ'_μ which are linear combinations of the first set. That is,

$$\psi'_\mu = \sum_{\nu=1}^{l} \psi_\nu \alpha_{\nu\mu} \qquad \text{or} \qquad \psi_\kappa = \sum_{\lambda=1}^{l} \psi'_\lambda \alpha^{-1}{}_{\lambda\kappa}$$

Then

$$\begin{aligned}
P_R \psi'_\mu &= P_R \sum_\nu \psi_\nu \alpha_{\nu\mu} = \sum_{\kappa,\nu} \psi_\kappa \Gamma(R)_{\kappa\nu} \alpha_{\nu\mu} \\
&= \sum_{\lambda,\kappa,\nu} \psi'_\lambda \alpha^{-1}{}_{\lambda\kappa} \Gamma(R)_{\kappa\nu} \alpha_{\nu\mu} = \sum_\lambda \psi'_\lambda [\boldsymbol{\alpha}^{-1} \mathbf{\Gamma}(R) \boldsymbol{\alpha}]_{\lambda\mu} \\
&= \sum_\lambda \psi'_\lambda \Gamma'(R)_{\lambda\mu}
\end{aligned}$$

where $\mathbf{\Gamma}'$ is the new representation matrix. Thus we see that

$$\mathbf{\Gamma}'(R) = \boldsymbol{\alpha}^{-1} \mathbf{\Gamma}(R) \boldsymbol{\alpha} \tag{3-24}$$

and the different choice of basis functions merely produces a representation *equivalent* to the old one. Thus, within a similarity transformation, *there is a unique representation of the group of the Schrödinger equation corresponding to each eigenvalue of the Hamiltonian.* A set of eigenfunctions can always be classified uniquely according to the irreducible representation to which it belongs, i.e., the one for which the eigenfunctions form a set of basis vectors.

If a particular choice of matrices (within the range allowed by the similarity transformation) is made, then a function may be characterized even more precisely by giving its row index within the representation. In this way group theory provides "good quantum numbers" for any problem in the form of the labels of the representations and the rows within each one. The associated degeneracy is simply the dimensionality of the representation. Thus, by finding the dimensionalities of all the irreducible representations of the group of the Schrödinger equation (as described in Sec. 3-4), we are able to determine unequivocally the degrees of (nonaccidental) degeneracy possible in any problem. From this observation it follows that a perturbation can lift degeneracies if, and only if, its inclusion in the Hamiltonian reduces the symmetry group and hence changes the possible irreducible representations. Moreover, if representation matrices are worked out, they contain the transformation properties of all eigenfunctions under all the symmetry operators of the group.

An example. As an example using our standard group of order 6, imagine that we are interested in finding the eigenstates of an electron moving in the potential field of three protons located at the corners of an equilateral triangle. In this case the group of the Schrödinger equation contains all six rotational operations considered in this example group. (It also contains six more operations involving a reflection in the plane, but as we shall see later these extra operations do not affect the degeneracies.) This group has three irreducible representations of dimensionality 1, 1, and 2. Thus only nondegenerate and doubly degenerate states are possible. All higher degeneracy is excluded by group theory alone. Those eigenfunctions belonging to the identical representation $\Gamma^{(1)}$ are invariant under all the group operations. Similarly, basis functions of $\Gamma^{(2)}$ are invariant under E, D, and F, but they change sign under the 180° rotations A, B, and C. This can be seen from the character table, since for a one-dimensional representation $\chi(R) = \mathbf{\Gamma}(R)$. The doubly degenerate eigenfunctions of $\Gamma^{(3)}$ symmetry can be chosen so as to transform between themselves in accordance with the 2×2 matrix representation. For example, an eigenfunction ψ_1 belonging to the first row of $\Gamma^{(3)}$ will transform into $-\frac{1}{2}\psi_1 + (\sqrt{3}/2)\psi_2$ under P_B. Of course, a different choice of the degenerate eigenfunctions would transform according to a set of matrices related to those given above by a similarity transformation, which will also be unitary if the new linear combinations are chosen to preserve orthonormality.

3-7 Illustrative Representations of Abelian Groups

In an Abelian group, each element forms a class by itself. Therefore the number of classes, and hence the number of irreducible representations, equals the number of group elements h. But in this case, (3-12) requires that

$$\sum_{i=1}^{h} l_i^2 = h$$

This is possible only by choosing $l_1 = l_2 = \cdots = l_h = 1$. Thus *an Abelian group of order h has h one-dimensional representations and no others.* Each of these representations is simply a set of complex numbers, one number being associated with each group element. Note that the absence of any larger irreducible representations implies that there are no degeneracies if the symmetry group of the Hamiltonian is Abelian.

Cyclic groups. Cyclic groups are Abelian groups with elements $A_1 = A$, $A_2 = A^2, \ldots, A^h = E$. Let the number representing A itself in some representation of this group be denoted $\Gamma(A) = r$. Then $\Gamma(A_n) = \Gamma(A)^n = r^n$, and in particular $\Gamma(E) = 1$ requires that

$$\Gamma(A)^h = r^h = 1$$

or

$$r = e^{2\pi i p/h} \qquad p = 1, 2, 3, \ldots, h$$

since these h values of r form the hth roots of unity. In this way we have found all h of the irreducible representations. They can be written in the form

$$\Gamma^{(p)}(A) = e^{2\pi i p/h} \qquad p = 1, 2, 3, \ldots, h \qquad \blacktriangleright (3\text{-}25)$$

Bloch's theorem. The cyclic group of order h is the symmetry group of the Hamiltonian for a periodic potential with h periods in a ring or in a linear arrangement with periodic boundary conditions applied at walls h periods apart. In this application the group element A represents a displacement through one period. For definiteness, let A represent a displacement by a in coordinates (or by $-a$ in the contours of the function) so that $P_A\psi(x) = \psi(x + a)$. By our general theorem, all eigenfunctions of a Hamiltonian having this symmetry must transform according to some representation of the group. For example, all solutions from the pth representation must have the property

$$\psi_p(x + a) = P_A\psi_p(x) = \Gamma^{(p)}(A)\psi_p(x) = e^{2\pi i p/h}\psi_p(x)$$

Upon introducing the total length $L = ah$, this can be written as

$$\psi_p(x + a) = e^{2\pi i p a/L}\psi_p(x) = e^{ika}\psi_p(x)$$

where k is related to p by $k = 2\pi p/L$. Relabeling the function with the equivalent index k, we have

$$\psi_k(x + a) = e^{ika}\psi_k(x) \qquad (3\text{-}26)$$

This equation gives the transformation property imposed by the translational-symmetry group. As is easily seen, any function $\psi_k(x)$ satisfying (3-26) can be written in the form

$$\psi_k(x) = u_k(x)e^{ikx} \qquad (3\text{-}27)$$

where $u_k(x)$ is periodic with the period a. This result is the celebrated Bloch theorem of solid-state physics. Clearly it is based purely on symmetry through the machinery of group theory. Therefore it is a rigorous result, free of special approximations, and k defined in this way is a "good quantum number" for characterizing eigenfunctions for a periodic potential.

Two-dimensional rotation group. Any group composed of rotations about a fixed axis is clearly an Abelian group. If all angles of rotation φ are

allowed, the group is of infinite order. However, it is so simple that we can handle it anyway. Being Abelian, its representations are just numbers. The group-multiplication property for successive rotations implies that the representations satisfy

$$\Gamma(\varphi_1)\Gamma(\varphi_2) = \Gamma(\varphi_1 + \varphi_2)$$

This can be satisfied only by an exponential relation of the sort

$$\Gamma^{(m)}(\pm\varphi) = e^{im\varphi} \qquad (3\text{-}28)$$

the plus sign referring to a rotation of axes and the negative sign to a rotation of the contours of the function. We choose the latter convention in discussing rotations. The representation index m is restricted to the values $m = 0, \pm 1, \pm 2, \ldots$ by the requirement that $\Gamma^{(m)}(2\pi) = \Gamma^{(m)}(E) = 1$. It is readily verified that any function satisfying

$$\begin{aligned}\psi_m(r, \theta, \varphi - \varphi_0) &= P_{\varphi_0}\psi_m(r, \theta, \varphi)\\ &= \Gamma^{(m)}(\varphi_0)\psi_m(r, \theta, \varphi) = e^{-im\varphi_0}\psi_m(r, \theta, \varphi)\end{aligned}$$

depends on φ only through a factor $e^{im\varphi}$. Hence any eigenfunction for a Hamiltonian whose symmetry group is the group of all rotations about an axis must have the form

$$\psi_m(r, \theta, \varphi) = f(r, \theta)e^{im\varphi} \qquad m = 0, \pm 1, \pm 2, \ldots$$

This result is a familiar consequence of the fact that angular momentum along an axis of symmetry is conserved and hence has a good quantum number m associated with it.

3-8 Basis Functions for Irreducible Representations

The foregoing simple examples have given a small indication of the way in which irreducible-representation labels serve as good quantum numbers in physical applications. We now wish to develop methods for dealing with the representations of dimensionality greater than 1, which arise when the symmetry group contains noncommuting elements leading to the possibility of degeneracy. In this case we need *two* labels for a basis function, one for the irreducible representation and one for the row (or column) within the representation. Naturally the second label retains a definite significance only as long as we confine ourselves to a particular choice of representation matrices from among all the equivalent sets related by a similarity transformation.

Let a basis function belonging to the κth row of the jth irreducible representation be denoted $\varphi_\kappa^{(j)}$. The other functions $\varphi_\lambda^{(j)}$ required to complete the basis for the representation are called the *partners* of the given function. Then by definition the result of operating with any element of the group on $\varphi_\kappa^{(j)}$ can be expressed as a linear combination of $\varphi_\kappa^{(j)}$ and its partners as follows,

$$P_R\varphi_\kappa^{(j)} = \sum_{\lambda=1}^{l_j} \varphi_\lambda^{(j)}\Gamma^{(j)}(R)_{\lambda\kappa} \tag{3-29}$$

where l_j is the dimensionality of the representation. Now, if we multiply through by $\Gamma^{(i)}(R)^*_{\lambda'\kappa'}$, sum over R, and use the great orthogonality theorem (3-8), we obtain

$$\sum_R \Gamma^{(i)}(R)^*_{\lambda'\kappa'}P_R\varphi_\kappa^{(j)} = \frac{h}{l_j}\,\delta_{ij}\delta_{\kappa\kappa'}\varphi_{\lambda'}^{(j)} \tag{3-30}$$

From this equation we conclude that application of the operator

$$\mathscr{P}_{\lambda\kappa}^{(j)} = \frac{l_j}{h}\sum_R \Gamma^{(j)}(R)_{\lambda\kappa}{}^*P_R \tag{3-31}$$

to a basis function has the property of yielding zero unless the function being operated on belongs to the κth row of $\Gamma^{(j)}$. Moreover, we see that, if this condition *is* satisfied, then the result of the operation is $\varphi_\lambda^{(j)}$. This gives us a prescription for generating all the partners of any given basis function. Also, if we set $\lambda = \kappa$, we obtain

$$\mathscr{P}_{\kappa\kappa}^{(j)}\varphi_\kappa^{(j)} = \varphi_\kappa^{(j)} \tag{3-32}$$

In other words, $\varphi_\kappa^{(j)}$ is an eigenfunction of $\mathscr{P}_{\kappa\kappa}^{(j)}$ with eigenvalue unity. This property serves to identify uniquely the labels of any basis function. Note that, since $\mathscr{P}_{\kappa\kappa}^{(j)}$ is a linear operator, any linear combination of functions belonging to the κth row of $\Gamma^{(j)}$ (but coming from different choices of basis functions) such as $a\varphi_\kappa^{(j)} + b\psi_\kappa^{(j)}$ will also belong to that row and representation.

THEOREM: If $\Gamma^{(1)}, \Gamma^{(2)}, \ldots, \Gamma^{(c)}$ are all of the distinct irreducible representations of a group of operators P_R, then any function F in the space operated on by P_R can be decomposed into a sum of the form

$$F = \sum_{j=1}^{c}\sum_{\kappa=1}^{l_j} f_\kappa^{(j)} \tag{3-33}$$

where $f_\kappa^{(j)}$ belongs to the κth row of the jth irreducible representation.

PROOF: Consider the set of all functions $F, F_2', \ldots, F_h'$ formed by operation with the operators $P_E, P_{A_2}, \ldots, P_{A_h}$ on F. Discard all functions which are not linearly independent of the others, and orthogonalize the remainder (e.g., by the Schmidt procedure). Denote the resulting set of n functions by $F, F_2, \ldots, F_n$. These functions form the basis for a unitary representation of the group, since the result of successive operations must always be expressible as a linear combination of the set. This follows since the equation $P_SP_RF = P_{SR}F$ is in the space spanned by the set, by construction.

Call this n-dimensional representation Γ, so that

$$P_RF_k = \sum_{i=1}^{n} F_i\Gamma(R)_{ik}$$

There are now two possibilities: either Γ is one of the irreducible representations, or it is not. If it is, then F has been shown to belong to a particular row of that representation and the theorem is proved. If it is not, then it can be brought to block form in terms of the chosen irreducible representation matrices by a similarity transformation, so that

$$\boldsymbol{\alpha}^{-1}\boldsymbol{\Gamma}(R)\boldsymbol{\alpha} = \begin{pmatrix} \boldsymbol{\Gamma}^{(i)}(R) & 0 & 0 \\ 0 & \boldsymbol{\Gamma}^{(j)}(R) & 0 \\ 0 & 0 & \cdots \end{pmatrix} \tag{3-34}$$

The matrix $\boldsymbol{\alpha}$ now defines a set of functions F_k'' which transform according to (3-34) and hence are functions of the type $f_\kappa^{(j)}$ for various values of j and κ. Using the inverse $\boldsymbol{\alpha}^{-1}$, we may express the F_k, and in particular F, as linear combinations of the F_k'' or $f_\kappa^{(j)}$. This completes the proof.

Having established the validity of (3-33), we may now use the operators $\mathscr{P}_{\kappa\kappa}^{(j)}$ defined in (3-31) to determine the individual terms in the sum in (3-33). We have noted that

$$\mathscr{P}_{\kappa\kappa}^{(j)}f_{\kappa'}^{(j')} = \delta_{\kappa\kappa'}\delta_{jj'}f_\kappa^{(j)} \tag{3-35}$$

Therefore

$$\mathscr{P}_{\kappa\kappa}^{(j)}F = f_\kappa^{(j)} \tag{3-36}$$

and $\mathscr{P}_{\kappa\kappa}^{(j)}$ is a *projection operator* which projects out the part of any function which belongs to the κth row of the jth representation. Such a projection operator is called *idempotent* because of the property that

$$\mathscr{P}_{\kappa\kappa}^{(j)}\mathscr{P}_{\kappa\kappa}^{(j)} = \mathscr{P}_{\kappa\kappa}^{(j)}$$

i.e., all powers of the operator are equal.

We now are able to form a set of basis functions for any representation at will. Starting with an arbitrary function F, we can project out one $f_\kappa^{(j)}$, which after normalization is a suitable basis function $\varphi_\kappa^{(j)}$. Then use of the transfer operators $\mathscr{P}_{\lambda\kappa}^{(j)}$ yields all its partners, since $\mathscr{P}_{\lambda\kappa}^{(j)}\varphi_\kappa^{(j)} = \varphi_\lambda^{(j)}$. Van Vleck has appropriately styled this procedure as the *basis-function generating machine*.

THEOREM: Two functions which belong to different irreducible representations or to different rows of the same unitary representation are orthogonal.

PROOF: Consider the scalar product

$$(\varphi_\kappa^{(j)}, \psi_{\kappa'}^{(j')}) = (P_R\varphi_\kappa^{(j)}, P_R\psi_{\kappa'}^{(j')})$$
$$= \sum_{\lambda,\lambda'} \Gamma^{(j)}(R)^*_{\lambda\kappa}\Gamma^{(j')}(R)_{\lambda'\kappa'}(\varphi_\lambda^{(j)}, \psi_{\lambda'}^{(j')})$$

We may sum the right member over all R and divide by h, since it must be independent of R. Applying the great orthogonality theorem, we obtain

$$(\varphi_\kappa^{(j)}, \psi_{\kappa'}^{(j')}) = \delta_{jj'}\delta_{\kappa\kappa'} \sum_{\lambda=1}^{l_j} (\varphi_\lambda^{(j)}, \psi_\lambda^{(j)}) l_j^{-1}$$

Thus, not only have we proved the theorem, but we have also shown that the scalar product $(\varphi_\kappa^{(j)}, \psi_\kappa^{(j)})$ is independent of κ.

The results derived above have required knowledge of the complete representation matrices $\mathbf{\Gamma}^{(j)}(R)$ or at least all the diagonal values $\Gamma^{(j)}(R)_{\kappa\kappa}$. We can get similar but less detailed results with knowledge of only the characters of the representations. To do this, we set $\lambda = \kappa$ in (3-31) and sum over κ. This defines a new projection operator

$$\mathscr{P}^{(j)} = \sum_\kappa \mathscr{P}_{\kappa\kappa}^{(j)} = \frac{l_j}{h} \sum_R \chi^{(j)}(R)^* P_R \tag{3-37}$$

Following arguments similar to those above, we see that any function $f^{(j)}$ expressible as a sum of functions belonging only to rows within the jth representation will satisfy $\mathscr{P}^{(j)} f^{(j)} = f^{(j)}$ and that

$$\mathscr{P}^{(j)} F = f^{(j)} \tag{3-38}$$

That is, from an arbitrary function $\mathscr{P}^{(j)}$ projects out the part belonging to the jth representation. These results are of course unaffected by similarity transformations which scramble the basis functions, and hence the rows, in any given representation.

As a rather trivial example of these results, consider the group consisting of the identity and the reflection operator σ which takes x into $-x$. This group has two classes, hence two one-dimensional irreducible representations. The character table is

	E	σ
$\Gamma^{(1)}$	1	1
$\Gamma^{(2)}$	1	-1

Hence, the projection operator for $\Gamma^{(1)}$ is $\mathscr{P}^{(1)} = (\frac{1}{2})(P_E + P_\sigma)$, and that for $\Gamma^{(2)}$ is $\mathscr{P}^{(2)} = (\frac{1}{2})(P_E - P_\sigma)$. Operating on an arbitrary function $F(x)$, these yield $\mathscr{P}^{(1)}F(x) = (\frac{1}{2})[F(x) + F(-x)]$ and $\mathscr{P}^{(2)}F(x) = (\frac{1}{2})[F(x) - F(-x)]$. Clearly these projected functions are, respectively, even and odd under reflection, as required for them to belong to $\Gamma^{(1)}$ and $\Gamma^{(2)}$, respectively. Our other theorems are illustrated by the facts that any function can be expressed as the sum of odd and even parts constructed as above and that any odd function is orthogonal to any even one.

The techniques developed in this section are useful in setting up proper zero-order symmetry orbitals which belong to a given row of a given representation. We shall later prove that, since the Hamiltonian commutes with the entire group of symmetry operators, then it can have matrix elements only between functions of the same representational classification. This leads to a maximum reduction in the size of the secular equations that must be solved.

3-9 Direct-product Groups

It often occurs that the complete symmetry of the system under consideration can be broken up into two or more types such that the operators of one type commute with those of any other. An important example is that in which the two types of operators operate on entirely different coordinates. For example, in H_2O we can permute the two protons, permute the 10 electrons, and rotate the molecule as a whole. One of each of these three types of operations could be carried out in any order with the same final result. A second example is the separation of orbital and spin operators. A third example is the inversion operator and the group of proper rotations.

Although such cases could be treated with no special attention, we can simplify our work considerably by taking advantage of these properties by introducing the concept of *direct-product groups*. If we have two groups of operators, $\mathscr{G}_a = E, A_2, \ldots, A_{h_a}$ and $\mathscr{G}_b = E, B_2, \ldots, B_{h_b}$ such that all of $\mathscr{G}_a$ commute with all of $\mathscr{G}_b$, then

$$\mathscr{G}_a \times \mathscr{G}_b = E, A_2, \ldots, A_{h_a}, B_2, A_2B_2, \ldots, A_{h_a}B_2, \ldots, A_{h_a}B_{h_b}$$

forms a group of $h_a h_b$ elements, assuming that the only common element in the groups is the identity. To check that this is so, we consider the multiplication of two elements

$$A_k B_l A_{k'} B_{l'} = (A_k A_{k'})(B_l B_{l'})$$

since B_l and $A_{k'}$ commute. But the right member is found in the direct-product group defined above since $\mathscr{G}_a$ and $\mathscr{G}_b$ are separately groups closed under multiplication. Therefore $\mathscr{G}_a \times \mathscr{G}_b$ is also closed, as required.

Representations. It is natural to suppose that the direct-product matrices of the irreducible representations of the component groups might form irreducible representations of the direct-product group. This in fact is the case. As described in Appendix A, the direct product of two matrices **A** and **B** is a matrix **A × B** whose elements are all the products of an element of **A** and one of **B**. Each element bears a double set of subscripts. For example, the element obtained from $A_{ij}B_{kl}$ is labeled $(A \times B)_{ik,jl}$, the two initial indices being given before the comma. The fact that these direct-product matrices in fact have the requisite group-multiplication property follows from the commutivity of ordinary matrix multiplication and the direct-product operation. Thus

$$\begin{aligned}\mathbf{\Gamma}^{(a\times b)}(A_kB_l)\mathbf{\Gamma}^{(a\times b)}(A_{k'}B_{l'}) &= [\mathbf{\Gamma}^{(a)}(A_k)\times\mathbf{\Gamma}^{(b)}(B_l)][\mathbf{\Gamma}^{(a)}(A_{k'})\times\mathbf{\Gamma}^{(b)}(B_{l'})]\\ &= [\mathbf{\Gamma}^{(a)}(A_k)\mathbf{\Gamma}^{(a)}(A_{k'})]\times[\mathbf{\Gamma}^{(b)}(B_l)\mathbf{\Gamma}^{(b)}(B_{l'})]\\ &= \mathbf{\Gamma}^{(a)}(A_kA_{k'})\times\mathbf{\Gamma}^{(b)}(B_lB_{l'})\\ &= \mathbf{\Gamma}^{(a\times b)}(A_kA_{k'}B_lB_{l'})\end{aligned}$$

By an application of Schur's lemma it can be shown[1] that the direct product of two *irreducible* representations forms an *irreducible* representation of the direct product group. We now show that we get *all* the irreducible representations of the direct-product group in this way. Let $l_1^a, l_2^a, \ldots$ and $l_1^b, l_2^b, \ldots$ be the dimensionalities of the irreducible representations of $\mathscr{G}_a$ and $\mathscr{G}_b$. By our dimensionality theorem (3-12),

$$\sum_i (l_i^a)^2 = h_a, \quad\text{and}\quad \sum_j (l_j^b)^2 = h_b.$$

By the definition of the direct-product matrices, their dimensionalities will be $l_{ij} = l_i^a l_j^b$. Then applying (3-12) to the product group

$$\begin{aligned}\sum_{i,j} l_{ij}^2 &= \sum_{i,j}(l_i^a l_j^b)^2 = \sum_i (l_i^a)^2 \sum_j (l_j^b)^2\\ &= h_a h_b = h\end{aligned}$$

where h is the order of the direct-product group. Since $\sum_{i,j} l_{ij}^2 = h$, there can be no other irreducible representations than those expressible as direct products. Note that these direct-product representations carry a double set of representation and row labels. This illustrates how extra quantum numbers arise when there are extra independent degrees of freedom characterized by extra commuting symmetry operators.

Class structure and characters. The class structure of the product group is easily obtained from knowledge of the class structure of the component groups since elements from $\mathscr{G}_a$ commute with those of $\mathscr{G}_b$. Therefore, the number of classes is simply the product of the numbers of classes in $\mathscr{G}_a$ and in $\mathscr{G}_b$, in agreement with the number of irreducible representations in the product group.

An important observation is that the character of any direct-product representation is the product of the characters of the component representations. This is proved by simple inspection of the character,

$$\begin{aligned}\chi^{(a\times b)}(A_kB_l) &= \sum_{i,j}\Gamma^{(a\times b)}(A_kB_l)_{ij,ij}\\ &= \sum_{i,j}\Gamma^{(a)}(A_k)_{ii}\Gamma^{(b)}(B_l)_{jj} = [\sum_i \Gamma^{(a)}(A_k)_{ii}][\sum_j \Gamma^{(b)}(B_l)_{jj}]\\ &= \chi^{(a)}(A_k)\chi^{(b)}(B_l)\end{aligned}$$

[1] Wigner, *op. cit.*, chap. 16.

This allows us to write out the character table of any group which can be expressed as a direct product with knowledge of only the character tables of the smaller groups from which it is composed. Naturally this provides a great practical simplification.

Example. Let us consider the direct-product group composed of the rotation group of the equilateral triangle (called D_3 in standard notation) and the group $\mathscr{S} = (E, \sigma_h)$. In the latter group, σ_h is the operation of reflection in the plane of the triangle. In standard notation, the direct-product group is called D_{3h}. It is the symmetry group for an equilateral triangle of finite thickness, so that we have an additional six inequivalent positions in which the "numbers on the triangle" have been reflected through onto the other surface. There are now 12 group elements, the original 6 from D_3, each multiplied both by the identity and by σ_h. This is what we mean by the notation $D_{3h} = D_3 \times \mathscr{S}$. The elements of D_3 and $\mathscr{S}$ commute because it makes no difference whether the triangle is first rotated and then subjected to reflection in the plane, or vice versa.

The multiplication table of $\mathscr{S}$ is

	E	σ_h
E	E	σ_h
σ_h	σ_h	E

The group is Abelian; so there are two classes and two one-dimensional irreducible representations. Upon denoting the two representations Γ^+ and Γ^- for even and odd, the character table is simply

$\mathscr{S}$	E	σ_h
Γ^+	1	1
Γ^-	1	−1

Multiplying this table by that for D_3 given in Sec. 3-3, we obtain the character table for the product group D_{3h}.

D_{3h}	E	(A, B, C)	(D, F)	σ_h	$\sigma_h(A, B, C)$	$\sigma_h(D, F)$
$\Gamma^{(1+)}$	1	1	1	1	1	1
$\Gamma^{(2+)}$	1	−1	1	1	−1	1
$\Gamma^{(3+)}$	2	0	−1	2	0	−1
$\Gamma^{(1-)}$	1	1	1	−1	−1	−1
$\Gamma^{(2-)}$	1	−1	1	−1	1	−1
$\Gamma^{(3-)}$	2	0	−1	−2	0	1

For clarity, we have labeled the columns by giving the actual group elements in the class rather than using arbitrary class labels $\mathscr{C}_1, \ldots, \mathscr{C}_6$. Now that the table is worked out, we could dispense completely with the observation that the group D_{3h} may be viewed as a direct product and simply treat it as an ordinary group of order 12. However, the distinction is very worthwhile in reducing the effort required to work out the table. We note in passing that going from D_3 to D_{3h} has not changed the degeneracies (one or two) which are possible in view of the dimensionalities of the irreducible representations. This verifies the assertion made in the example treated at the end of Sec. 3-6.

3-10 Direct-product Representations within a Group

A distinct, although related, example of the use of the direct product is in the formation of a new representation Γ of a given group from two representations $\Gamma^{(1)}$ and $\Gamma^{(2)}$ of the same group. This is done by using as basis functions all possible products of the basis functions from the two initial representations. Let the two bases be

$$\varphi_1, \ldots, \varphi_n \qquad \text{and} \qquad \psi_1, \ldots, \psi_m$$

where n and m are the dimensionalities of $\Gamma^{(1)}$ and $\Gamma^{(2)}$, respectively. Then the functions $\varphi_\kappa\psi_\lambda$ form a basis for an nm-dimensional representation Γ. This may be verified by considering the effect of a transformation operator,

$$\begin{aligned} P_R(\varphi_\kappa\psi_\lambda) &= \sum_{\kappa'} \varphi_{\kappa'}\Gamma^{(1)}(R)_{\kappa'\kappa} \sum_{\lambda'} \psi_{\lambda'}\Gamma^{(2)}(R)_{\lambda'\lambda} \\ &= \sum_{\kappa',\lambda'} \varphi_{\kappa'}\psi_{\lambda'}[\Gamma^{(1)}(R)_{\kappa'\kappa}\Gamma^{(2)}(R)_{\lambda'\lambda}] \\ &= \sum_{\kappa',\lambda'} \varphi_{\kappa'}\psi_{\lambda'}\Gamma(R)_{\kappa'\lambda',\kappa\lambda} \end{aligned}$$

where $\mathbf{\Gamma}(R) = \mathbf{\Gamma}^{(1)}(R) \times \mathbf{\Gamma}^{(2)}(R)$. Thus the direct-product matrices $\mathbf{\Gamma}(R)$ form a representation of the group based on the functions $\varphi_\kappa\psi_\lambda$.

As in the previous section, the character is obtained by taking the product of the characters of the component representations. That is,

$$\chi(R) = \chi^{(1)}(R)\chi^{(2)}(R)$$

where χ is the character for the representation Γ.

An important difference between these direct-product representations and those treated in the previous section is that in the present case the representations are in general reducible. This is obviously true, in view of the limited total number of distinct *irreducible* representations for any given group. If one then forms a new nm-dimensional representation, it must

in general be reducible to a sum of irreducible representations. We express this schematically by writing

$$\Gamma^{(i)} \times \Gamma^{(j)} = \sum_k a_{ijk}\Gamma^{(k)} \tag{3-39}$$

As before, this notation means that, if $\mathbf{\Gamma}^{(i)}(R) \times \mathbf{\Gamma}^{(j)}(R)$ is brought to block form, $\mathbf{\Gamma}^{(k)}(R)$ appears a_{ijk} times along the diagonal. We may find the coefficients a_{ijk} by using our standard formula (3-20) for the decomposition of a reducible representation. Since

$$\chi(R) = \chi^{(i)}(R)\chi^{(j)}(R) = \sum_k a_{ijk}\chi^{(k)}(R)$$

$$\begin{aligned} a_{ijk} &= h^{-1} \sum_R \chi^{(i)}(R)\chi^{(j)}(R)\chi^{(k)}(R)^* \\ &= h^{-1} \sum_l N_l\chi^{(i)}(\mathscr{C}_l)\chi^{(j)}(\mathscr{C}_l)\chi^{(k)}(\mathscr{C}_l)^* \end{aligned} \tag{3-40}$$

Note that if, as is usual, the $\chi^{(k)}(\mathscr{C}_l)$ are real, then a_{ijk} is independent of the order of the indices.

This technique of decomposing a direct-product representation will prove of great usefulness in determining selection rules and in other applications.

EXERCISES

3-1 (*a*) How many inequivalent irreducible representations of D_4, the symmetry group of the square considered in Exercise 2-1, exist? What are their dimensionalities?

(*b*) Work out the character table of this group by inspection, using the rules given in Sec. 3-4. Verify the formula based on the c_{ijk} in several instances.

3-2 Show in general that $\sum_R \chi^{(j)}(R) = 0$ for all representations except the identical representation $\Gamma^{(1)}$, in which all elements are represented by 1. What is the value of the sum for $\Gamma^{(1)}$?

3-3 Write out the matrices of the regular representation of the group D_4 for the elements E, F, G, H. Using these matrices, verify by direct matrix multiplication that $FG = H$.

3-4 Using the regular representation, prove that

$$\sum_j l_j\chi^{(j)}(R) = h$$

if $R = E$ and is zero otherwise. In this l_j is the dimensionality of the jth representation. This result is an additional aid in working out the character tables.

3-5 Work out the orthogonal transformation matrices $R_x(\theta_x)$, $R_y(\theta_y)$, and $R_z(\theta_z)$ for rotations of axes by angles θ_x, θ_y, θ_z about the x, y, z axes, respectively. Take the sense of rotation so that the y axis is rotated toward x in R_z, etc. Using them, compute the matrices $R_x(\theta_x)R_y(\theta_y)$ and $R_y(\theta_y)R_x(\theta_x)$. Note that these rotations do not commute. What is the matrix for $R_xR_y - R_yR_x$? Show that this matrix vanishes as θ^2 if $\theta_x = \theta_y = \theta$ is much less than 1 and corresponds to the *change* $(R_z - E)$ produced by a rotation through θ^2 about the z axis.

3-6 (*a*) Find the transformed functions P_Rf, P_Sf, $P_S(P_Rf)$, $P_{SR}f$, and $P_{RS}f$, where $f = x$, $R = R_y(\theta_y)$, and $S = R_z(\theta_z)$. Note that $\mathbf{R}^{-1} = \mathbf{R}^\dagger = \tilde{\mathbf{R}}$. Generalizing from your results, you may observe that the three p-like functions x, y, z form a basis for a three-dimensional representation of the complete rotation group since

$$P_R p_i = \sum_j p_j \Gamma(R)_{ji}$$

where $i, j = x, y, z$ and R represents any arbitrary rotation. This property is true of the $(2l + 1)$ polynomials equivalent to the spherical harmonics corresponding to any l and of the spherical harmonics themselves.

(*b*) Repeat (*a*) for $f = xy$. Find a convenient set of partners to xy in a basis for representing an arbitrary rotation.

3-7 (*a*) Form a representation of D_3, the rotational symmetry group of the equilateral triangle, which has $F = x^2zg(r)$ as part of its basis. The z axis is the three-fold axis, and $g(r)$ is such as to assure radial convergence in the normalization integral. What are the other basis functions?

(*b*) If this representation is reducible, into what irreducible representations does it reduce?

(*c*) If your basis functions are not orthonormal, choose a new set of linear combinations of them that are. (You need orthonormalize only the angular part.) By applying the corresponding similarity transformation to the matrices of your representation, transform it into a unitary representation. If you have chosen your orthonormal functions wisely, the matrices will now be in block form. If not, reduce them to block form by a suitable unitary transformation to a new orthonormal basis.

(*d*) Express $F = x^2zg(r)$ explicitly as a sum of parts $\sum_{j,\kappa} f_\kappa^{(j)}$, each of which transforms according to a particular row of one of the irreducible representations.

3-8 Write out the character table of D_{4h}, taking advantage of the fact that $D_{4h} = D_4 \times i$, where i is the group containing only the inversion and the identity.

3-9 (*a*) Find unitary matrices for all the irreducible representations of D_4. (HINT: Consider the transformation properties of the coordinates x and y in the plane of the square.)

(*b*) How could you now obtain matrices for all the irreducible representations of D_{4h}?

3-10 Work out all direct products $\Gamma^{(i)} \times \Gamma^{(j)} = \sum_k a_{ijk}\Gamma^{(k)}$ of the irreducible representations of the group D_3. Note that a_{ijk} is independent of the subscript order since all the characters involved are real.

3-11 Repeat Exercise 3-10 for the groups D_4 and O, O being the octahedral group discussed in Sec. 4-6, where a character table is given.

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