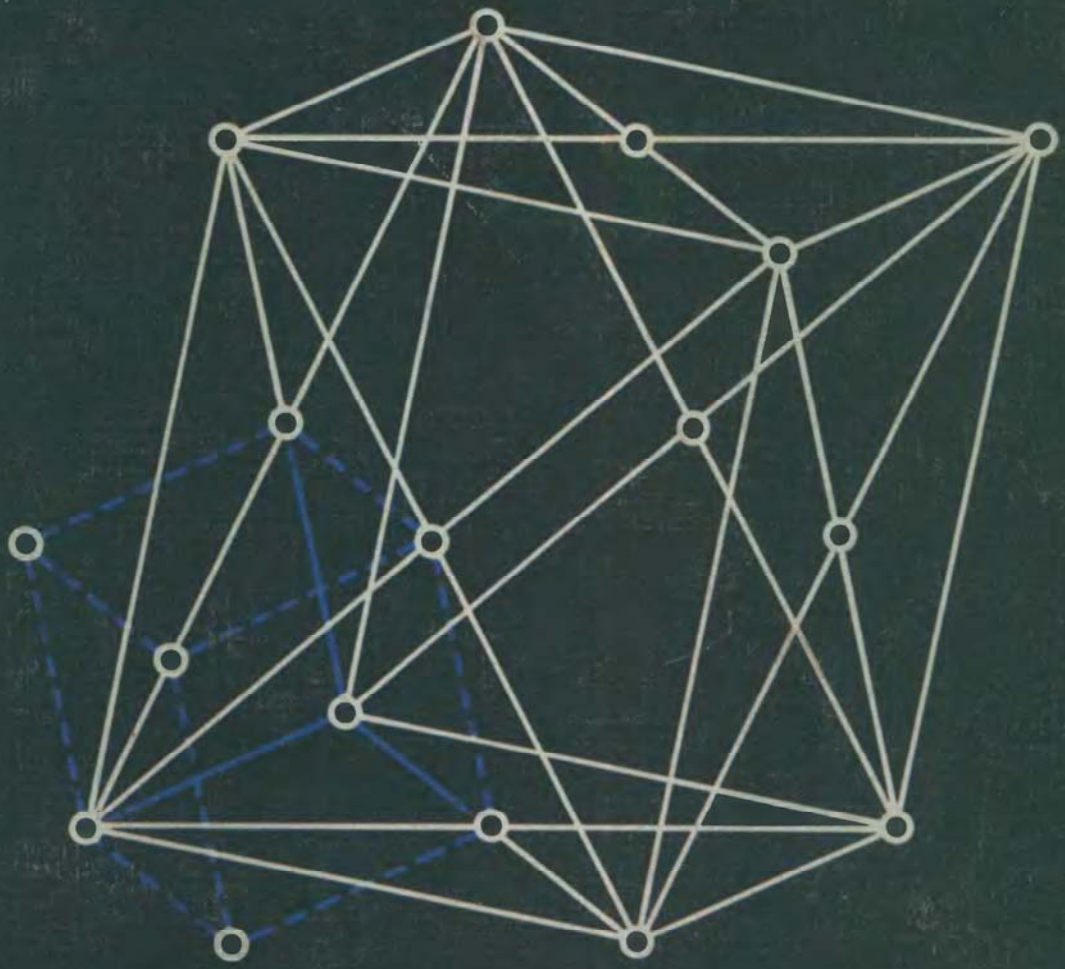
G. L. Bir and G. E. Pikus

SYMMETRY AND STRAIN-INDUCED EFFECTS IN SEMICONDUCTORS



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CONTENTS

FOREWORD TO ENGLISH EDITION

It is with great anticipation that we, who have worked on one aspect or another of the band structure of semiconductors, have looked forward to the appearance of the English translation of the Bir-Pikus book. It is a landmark! No other term, I think, fits so aptly. And now it will become accessible through the good offices of the Israel Program for Scientific Translations to a much larger readership outside of the Soviet Union. Its impact on semiconductor physics will be great and long lasting.

This book is distinguished in many ways. Much could be said about the wealth of material it holds, a great deal of which is exposed to easy access for the first time, or about the thorough exposition of the methods of group theory formal enough to satisfy the theorist yet cast in a pedagogical style to teach the experimental physicist. But the *tour de force* which sets this book apart from all others is its elegant and definitive treatment of the theory of deformation effects in crystals, which organizes and elevates this subject to its rightful place of importance in solid state physics. Certainly no one is better qualified than the authors to do this. Bir and Pikus effectively opened this field in the late 1950s with their now classical papers on the effects of uniaxial deformation on the degenerate valence bands of cubic semiconductors. Since that event, and stimulated to a large extent by a continuing flow of theoretical work from Bir and Pikus, the subject has expanded immensely, so that today uniaxial stress occupies a role alongside large external magnetic and electric fields as a standard tool for perturbing and studying energy spectra in solids. This book crowns their accomplishments.

One topic which receives special emphasis is the theory of invariants. This beautiful and rigorous theory based on symmetry was pioneered nearly 20 years ago by J. M. Luttinger, but has failed to receive the widespread application it deserves. This is surprising because one needs only to recount how much the explosive growth of electron paramagnetic resonance in the 1950s owes to the single development of the Spin Hamiltonian to realize how important the analogous construct could be for the representation of energy spectra of electrons and phonons, especially in the presence of crystal deformations and magnetic fields. In the hands of Bir and Pikus the theory of invariants is developed with such clarity and applied so generally that its simplicity, elegance, and impressive power can no longer be overlooked.

The authors include some experimental results for illustration. The speed at which these parts become dated will be a measure of the book's success.

J. C. Hensel

PREFACE

In recent years, group-theoretic methods have found wide application in solid state physics and the use of these methods has become a prerequisite for experimental as well as theoretical physicists.

By tradition, however, most books on group theory are devoted primarily to questions arising in atomic and molecular theory. Much work, including important results, with a bearing on the application of group theory to solid state physics cannot be found in any of these books.

The present authors' goal was to write a book devoted specifically to the applications of group theory to solid state physics, presenting, on the one hand, a detailed exposition of those parts of group theory which find application in solid state physics and, on the other, leading up to an examination of specific physical effects. Major attention has been paid to strain-induced effects, more precisely, effects produced by strains which break the symmetry of the crystal, since the relevant theory may be based almost entirely on symmetry theory.

The first part of the book, Chapters I–III, presents an exposition of the requisite parts of group theory. In distinction from other monographs, we make systematic use of projective representations to construct representations of the space groups. In this connection a detailed description is given of Schur's classical method for construction of projective representations, and their properties are described in detail. Using this method, we construct projective representations of all the point groups, which then lead easily to the representation matrices of all the space groups.

Consideration is also given in this part of the book to the role of time inversion and to selection rules for space groups allowing for time inversion. Hitherto, material on these questions has been available only in the original papers.

The second part of the book, Chapters IV and V, gives a description of group-theoretic methods for construction of electron or phonon spectra in the vicinity of singular points, including spectra in strained crystals. Apart from the so-called $\boldsymbol{kp}$ theory, which is essentially a modification of the usual perturbation theory for a degenerate spectrum, we make wide use of the theory of invariants. The latter method is employed not merely for its computational advantages. Unlike $\boldsymbol{kp}$-theory, which is based on the self-consistent field approximation, the theory of invariants usually assumes, apart from the general elements of symmetry theory, only the existence of quasi-particles, which is not open to question, at least when the number of particles is sufficiently small and their interaction therefore negligible. For this reason, comparison of the results obtained by both methods enables one to determine which of the conclusions of $\boldsymbol{kp}$-theory are indeed based on the assumption that the self-consistent field exists and which are not. For example, the two-band model of $\boldsymbol{kp}$-theory is based on the assumption that the self-consistent

potential is the same for electrons at the bottom of the conduction band and at the top of the valence band. Results obtained by the theory of invariants show that practically all conclusions following from the $\boldsymbol{kp}$-theory remain valid independently of this assumption.

The third part of the book (Chapters VI and VII) examines various strain-induced effects in semiconductors. From the extremely broad range of such effects, we have selected mainly optical and resonance phenomena which are most directly linked with the structure of the current carrier spectrum and the changes it experiences under strain, and which yield the most reliable determination of this spectrum. An exception is §34, in which we consider the effect of strain on the electric conductivity of semiconductors. This effect, which has been studied most extensively, is the basis for many more complex effects widely applied for investigation of semiconductors, and is exploited in various semiconductor devices. The piezoresistance effect and the various secondary effects that it produces, such as concentration effects in intrinsic semiconductors, are widely used in strain gauges of various types.

Unlike the first two parts of the book, which discuss general material, the last part is more specialized in nature. We have nevertheless seen fit to include these sections, since they provide good examples of the use of general methods to solve specific problems with a direct bearing on experiment, and are moreover of independent interest owing to the increasing use of strain-based methods to investigate semiconductors. Most of our attention in this part of the book is devoted to theoretical questions. The experimental material presented in the tables and figures is mainly illustrative and far from complete.

In describing methods for construction of spectra and examining specific effects we naturally could not consider all groups of conductors. We have therefore confined ourselves consistently throughout this part of the book to the semiconductors best studied and most widely used in technology: cubic lattices of the diamond type (Ge, Si) and the zinc blende type, and hexagonal lattices of the wurtzite type. The wurtzite lattice is characteristic for most semiconductors of A_3B_5 and A_2B_6 types. Brief consideration is also given to the NaCl cubic lattice. This structure is characteristic for PbSe, PbTe, PbS and other semiconductors.

The literature used in writing the book and various papers significantly complementing and extending the material are listed in the bibliography. This bibliography naturally lays no claim to completeness. The items are classified according to the specific sections of the book to which they are relevant. For this reason, specific references are generally omitted in the text.

As stated above, familiarization with the methods of group theory is a sine qua non not only for theoreticians but also for experimental physicists. The authors have therefore striven to present the material in the most systematic and accessible form. To what degree they have achieved this goal must be judged by the reader.

In conclusion, it is our pleasant duty to thank D.K. Faddeev, E.I. Rashba and E.L. Ivchenko, who read through the manuscript fully or in part and offered many useful comments.

The authors

Chapter I

CRYSTAL SYMMETRY

§1. ELEMENTS OF ABSTRACT GROUP THEORY

The symmetry of a body is characterized by the transformations which leave it invariant, i.e., bring it into coincidence with itself.

The set of symmetry elements has a number of properties which follow directly from the definition. Thus, the set of symmetry elements always contains the identity (or unit) transformation. If there are no other elements, the body is totally devoid of symmetry.

If we apply two symmetry transformations to a body in succession, it is again left invariant, i.e., successive application of two symmetry transformations is also a symmetry element.

Applying one of the symmetry transformations to a body, we bring it into coincidence with itself. The inverse transformation again brings it into coincidence with itself. Thus, for each symmetry transformation there is an inverse, which is also a symmetry element, and successive application of a transformation and its inverse is equivalent to the identity transformation.

A set of elements with the above properties forms a group.

Let us present the definition of a group. A group $\mathcal{G}$ is a (finite or infinite) set of elements g having the following properties:

1. A multiplication operation is defined for all elements $g \in \mathcal{G}$,* so that for any g_1 and g_2 in $\mathcal{G}$ there exists $g_3 \in \mathcal{G}$ such that $g_1 g_2 = g_3$. In other words, the multiplication operation associates with any two elements of the group $\mathcal{G}$ (taken in a definite order) a third element of the group.

Thus, multiplication of symmetry operations means successive application of symmetry transformations, the operation appearing on the right being the first performed. In the general case, $g_1 g_2 \neq g_2 g_1$. Groups in which $g_1 g_2 = g_2 g_1$ for all elements are known as commutative or abelian groups.

2. The associative law of multiplication holds: $(g_1 g_2) g_3 = g_1 (g_2 g_3)$.**

3. Among the elements of a group there is one and only one element, called the identity or unit element e, which has the property $ge = eg = g$ for every $g \in \mathcal{G}$.

4. Each group element g has an inverse g^{-1} such that $gg^{-1} = e$. Using properties 2 and 3, we easily show that also $g^{-1}g = e$.

The definition of the inverse implies

$$(g_1 g_2 \cdots g_n)^{-1} = g_n^{-1} \cdots g_2^{-1} g_1^{-1}. \tag{1.1}$$

* The symbol $g \in \mathcal{G}$ means: g belongs to $\mathcal{G}$, and the symbol $g \bar{\in} \mathcal{G}$ means: g does not belong to $\mathcal{G}$.

** This property is obvious for symmetry transformations.

In fact, by definition we have $(g_1g_2\ldots g_n)(g_1g_2\ldots g_n)^{-1}=e$. Multiplying this equality from the left by g_1^{-1}, g_2^{-1}, ..., g_n^{-1} successively, we obtain (1.1).

These group postulates conform exactly to the properties of the set of symmetry elements, which followed from intuitive considerations. Indeed, the fact that the set of symmetry elements forms a group is the reason for the prominent role of group theory in physics.

An example of a group which is fundamental in physical applications of group theory is the group of n-th order square matrices $\boldsymbol{A}$ with nonzero determinant, Det $\boldsymbol{A}\neq 0$. If we take the usual multiplication of square matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ as the group multiplication,

$$(AB)_{ij}=\sum_s A_{is}B_{sj},$$

and let the identity element be the identity matrix $\boldsymbol{I}$ with elements $I_{ij}=\delta_{ij}$, where δ_{ij} is the Kronecker symbol:

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

it is easy to prove that all the group postulates are fulfilled.

The condition Det $\boldsymbol{A}\neq 0$ is known to be necessary and sufficient for the matrix $\boldsymbol{A}$ to have an inverse.

The number of elements comprising a group may be finite or infinite. Accordingly, the group is said to be finite or infinite. The number of elements in a finite group is called its order h.

Let us consider a few properties of finite groups.

Take any element g_i of the group $\mathcal{G}$ and form every possible product gg_i, $g\in\mathcal{G}$. All these elements obviously belong to $\mathcal{G}$, and their number equals the order h of the group $\mathcal{G}$. It is easy to see that the set of elements gg_i yields the whole group $\mathcal{G}$, but in a different order. It is sufficient to show that no two of the elements gg_i are equal. In fact, the equality $g_1g_i=g_2g_i$ would imply that $g_1=g_2$.

Thus, the set of elements $g_i^{-1}gg_i$ again yields the whole group $\mathcal{G}$, where g runs through all elements of the group and g_i is any fixed element.

These group properties are very useful in summation of some function over the group, i.e., a function $\varphi(g)$ which depends on the elements $g\in\mathcal{G}$, since on the basis of the preceding properties

$$\sum_{g\in\mathcal{G}}\varphi(g)=\sum_{g\in\mathcal{G}}\varphi(g_ig)=\sum_{g\in\mathcal{G}}\varphi(gg_i)=\sum_{g\in\mathcal{G}}\varphi(g_i^{-1}gg_i) \tag{1.2}$$

for any fixed $g_i\in\mathcal{G}$. Equalities (1.2) are obvious, since the sums on the left and right of each equality contain the same terms, taken in a different order.

Consider some fixed element g of the group $\mathcal{G}$ and form the sequence of elements

$$e,\ g,\ g^2,\ g^3,\ \ldots,\ g^k,\ \ldots \tag{1.3}$$

Because of the finite number of elements in the group, one of the terms in this sequence must appear a second time after a certain number of powers. Let the first repeating element be $g^m=g^p$ (where $m>p$). It is obvious that $p=0$ and $g^m=e$, since if $p>0$ we would have $g^{m-1}=g^{p-1}$, i.e., the element g^{m-1}, equal to g^{p-1}, would appear earlier in the sequence (1.3) and g^m would not be the first repeating element, contrary to hypothesis.

Thus the first repeated element in (1.3) is the identity element e.

The smallest number m for which $g^m = e$ is called the order of the element g, and the sequence

$$e, g, g^2, \ldots, g^{m-1} \tag{1.4}$$

is its period. It is easy to see that $g^{m-1} = g^{-1}$, $g^{m-2} = g^{-2}$, etc. If we extend the sequence (1.3) to $k > m$, it will simply repeat the period (1.4) periodically. The period (1.4) of any element g forms a cyclic group.*

Any set of elements of the group $\mathcal{G}$ which itself comprises a group is called a subgroup. Thus, the period of each element g of $\mathcal{G}$ is a cyclic subgroup of $\mathcal{G}$. To show that some subset of a group $\mathcal{G}$ is a subgroup, it is sufficient to verify that it contains all products of its elements. Indeed, the associative law holds for every group element, including, of course, the elements of the set under discussion. Next, since together with an element g the set also contains all products of its elements, it also contains every power of an element g, in particular, $g^m = e$, where m is the order of g. Thus, the set contains the identity element. It also contains g^{-1}, since $g^{-1} = g^{m-1}$.

We now show that the order of a subgroup $\mathcal{F}$ is a divisor of the order of the group (Lagrange's theorem).

To prove this theorem, consider some element g_1 belonging to the group $\mathcal{G}$ but not to its subgroup $\mathcal{F}$, and form all its right multiples fg_1, $f \in \mathcal{F}$, or left multiples $g_1 f$, respectively. The set $\mathcal{F}g_1$ ($g_1\mathcal{F}$) is called the right (left) coset of g_1 by $\mathcal{F}$. The elements fg_1 belong to $\mathcal{G}$ but not to $\mathcal{F}$. In fact, if fg_1 belonged to $\mathcal{F}$, then g_1 would also belong to $\mathcal{F}$, and this would contradict the assumption. Now let g_2 be an element belonging neither to $\mathcal{F}$ nor to $\mathcal{F}g_1$, and form the set fg_2. It is readily seen that no element $\mathcal{F}g_2$ is in $\mathcal{F}$ or in $\mathcal{F}g_1$. For suppose, say, that $f_1 g_2 = f_2 g_1$, $f_1, f_2 \in \mathcal{F}$; then $g_2 = f_1^{-1} f_2 g_1$, so that g_2 belongs to the set $\mathcal{F}g_1$, contrary to assumption.

Thus, the cosets $\mathcal{F}g_1$ and $\mathcal{F}g_2$ are disjoint. Continuing this process until we exhaust the entire group, we conclude that $\mathcal{G}$ can be partitioned into complexes having no common elements:

$$\mathcal{F}, \mathcal{F}g_1, \mathcal{F}g_2, \ldots, \mathcal{F}g_{l-1}, \tag{1.5}$$

where l is an integer. Since each coset of $\mathcal{F}g_i$ contains a number of elements equal to the order s of the subgroup $\mathcal{F}$, it follows from (1.5) that

$$h = ls. \tag{1.6}$$

The number l, which is equal to h/s, is called the index of the subgroup $\mathcal{F}$ in $\mathcal{G}$.

Since the period of each element is a subgroup with number of elements equal to the order of the element, it follows that the order of each element must divide the order of the group. In particular, it follows from (1.6) that

$$g^h = e \tag{1.7}$$

for any $g \in \mathcal{G}$.

* A group consisting of elements $e, a, a^2, \ldots, a^{n-1}$ $(a^n = e)$ is said to be cyclic. It is clear from the definition that a cyclic group is commutative.

If the order is a prime number, then what has been said implies that in such a group there are no subgroups besides the trivial ones: e and the whole group. In this case $\mathcal{G}$ is a cyclic group.

Let us introduce the concept of conjugate elements.

Elements g_1 and g_2 are said to be conjugate if there exists an element $x \in \mathcal{G}$ such $xg_1x^{-1} = g_2$. It is clear from the definition that the relation of conjugacy is (a) symmetric and (b) transitive, i.e.: (a) if g_1 is conjugate to g_2, then g_2 is conjugate to g_1; (b) if g_1 is conjugate to g_2 and g_2 is conjugate to g_3, then g_1 is conjugate to g_3.

In fact: (a) By definition, if g_1 is conjugate to g_2, there exists $x \in \mathcal{G}$ such that $xg_1x^{-1} = g_2$, whence we obtain $g_1 = x^{-1}g_2x = (x^{-1})g_2(x^{-1})^{-1}$, and since $x^{-1} \in \mathcal{G}$, symmetry is proved. (b) Let $xg_1x^{-1} = g_2$ and $yg_2y^{-1} = g_3$, where $x, y \in \mathcal{G}$. From the second equality we obtain $g_2 = y^{-1}g_3y$. Substituting g_2 into the first equality, we find $xg_1x^{-1} = y^{-1}g_3y$ or $yxg_1(yx)^{-1} = g_3$. Since $x, y \in \mathcal{G}$, we have $yx \in \mathcal{G}$, and so g_1 is indeed conjugate to g_3.

These properties imply that the elements in a group may be partitioned into sets of conjugate elements, known as conjugate classes or just classes, each element appearing in one and only one class.

Forming the h products gg_1g^{-1}, we obtain all the elements of the class ρ_{g_1} containing g_1. The number of elements in the class ρ is denoted by h_ρ. Not all the products gg_1g^{-1} are different. We shall show that each element of ρ_{g_1} appears as gg_1g^{-1} the same number of times, namely, h/h_ρ times.

Let the element g' appear in the class p times. Then there exist p elements $x_1, x_2, \ldots, x_p$, forming a set X, say, such that $xg_1x^{-1} = g'$. Let the element g'' appear q times as gg_1g^{-1} and let $y_1, y_2, y_3, \ldots, y_q$ be all the elements, forming a set Y, for which $yg_1y^{-1} = g''$. Since g' and g'' belong to the same class ρ, there exists $g_0 \in \mathcal{G}$ such that $g' = g_0g''g_0^{-1}$, or $g'' = g_0^{-1}g'g_0$. Hence $(g_0y)g_1(g_0y)^{-1} = g$, which implies that the set X must contain q elements of the form g_0y_i $(i = 1, \ldots, q)$, so that $p \geqslant q$. On the other hand, in exactly the same manner we may show that the set Y contains p elements $g_0^{-1}x_i$ $(i = 1, 2, \ldots, p)$, so that $q \geqslant p$. This implies that $p = q$, i.e. each element of the class ρ appears as gg_1g^{-1} the same number h/h_ρ of times. Therefore,

$$\sum_{g \in \mathcal{G}} \varphi(gg_1g^{-1}) = \frac{h}{h_\rho} \sum_{g \in \rho_{g_1}} \varphi(g), \tag{1.8}$$

where φ is any single-valued function on the group.

All elements of the same class have the same order. In fact, if the order of an element g is m, i.e. $g^m = e$, then $(xgx^{-1})^m = xg^mx^{-1} = e$.

The identity element e alone forms a class, since it is not the conjugate of any other element.

Each class of an abelian group consists of one element, since $xgx^{-1} = g$ for all x.

We have considered the partition of a group $\mathcal{G}$ into subgroups and classes. It is essential to note, however, that classes (other than the identity element) are not subgroups, since they do not contain the identity element. On the other hand, in the general case any subgroup of the group $\mathcal{G}$ contains elements from different classes, but not necessarily complete classes. The invariant subgroups of the group $\mathcal{G}$ represent a special case.

An invariant (or normal, self-conjugate) subgroup is a subgroup $\mathcal{R}$ of $\mathcal{G}$ consisting of complete classes of $\mathcal{G}$, i.e., if $\mathcal{R}$ is an invariant

subgroup and $r \in \mathcal{R}$, then $grg^{-1} \in \mathcal{R}$ for every $g \in \mathcal{G}$. We have already defined the right and left cosets by a subgroup $\mathcal{F}$. If $\mathcal{F} = \mathcal{R}$ is an invariant subgroup, the right and left cosets coincide. In fact, the right coset of an element $g \in \mathcal{R}$ consists of the elements $eg = g, r_2 g, \ldots, r_l g$ ($r_i \in \mathcal{R}$, $i = 1, 2, \ldots, l$; $r_1 = e$). But since $r_i g = gg^{-1} r_i g$ and $g^{-1} r_i g = r_k \in \mathcal{R}$ by the definition of an invariant subgroup, we have $r_i g = g r_k$. Therefore, when r_i runs through all the elements of $\mathcal{R}$, r_k runs through the same elements but in a different order, i.e., the sets $r_i g$ and $g r_k$ coincide, and so the right and left cosets coincide.

Consider two cosets $\mathcal{R}g_1$ and $\mathcal{R}g_2$ and choose any representatives $\tilde{g}_1 \in \mathcal{R}g_1$ and $\tilde{g}_2 \in \mathcal{R}g_2$. It is easily proved that the product $\tilde{g}_1 \tilde{g}_2$, where $\tilde{g}_1 \in \mathcal{R}g_1$ and $\tilde{g}_2 \in \mathcal{R}g_2$, belongs to the coset $\mathcal{R}g_1 g_2$.

In fact, $\tilde{g}_1$ and $\tilde{g}_2$ may be written $\tilde{g}_1 = r_i g_1$ and $\tilde{g}_2 = r_k g_2$, where r_i and r_k are any elements of $\mathcal{R}$. Thus

$$\tilde{g}_1 \tilde{g}_2 = r_i g_1 r_k g_2 = r_i g_1 r_k g_1^{-1} g_1 g_2 = r_i r'_k g_1 g_2 = r''_k g_1 g_2 \in \mathcal{R}g_1 g_2,$$

since $r'_k = g_1 r_k g_1^{-1} \in \mathcal{R}$ by the definition of an invariant subgroup and $r_i r'_k = r''_k \in \mathcal{R}$. Conversely, each representative $\tilde{g}$ of the coset $\mathcal{R}g_1 g_2$ may be written as a product of representatives $\tilde{g}_1 \in \mathcal{R}g_1$ and $\tilde{g}_2 \in \mathcal{R}g_2$, where we may choose rg_1 as $\tilde{g}_1$ and g_2 as $\tilde{g}_2$. Thus all the products $\tilde{g}_1 \tilde{g}_2$, $\tilde{g}_1 \in \mathcal{R}g_1$, $\tilde{g}_2 \in \mathcal{R}g_2$, belong to the coset $\mathcal{R}g_1 g_2$ and completely exhaust it.

Thanks to this property of the cosets of an invariant subgroup $\mathcal{R}$, we may treat each coset $\mathcal{R}g$ as an element of a new group, called the factor group by the subgroup $\mathcal{R}$, with multiplication defined by $\mathcal{R}g_1 \cdot \mathcal{R}g_2 = \mathcal{R}g_1 g_2$. The associative law for multiplication of cosets follows from the associative law for multiplication of elements of $\mathcal{G}$.

Furthermore, each element of the factor group $\mathcal{R}g$ has an inverse, namely, the coset $\mathcal{R}g^{-1}$. Since $r_1 g r_2 g^{-1} = r_1 (g r_2 g^{-1}) \in \mathcal{R}$, the product of $\mathcal{R}g$ and $\mathcal{R}g^{-1}$ is the subgroup $\mathcal{R}$ itself, which acts as the identity element in the factor group. The order of the factor group is the number of cosets by $\mathcal{R}$, i.e., the index of $\mathcal{R}$.

We now introduce the concepts of isomorphism and homomorphism of groups.

Two groups $\mathcal{G}$ and $\tilde{\mathcal{G}}$ of the same order are said to be isomorphic if we can establish a one-to-one mapping or correspondence $g_i \leftrightarrow \tilde{g}_i$ between their elements $g \in \mathcal{G}$ and $\tilde{g} \in \tilde{\mathcal{G}}$ such that if $g_1 \leftrightarrow \tilde{g}_1$ and $g_2 \leftrightarrow \tilde{g}_2$, then $g_1 g_2 \leftrightarrow \tilde{g}_1 \tilde{g}_2$. It is easily shown that the identity element e of $\mathcal{G}$ corresponds to the identity element $\tilde{e}$ of $\tilde{\mathcal{G}}$, and that the inverse g^{-1} corresponds to $\tilde{g}^{-1}$.

Isomorphic groups obviously have exactly the same structure, and from the standpoint of group theory they are generally not distinguished from one another, although in reality such groups may be quite different as to the physical or geometric meaning of their elements.

A more general type of correspondence between two groups is homomorphism; here, as opposed to isomorphism, the mapping is not required to be one–one. A group $\mathcal{G}$ is homomorphic to a group $\mathcal{F}$ if each element of $\mathcal{G}$ is mapped onto an element of $\mathcal{F}$; several (but at least one) elements of $\mathcal{G}$ may be mapped onto each element of $\mathcal{F}$. The mapping is such that if $g_1 \to f_1$ $g_2 \to f_2$, $g_1, g_2 \in \mathcal{G}$, $f_1, f_2 \in \mathcal{F}$, then $g_1 g_2 \to f_1 f_2$.

Homomorphism is therefore not a symmetric relation.

The number of elements in the group $\mathcal{G}$ is obviously not less than the number of elements in the group $\mathcal{F}$. If the number of elements is equal, the homomorphism becomes an isomorphism.

Let us consider the structure of the group $\mathcal{G}$. Consider the set of all elements $e_1, e_2, \ldots, e_n \in \mathcal{G}$ mapped onto the identity element e of the group $\mathcal{F}$. This set $\mathcal{E}$ is called the kernel of the homomorphism. We shall show that the kernel of a homomorphism is an invariant subgroup of $\mathcal{G}$.

First, any product $e_i e_j$ is also in $\mathcal{E}$, so that $\mathcal{E}$ is a subgroup of $\mathcal{G}$. In fact, any product $e_i e_j$ is mapped onto $e \cdot e = e$, the identity element of $\mathcal{F}$, and every element of $\mathcal{G}$ which is mapped onto e in $\mathcal{F}$ is contained in $\mathcal{E}$. In order to show that $\mathcal{E}$ is an invariant subgroup of $\mathcal{G}$, we consider any element ge_ig^{-1}, $e_i \in \mathcal{E}$, where g is an arbitrary element of $\mathcal{G}$ mapped onto an element f (say) of $\mathcal{F}$. The element of $\mathcal{F}$ onto which ge_ig^{-1} is mapped is $f_1 e f_1^{-1} = e$. Thus, the element ge_ig^{-1} belongs to $\mathcal{E}$, i.e., $\mathcal{E}$ is an invariant subgroup of $\mathcal{G}$.

We now determine the set of elements of $\mathcal{G}$ mapped onto a fixed element f of $\mathcal{F}$ (by the definition of a homomorphism, there is at least one such element). Let g be any element of $\mathcal{G}$ which is mapped onto f. It is evident that the entire coset by $\mathcal{E}$, i.e., the coset $g\mathcal{E}$, is also mapped onto f, since the image in $\mathcal{F}$ of each element ge_i is $fe = f$. Conversely, each element of $\mathcal{G}$ which is mapped onto $f \in \mathcal{F}$ belongs to the coset $g\mathcal{E}$. In fact, let g_1 be an element of the group other than g, which is mapped onto the element f in $\mathcal{F}$. Consider the element $g_1 g^{-1}$. The corresponding element of $\mathcal{F}$ is the identity element $ff^{-1} = e$. Thus $g_1 g^{-1} \in \mathcal{E}$, so that $g_1 \in \mathcal{E}g$. Hence the number of elements in $\mathcal{G}$ mapped onto the element $f \in \mathcal{F}$ is just n, the order of the subgroup $\mathcal{E}$, and they form a coset $g\mathcal{E}$ of the group $\mathcal{G}$. These cosets exhaust the group $\mathcal{G}$.

In contrast to an isomorphism, which is a one–one correspondence between the elements of two groups $\mathcal{F}$ and $\mathcal{G}$, in a homomorphism we have a single-valued mapping of the elements of $\mathcal{G}$ onto those of $\mathcal{F}$ and an n-valued mapping of $\mathcal{F}$ onto $\mathcal{G}$. Each element $f \in \mathcal{F}$ is the image of n elements of $\mathcal{G}$, which form a coset by $\mathcal{E}$. Thus the correspondence between the elements of $\mathcal{F}$ and the cosets is one–one. Since the cosets by $\mathcal{E}$ are the elements of the factor group, it follows that $\mathcal{F}$ is isomorphic to the factor group of $\mathcal{G}$ by its subgroup $\mathcal{E}$.

The set of all elements of a group $\mathcal{G}$ which commute with every element $g \in \mathcal{G}$ is a subgroup $\mathcal{F}$ called the center of $\mathcal{G}$. The center is an abelian invariant subgroup of $\mathcal{G}$.

Consider two groups $\mathcal{F}$ and $\mathcal{H}$ with elements $f \in \mathcal{F}$ and $h \in \mathcal{H}$. The set of all pairs of elements (f, h) is a new group $\mathcal{G}$, under the multiplication defined by $(f_1, h_1)(f_2, h_2) = (f_1 f_2, h_1 h_2)$. This group $\mathcal{G}$ is called the direct product of $\mathcal{F}$ and $\mathcal{H}$:

$$\mathcal{G} = \mathcal{F} \times \mathcal{H}.$$

The number of elements in this new group is the product of the order of $\mathcal{F}$ and the order of $\mathcal{H}$. Since

$$(f, h)(f_1, h_1)(f, h)^{-1} = (ff_1f^{-1}, hh_1h^{-1}),$$

the number of classes in $\mathcal{G}$ is the product of the numbers of classes in $\mathcal{F}$ and in $\mathcal{H}$.

If the only common element of the groups $\mathcal{F}$ and $\mathcal{H}$ is the identity element e and every element of $\mathcal{F}$ commutes with every element of $\mathcal{H}$, the group $\mathcal{G} = \mathcal{F} \times \mathcal{H}$ may be viewed as the set of elements $g = fh$, with multiplication

defined by

$$g_1g_2 = f_1h_1f_2h_2 = (f_1f_2)\,(h_1h_2).$$

In the sequel we shall have to deal with direct products of groups only in this situation.

To define a group, we must list all of its elements and specify the multiplication law. For finite groups this may be done by providing a multiplication table. In certain cases, however, it is more convenient to specify a group through generators and defining relations.

In fact, each element of a finite group may be represented as a power or product of powers of a certain finite number of elements a, b, c, ... called generators of the group. These generators satisfy relations of the type

$$a^p b^q c^r \ldots = e, \tag{1.9}$$

where p, q, and r are positive integers or zero, and e is the identity element of the group. These relations are called defining relations. In the case of symmetry groups they depend on the mutual arrangement of the symmetry elements.

Specification of generators and defining relations completely determines the group. For example, a cyclic group of order n is defined by one generator a and one relation $a^n = e$.

The same group may generally have different systems of generators. The defining relations will also differ accordingly.

Obviously, if we can set up a correspondence between two groups so that they have the same number of generators and the same defining relations, they are isomorphic.

§2. SYMMETRY TRANSFORMATIONS

We now consider symmetry transformations in greater detail. Any transformation which brings a body into coincidence with itself preserves the distance between any two of its points; a symmetry transformation may therefore be decomposed into elementary transformations: (1) rotation about an axis, (2) reflection in a plane, (3) translation t_a (parallel displacement) by some vector a.

A rotation $c_l(\alpha)$ is defined by specifying the direction of the rotation axis l and the angle of rotation α. A reflection σ in a plane is defined by specifying the reflection plane. A translation by a vector a displaces each point along the vector a.

These three elementary transformations have different sets of fixed points. Thus, under rotation about an axis all points on the axis remain fixed, and reflection in a plane fixes the points on the reflection plane; a translation does not have fixed points at all.

Note that although reflections in a plane and rotations about an axis have fixed points, their products may lack fixed points in the general case. For example, it is easy to see that two reflections in parallel planes σ_1 and σ_2

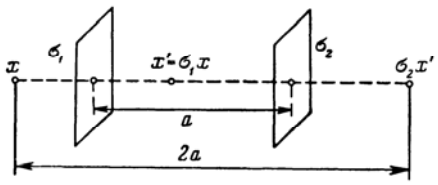


FIGURE 1. Successive reflection in parallel planes.

separated by a distance a are equivalent to translation by the vector $2a$, i.e., $\sigma_2\sigma_1 = t_{2a}$ (Figure 1).

The symmetry group of a body of finite dimensions (such as an atom or molecule) cannot contain a translation, since for any finite body there must be a fixed point, namely, the center of gravity of the object.

A symmetry group in which there is a fixed point common to all transformations of the group is called a point group.

All rotation axes and reflection planes in a point group intersect at the fixed point. Thus, a point group may be the symmetry group of a finite body only.

Symmetry groups of infinite bodies, such as a crystal lattice, may contain translations, since a lattice is obviously invariant under displacements as well as rotations and reflections.

Before proceeding to discuss the various symmetry groups, let us consider the basic properties of rotations, reflections and translations.

Successive application of m rotations about an axis l through an angle α is equivalent to rotation through the angle $m\alpha$:

$$c_l^m(\alpha) = c_l(m\alpha).$$

Let α be a rational fraction of 2π, say, $\alpha = 2\pi/n$, where n is an integer; then n rotations are equivalent to the identity transformation $c_l^n(\alpha) = c_l(n\alpha) = c_l(2\pi)$. Therefore, the set of rotations through such angles contains a finite number n of elements and forms a cyclic group, known as C_n.

If α is not commensurable with 2π, no two rotations $c^p(\alpha)$ are equal, and they are dense in the set of all rotations about the given axis (through all possible angles from 0 to 2π). It follows that rotation angles which are irrational in 2π signify the existence of axial symmetry. The corresponding symmetry groups are infinite and allow rotations through arbitrarily small angles.

Rotations through infinitesimal angles are impossible in a crystal lattice, in view of the discrete nature of its structure, and therefore only elements of the finite point groups can be symmetry elements of a crystal lattice.

The product of any number of rotations about different axes which intersect at a point is again a rotation about an axis through the same point.

Rotations about different axes are in general not commutative. Commutativity holds only in the special case of rotations through π about two mutually perpendicular axes, since the product of such rotations is a rotation through π about a third axis perpendicular to the first two axes.

Let $c_l(\alpha)$ be rotation about an axis l through an angle α and f any rotation We claim that the operation $fc_l(\alpha)f^{-1}$ is rotation through the angle α about a

new axis $f\boldsymbol{l}$, i.e., the image of the axis $\boldsymbol{l}$ under the transformation f:

$$fc_l(\alpha)f^{-1} = c_{f\boldsymbol{l}}(\alpha). \tag{2.1}$$

In fact, the axis $f\boldsymbol{l}$ remains fixed under the transformation $fc_l(\alpha)f^{-1}$, since $fc_l(\alpha)f^{-1}(f\boldsymbol{l}) = fc_l(\alpha)\boldsymbol{l} = f\boldsymbol{l}$. Consequently, $fc_l(\alpha)f^{-1}$ is a rotation about $f\boldsymbol{l}$. We now show that $fc_l(\alpha)f^{-1}$ is a rotation through the angle α. Let $\boldsymbol{x}$ be an arbitrary vector through the axis $\boldsymbol{l}$ and perpendicular to it: $\boldsymbol{x} \perp \boldsymbol{l}$. Then $\alpha = \widehat{(\boldsymbol{x}, c_l(\alpha)\boldsymbol{x})}$. Since f does not change angles between vectors, it follows that $f\boldsymbol{x} \perp f\boldsymbol{l}$ and the angle of the rotation $c_{f\boldsymbol{l}}(\alpha)$, i.e., the angle between the vectors $f\boldsymbol{x}$ and $c_{f\boldsymbol{l}}(\alpha)\boldsymbol{x} = fc_l(\alpha)f^{-1}f\boldsymbol{x} = fc_l(\alpha)\boldsymbol{x}$, is $\widehat{(f\boldsymbol{x}, fc_l(\alpha)\boldsymbol{x})} = \alpha$.

We now show that the product of two rotations through π about axes $\boldsymbol{l}$ and $\boldsymbol{l}'$ which make an angle φ is rotation about a third axis $\boldsymbol{l}''$ perpendicular to $\boldsymbol{l}$ and $\boldsymbol{l}'$, through the angle 2φ, i.e.,

$$c_{f\boldsymbol{l}}(\pi)c_l(\pi) = f^2, \tag{2.2}$$

where $f = c_{l''}(\varphi)$, $\boldsymbol{l}' = c_{l''}(\varphi)\boldsymbol{l} = f\boldsymbol{l}$.

In fact, by (2.1), $c_{f\boldsymbol{l}}(\pi)c_l(\pi) = fc_l(\pi)f^{-1}c_l(\pi)$, and $c_l(\pi)f^{-1}c_l(\pi) = f$, since rotation of the axis $\boldsymbol{l}''$ through π about any perpendicular axis reverses its direction.

We now turn to the basic properties of reflections. Twofold reflection in the same plane yields the identity transformation:

$$\sigma^2 = e. \tag{2.3}$$

Successive application of rotations and reflections gives rise to new symmetry elements, known as improper rotations s_n.

An improper rotation s_n is a transformation made up of a rotation c_n and a reflection σ_h* in the plane perpendicular to the rotation axis:

$$s_n = \sigma_h c_n = c_n \sigma_h, \tag{2.4}$$

since, as is easily proved, any rotation commutes with any reflection in a plane perpendicular to the rotation axis.

It follows from (2.4) that

$$s_n^2 = c_n^2, \quad \sigma_h s_n = c_n. \tag{2.5}$$

An improper rotation has only one fixed point, the point at which the rotation axis intersects the reflection plane.

An improper rotation of order 2 is a special case, known as inversion, i:

$$s_2 = c_2\sigma_h = i, \quad i^2 = e, \quad i\sigma_h = c_2, \quad ic_2 = \sigma_h. \tag{2.6}$$

Inversion maps each point in space onto its reflection relative to a certain point, known as the center of inversion, which is the point of intersection of the rotation axis and the reflection plane.

Under inversion, each vector $\boldsymbol{a}$ reverses its direction, $i\boldsymbol{a} = -\boldsymbol{a}$. Thus inversion converts a right-handed coordinate system into a left-handed coordinate system.

Geometric considerations show that inversion commutes with all rotations and reflections. The elements of a point group not involving reflections, i.e., rotations, are called elements of the first kind. The remaining elements, which do contain reflections, are called elements of the second kind. Each

* A reflection plane perpendicular to the rotation axis is usually denoted by σ_h. If the rotation axis lies in the reflection plane, the latter is denoted by σ_v.

element of the second kind h may be expressed as the product of a certain rotation f and inversion i:

$$h = if = fi.$$

For example,

$$s_l(\beta) = \sigma_h c_l(\beta) = ic_l(\pi)\, c_l(\beta) = ic_l(\pi + \beta). \tag{2.7}$$

Since the product of two rotations is a rotation, the product of any number of elements of the first kind is again an element of the first kind. Consequently, a set consisting only of rotations may be a group.

The product of two elements of the second kind is an element of the first kind; therefore, the product of an even number of elements of the second kind is a rotation, and the product of an odd number of elements of the second kind is again an element of the second kind.

Point groups consisting only of elements of the first kind are called groups of the first kind, and groups containing elements of both the first and second kind are groups of the second kind.

Conjugate elements of the second kind satisfy relations similar to (2.1).

If $c_l(\alpha)$ is rotation through an angle α about an axis l, and $h = if$ is any element of the second kind (f is a rotation), then

$$hc_l(\alpha)\, h^{-1} = c_{-hl}(\alpha) = c_{hl}(-\alpha). \tag{2.8}$$

In fact,

$$hc_l(\alpha)\, h^{-1} = ifc_l(\alpha)\, if^{-1} = c_{fl}(\alpha) = c_{-hl}(\alpha) = c_{hl}(-\alpha).$$

We can also prove the following equalities in a similar manner:

$$fs_l(\alpha)\, f^{-1} = s_{fl}(\alpha), \tag{2.9}$$

$$hs_l(\alpha)\, h^{-1} = s_{-hl}(\alpha). \tag{2.10}$$

In particular, if we note that when $\alpha = 0$, $s_l(\alpha)$ is the reflection σ in the plane perpendicular to the axis l, then by (2.9)

$$f\sigma f^{-1} = \sigma', \tag{2.11}$$

where σ' is reflection in the image of the plane σ under the rotation f.

It follows from (2.11) that the product of two reflections in intersecting planes σ and σ' making an angle φ is rotation through the angle 2φ about the line of intersection of the planes. In fact,

$$\sigma'\sigma = f\sigma f^{-1}\sigma = f^2, \tag{2.12}$$

since by (2.8)

$$\sigma_v c_l(\alpha)\, \sigma_v = c_{-l}(\alpha) = c_l^{-1}(\alpha). \tag{2.13}$$

Axes of rotation (or improper rotation) and reflection planes which are mapped onto each other by one of the group elements are said to be equivalent. We must remember here that, by (2.8), (2.10), and (2.13), improper rotations and reflections in a plane also reverse the direction of the rotation axis.

It follows from (2.1), (2.8), and (2.9) that rotations through identical angles about equivalent axes, or reflections in equivalent planes, lie in the same conjugate class.

A symmetry axis is said to be two-sided if rotations about this axis through equal angles in opposite directions are conjugate. As follows from (2.1), (2.8), (2.9), and (2.13), for this to be true the point group must contain a rotation which reverses the direction of the rotation axis or an improper rotation (in particular, a reflection) which does not change the direction of the rotation axis. Examples are rotations through the angle π about a perpendicular axis or reflections σ_v in a plane containing the original axis.

We now consider the properties of translations.

By the definition of a translation, successive translation by vectors $\boldsymbol{a}$ and $\boldsymbol{b}$ is translation by the vector $\boldsymbol{a}+\boldsymbol{b}$:

$$t_a t_b = t_{a+b}. \tag{2.14}$$

It follows from (2.14) that any two translations commute:

$$t_a t_b = t_b t_a = t_{a+b}. \tag{2.15}$$

The inverse of a translation t_a is the translation t_{-a}:

$$(t_a)^{-1} = t_{-a}, \tag{2.16}$$

since $t_a t_{-a} = e$, where e is the identity transformation.

These properties of parallel displacements imply that the set of translations forms an abelian group.

The group of translations is isomorphic to the vector group $\mathscr{F}$ whose elements are vectors $\boldsymbol{a}$, $\boldsymbol{b}$ and the group operation is vector addition. The zero vector acts as the identity in the group $\mathscr{F}$, and the inverse of the vector $\boldsymbol{a}$ is $-\boldsymbol{a}$. If all vectors in $\mathscr{F}$ lie on one straight line, the group is said to be one-dimensional; if all vectors lie in one plane, it is two-dimensional. If there are three non-coplanar vectors in $\mathscr{F}$, it is said to be three-dimensional.

The symmetry group of an infinite body – space group – may contain rotations, reflections and translations, and so a symmetry element of an infinite body may be written

$$g = t_a r \tag{2.17}$$

or

$$g = (r \mid \boldsymbol{a}), \tag{2.17a}$$

where t_a is translation by the vector $\boldsymbol{a}$ and r is a "rotational" element: rotation, reflection or improper rotation.

New symmetry elements arise in a space group: screw displacements and glide reflections. Screw displacements arise as a result of the addition of rotations and translations.

Let r be the rotation $c_l(\alpha)$.

We resolve the vector $\boldsymbol{a}$ into its components $\boldsymbol{a}_\parallel$ and $\boldsymbol{a}_\perp$:

$$\boldsymbol{a} = \boldsymbol{a}_\parallel + \boldsymbol{a}_\perp,$$

where $\boldsymbol{a}_\parallel \parallel \boldsymbol{l}$ and $\boldsymbol{a}_\perp \perp \boldsymbol{l}$. Then

$$g = t_{a_\parallel} t_{a_\perp} c_l(\alpha).$$

The transformation $t_{a_\perp} c_l(\alpha)$ is a plane transformation, since it leaves every point lying in the plane perpendicular to the $\boldsymbol{l}$-axis in the same plane.

According to Chasles's theorem, any plane transformation is either a pure rotation about some axis l' perpendicular to the plane, when $\alpha \neq 0$ (the point of intersection of this axis and the plane, which is the fixed point of the transformation $t_{a_\perp} c_l(\alpha)$, is called the Chasles center) or a pure translation, when $\alpha = 0$.

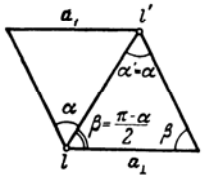


FIGURE 2. Plane transformation $t_{a_\perp} c_l(\alpha)$.

Let us determine the position of the Chasles center and the angle of rotation about l'. In Figure 2 the points l and l' denote the points at which the axes l and l' cut the plane perpendicular to them. The transformation $t_{a_\perp} c_l(\alpha)$ fixes the point l' and displaces l by the vector $a_\perp$. It is clear from Figure 2 that the rotation angle about l' is $\alpha' = \alpha$. To determine the position of the Chasles center, draw the vector $a_\perp$ from the point l and then draw straight lines from the end of the vector $a_\perp$ and the point l, making an angle $\beta = (\pi - \alpha)/2$ with the vector $a_\perp$. Their point of intersection is the Chasles center l'.

Thus, $t_{a_\perp} c_l(\alpha) = c_{l'}(\alpha)$ and the transformation $g = t_a c_l(\alpha)$ may be written

$$g = t_{a_\parallel} c_{l'}(\alpha). \tag{2.18}$$

A transformation involving rotation about an axis l' through an angle α and subsequent translation by a vector $a_\parallel$ parallel to the rotation axis (Figure 3, a) is called a screw displacement, and the axis l' is called the screw axis. Screw displacements obviously do not have fixed points.

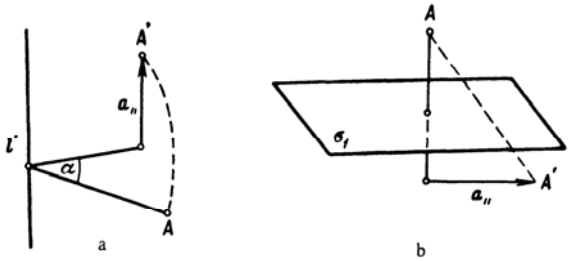


FIGURE 3. a) Screw displacement. b) Glide reflection.

Glide planes are produced by reflections in a plane followed by translations in the same plane. Let r be reflection in some plane σ. We again resolve a into two components, $a_\parallel$ and $a_\perp$, respectively parallel and perpendicular to the plane σ:

$$a = a_\parallel + a_\perp, \quad t_a = t_{a_\parallel} t_{a_\perp}.$$

As shown above (see Figure 1), $t_{a_\perp} \sigma = \sigma_1$, where σ_1 is reflection in a plane parallel to σ at a distance $a_\perp/2$. Therefore,

$$g = t_{a_\parallel}\sigma_1. \tag{2.19}$$

The transformation g involves reflection in the plane σ_1 and subsequent translation by the vector $a_\parallel$, which is parallel to the reflection plane (Figure 3, b). This transformation is called a glide reflection and σ_1 is the glide plane.

In the general case, then, each space group element is either a screw displacement or a glide reflection, special cases of which are either pure translations, pure rotations or reflections in a plane.

The translations by vectors obtained from a by applying all the "rotational" point group operations r comprise the conjugate class of t_a, since rt_ar^{-1} is translation by the vector ra:

$$rt_ar^{-1} = t_{ra}. \tag{2.20}$$

In fact, successive application of transformations rt_ar^{-1} to the point with the radius-vector x yields

$$rt_ar^{-1}x = r(r^{-1}x + a) = x + ra,$$

so that the resultant transformation is translation by the vector ra.

Equality (2.20) implies that

$$rt_a = t_{ra}r. \tag{2.21}$$

The multiplication rule for elements $g_1 = t_{a_1}r_1$ and $g_2 = t_{a_2}r_2$ follows from (2.21):

$$t_{a_1}r_1t_{a_2}r_2 = t_{a_1}(r_1t_{a_2})r_2 = t_{a_1}t_{r_1a_2}r_1r_2,$$

i.e.,

$$t_{a_1}r_1t_{a_2}r_2 = t_{a_1+r_1a_2}r_1r_2, \tag{2.22}$$

or, in the notation of (2.17a),

$$(r_1 \mid a_1)(r_2 \mid a_2) = (r_1r_2 \mid a_1 + r_1a_2). \tag{2.22a}$$

So far we have considered the symmetry elements geometrically, indicating the effect of the transformations on points. However, these transformations may also be described by methods of analytic geometry. The position of each point is given through its cartesian coordinates $x_i = x, y, z$ in some fixed coordinate system. A symmetry transformation moves the point to a new position, whose coordinates in the same coordinate system are $x_i' = x', y', z'$. By specifying the transformation law for the coordinates, i.e., the dependence of x_i' on x, y, z, one obtains an analytical expression for the symmetry element.

A convenient choice of origin for point group transformations is the fixed point. Then any point group transformation r is described by a linear homogeneous coordinate transformation:

$$x' = rx = \mathcal{R}(r)x \text{ or } x_i' = \sum_s \mathcal{R}_{is}(r)x_s, \tag{2.23}$$

where $\mathcal{R}(r)$ is a real 3×3 matrix.

Since rotations and reflections do not change the length of vectors or the angles between them, the matrix $\mathcal{R}$ satisfies the orthogonality conditions:

$$\sum_s \mathcal{R}_{si}(r)\mathcal{R}_{sk}(r) = \delta_{ik}. \tag{2.24}$$

This means that the sum of squares of the elements of each column of the matrix $\mathcal{R}$ is unity, and the [scalar] product of any two distinct columns is zero. Such matrices are said to be orthogonal.

It follows from (2.24) that

$$\sum_s \tilde{\mathcal{R}}_{is}(r)\,\mathcal{R}_{sk}(r) = (\tilde{\mathcal{R}}\mathcal{R})_{ik} = \delta_{ik}, \tag{2.25}$$

where $\tilde{\mathcal{R}}$ is the transpose of $\mathcal{R}$, i.e., the matrix in which the rows and columns are interchanged:

$$\tilde{\mathcal{R}}_{ij} = \mathcal{R}_{ji}. \tag{2.26}$$

Equation (2.25) implies that

$$\tilde{\mathcal{R}}(r) = \mathcal{R}^{-1}(r), \tag{2.27}$$

i.e., the transpose of an orthogonal matrix is its inverse. By (2.27), $(\mathcal{R}\tilde{\mathcal{R}})_{ik} = \delta_{ik}$, from which it follows that the orthogonality relations hold not only for the columns of orthogonal matrices (2.24), but also for their rows:

$$\sum_s \mathcal{R}_{is}(r)\,\mathcal{R}_{ks}(r) = \delta_{ik}. \tag{2.28}$$

We have already discussed how the coordinates of a point in a fixed coordinate system transform under symmetry transformations. Let us now consider how the coordinates of the fixed point A vary when a symmetry operation is applied to the coordinate system itself. Let the coordinates of A in the coordinate system xyz be (x, y, z). Now change over to a new coordinate system $x'y'z$, obtained from the coordinate system xyz by a transformation r. Obviously, the coordinates of the point $A(x', y', z')$ in the new coordinate system $x'y'z'$ are simply the coordinates of the vector $r^{-1}A$ in the old coordinate system, since the same rotation of both the coordinate system and the vector A leaves its coordinates unchanged. Consequently, by (2.23) and (2.27), the coordinates of A in the new coordinate system $x'y'z'$ will be

$$x'_i = (r^{-1}x)_i = \sum_s \mathcal{R}(r^{-1})_{is}\,x_s = \sum_s \mathcal{R}(r)_{si}\,x_s. \tag{2.29}$$

Evidently, the matrix of the transformation of the coordinates of a fixed point under a rotation of the coordinate system is the transpose of the matrix $\mathcal{R}(r)$ of (2.23), which describes the change of the coordinates for the motion of a point in a fixed coordinate system.

Since $\operatorname{Det}\tilde{\mathcal{R}} = \operatorname{Det}\mathcal{R}$, it follows from (2.25) that $(\operatorname{Det}\mathcal{R})^2 = 1$, i.e., $\operatorname{Det}\mathcal{R} = \pm 1$.

It is easy to show that for rotations the determinant of the matrix $\mathcal{R}$ is unity. The identity matrix I with elements $I_{ik} = \delta_{ik}$ corresponds to the identity transformation. The matrix $-I$ corresponds to inversion, which changes the signs of the coordinates. The determinant of this matrix is obviously -1. Since multiplication of transformations corresponds to multiplication of matrices, as will be shown below, and the determinant of a product of matrices is the product of their determinants, it follows that the determinant of the matrix of any element of the second kind is -1.

Viewing a point group of transformations in the setting of analytical geometry, we obtain a group of orthogonal matrices $\mathcal{R}$.

If we define the group operation to be the usual matrix multiplication, the group of matrices $\mathscr{R}(r)$ is clearly isomorphic to the point group $\mathscr{G}$, since the matrix of the transformation $\mathscr{R}(r_2r_1)$ is the product of the matrices $\mathscr{R}(r_2)\mathscr{R}(r_1)$. Indeed, if $x''=r_2r_1x=r_2x'$, we have

$$x''_k=\sum_s \mathscr{R}(r_2)_{ks}x'_s=\sum_{st}\mathscr{R}(r_2)_{ks}\mathscr{R}(r_1)_{st}x_t=\sum_s \mathscr{R}(r_2r_1)_{ks}x_s.$$

Consequently,

$$\mathscr{R}(r_2r_1)=\mathscr{R}(r_2)\mathscr{R}(r_1). \tag{2.30}$$

Translation operations may also be specified by a coordinate transformation: a translation t_a corresponds to addition of a vector a to the radius-vector x of the point:

$$x'=x+a, \quad x'_i=x_i+a_i. \tag{2.31}$$

Any transformation t_ar (2.17) involving a rotational element r and translation by a vector a may be written as an inhomogeneous linear coordinate transformation:

$$x'=a+\mathscr{R}(r)x, \tag{2.32}$$

where $\mathscr{R}$ is the orthogonal matrix of the rotational transformation r.

§3. POINT GROUPS

We now consider the possible types of point groups.

Every point group can be built up from the simplest groups C_n by adding new symmetry elements: rotations around other axes and reflections in planes. The addition of one of the new elements entails the appearance of other symmetry elements.

It should be stressed that in building up finite point groups these new symmetry elements cannot be added arbitrarily. For example, new symmetry axes cannot intersect the old ones at arbitrary angles.

Indeed, the product of two rotations through angles commensurate with 2π about axes intersecting at an arbitrary angle may produce a rotation about a third axis, through an angle not commensurate with 2π; as shown in §2, this results in an infinite group.

This is precisely the reason for the existence of finitely many types of point group.

There are altogether fourteen types of finite point groups. These are the groups C_n, S_{2n}, C_{nh}, C_{nv}, D_n, D_{nh}, D_{nd}, T, T_d, T_h, O, O_h, Y, Y_h.

Group C_n. This is the group of rotations about an axis through angles $\frac{2\pi}{n}k$ ($k=0,1,2,\ldots,n-1$). The group is cyclic, and the number of classes equals the number of elements n. The group C_n is defined by one generator $a=c_n$ and one defining relation

$$a^n=e. \tag{3.1}$$

Group C_{nh}. The groups C_{nh} have an n-fold axis and a reflection plane σ_h perpendicular to it (Figure 4, a). The group C_{nh} has $2n$ elements: the

n elements of the group C_n

$$c_n^k \qquad (k=0,\ 1,\ \ldots,\ n-1)$$

and n improper rotations

$$s_n^k = c_n^k \sigma_h \qquad (k=0,\ 1,\ \ldots,\ n-1).$$

When n is even, the group contains an inversion $i=\sigma_h c_n^{n/2}$. All these groups are abelian, since rotations about an axis commute with reflections in a perpendicular plane. The number of classes equals the number of elements. The group $C_{0h} \equiv C_s$ consists of two elements, e and σ_h.

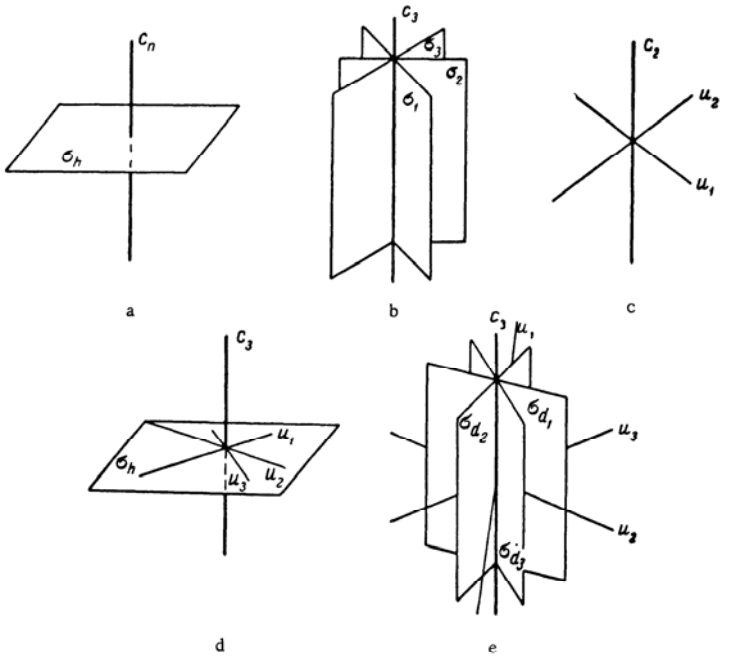


FIGURE 4. Symmetry elements of point groups:

a) C_{nh}; b) C_{3v}; c) D_2; d) D_{3h}; e) D_{3d}.

C_{nh} is the direct product of the groups C_n and C_s:

$$C_{nh} = C_n \times C_s, \tag{3.2}$$

and for even $n = 2p$

$$C_{2p,h} = C_n \times C_i,$$

where C_i is the group consisting of the two elements, e and i.

The group C_{nh} is defined by two generators $a = c_n$ and $b = \sigma_h$, and the relations

$$a^n = e, \quad b^2 = e, \quad ab = ba. \tag{3.3}$$

When n is even, the inversion i may be chosen as the generator b.

Group S_n is formed by the powers of an improper rotation: e, s_n, $s_n^2 = c_n$, $s_n^3 = \sigma_h c_n^3$, etc. If n is odd, S_n is of order $2n$, since $s_n^{2n} = c_n^{2n} = e$, and $s_n^n = \sigma^n = \sigma_h$. Thus, if n is odd, S_n is generated by c_n and σ_h and coincides with the group C_{nh}. For odd n, therefore, the groups C_{nh} are actually the cyclic groups S_{2n}.

When n is even, S_n is of order n, since $s_n^n = c_n^n = e$. Thus, the rotation c_n and reflection σ_h do not appear separately in this group; s_n acts as the independent element, and S_n consists of the powers s_n^k $(k = 0, 1, \ldots, n-1)$. Here $s_n^{2k} = c_n^{2k}$. The group S_2 is just the group C_i introduced above.

The group S_{2p} is isomorphic to C_{2p} and is defined by one generator $a = s_{2p}$ and the condition $a^{2p} = e$.

Group C_{nv}. The groups C_{nv} have an n-fold axis and n reflection planes through this axis (see Figure 4, b, where the arrangement of the symmetry elements is depicted for the group C_{3v}). Each group contains $2n$ elements, n of them being the elements of the group C_n, and the others reflections in n vertical planes. Since there is a reflection plane through the axis c_n, this axis is two-sided, i.e., the rotations c_n^k and c_n^{n-k} are conjugate.

If n is odd, the rotations c_n^k $(k = 0, 1, \ldots, n-1)$ take each of the planes σ_v successively onto all the others, and so all the reflections in the planes σ_v are in one class. If n is even, say $n = 2p$, the rotations c_n^k take each plane σ_v successively onto the next but one, and so the reflections in the planes are divided into two classes, each containing p reflections.

If n is even, the group $C_{2p,v}$ has $p+3$ classes: $p-1$ classes (c_{2p}^k, c_{2p}^{-k}) $(k = 1, \ldots, p-1)$, the class c_{2p}^p, the identity element e, and two classes each containing p reflections in the planes $c_{2p}^k \sigma_v c_{2p}^{-k}$ and $c_{2p}^k \sigma_v' c_{2p}^{-k}$, respectively, $k = 0, 1, \ldots, p-1, \sigma_v' = c_n \sigma_v$.

If $n = 2p+1$ is odd, then all the planes are equivalent and the corresponding reflections constitute a single class. In addition, there are p classes of rotations $(c_{2p+1}^k, c_{2p+1}^{-k})$ $(k = 1, \ldots, p)$, and the class consisting of the identity element, a total of $p+2$ classes.

The group C_{nv} is also defined by two generators, $a = c_n$ and $b = \sigma_v$. It follows from (2.13) that $\sigma_v c_n \sigma_v = c_n^{-1} = c_n^{n-1}$, so that the generators of C_{nv} satisfy the relations

$$a^n = e, \quad b^2 = e, \quad ba = a^{n-1} b. \tag{3.4}$$

Group D_n. The groups D_n have one n-fold axis and n twofold axes perpendicular to it (we denote the latter by u_2). Figure 4, c shows the system of axes for D_2. The group D_n contains $2n$ elements: the n elements of the group C_n and n rotations about the twofold axes. The n-fold axis is two-sided, owing to the presence of the perpendicular twofold axes. The groups D_n are isomorphic to the groups C_{nv}, the isomorphism being given by $c_n \leftrightarrow c_n$, $u_2 \leftrightarrow \sigma_v$. As in the groups C_{nv}, when n is odd all the twofold axes of D_n are equivalent. When n is even, each twofold axis is taken successively onto the next but one, and there are two sets of $n/2$ equivalent twofold axes. The distribution of elements among the classes is similar to that in C_{nv}. The groups D_n are defined by two generators $a = c_n$ and $b = u_2$, satisfying the relations (3.4).

Groups D_{nh}. The groups D_{nh} are obtained from D_n by adding a reflection plane σ_h perpendicular to the n-fold axis. The group D_{nh} contains $4n$ elements: the $2n$ elements of D_n and the $2n$ products $u_2\sigma_h$; by (2.12) the latter are reflections σ_v in planes through the axis c_n and the twofold axis u_2. Thus, addition of a horizontal reflection plane gives rise to n vertical reflection planes passing through the n-fold axis. It follows that the group D_{nh} may be obtained from either C_{nv} or C_{nh}, by adding a reflection plane σ_h or a twofold axis, respectively. Figure 4, d shows the arrangement of the elements in D_{3h}. The $4n$ elements of D_{nh} include n rotations c_n^k ($k=0, 1, \ldots, n-1$), n rotations through π about twofold axes $u_2c_n^k$ (these are elements of D_n), n improper rotations $s_n^k=\sigma_hc_n^k$, and n reflections in vertical planes $\sigma_vc_n^k$.

Since σ_h commutes with each element of D_n, D_{nh} is the direct product of D_n and C_s:

$$D_{nh}=D_n\times C_s.$$

Therefore, the number of classes in D_{nh} is twice the number of classes in D_n and the classes of D_{nh} are obtained by multiplying the classes of D_n by e and σ_h.

When n is even, D_{nh} contains the inversion $c_n^{n/2}\sigma_h=c_2\sigma_h=i$; thus, when $n=2p$ the group $D_{2p,h}$ may be written as a direct product

$$D_{2p,h}=D_{2p}\times C_i.$$

The groups D_{nh} are defined by three generators $a=c_n$, $b=u_2$, and $c=\sigma_h$ or i for even n. These satisfy the relations

$$a^n=e,\quad b^2=e,\quad c^2=e,\quad ba=a^{n-1}b,\cdot\ ac=ca,\quad cb=bc. \tag{3.5}$$

When n is odd, D_{nh} is isomorphic to D_{2n}, and it may be defined by two generators $a=s_n$ and $b=u_2$. The defining relations are similar to (3.4):

$$a^{2n}=e,\quad b^2=e,\quad ba=a^{2n-1}b.$$

Groups D_{nd}. The groups D_{nd} are obtained from the groups D_n by adding n "diagonal" reflection planes through the n-fold axis midway between each two twofold axes (see Figure 4,e, which illustrates the axes and planes of the group D_{3d}).

The group D_{nd} contains $4n$ elements: besides the $2n$ elements of D_n, there are $2n$ new elements, obtained from the elements of D_n through multiplying by reflection σ_d in the diagonal planes. These $2n$ elements comprise n reflections σ_d in different planes $c_n^k\sigma_d$ and n products σ_du_2.

By (2.12), the product σ_du_2 may be rewritten as $\sigma_du_2=\sigma_d\sigma_v\sigma_h=\sigma_hc_{2n}=s_{2n}$, since $u_2=\sigma_v\sigma_h$, and $\sigma_d\sigma_v$ is rotation about the axis c_n (which is the line of intersection of the planes σ_v and σ_d), the rotation angle being twice that between neighboring planes σ_v and σ_d, i.e., $2\pi/2n=\pi/n$. All the other products $\sigma_du_2c_n^k$ ($k=0, 1, \ldots, n-1$) are improper rotations s_{2n}^{2k+1}. Consequently, the axis c_n in D_{nd} becomes a $2n$-fold improper rotation axis.

Since reflections in the diagonal planes take each twofold axis successively onto the next, all the twofold axes are equivalent, as are the reflection planes. The improper rotations s_{2n}^{2k+1} and s_{2n}^{-2k-1} are conjugate. Therefore, if $n=2p$ each group $D_{2p,d}$ contains $2p+3$ classes: e, c_{2p}^p, $p-1$ classes each containing two rotations about the n-fold axis, the class of $2p=n$ rotations around the twofold axes, p classes each containing two improper rotations

of the form s_{2n}^{2k+1} and s_{2n}^{-2k-1} $(k = 0, 1, 2, \ldots, p-1)$, and the class of $n = 2p$ reflections σ_d in the diagonal planes.

For odd $n = 2p+1$, the group $D_{2p+1,d}$ contains the inversion, since then for each twofold axis u_2 there is one plane σ_d perpendicular to it. When n is odd, therefore, the group $D_{2p+1,d}$ may be written as a direct product

$$D_{2p+1,d} = D_{2p+1} \times C_i.$$

Thus $D_{2p+1,d}$ contains $2(p+2) = 2p+4$ classes, obtained from the $p+2$ classes of D_{2p+1} through multiplying by e and inversion i.

The group D_{nd} may be obtained by adding the twofold axis u_2 or the reflection plane σ_v to the group S_{2n}. Hence, D_{nd} has two generators: $a = s_{2n}$, a $2n$-fold improper rotation axis, and $b = u_2$, a twofold axis, satisfying the relations

$$a^{2n} = e, \quad b^2 = e, \quad ba = a^{2n-1}b. \tag{3.6}$$

Thus D_{nd} is isomorphic to D_{2n}.

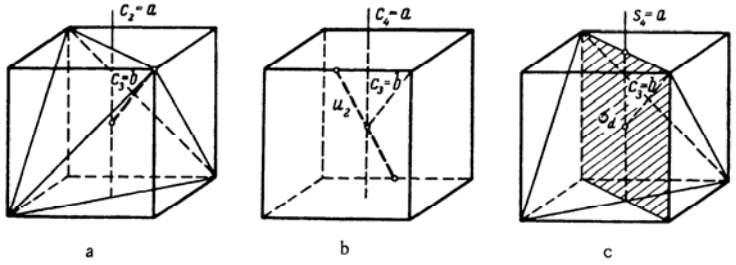


FIGURE 5. Symmetry elements of the cubic groups:

a) T; b) O; c) T_d.

Group T. The group T is the group of rotations which leave a tetrahedron invariant (Figure 5, a). This group has three mutually perpendicular twofold axes joining the midpoints of opposite edges of the tetrahedron, and four threefold axes joining each vertex of the tetrahedron to the midpoint of the opposite face. The group T may be obtained from D_2 by adding a threefold axis. The tetrahedral group has twelve elements: e, $3c_2$, $4c_3$ and $4c_3^2$. The three twofold axes are equivalent, since they go into each other under rotations about the threefold axis. The threefold axes are also equivalent, since they go into each other under rotations about the axes c_2. The elements of the group T comprise four classes: e, $(3c_2)$, $(4c_3)$, $(4c_3^2)$. T is defined by two generators, the twofold axis $a = c_2$ and the threefold axis $b = c_3$. To derive the relations defining the mutual arrangement of these elements, we note that the other twofold axes are obtained from a by rotations about either of the threefold axes $c_2' = c_3 c_2 c_3^{-1}$ and $c_2'' = c_3^2 c_2 c_3^{-2}$. Since the axes c_2 and c_2' are mutually perpendicular, the product of c_2 and c_2' gives rotation through π about the third axis $c_2'' = c_2' c_2$, i.e., $ab^{-1}a = bab^{-2}$. This yields the following defining relations for T:

$$a^2 = e, \quad b^3 = e, \quad bab = ab^2a. \tag{3.7}$$

The elements of T are expressed in terms of the generators as follows:

$$\begin{array}{llll} c_2 = a, & c_2' = bab^2, & c_2'' = b^2ab; & \\ c_3 = b, & c_3' = aba, & c_3'' = ab, & c_3''' = ba; \\ c_3'^2 = ab^2a, & c_3''^2 = b^2a, & c_3'''^2 = ab^2, & c_3^2 = b^2. \end{array} \tag{3.8}$$

Group T_h is obtained from T by adding inversion, with the inversion center at the center of the tetrahedron:

$$T_h = T \times C_i.$$

Since $c_2 i = \sigma_h$, T_h has three mutually perpendicular reflection planes. In addition, we get improper rotations s_6 and s_6^5, since

$$c_3 i = c_3 c_2 \sigma_h = c_6^5 \sigma_h = s_6^5 \quad \text{and} \quad c_3^2 i = c_3^2 c_2 \sigma_h = s_6,$$

i.e., the threefold axes become sixfold improper rotation axes. The number of classes in the group is twice the number of classes in T, i.e., 8. These conjugate classes are obtained from those of T through multiplying by e and i, respectively. The group T_h may be defined by two generators, $a = c_2$ and $s = s_6$.

Since the rotation s_6 takes the axis c_2 into $c_2'' = s_6 c_2 s_6^{-1}$, and $c_3 = s_6^2$ takes the axis c_2 into $c_2' = c_3 c_2 c_3^{-1}$ and $c_2' c_2 = c_2''$, it follows that $sas^{-2} = as^{-1}a^{-1}$, whence we obtain defining relations for T_h:

$$a^2 = e, \quad s^6 = e, \quad sas = as^2a. \tag{3.9}$$

Group O is the group of rotations which leave a cube invariant. It contains three fourfold axes joining the centers of opposite faces, four threefold axes c_3 joining opposite vertices of the cube, and six twofold axes u_2 joining the centers of opposite edges (Figure 5, b).

This group may be obtained by adding a threefold axis to D_4. In the group O axes of the same order are equivalent, and they are all two-sided. The 24 elements of O are distributed among five classes:

$$(e), \quad (4c_3, 4c_3^2), \quad (3c_4, 3c_4^3), \quad (3c_4^2), \quad (6u_2). \tag{3.10}$$

The octahedral group has two generators, which may be taken as rotation about a fourfold axis $a = c_4$ and rotation about a threefold axis $b = c_3$, satisfying the following relations:

$$a^4 = e, \quad b^3 = e, \quad aba = b^2; \tag{3.11}$$

the last relation follows from the fact that $u_2^2 = (ab)^2 = e$. All the other elements in the group of the octahedron may be expressed in terms of different powers and products of the generators:

$$\begin{array}{llll} c_4 = a, & c_4' = bab^2, & c_4'' = b^2ab, & \\ c_4^2 = a^2, & c_4'^2 = ba^2b^2, & c_4''^2 = b^2a^2b, & \\ c_4^3 = a^3, & c_4'^3 = b^2a, & c_4''^3 = ab^2, & \\ c_3 = b, & c_3' = aba^3, & c_3'' = a^2ba^2, & c_3''' = a^3ba, \\ c_3^2 = b^2, & c_3'^2 = a^2b, & c_3''^2 = a^2b^2a^2, & c_3'''^2 = ba^2, \ u_2''' = ba, \\ u_2 = ab, & u_2' = a^2ba^3, & u_2'' = a^3ba^2, & u_2^{(IV)} = ba^2b^2a, \ u_2^{(V)} = b^2ab^2. \end{array} \tag{3.12}$$

Group T_d is the full symmetry group of the tetrahedron. In addition to the elements of the group T it contains reflections, one for each plane through two vertices and the midpoint of the opposite edge (see Figure 5, c). There are 24 elements in T_d: 12 elements of T,

$$e, \quad 3c_2, \quad 4c_3, \quad 4c_3^2,$$

six reflections in the planes σ_d, and six improper rotations s_4 and s_4^3. These improper rotations arise, as in D_{2d}, because the reflection planes for the twofold axes are diagonal. The symmetry planes contain the axis c_3; in T_d, therefore, as opposed to T, these axes are two-sided. As in the group D_{2d}, the improper rotations s_4 and s_4^3 are conjugate and appear in one class. Thus the elements of T_d are distributed among five classes:

$$(e), \quad (4c_3, 4c_3^2), \quad (6\sigma), \quad (3s_4, 3s_4^3), \quad (3c_2).$$

The group T_d is isomorphic to the group O, via the correspondence $s_4 \leftrightarrow c_4$, $c_3 \leftrightarrow c_3$, $u_2 \leftrightarrow \sigma$. Hence the defining relations for T_d are the same as for O, i.e., equations (3.11), if we take $a = s_4$ and $b = c_3$ as generators. All the elements of T_d are expressed in terms of the generators as in (3.12).

The group O_h is the full symmetry group of the cube. It is obtained by adding an inversion center to O:

$$O_h = O \times C_i.$$

The number of elements in O_h is 48. The threefold axes are the diagonals of the cube; as in the group T_d, these become sixfold improper rotation axes, and three reflection planes σ_h appear perpendicular to the fourfold axes. In addition, there are six reflection planes σ_d, one through each pair of opposite edges. The number of classes in the group O_h is 10; five of them coincide with those of the group O, and the others are obtained from them through multiplying by the inversion i. These classes are:

$$(i), \quad (4s_6, 4s_6^5), \quad (3s_4, 3s_4^3), \quad (3\sigma_h), \quad (6\sigma_d).$$

The group O_h may also be obtained by adding the inversion to the group T_d:

$$O_h = T_d \times C_i.$$

We may take the rotation $c_4 = a$ and improper rotation $s_6 = s$ as the generators of O_h. These elements satisfy the following defining relations:

$$a^4 = e, \quad s^6 = e, \quad as^3 = s^3a, \quad sa^3s = a. \tag{3.13}$$

The third of these relations is the commutativity of inversion $i = s^3$ and c_4; the last follows from the easily verified fact that $sa^3 = s_6c_4^3 = ic_3^2c_4^3$ is reflection in one of the planes σ_d, and $\sigma_d^2 = e$.

Each element of O_h is either an element of O or the product of an element of O and the inversion $i = s^3$. Therefore, half of the elements of O_h are expressed in terms of the generators a and b as in equations (3.12), except that b must be replaced by s^2, and the other half is obtained through multiplication by the inversion s^3.

We shall show in §5 that the icosahedral groups Y and Y_h are not crystal symmetry groups and therefore we shall not discuss them.

§4. FULL ROTATION GROUP

We now consider the symmetry group of a sphere, the spherical group $\mathscr{K}$, which consists of all possible rotations through arbitrary angles about an arbitrary axis through the center of the sphere and thus contains a continuous set of elements. This group is also known as the full rotation group. Although the full rotation group is not a crystal symmetry group, it is important in many applications of solid state theory, and we shall therefore discuss its basic properties briefly.

Each element of $\mathscr{K}$ is a rotation $c_l(\varphi)$, characterized by the direction of the rotation axis l and the angle of rotation φ. We shall describe the rotation $c_l(\varphi)$ by a vector $\boldsymbol{\varphi}$ with components φ_x, φ_y, φ_z directed along the rotation axis l. The length of the vector $\boldsymbol{\varphi}$ is the angle of rotation φ:

$$|\boldsymbol{\varphi}| = \sqrt{\varphi_x^2 + \varphi_y^2 + \varphi_z^2}.$$

Thus each element of the full rotation group is a function of three parameters φ_x, φ_y, φ_z, which satisfy the inequality

$$\sqrt{\varphi_x^2 + \varphi_y^2 + \varphi_z^2} \leqslant 2\pi.$$

The Euler angles θ, φ, ψ are frequently used as the three independent parameters characterizing rotations.

All the general theorems proved in §1 for finite groups which are based on group properties are applicable to the full rotation group, provided the conclusion does not involve the number of elements.

All rotation axes in the spherical group are two-sided and equivalent, and so all rotations through the same angle $|\boldsymbol{\varphi}|$ about all possible axes lie in a single conjugate class.

If we add the inversion i to the full rotation group $\mathscr{K}$, we obtain the full orthogonal group

$$\mathscr{K}_h = \mathscr{K} \times C_i,$$

in which each plane through the center of the sphere is a reflection plane. Each element of the orthogonal group $\mathscr{K}_h$ is either a rotation or the product of inversion and a rotation.

Every finite point group is clearly a subgroup of the orthogonal group.

Rotations through infinitesimal angles play a decisive role in the full rotation group, since any rotation through a finite angle about a given axis may be obtained as a result of continuous successive rotations through infinitesimal angles. Thus the properties of rotations in the full rotation group are determined by the properties of infinitesimal rotations.

Consider an infinitesimal rotation $\boldsymbol{\varphi}$. Simple geometric considerations show that, up to first order terms in $|\boldsymbol{\varphi}|$, this rotation takes the radius-vector $\boldsymbol{x}'$ of an arbitrary point in a fixed coordinate system to the new position:

$$\boldsymbol{x}' = \boldsymbol{x} + [\boldsymbol{x}\boldsymbol{\varphi}].^* \tag{4.1}$$

* Accordingly, by (2.29), the change in the radius-vector of the point under a small rotation $\boldsymbol{\varphi}$ of the coordinate system is $\boldsymbol{x}' = \boldsymbol{x} - [\boldsymbol{x}\boldsymbol{\varphi}]$.

For infinitesimal rotations about the x-, y- and z-axes, respectively, formula (4.1) gives

$$\begin{aligned} &\varphi=\varphi_x, \quad x'=x, && y'=y+z\varphi_x, && z'=z-y\varphi_x;\\ &\varphi=\varphi_y, && x'=x-z\varphi_y, && y'=y, && z'=z+x\varphi_y;\\ &\varphi=\varphi_z, && x'=x+y\varphi_z, && y'=y-x\varphi_z, && z'=z. \end{aligned} \tag{4.2}$$

Let $\mathcal{F}(x, y, z)$ be a single-valued differentiable function of the coordinates. Consider its variation under an infinitesimal rotation φ of the coordinate system:

$$\mathcal{D}(\varphi)\mathcal{F}(x, y, z) = \mathcal{F}(\varphi^{-1}\boldsymbol{x}) = \mathcal{F}(x+z\varphi_y-y\varphi_z,\ y-z\varphi_x+x\varphi_z,\ z+y\varphi_x-x\varphi_y).$$

Expanding $\mathcal{F}(\varphi^{-1}\boldsymbol{x})$ in a Taylor series up to first order in φ, we obtain

$$\begin{aligned} \mathcal{D}(\varphi)\mathcal{F}(x, y, z) &= \mathcal{F}(x, y, z)+(\varphi_y z-y\varphi_z)\frac{\partial\mathcal{F}}{\partial x}(x, y, z)+\\ &+(x\varphi_z-z\varphi_x)\frac{\partial\mathcal{F}(x, y, z)}{\partial y}+(y\varphi_x-x\varphi_y)\frac{\partial\mathcal{F}}{\partial z}(x, y, z)=\\ &=(1+i\boldsymbol{L}\varphi)\mathcal{F}(x, y, z), \end{aligned} \tag{4.3}$$

where $\boldsymbol{L}$ is the vector operator $-i[\boldsymbol{x}\nabla]$ with components

$$\begin{aligned} L_x=-i\left\{y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right\}, \quad L_y=-i\left\{z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right\},\\ L_z=-i\left\{x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right\}. \end{aligned} \tag{4.4}$$

$\boldsymbol{L}$ is known as the infinitesimal rotation operator; it coincides with the angular momentum operator of quantum mechanics

A direct check shows that the operators L_x, L_y and L_z satisfy the following commutation relations:

$$L_xL_y-L_yL_x=iL_z, \quad L_yL_z-L_zL_y=iL_x, \quad L_zL_x-L_xL_z=iL_y. \tag{4.5}$$

Using the group properties of rotations, we shall show that the operator

$$\mathcal{D}(\varphi)\mathcal{F}(x, y, z)=\mathcal{F}(\varphi^{-1}\boldsymbol{x}), \tag{4.6}$$

which describes how the function $\mathcal{F}(x, y, z)$ transforms under a rotation through any finite angle φ, is uniquely determined by the infinitesimal rotation operator $\boldsymbol{L}$ and the angle φ.

To this end, we consider two rotations about the same axis through angles $s\varphi$ and $t\varphi$. Since the product of $s\varphi$ and $t\varphi$ is a rotation about the same axis, through the angle $(s+t)\varphi$, successive application of the operators $\mathcal{D}(s\varphi)$ and $\mathcal{D}(t\varphi)$ yields the transformation effected by the operator $\mathcal{D}((s+t)\varphi)$:

$$\mathcal{D}(s\varphi)\mathcal{D}(t\varphi)=\mathcal{D}((s+t)\varphi). \tag{4.7}$$

Differentiating with respect to s and setting $s=0$, we obtain

$$\mathcal{D}(t\varphi)\frac{d\mathcal{D}(s\varphi)}{ds}\Big|_{s=0}=\frac{d\mathcal{D}((s+t)\varphi)}{ds}\Big|_{s=0}=\frac{d\mathcal{D}(t\varphi)}{dt}.$$

By (4.3)

$$\frac{d\mathcal{D}(s\varphi)}{ds}\Big|_{s=0}=i\boldsymbol{L}\varphi,$$

and hence the following equation for $\mathcal{D}(t\varphi)$:

$$\frac{d\mathcal{D}(t\varphi)}{dt} = i(\boldsymbol{L}\varphi)\,\mathcal{D}(t\varphi). \tag{4.8}$$

Since when $t = 0$ we have $\mathcal{D}(0) = 1$, the identity operator, it follows from (4.8) that

$$\mathcal{D}(t\varphi) = e^{i(\boldsymbol{L}\varphi)t}.$$

Setting $t = 1$, we obtain an expression for $\mathcal{D}(\varphi)$ in terms of the infinitesimal rotation operator $\boldsymbol{L}$:

$$\mathcal{D}(\varphi) = e^{i(\boldsymbol{L}\varphi)}. \tag{4.9}$$

The operator $e^{i\boldsymbol{L}\varphi}$ is defined through the series expansion

$$e^{i(\boldsymbol{L}\varphi)} = 1 + i(\boldsymbol{L}\varphi) + \frac{(i(\boldsymbol{L}\varphi))^2}{2} + \ldots + \frac{(i(\boldsymbol{L}\varphi))^n}{n!} + \ldots; \tag{4.10}$$

thus formula (4.3) is the first term in the expansion of $\mathcal{D}(\varphi)$ in powers of the small parameter φ.

With any rotation of space we may associate a certain transformation of the plane. Indeed, let us consider the stereographic projection of the sphere onto the plane (Figure 6). Take a sphere of unit radius with center at the point $O(0, 0, 0)$. With each point P of the sphere we associate the point P' in the $\xi\eta$-plane at which the line $O'P$ intersects the $\xi\eta$ plane. This correspondence is clearly one–one, provided we associate the point $O'(0, 0, 1)$ with the point at infinity on the plane. For any rotation of the sphere, taking a point P onto some point M on the sphere, we have a certain transformation of the $\xi\eta$-plane, taking the point P' onto the corresponding point M' in the $\xi\eta$-plane.

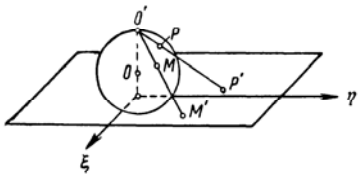


FIGURE 6. Stereographic projection of sphere onto plane.

If we introduce the complex variable $\zeta = \xi + i\eta$, we can show /I. 8/ that any rotation of the sphere induces a certain linear-fractional transformation of ζ in the $\xi\eta$-plane:

$$\zeta' = \frac{\alpha\zeta + \beta}{\gamma\zeta + \delta}, \tag{4.11}$$

defined by the matrix

$$u = \begin{Vmatrix} \alpha & \beta \\ \gamma & \delta \end{Vmatrix}$$

with complex parameters α, β, γ, δ, which depend on the components φ_x, φ_y, φ_z of the rotation vector. The matrix u is unitary, and its determinant is unity.*

Thus, with every rotation of the sphere we can associate a unitary matrix with determinant unity, which defines the corresponding linear-fractional transformation of the $\xi\eta$-plane. Moreover, the product of two rotations corresponds to the product of the corresponding matrices u. Since the product of two unitary matrices with determinant unity is again a unitary matrix with determinant unity, the matrices u form a group $\mathcal{U}$, which is known as the unitary group or group of motions. We have thus established a correspondence between the rotations of a sphere, which form the full rotation group $\mathcal{K}$, and the unitary matrices u with determinant unity, which are the elements of the unitary group $\mathcal{U}$.

However, this correspondence is not one–one. In fact, each matrix u corresponds to a definite transformation (4.11) of the $\xi\eta$-plane and thus to a definite rotation of the sphere. Therefore, each matrix u uniquely determines a rotation of the sphere. However, to each rotation of the sphere there correspond not one but two unitary matrices with determinant unity, namely the matrices u and $-u$, since it is clear from (4.11) that both these matrices correspond to the same transformation of the $\xi\eta$-plane. Thus the unitary group $\mathcal{U}$ is homomorphic to the full rotation group $\mathcal{K}$. The kernel of the homomorphism is the group of two elements I and $-I$, where I is the 2×2 identity matrix. This group is the center of the group $\mathcal{U}$. The corresponding factor group is isomorphic to the full rotation group $\mathcal{K}$.

It can be shown /I.8/ that the matrix u corresponding to a rotation φ with components φ_x, φ_y, φ_z is

$$u(\varphi) = e^{i(\sigma_x\varphi_x + \sigma_y\varphi_y + \sigma_z\varphi_z)/2} = e^{i(\sigma\varphi)/2}, \tag{4.12}$$

where the "vector" σ is a 2×2 matrix with components

$$\sigma_x = \begin{Vmatrix} 0 & 1 \\ 1 & 0 \end{Vmatrix}, \quad \sigma_y = \begin{Vmatrix} 0 & -i \\ i & 0 \end{Vmatrix}, \quad \sigma_z = \begin{Vmatrix} 1 & 0 \\ 0 & -1 \end{Vmatrix}. \tag{4.13}$$

σ_x, σ_y and σ_z are known as the Pauli matrices; they play an important role in the theory of representations of the rotation group and in applications of group theory in physics. It follows from the definition of the Pauli matrices (4.13) that they satisfy the relations

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1, \quad \sigma_x\sigma_z = -\sigma_z\sigma_x, \quad \sigma_x\sigma_y = -\sigma_y\sigma_x, \quad \sigma_y\sigma_z = -\sigma_z\sigma_y. \tag{4.14}$$

Formula (4.12) for $u(\varphi)$ is a symbolic notation for a 2×2 matrix and is defined through series expansion of the exponential in (4.12). Expanding $e^{i(\sigma\varphi)/2}$ in series (see (4.10)) and using (4.14), we easily show that

$$u(\varphi) = e^{i(\sigma\varphi)/2} = I\cos\frac{\varphi}{2} + i\frac{(\sigma\varphi)}{\varphi}\sin\frac{\varphi}{2}, \tag{4.15}$$

where I is the identity matrix.

It follows from (4.15) that the matrix of a rotation about the z-axis through an angle φ (i.e., $\varphi = \varphi_z$) is

$$u(\varphi_z) = I\cos\frac{\varphi}{2} + i\sigma_z\sin\frac{\varphi}{2} = \begin{Vmatrix} e^{i\varphi/2} & 0 \\ 0 & e^{-i\varphi/2} \end{Vmatrix}. \tag{4.16}$$

* The matrix u is unitary if $|\alpha|^2 + |\beta|^2 = |\gamma|^2 + |\delta|^2 = 1$ and $\alpha^*\gamma + \beta^*\delta = 0$. For further details on unitary matrices, see §7.

Formulas (4.15) and (4.16) demonstrate why the correspondence between $u(\varphi)$ and φ is not one–one. In fact, the rotations φ and $\varphi + 2\pi$ are indistinguishable; however, as is clear from (4.15) and, in the special case of rotation about the z-axis, from (4.16), the matrices $u(\varphi)$ and $u(\varphi + 2\pi)$ differ in sign. For example, the matrices I and $-I$ both correspond to rotations about the z-axis through angles 0 and 2π.

§5. BRAVAIS LATTICES

In this and in the following sections we shall discuss the crystal symmetry groups. We shall not list all the space groups* but only explain their structure and indicate the elements that must be specified in order completely to define the symmetry group of a crystal.

The crystal symmetry groups may be constructed by purely mathematical reasoning, starting from simple axioms which embody the hypothesis of the atomic structure of crystals. These groups were constructed by Fedorov and somewhat later by Schoenflies, who showed that there are altogether 230 space groups for crystal lattice symmetry.

We shall call points of a crystal equivalent if they are indistinguishable by their physical and geometric properties.

The symmetry group of a crystal consists of all transformations which take every point of the crystal onto an equivalent point.

Every crystal lattice possesses the fundamental property of translational periodicity, which may be taken as the basis for the definition of a crystal lattice. To elucidate: the symmetry group of a lattice always contains a three-dimensional group of translations T by vectors a, which form a three-dimensional vector group $\mathcal{F}$. By virtue of the atomic structure of a crystal lattice, the lengths of the translation vectors $a \in \mathcal{F}$ are bounded below by some positive quantity, since the distance between the atoms (ions) in a crystal lattice cannot be arbitrarily small. A vector group $\mathcal{F}$ is said to be discrete if the length of any vector $a \in \mathcal{F}$ is greater than some number d.

Every three-dimensional discrete group contains three noncoplanar vectors a_1, a_2, a_3 such that any vector $a \in \mathcal{F}$ may be expressed as

$$a = m_1 a_1 + m_2 a_2 + m_3 a_3, \tag{5.1}$$

where m_1, m_2 and m_3 are integers (positive, negative or zero). The parallelepiped whose sides are the basic vectors a_1, a_2, a_3 is called the basic parallelepiped or primitive cell of the crystal. We note that the choice of the basic vectors a_1, a_2, a_3 is to some degree arbitrary.

Any of the primitive cells may be constructed in the following manner.

Choose an arbitrary vector $a \in \mathcal{F}$, and define a_1 to be a vector in the group $\mathcal{F}$, parallel to a, of minimal length. Now choose an arbitrary vector $b \in \mathcal{F}$ not parallel to a_1. The vectors a_1 and b define a plane $a_1 b$. Let a_2 be any vector in $\mathcal{F}$, in the plane $a_1 b$, with minimal projection on the straight line perpendicular to a_1 in the plane $a_1 b$. The two vectors a_1 and a_2 define a face of the primitive cell. Finally, a_3 will be a vector of $c \in \mathcal{F}$ which does not lie in the plane $a_1 a_2$ and has minimal projection on the straight line perpendicular to this plane.

* The space groups are described, for example, in the monographs /I.3, I.10/ and the handbooks /I.19, I.18/.

It is clear from the above construction that one edge of the primitive cell may be directed along any vector $a \in \mathcal{F}$, and one of its faces may lie in the plane defined by any two vectors a and $b \in \mathcal{F}$. The volume of the primitive cell based on vectors a_1, a_2, a_3 is $(a_1 [a_2 \times a_3]) = \Omega_0$; all parallelepipeds determined by three basic vectors chosen as just described have the same volume.

A crystal lattice may be considered as constructed from identical primitive cells. The vertices of the parallelepipeds which form the cells, i.e., the ends of the vectors a (5.1), are called Bravais points, and the lattice formed by the Bravais points is called a Bravais lattice.

It should be noted that the points of the Bravais lattice are in general not real points of the crystal lattice, i.e., locations of atoms or ions. In fact, in order to construct a Bravais lattice in the general case one can start from an arbitrary point of the crystal lattice as zero point, and therefore the other points of the Bravais lattice may lie at arbitrary but equivalent points of the lattice.

If there is one atom for each primitive cell of the crystal, it is convenient to locate the points of the Bravais lattice at the positions of the atoms, and then the Bravais lattice coincides with the real lattice of the crystal. But if there are several atoms for each cell, i.e., the lattice is compound, then of course only one of the atoms of the primitive cell may determine the zero point of the Bravais lattice; thus the number of points in the Bravais lattice is less than the number of real points in the crystal lattice.

We may view a compound lattice of this kind as a lattice formed by several interpenetrating Bravais lattices (the exact number depends on the number of atoms in the primitive cell), whose zero points coincide with the positions of the atoms in the primitive cell. However, the translational symmetry of the crystal is characterized, of course, by only one of the Bravais lattices.

In the general case the parallel displacements (5.1) do not exhaust all the symmetry transformations of the crystal, since the latter may contain equivalent points which cannot be brought into coincidence by any of the translations (5.1); thus the symmetry group of the lattice may contain rotational elements: rotations, reflections and improper rotations.

Symmetry of Bravais Lattices

The totality of reflections and rotations (improper rotations) which map the Bravais lattice onto itself and have a fixed point form a certain point group. This symmetry point group of the Bravais lattice, $\mathcal{H}$, is also the symmetry group of the vector group $\mathcal{F}$ which characterizes the translational symmetry of the crystal. Each element $r \in \mathcal{H}$ maps a vector $a \in \mathcal{F}$ onto another vector $a' = ra \in \mathcal{F}$. A necessary and sufficient condition for this to be true in a discrete vector group is that each basic vector a_1, a_2, a_3 remain in the group $\mathcal{F}$ under any transformation r, i.e.

$$\begin{aligned} ra_1 &= m_1 a_1 + m_2 a_2 + m_3 a_3, \\ ra_2 &= n_1 a_1 + n_2 a_2 + n_3 a_3, \\ ra_3 &= l_1 a_1 + l_2 a_2 + l_3 a_3, \end{aligned} \tag{5.2}$$

where m_i, n_i, l_i are arbitrary integers. The actual meaning of condition (5.2) is that rotations and translations by whole periods must be compatible.

The compatibility condition (5.2) for rotations and translations implies that not every point group may be the symmetry group of a vector group. In order to ascertain which point groups may be symmetry groups of a three-dimensional discrete vector group, let us examine the elements which the group $\mathcal{H}$ contains.

Together with any vector $\boldsymbol{a}$, a vector group $\mathcal{T}$ also contains $-\boldsymbol{a}$; thus any group $\mathcal{H}$ must contain inversion.

Let c_n be an n-fold rotation appearing in the group $\mathcal{H}$. For any $\boldsymbol{a} \in \mathcal{T}$, the vector $c_n\boldsymbol{a} - c_n^{-1}\boldsymbol{a}$ lies in a plane perpendicular to the axis c_n; thus, the three-dimensional discrete vector group $\mathcal{T}$ induces a certain discrete group on this plane. Let $\boldsymbol{e}$ be the shortest vector in the latter group. The vector $c_n\boldsymbol{e} + c_n^{-1}\boldsymbol{e}$ is obviously parallel to $\boldsymbol{e}$, and so it is a multiple of $\boldsymbol{e}$ of length at most $2e$. Therefore

$$c_n\boldsymbol{e} + c_n^{-1}\boldsymbol{e} = m\boldsymbol{e} \qquad (m = 0, \pm 1, \pm 2). \tag{5.3}$$

The length of this vector is $|c_n\boldsymbol{e} + c_n^{-1}\boldsymbol{e}| = 2e\cos(2\pi/n)$, where e is the length of the vector $\boldsymbol{e}$. Hence we obtain the equation

$$2\cos\frac{2\pi}{n} = m \qquad (m = 0, \pm 1, \pm 2). \tag{5.4}$$

Formula (5.4) can hold only for $n = 2, 3, 4$ and 6. Thus condition (5.2) implies that the symmetry group of any three-dimensional Bravais lattice may have been only twofold, threefold, fourfold, and sixfold axes. It can also be shown that if the group $\mathcal{H}$ contains a subgroup C_n with $n > 2$, there is also a reflection plane σ_v passing through the axis c_n, i.e., the group $\mathcal{H}$ contains a subgroup C_{nv}.

Therefore, every symmetry group of a vector group contains inversion and may contain only twofold, threefold, fourfold, and sixfold axes; moreover, for any of these threefold, fourfold, and sixfold axes there is always a reflection plane containing the axis.

It is readily checked directly that only seven groups have these properties. These are the groups S_2, C_{2h}, D_{2h}, D_{3d}, D_{4h}, D_{6h}, O_h. We shall show below that for each of these seven point groups we may actually construct the vector group $\mathcal{T}$ and a Bravais lattice whose symmetry group is this point group. Note that the same symmetry group $\mathcal{H}$ may correspond to different vector groups, and accordingly different Bravais lattices. The totality of all vector groups having the same symmetry group is called a system or holohedry.

Thus there are altogether seven systems. These systems are given the following names: triclinic T (group S_2), monoclinic M (group C_{2h}), orthorhombic O (group D_{2h}), rhombohedral or trigonal R (group D_{3d}), tetragonal or quadratic Q (group D_{4h}), hexagonal H (group D_{6h}) and cubic K (group O_h).

Thus, there are altogether seven symmetry groups $\mathcal{H}$ for all crystals, i.e., seven systems of Bravais lattices.

Lattice Types

Two vector groups belonging to one system are said to be of the same type if one of them can be obtained from the other by a continuous transformation

of the basic vectors which does not lower the symmetry of the vector group. It follows from this definition that different vector groups which can be obtained from one another by a continuous variation of the parameters permitted by the symmetry group, for example, by changing the scale of the vectors a_1, a_2, a_3, belong to the same type.

As we shall see below, for each system there may be several types of Bravais lattices (lattice types), i.e., several arrangements of the basic vectors, satisfying condition (5.2), which cannot be taken into each other by a continuous transformation. Altogether, the seven systems subdivide into fourteen types of vector groups, i.e., fourteen lattice types.

We now consider the lattice types.

Triclinic system T (group S_2). The symmetry group S_2 contains only two elements, e and i, and so any triple of noncoplanar vectors a_1, a_2, a_3 may be a basis in the group $\mathcal{F}$ (Figure 7). Since any other triple of noncoplanar vectors may be taken onto the given vectors a_1, a_2 a_3 by a continuous transformation, it follows that for the triclinic system there is only one lattice type, called a primitive lattice and denoted by Γ_t. Each Bravais lattice of type Γ_t is determined by six parameters: the lengths of the vectors a_1, a_2, a_3 and the three angles between them.

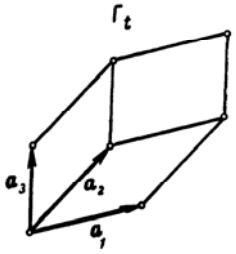


FIGURE 7. Basic vectors of the Bravais lattice of the triclinic system.

The primitive cell for type Γ_t is an arbitrary parallelepiped (see Figure 7) with the points of the Bravais lattice at its vertices. It is invariant under transformations of the group S_2.

Monoclinic system M (group C_{2h}). The monoclinic system contains two lattice types. The first type Γ_m, called a primitive lattice, is shown in Figure 8, a. The arrangement of the basic vectors for this type is characterized by the conditions

$$a_3 \perp a_1, \quad a_3 \perp a_2.$$

The vector a_3 is parallel to the twofold axis c_2, and the vectors a_1 and a_2 lie in the reflection plane σ_h. The primitive cell in type Γ_m is a right parallelepiped with an arbitrary base. It is invariant under every operation of the group C_{2h}. The points of the Bravais lattice are located at the vertices of the primitive cell.

The arrangement of the basic vectors for the second lattice type of the monoclinic system, shown in Figure 8, b, is characterized by the conditions

$$2a_3 - a_1 \perp a_1, \quad 2a_3 - a_1 \perp a_2.$$

This type is known as a base-centered lattice, denoted by Γ_m^b. The primitive cell (dashed lines in Figure 8, b) is not invariant under the transformations of the group C_{2h}, although, of course, a lattice composed of these cells is mapped onto itself by these transformations: each of the basic vectors a_1, a_2, a_3 is transformed into a linear combination (5.2) with integer coefficients.

Type Γ_m^b lattices nevertheless contain a parallelepiped invariant under C_{2h}, built up from the vectors a_1, a_2, a_3. This is the right parallelepiped with sides a_1, a_2, $2a_3 - a_1$ (bold lines in Figure 8, b), known as the Bravais parallelepiped. In the case of a primitive lattice the Bravais parallelepiped coincides

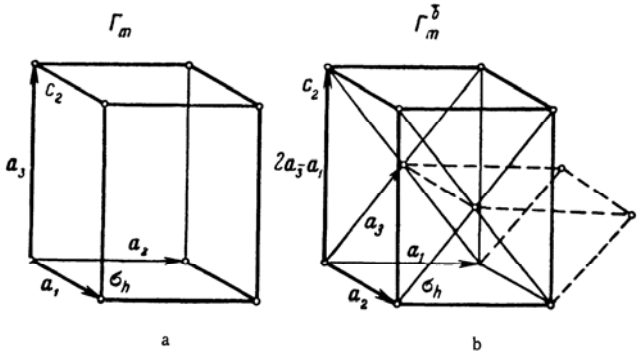


FIGURE 8. Basic vectors of Bravais lattice in monoclinic system:

a) primitive lattice Γ_m; b) base-centered lattice Γ_m^b (dashed lines: primitive cell).

with the primitive cell; the points of the Bravais lattice are located at its vertices and there is one point for each parallelepiped. In the type Γ_m^b lattice there are also points of the Bravais lattice, at the midpoints of the lateral faces (with respect to the axis c_2); this is the reason type Γ_m^b lattices are known as base-centered lattices. Here the Bravais parallelepiped contains two lattice points.

The Bravais parallelepiped for the monoclinic system is determined by four parameters: the height, lengths of edges of base, and angle between them; thus the type Γ_m and Γ_m^b lattices of the monoclinic system are determined by these four parameters. It should be clear from Figure 8, b that type Γ_m and Γ_m^b lattices cannot be taken into one another by any continuous transformation (i.e., a continuous variation of the four parameters) without lowering their symmetry.

For each of the Bravais lattices belonging to one of six systems (the exception is the hexagonal system) we may construct a Bravais parallelepiped, i.e., an invariant parallelepiped of minimal volume built from the basic vectors. In the general case, there will be points of the Bravais lattice not only at the vertices of the parallelepiped, but also (possibly) at the midpoint of the parallelepiped and the midpoints of its faces. The Bravais lattice of a crystal may be built up from identical Bravais parallelepipeds. In a certain sense invariant parallelepipeds are more convenient for describing Bravais lattices than primitive cells, since the form of the latter depends on the specific choice of basic vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$.

In the general case, the Bravais parallelepiped does not coincide with the primitive cell. This is demonstrated in the monoclinic system, where the volume of the Bravais parallelepiped for type Γ_m^b lattices is twice that of the primitive cell. However, the primitive cell for primitive Γ_m lattices (and, of course, for Γ_t) coincides with the Bravais parallelepiped.

Henceforth, our examination of the possible lattice types belonging to a given system will start from the appropriate Bravais parallelepiped.

Orthorhombic system O (group D_{2h}). In the orthorhombic system there are three mutually perpendicular twofold axes; the Bravais parallelepiped

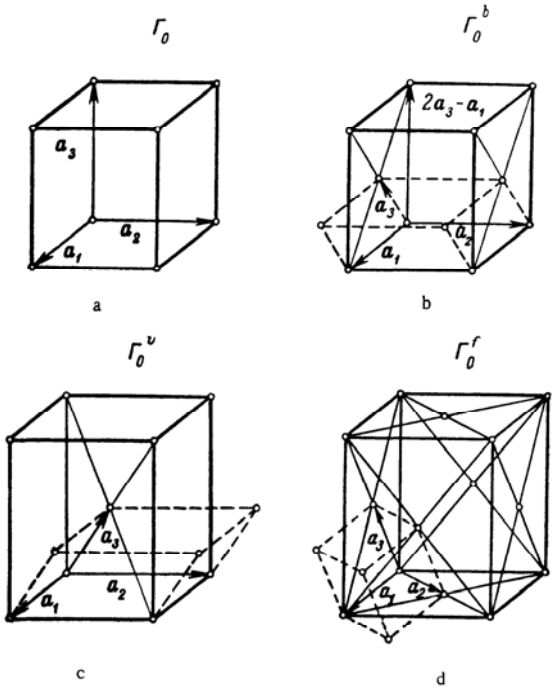


FIGURE 9. Basic vectors in orthorhombic system:

a) primitive lattice Γ_0; b) base-centered lattice Γ_0^b; c) body-centered lattice Γ_0^v; d) face-centered lattice Γ_0^f.

is therefore a parallelepiped with mutually perpendicular edges (Figure 9). There are four lattice types, determined by the possible location of the lattice points in the Bravais parallelepiped.

The primitive lattice Γ_0 is obtained when the lattice points lie at the vertices of the Bravais parallelepiped (Figure 9, a). As basic vectors $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$ we may choose three mutually perpendicular edges of the parallelepiped,

$$\boldsymbol{a}_1 \perp \boldsymbol{a}_2, \quad \boldsymbol{a}_2 \perp \boldsymbol{a}_3, \quad \boldsymbol{a}_1 \perp \boldsymbol{a}_3.$$

The primitive cell for the Γ_0 lattice, which coincides with the Bravais parallelepiped, is invariant under the transformations of the group D_{2h}.

The base-centered lattice Γ_0^b (Figure 9, b) is similar to the type Γ_m^b lattice of the monoclinic system; two points of the Bravais lattice are located at the centers of any two opposite faces. The basic vectors for type Γ_0^b lattices may be chosen as shown in Figure 9, b: $\boldsymbol{a}_1$ and $\boldsymbol{a}_2$ are edges of the parallelepiped, and the end of the vector $\boldsymbol{a}_3$ lies at the midpoint of an adjacent face, i.e.,

$$\boldsymbol{a}_1 \perp \boldsymbol{a}_2 \perp 2\boldsymbol{a}_3 - \boldsymbol{a}_1 \perp \boldsymbol{a}_1.$$

In the orthorhombic system there are two new lattice types not met with in the monoclinic system: body-centered and face-centered.

In the body-centered lattice Γ_0^v one of the lattice points is located at the midpoint of the Bravais parallelepiped (Figure 9, c). The basic vectors may be chosen in the following manner: a_1 and a_2 along edges of the Bravais parallelepiped, the end of a_3 lying at the midpoint of the Bravais parallelepiped:

$$a_1 \perp a_2 \perp 2a_3 - a_1 - a_2 \perp a_1.$$

In the face-centered lattice Γ_0^f there are lattice points at the midpoint of each face of the Bravais parallelepiped (Figure 9, d). The basic vectors may be chosen as in Figure 9, d; they are determined by the conditions

$$a_1 \perp 2a_2 - a_1 \perp 2a_3 - a_1 \perp a_1.$$

The Bravais parallelepiped in the orthorhombic system is determined by three independent parameters: the lengths of three of its edges; thus any lattice of the orthorhombic system is determined by these three parameters. It is easily seen that the lattice types enumerated above cannot be reduced to one another by any variation of the lengths of the edges of the Bravais parallelepiped.

The primitive cells for type Γ_0^b, Γ_0^v and Γ_0^f lattices, indicated in Figures 9, b, c, d by dashed lines, are not invariant under the transformations of the group D_{2h}; their volumes comprise respectively 1/2, 1/4, and 1/8 of the volume of the Bravais parallelepiped.

Note that we could have chosen a right parallelepiped with rhombic rather than rectangular base, which is also invariant under D_{2h}, to play the part of the Bravais parallelepiped. Of course, this would again have given four lattice types; an examination of Figure 10 reveals the following correspondence between the two sets of lattice types:

	Rectangular base	Rhombic base
Figure 10, a	Primitive Γ_0	Base-centered
Figure 10, b	Body-centered Γ_0^v	Face-centered
Figure 10, c	Base-centered Γ_0^b	Primitive
Figure 10, d	Face-centered Γ_0^f	Body-centered

Since the Bravais parallelepiped in the monoclinic system may be any right parallelepiped, there is no distinction between right parallelepipeds with rhombic and rectangular bases. This is why the face-centered and body-centered lattices of type Γ_m^b are equivalent in this system.

Tetragonal system Q (group D_{4h}). In the group D_{4h} one of the twofold axes of the group D_{2h} becomes a fourfold axis, and so the appropriate Bravais parallelepiped is a right parallelepiped with a square base (Figure 11).

In transition from the orthorhombic system to the tetragonal, the rectangle and rhombus forming the bases of the two possible Bravais parallelepipeds become squares, so that the distinction between these parallelepipeds again disappears. Therefore, as is clear from Figure 10 and the above table, the base-centered lattice of the tetragonal system is equivalent to the primitive lattice, and the face-centered and body-centered lattices are equivalent. Thus, only two lattice types are possible: primitive Γ_q (Figure 11, a) and body-centered Γ_q^v (Figure 11, b).

The primitive lattice is similar to the primitive lattice of the group D_{2h}. Its basic vectors satisfy the conditions

$$a_1 \perp a_2 \perp a_3 \perp a_1, \quad a_1 = a_2.$$

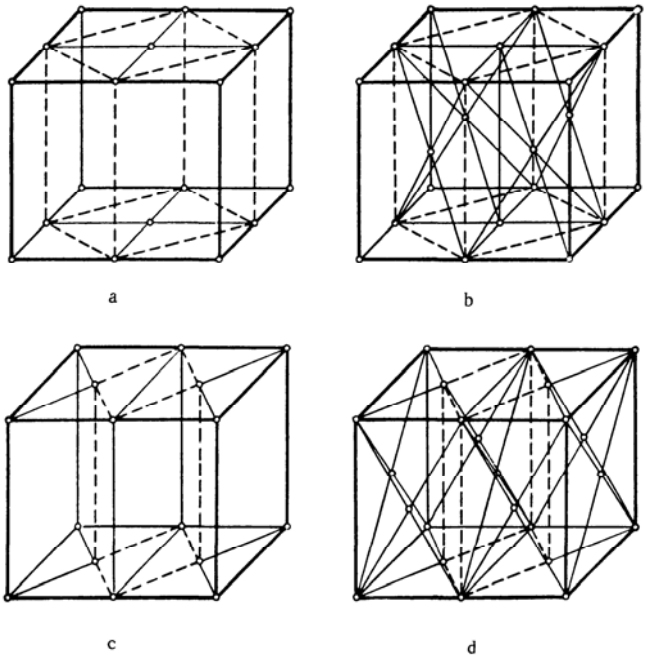


FIGURE 10. Bravais lattices in orthorhombic system with different choice of Bravais parallelepiped.

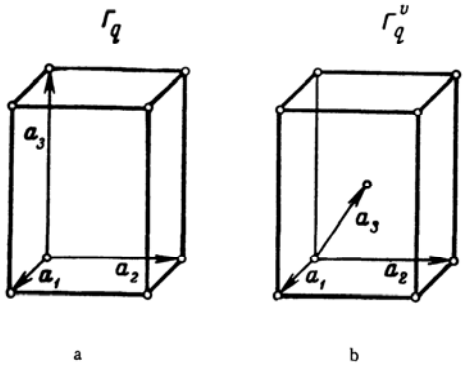


FIGURE 11. Basic vectors in tetragonal system:

a) primitive lattice Γ_q; b) body-centered lattice Γ_q^v.

The body-centered lattice Γ_q^v is also similar to the type Γ_0^v lattice. The basic vectors may be chosen as for type Γ_0^v:

$$\boldsymbol{a}_1 \perp \boldsymbol{a}_2 \perp 2\boldsymbol{a}_3 - \boldsymbol{a}_1 - \boldsymbol{a}_2 \perp \boldsymbol{a}_1,$$

but the presence of a fourfold axis adds one other condition:

$$a_1 = a_2.$$

Since the Bravais parallelepiped is determined by two parameters: length of edge and height, all lattices in the tetragonal system are also determined by these parameters.

Cubic system K (group O_h). In the cubic system the Bravais parallelepiped is a cube. Therefore, in the primitive cubic lattice Γ_c the primitive cell is a cube, and the basic vectors a_1, a_2, a_3 may be chosen mutually orthogonal and of equal lengths (Figure 12, a):

$$a_1 \perp a_2 \perp a_3 \perp a_1, \quad a_1 = a_2 = a_3.$$

In the body-centered lattice Γ_c^v there is a lattice point at the midpoint of the cube. The basic vectors indicated in Figure 12, b are characterized by the conditions

$$a_1 \perp a_2, \quad a_1 \perp 2a_3 - a_2 - a_1 \perp a_2, \quad a_1 = a_2 = |2a_3 - a_2 - a_1|.$$

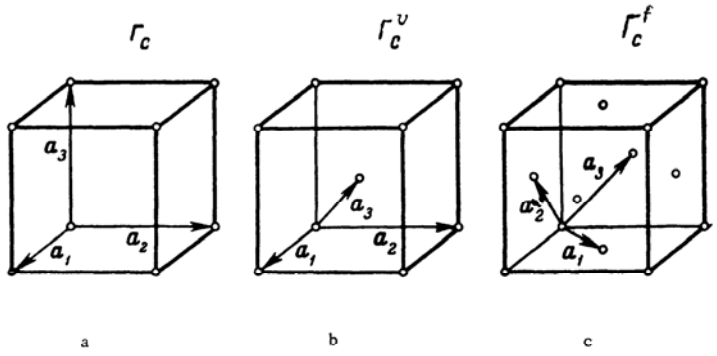


FIGURE 12. Bravais lattices in cubic system:

a) primitive lattice Γ_c; b) body-centered lattice Γ_c^v; c) face-centered Γ_c^f.

We showed above that in the tetragonal system the face-centered lattice is equivalent to the body-centered lattice, but in the cubic system there is no such equivalence, since the resulting parallelepiped with square base is not a cube; in the cubic system, then, the face-centered lattice again becomes an independent type, with lattice points at the midpoints of each face of the cube (Figure 12, c). The basic vectors a_1, a_2, a_3 may be chosen to satisfy the conditions

$$a_1 + a_2 - a_3 \perp a_3 + a_2 - a_1, \quad a_3 + a_2 - a_1 \perp a_1 - a_2 + a_3,$$
$$a_1 + a_2 - a_3 \perp a_1 - a_2 + a_3, \quad a_1 = a_2 = a_3.$$

Since a cube is determined by only one parameter, the length of the edge, all cubic lattices are determined by one parameter – the lattice constant.

Rhombohedral (trigonal) system R (group D_{3d}). D_{3d} symmetry is characteristic of a rhombohedron – a parallelepiped obtained by stretching or compressing a cube along its diagonal (Figure 13).

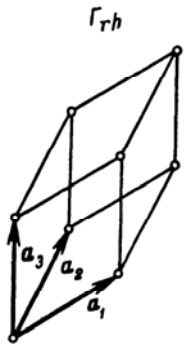


FIGURE 13. Bravais parallelepiped of rhombohedral lattice Γ_{rh}.

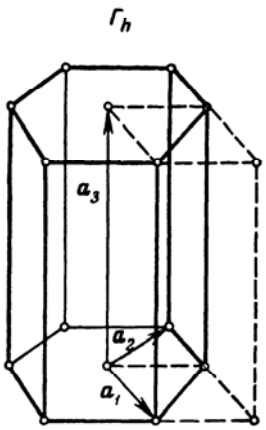


FIGURE 14. Bravais prism of hexagonal lattice Γ_h.

In the rhombohedral system there is only one possible lattice type, the primitive lattice Γ_{rh}, with the lattice points situated at the vertices of a rhombohedron. A simple construction will show that in the rhombohedral system both face-centered and body-centered types are equivalent to the primitive lattice. The arrangement of the basic vectors of the Γ_{rh} lattice, shown in Figure 13, is characterized by the conditions

$$a_1 = a_2 = a_3, \quad \widehat{a_1 a_2} = \widehat{a_1 a_3} = \widehat{a_2 a_3}.$$

Lattices of the rhombohedral system are uniquely described by two parameters: the length of the edges and the angle between them.

Hexagonal system H (group D_{6h}). Since the group D_{6h} admits a sixfold axis, it can have no invariant parallelepiped. The figure invariant under the transformations of D_{6h} is a hexagonal prism (Figure 14), known as the Bravais prism.

In the hexagonal system there is again only one lattice type, Γ_h; the lattice points are located at the vertices of the Bravais prism and at the centers of its bases (see Figure 14). The basic vectors in a type Γ_h lattice satisfy the conditions

$$a_3 \perp a_2, \quad a_3 \perp a_1, \quad \widehat{a_1 a_2} = 2\pi/3.$$

The primitive cell is shown in Figure 14 by dashed lines; it is a right parallelepiped on a rhombic base. The angle between the edges of the rhombus is $2\pi/3$.

Type Γ_h lattices are determined by two independent parameters: height of the prism and length of edge of the base.

The Bravais lattices listed above exhaust all the possible types of discrete three-dimensional lattices.

TABLE 5.1

System	Type	Basic vectors		Parameters of Bravais parallelepiped
Triclinic T (S_2)	Primitive Γ_t	Arbitrary $\boldsymbol{a}_1, \boldsymbol{a}_2, \boldsymbol{a}_3$	(Fig. 7)	$a_1, a_2, a_3, \widehat{a_1a_2}, \widehat{a_1a_3}, \widehat{a_2a_3}$
Monoclinic M (C_{2h})	Primitive Γ_m	$\boldsymbol{a}_3 \perp \boldsymbol{a}_1$, $\boldsymbol{a}_3 \perp \boldsymbol{a}_2$	(Fig. 8,a)	$a_1, a_2, a_3, \widehat{a_1a_2}$
	Base-centered Γ_m^b	$2\boldsymbol{a}_3 - \boldsymbol{a}_1 \perp \boldsymbol{a}_1$, $2\boldsymbol{a}_3 - \boldsymbol{a}_1 \perp \boldsymbol{a}_2$	(Fig. 8,b)	
Orthorhombic O (D_{2h})	Primitive Γ_0	$\boldsymbol{a}_1 \perp \boldsymbol{a}_2 \perp \boldsymbol{a}_3 \perp \boldsymbol{a}_1$	(Fig. 9,a)	a_1, a_2, a_3
	Base-centered Γ_0^b	$\boldsymbol{a}_1 \perp \boldsymbol{a}_2 \perp 2\boldsymbol{a}_3 - \boldsymbol{a}_1 \perp \boldsymbol{a}_1$	(Fig. 9,b)	
	Body-centered Γ_0^v	$\boldsymbol{a}_1 \perp \boldsymbol{a}_2 \perp 2\boldsymbol{a}_3 - \boldsymbol{a}_1 - \boldsymbol{a}_2 \perp \boldsymbol{a}_1$	(Fig. 9,c)	
	Face-centered Γ_0^f	$\boldsymbol{a}_1 \perp 2\boldsymbol{a}_2 - \boldsymbol{a}_1 \perp 2\boldsymbol{a}_3 - \boldsymbol{a}_1 \perp \boldsymbol{a}_1$	(Fig. 9,d)	
Tetragonal Q (D_{4h})	Primitive Γ_q	$\boldsymbol{a}_1 \perp \boldsymbol{a}_2 \perp \boldsymbol{a}_3 \perp \boldsymbol{a}_1$, $a_1 = a_2$	(Fig. 11,a)	a_3, a_1
	Body-centered Γ_q^v	$\boldsymbol{a}_1 \perp \boldsymbol{a}_2 \perp 2\boldsymbol{a}_3 - \boldsymbol{a}_1 - \boldsymbol{a}_2 \perp \boldsymbol{a}_1$, $a_1 = a_2$	(Fig. 11,b)	
Rhombohedral R (D_{3d})	Primitive Γ_{rh}	$a_1 = a_2 = a_3$, $\widehat{a_1a_2} = \widehat{a_1a_3} = \widehat{a_2a_3}$	(Fig. 13)	$a_1, \widehat{a_1a_2}$
Hexagonal H (D_{6h})	Primitive Γ_h	$\boldsymbol{a}_3 \perp \boldsymbol{a}_1$, $\boldsymbol{a}_3 \perp \boldsymbol{a}_2$, $\widehat{a_1a_2} = 2\pi/3$, $a_1 = a_2$	(Fig. 14)	a_1, a_3
Cubic K (O_h)	Primitive Γ_c	$\boldsymbol{a}_1 \perp \boldsymbol{a}_2 \perp \boldsymbol{a}_3 \perp \boldsymbol{a}_1$, $a_1 = a_2 = a_3$	(Fig. 12,a)	a_1
	Face-centered Γ_c^f	$\boldsymbol{a}_1 + \boldsymbol{a}_2 - \boldsymbol{a}_3 \perp \boldsymbol{a}_3 + \boldsymbol{a}_2 - \boldsymbol{a}_1$, $\boldsymbol{a}_3 + \boldsymbol{a}_2 - \boldsymbol{a}_1 \perp \boldsymbol{a}_1 - \boldsymbol{a}_2 + \boldsymbol{a}_3$, $\boldsymbol{a}_1 + \boldsymbol{a}_2 - \boldsymbol{a}_3 \perp \boldsymbol{a}_1 - \boldsymbol{a}_2 + \boldsymbol{a}_3$, $a_1 = a_2 = a_3$	(Fig. 12,c)	
	Body-centered Γ_c^v	$\boldsymbol{a}_1 \perp \boldsymbol{a}_2$, $\boldsymbol{a}_1 \perp 2\boldsymbol{a}_3 - \boldsymbol{a}_2 - \boldsymbol{a}_1 \perp \boldsymbol{a}_2$, $a_1 = a_2 = \lvert 2\boldsymbol{a}_3 - \boldsymbol{a}_2 - \boldsymbol{a}_1 \rvert$	(Fig. 12,b)	

Table 5.1 presents the basic characteristics of all fourteen Bravais lattice types.

Hierarchy of Systems

Of the point groups of crystal lattice symmetry, the groups O_h and D_{6h} possess the highest symmetry. All the other groups are subgroups of these. Thus, we can go from O_h to S_2 by successively lowering the symmetry: $O_h \to D_{4h} \to D_{2h} \to C_{2h} \to S_2$. Each group in this series is a subgroup of any preceding group. We can also go from O_h to C_{2h} through D_{3d}: $O_h \to D_{3d} \to C_{2h}$. A similar series goes from D_{6h} to S_2 through D_{2h} and C_{2h}: $D_{6h} \to D_{2h} \to C_{2h} \to S_2$.

Note that D_{3d} is a subgroup of D_{6h}; one would thus expect a continuous lattice transformation from D_{6h} to S_2 by the scheme $D_{6h} \to D_{3d} \to C_{2h} \to S_2$. However, as we shall show below, this continuous transformation of crystal structures is impossible.

To completely determine the symmetry of a Bravais lattice, we must specify not only its symmetry group but also the lattice type; we must therefore examine how a given lattice type of higher symmetry becomes a type of lower symmetry when the symmetry of the lattice is lowered.

We shall say that a system A is subordinate to a system B, $A \leftarrow B$, if the symmetry point group of the system A is a subgroup of that of the system B,

and each lattice type belonging to B may be converted into a lattice type of A by an infinitesimal continuous transformation of the basic vectors, which corresponds to reduction of the symmetry of the point group from B to A.

As we shall show below, except for the above-mentioned case of the groups D_{6h} and D_{3d}, the first condition implies the second.

We now consider the hierarchy of systems in greater detail.

If we dilate (or compress) a cube along one of its fourfold axes, it becomes a right parallelepiped on a square base, the Bravais parallelepiped for the system D_{4h}. In the process, a primitive cubic lattice obviously becomes a primitive tetragonal lattice: $\Gamma_c \to \Gamma_q$, and the lattices Γ_c^f and Γ_c^v become the body-centered lattice Γ_q^v, since we have already shown that in the tetragonal system face-centered and body-centered lattices are equivalent.

The Bravais parallelepiped for the tetragonal system may be converted into the Bravais parallelepiped for the orthorhombic system in two ways.

1. Dilation (or compression) on one of the lateral faces. The result is a right parallelepiped with rectangular faces, which is invariant under D_{2h}. Of the four twofold axes of D_{4h}, the two axes along the edges of the parallelepiped remain. This deformation converts type Γ_q lattices into Γ_0, and Γ_q^v into Γ_0^v.

2. The deformation is brought about by shearing the plane of the parallelepiped base, thus altering the angle between the edges of the base. The result is a rectangular parallelepiped with rhombic base, which is also invariant under D_{2h}, i.e., of the original four twofold axes the other two axes (the diagonals of the base) now remain. It is easy to see that under this deformation a type Γ_q lattice becomes Γ_0^b, and Γ_q^v becomes Γ_0^f.

The invariant parallelepiped of the system C_{2h} may be obtained from the Bravais parallelepiped of the orthorhombic system by deforming the base so that the angle between its edges is changed. As implied by our previous discussion of the relationships between the lattice types, this deformation transforms the lattice types of the orthorhombic and monoclinic systems in the following manner:

$$\Gamma_0^b,\ \Gamma_0 \to \Gamma_m \quad \text{and} \quad \Gamma_0^v,\ \Gamma_0^f \to \Gamma_m^b.$$

When the symmetry is lowered still more, removing the twofold axis, the group C_{2h} becomes S_2, and both monoclinic lattice types are converted to type Γ_t:

$$\Gamma_0^b,\quad \Gamma_0 \to \Gamma_t.$$

Now consider the transition from O_h to S_2 through D_{3d}. It is brought about by dilating (or compressing) a cube along one of its diagonals, as a result of which the cube becomes a rhombohedron. This deformation converts all three cubic lattices into the primitive lattice Γ_{rh}. Indeed, the primitive cell of types Γ_c^v and Γ_c^f is a rhombohedron, but the angles between the edges are not arbitrary. The deformation makes the primitive cell a rhombohedron, with an arbitrary angle between the edges. In the rhombohedron there are three twofold axes perpendicular to the threefold axis and three diagonal reflection planes containing a threefold axis. Each of the twofold axes is perpendicular to one of the reflection planes. When the symmetry is lowered from D_{3d} to C_{2h}, one of these twofold axes and the reflection plane perpendicular to it remain.

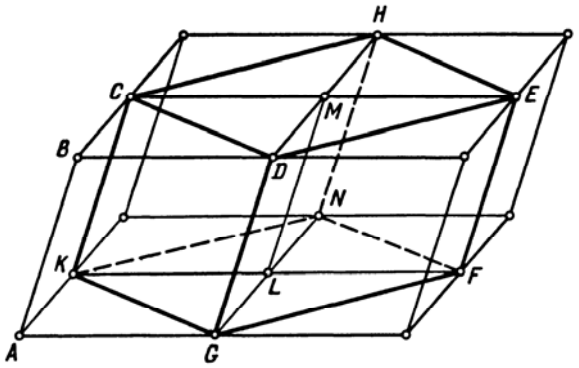


FIGURE 15. Correspondence of Bravais lattices in transformation from rhombohedral to monoclinic system.

This transformation may be brought about, for example, by a shearing deformation (Figure 15), altering one of the angles at a vertex, say *CBD*, and a change in the length of the edge *AB* and the parallel edges *CK*, *DG*, *ML*. The resulting parallelepiped, which is invariant under C_{2h}, is shown in Figure 15 by bold lines. Its face *EFGD* is an arbitrary parallelogram and lies in one of the reflection planes. The faces *CDEH* and *CDGK* are rectangles and are perpendicular to the plane of *EFGD*, since their edges *CD*, *HE*, *KG* and *NF* are parallel to the twofold axis.

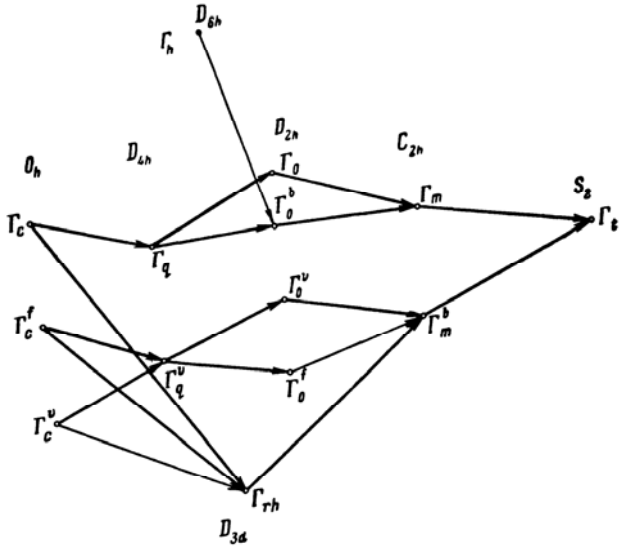


FIGURE 16. Hierarchy of systems.

As Figure 15 shows, in this case the lattice Γ_{rh} becomes a base-centered lattice Γ_0^b. This may be verified directly by comparing the primitive cells for type Γ_{rh}, Γ_0^b, and Γ_0 lattices (see Figures 9 and 13), since it is obvious that no small deformation of the basic vectors can convert a type Γ_{rh} lattice, where $\widehat{a_1a_2} = \widehat{a_1a_3} = \widehat{a_2a_3}$, into a primitive lattice Γ_{rh}, for which $a_3 \perp a_1$ and $a_3 \perp a_2$

Although D_{3d} is a subgroup of D_{6h}, it is impossible to convert a hexagonal lattice into a rhombohedral lattice by any infinitesimal transformation of the basic vectors, since the basic vectors for hexagonal lattices Γ_h satisfy the the conditions $a_3 \perp a_1$, $a_3 \perp a_2$, $a_1 = a_2 \neq a_3$, and no infinitesimal transformation will make them satisfy the conditions $\widehat{a_3a_1} = \widehat{a_1a_2} = \widehat{a_2a_3}$ and $a_1 = a_2 = a_3$, which must hold for lattices of the rhombohedral system.

The group D_{2h} is a subgroup of D_{6h}, since together with inversion D_{6h} has three mutually perpendicular twofold axes: c_6^3 and two horizontal twofold axes lying in a plane perpendicular to the sixfold axis.

A deformation along the horizontal twofold axes lowers the symmetry of D_{6h} to D_{2h}, and the primitive cell of Γ_h becomes a right parallelepiped with rhombic base, which (see table on p. 49) is equivalent to Γ_0^b. Therefore, in transition from the hexagonal to the orthorhombic system the primitive hexagonal lattice becomes a base-centered lattice Γ^b.

The hierarchy of systems and the relationships between lattice types in different systems is summarized in Figure 16.

§6. SPACE GROUPS

Crystal Classes

The system and lattice type characterize the symmetry group of a crystal incompletely, since they determine only the symmetry of its Bravais lattice. In compound crystals, having more than one atom in the primitive cell, the Bravais lattices may coincide without all equivalent points being the same. Thus the symmetry of a crystal lattice may in fact be lower than the symmetry of its Bravais lattice.

For example, although the Bravais lattice of any crystal contains inversion, inversion is not a symmetry element for all crystals.

Directions in a crystal along which all the physical properties of the crystal are identical will be called equivalent directions. Any two equivalent directions in a crystal clearly contain identical sequences of equivalent points of the crystal (e.g., identical sequences of atoms).

Let r be any element of the symmetry point group $\mathcal{H}$ of a Bravais lattice. According to the definition of the group $\mathcal{H}$, the Bravais lattice is invariant under the transformation r.

How do the other points of the crystal and the directions in the crystal transform? There are obviously three possibilities.

1. The transformation r takes every point of the crystal, and not only those of the Bravais lattice, onto equivalent points. When this is the case, of course, every direction is also mapped onto an equivalent direction. The element r then belongs to the crystal symmetry group G.

2. The transformation r maps every direction onto an equivalent direction, but not every point is mapped onto an equivalent one.

3. Not every direction is mapped onto an equivalent one.

In the last case, r is not an element of the crystal symmetry group.

We now consider a transformation r which maps any direction in the crystal onto an equivalent direction. Clearly, for this transformation to take all the points of the crystal onto equivalent points, we also need a parallel displacement (translation) by some vector α which is not a vector of the Bravais lattice. Therefore, although r itself is not an element of the crystal symmetry group G, the element $t_\alpha r$ is in G.

The elements of the point group $\mathcal{H}$ which take every direction in the crystal onto an equivalent one (i.e., the elements r in the first and second cases) form a certain point group F, which is a subgroup of $\mathcal{H}$. The group F is a crystallographic point group, also known as a crystal class.

The symmetry group of a macroscopic body is its crystallographic point group; thus the crystal class determines the macrosymmetry of the crystal. In particular, the number of independent components and the form of the macroscopic tensors are determined by the group F characterizing the crystal class.

Since each class is a subgroup of the symmetry group of a vector group, there are altogether 32 different crystal classes, according to the number of different subgroups in the symmetry groups of the Bravais lattices: e, S_2, C_s, C_2, C_{2h}, C_{2v}, D_2, D_{2h}, S_4, D_{2d}, C_4, C_{4v}, C_{4h}, D_4, D_{4h}, C_3, S_6, C_{3v}, D_3, D_{3d}, C_{3h}, D_{3h}, C_6, C_{6h}, C_{6v}, D_6, D_{6h}, T, T_h, T_d, O, O_h. Note that the same class may be a subgroup of different point groups determining the symmetry of a Bravais lattice. For example, S_2 is a subgroup of any of the seven point groups defining the system.

The crystal class is referred to the system with the lowest symmetry in which it first appears; in other words, a crystal class F belongs to system $\mathcal{H}$ if F is a subgroup of $\mathcal{H}$ and no system $\mathcal{H}_1$ subordinate to $\mathcal{H}$ contains F. This distribution of the classes among the systems is based on the following considerations. If the Bravais lattice of a crystal had a higher symmetry than required by the crystal class, it would be unstable, and any small effect (thermal expansion, changes in interatomic interaction, etc.) would lower the symmetry of the Bravais lattice to the lowest level permitted by the crystal class. Thus each crystal class belongs to one system. The only exception is the hexagonal system, whose lattice, as noted above, cannot be transformed into lattices of the rhombohedral system by any infinitesimal deformation. Hence the classes of the rhombohedral system also belong to the hexagonal system.

TABLE 6.1

System	Crystal classes						
Triclinic	e,	S_2					
Monoclinic	C_s,	C_2,	C_{2h}				
Orthorhombic	C_{2v},	D_2,	D_{2h}				
Tetragonal	S_4,	D_{2d},	C_4,	C_{4h},	C_{4v},	D_4,	D_{4h}
Rhombohedral	C_3,	S_6,	C_{3v},	D_3,	D_{3d}		
Hexagonal	C_{3h},	D_{3h},	C_6,	C_{6h},	C_{6v},	D_6,	D_{6h}
Cubic	T,	T_h,	T_d,	O,	O_h		

The distribution of the thirty-two crystal classes among the systems is presented in Table 6.1.*

Space Groups

Even the crystal class and lattice type are not enough to characterize the symmetry of a crystal. The crystal class characterizes the symmetry of the crystallographic point group, but in order to describe the space group which determines the microsymmetry of the crystal we must still specify the length of the translation vector α_r needed to bring all points of the crystal into coincidence with equivalent points. Hence, to each "rotational" element r of the crystallographic point group F (rotation, reflection, or improper rotation) corresponds a certain translation t_{α_r}, known as a nonprimitive translation.

Thus each element g of the space group G has the form

$$g = t_a t_\alpha r = t_{a+\alpha}\ r = (r \mid a + \alpha), \tag{6.1}$$

where r is a "rotational" element in the crystal class, and t_a the corresponding nonprimitive translation.

While a point group, in which all the symmetry elements have a common point, may be determined by simply listing all its symmetry elements, for a space group we must also specify the position of each rotational element within the primitive cell; this is the reason for specifying the vector α.

Since the "rotational" transformation r maps all the points of the Bravais lattice onto each other, while α is not a "whole" vector of the Bravais lattice, the transformation $t_\alpha r$ does not bring the lattice points into coincidence with each other. The presence of such an operation in the symmetry group of a crystal signifies that the crystal lattice is compound, i.e., there are at least two atoms of the same kind in each primitive cell. As remarked above, a lattice of this kind may be viewed as a system of interpenetrating identical Bravais lattices. The operations $t_\alpha r$, $\alpha \neq a$, map the points of each component lattice onto the identical points of another lattice.

The various space groups belonging to one class differ from each other as to the set of vectors α_r corresponding to the symmetry elements r in the group F. The vectors α may be expressed as linear combinations of a_1, a_2, and a_3:

$$\alpha = \gamma_1 a_1 + \gamma_2 a_2 + \gamma_3 a_3. \tag{6.2}$$

The numbers γ_1, γ_2, and γ_3 may be assumed nonnegative and less than unity**:

$$0 \leqslant \gamma_1 < 1, \quad 0 \leqslant \gamma_2 < 1, \quad 0 \leqslant \gamma_3 < 1. \tag{6.3}$$

The set of vectors α_i is not arbitrary, since they must satisfy certain relations, bound up with the fact that the rotational elements r_i themselves form a group. In fact, let the "rotational" element r_1 correspond to a nontrivial translation α_1, and r_2 to α_2. Since

$$t_{\alpha_1} r_1 t_{\alpha_2} r_2 = t_{\alpha_1 + r_1 \alpha_2} r_1 r_2,$$

*Crystals of the rhombohedral classes with hexagonal Bravais lattice belong to the rhombohedral system.

**If γ_1, γ_2, and γ_3 are not required to be nonnegative, they may be so chosen that

$$|\gamma_1| \leqslant 1/2, \quad |\gamma_2| \leqslant 1/2, \quad |\gamma_3| \leqslant 1/2.$$

it follows that the element $r_3 = r_1 r_2$ may correspond only to the vector $\alpha_3 = \alpha_1 + r_1\alpha_2 + a$, where a is a "whole" lattice vector, chosen so that α_3 satisfies condition (6.3)

Thus the nontrivial translation α_3 is uniquely determined for each rotational element α of the crystallographic point group by specifying nonprimitive translation vectors for the generators of the crystallographic point group. The defining relations between the "rotational" generators of the group F define the possible types of vectors for nonprimitive translations of the generators, hence also the possible types of space groups belonging to one crystal class.

Altogether, our 7 systems, 14 types, and 32 crystal classes consist of 230 different space groups.

Let us examine the structure of the space groups. Every space group contains an abelian subgroup T of translations by the fundamental lattice periods, with elements t_a. This subgroup is an invariant subgroup of the space group.

Indeed, all elements conjugate to t_a are also translations and therefore lie in T:

$$t_a r t_a (t_a r)^{-1} = t_a r t_a r^{-1} t_{-a} = t_{ra}. \tag{6.4}$$

Divide all the elements of the space group G into cosets modulo the translation subgroup and construct the corresponding factor group.

The elements of these cosets are all possible products of translations t_a and elements $t_{a_i} r_i$:

$$\{T\},\ \{Tt_{a_1} r_1\},\ \ldots,\ \{Tt_{a_n} r_n\}, \tag{6.5}$$

where a is any vector of type (5.1).

The factor group of any space group belonging to a given class is isomorphic to the crystallographic point group characterizing the crystal class. There is a one–one correspondence between the elements r_i of the group F and the cosets $Tt_{a_i} r_i$:

$$r_i \leftrightarrow \{Tt_{a_i} r_i\}. \tag{6.6}$$

Indeed, by (2.22), the product of representatives of cosets $\{Tt_{a_1} r_1\}$ and $\{Tt_{a_2} r_2\}$

$$t_a t_{a_1} r_1 t_{a'} t_{a_2} r_2 = t_{a + r_1 a' + r_1 a_2 + a_1} r_1 r_2$$

is an element of the coset $\{Tt_{a_3} r_3\}$, corresponding to the element $r_3 = r_1 \cdot r_2$.

Thus space groups belonging to one class are homomorphic to the group F characterizing the crystal class. The kernel of the homomorphism is the translation group T, and the corresponding factor group is isomorphic to F. This does not, of course, imply that space groups belonging to the same crystal class are isomorphic.

Chapter II

REPRESENTATIONS OF SYMMETRY GROUPS

§7. REPRESENTATION THEORY

Following on our discussion of symmetry groups, we now turn to the theory of representations of these groups. The special significance of representation theory is that in effect it provides the basis for all physical applications of group theory.

Let φ_1 be an arbitrary single-valued function of the coordinates of a point $x(x_1, x_2, x_3)$ in the coordinate system xyz. We transform to a new coordinate system $x'y'z'$, obtained from xyz by a symmetry transformation g_s. By (2.29) the coordinates of the point x in the new coordinate system, x'_1, x'_2, x'_3, are

$$x'_i = \sum_j \mathcal{R}_{ji}(g_s)\, x_j = (g_s^{-1}x)_i. \tag{7.1}$$

Now replace x_i in $\varphi_1(x)$ by x'_i and express x'_i in terms of x_i using (7.1). The result is a new function $\varphi_s(x)$. We shall treat this transformation as the result of applying an operator $\mathcal{D}(g_s)$ to the function $\varphi_1(x)$:

$$\mathcal{D}(g_s)\,\varphi_1(x) = \varphi_1(g_s^{-1}x) = \varphi_s(x). \tag{7.2}$$

Successively applying all the operations g to φ_1, we obtain h functions $\varphi_1, \varphi_2, \ldots, \varphi_h$. In the general case, however, these functions need not all be linearly independent and some of them may be expressed in terms of the others. Let the total number of linearly independent or basis functions φ_i be n; then each function $\varphi_s(x)$ may be expressed as a linear combination of these functions. If we apply the operator $\mathcal{D}(g)$ to one of the basis functions $\varphi_i(x)$, the new function $\varphi_i(g^{-1}x)$ may be expressed as a linear combination of the basis functions:

$$\mathcal{D}(g)\,\varphi_i(x) = \varphi_i(g^{-1}x) = \sum_j \mathcal{D}_{ji}(g)\,\varphi_j(x). \tag{7.3}$$

The actual form of the matrices $\mathcal{D}(g)$ and their order n depend on the choice of the function $\varphi_1(x)$. We note that the transformation (7.1) may also be viewed as the result of applying the operator $\mathcal{D}(g_s)$ to the vector functions x_1, x_2, x_3. In this interpretation, we have from (7.2) that $\mathcal{D}(g)x_i = (g^{-1}x)_i$, and it follows from (7.3) and (7.1) that $\mathcal{D}(g) = \mathcal{R}(g)$.

We claim that with this definition of the operator $\mathcal{D}(g)$ the operator $\mathcal{D}(g_s)$ corresponding to the operation $g_s = g_p g_q$ is the product of the corresponding operators:

$$\mathcal{D}(g_p g_q) = \mathcal{D}(g_p)\,\mathcal{D}(g_q). \tag{7.4}$$

In fact, it follows from (7.3) that

$$\mathcal{D}(g_p)\mathcal{D}(g_q)\varphi_i(\boldsymbol{x}) = \mathcal{D}(g_p)\varphi_i(\mathcal{R}(g_q)\boldsymbol{x}) = \\ = \varphi_i(\mathcal{R}(g_q)\mathcal{R}(g_p)\boldsymbol{x}) = \varphi_i(g_q^{-1}g_p^{-1}\boldsymbol{x}) = \\ = \varphi_i\left((g_pg_q)^{-1}\boldsymbol{x}\right) = \varphi_i(g_s^{-1}\boldsymbol{x}) = \mathcal{D}(g_s)\varphi_i(\boldsymbol{x}).$$

We now show that if the order of the summation indices is chosen as in (7.3) a similar rule holds for the matrices:

$$\mathcal{D}(g_p)\mathcal{D}(g_q)\varphi_i = \mathcal{D}(g_p)\sum_l \mathcal{D}_{li}(g_q)\varphi_l = \sum_l \mathcal{D}_{li}(g_q)\sum_k \mathcal{D}_{kl}(g_p)\varphi_k.$$

On the other hand,

$$\mathcal{D}(g_s)\varphi_i = \sum_k \mathcal{D}_{ki}(g_s)\varphi_k.$$

Consequently, by the usual rules of matrix multiplication,

$$\mathcal{D}(g_pg_q) = \mathcal{D}(g_p)\mathcal{D}(g_q). \tag{7.5}$$

Now suppose that with each element g of the group $\mathcal{G}$ we associate a square matrix $\mathcal{D}(g)$ of order n, so that for any p and q the product $g_s = g_pg_q$ is associated with the product $\mathcal{D}(g_s)$ of the matrices $\mathcal{D}(g_p)\mathcal{D}(g_q)$. The set of matrices $\mathcal{D}(g)$ is then called a representation of the group $\mathcal{G}$, of dimension (or degree) n, denoted by the symbol $\mathcal{D}$. A set of linearly independent functions φ_i $(i = 1, 2, \ldots, n)$ which transform according to (7.3) is called a basis of the representation $\mathcal{D}$. The set of operators $\mathcal{D}(g)$ defined as described above and satisfying condition (7.4) is an operator representation of the group $\mathcal{G}$.

Given any n linearly independent functions, we may always form n new functions (via linear combinations) which are orthogonal and normalized to unity. Henceforth, therefore, we shall always assume that the basis is a system of orthonormal functions, i.e., functions satisfying the condition

$$\langle\varphi_i\varphi_l\rangle = \int \varphi_i^*\varphi_l\,d\boldsymbol{x} = \delta_{il}. \tag{7.6}$$

Multiplying equation (7.3) by $\varphi_j^*(\boldsymbol{x})$ and integrating with respect to $\boldsymbol{x}$, we obtain in view of (7.6)

$$\mathcal{D}_{li}(g) = \int \varphi_l^*\mathcal{D}(g)\varphi_i\,d\boldsymbol{x} = \langle\varphi_l\mathcal{D}(g)\varphi_i\rangle. \tag{7.7}$$

Formula (7.7) recalls the usual definition of the matrix element of an operator in quantum mechanics.

The choice of the system of orthonormal functions is not unique. Given any system φ_i, we may always transform to a new system φ_i' via a linear transformation

$$\varphi_i' = S\varphi_i = \sum_l S_{li}\varphi_l. \tag{7.8}$$

A necessary condition for the new system of functions φ_l' to be orthonormal is that the matrix S be unitary, i.e.,

$$S^+ = \tilde{S}^* = S^{-1}, \text{ i.e., } S_{li}^{-1} = S_{il}^* \tag{7.9}$$

or

$$\tilde{S}^*S = S^*\tilde{S} = I. \tag{7.10}$$

Here S^+ denotes the hermitian conjugate of S:

$$S^+ = \tilde{S}^*,$$

where, as usual, the star denotes complex conjugation and the tilde ($\sim$) transposition.

Formula (7.10) shows that a unitary matrix has orthogonal columns and rows:

$$\sum_k S^*_{kl} S_{kj} = \delta_{lj}, \quad \sum_k S^*_{lk} S_{jk} = \delta_{lj}. \tag{7.10a}$$

When (7.10) holds, we have

$$\langle \varphi'_l \varphi'_j \rangle = \sum_{lk} S^*_{ll} S_{kj} \langle \varphi_l \varphi_k \rangle = \sum_{lk} S^*_{ll} S_{kj} \delta_{lk} = \delta_{lj}.$$

For real matrices the unitarity condition reduces to the orthogonality condition (2.24).

If the basis functions are orthonormal, the matrices $\mathcal{D}(g)$ in (7.3) are also unitary. Indeed, the value of the integral (7.6) is the same under any change of variables. Now, volume is invariant under symmetry transformations, i.e., $dx'_1\, dx'_2\, dx'_3 = dx_1\, dx_2\, dx_3$, since the Jacobian of the transformation is

$$\left| \frac{\partial (x'_1, x'_2, x'_3)}{\partial (x_1, x_2, x_3)} \right| = 1.$$

Thus, if we transform to the variables x' as in (7.1), it follows from (7.3) that

$$\int \varphi^*_i(x)\, \varphi_j(x)\, dx = \int \varphi^*_i(x')\, \varphi_j(x')\, dx' = \int \varphi^*_i(g^{-1}x)\, \varphi_j(g^{-1}x)\, dx =$$
$$= \sum_{kl} \mathcal{D}^*_{kl}(g)\, \mathcal{D}_{lj}(g) \int \varphi^*_k(x)\, \varphi_l(x)\, dx = \sum_k \mathcal{D}^*_{kl}(g)\, \mathcal{D}_{kj}(g) = \delta_{lj}.$$

Consequently,

$$\mathcal{D}^{-1}(g) = \mathcal{D}(g^{-1}) = \mathcal{D}^+(g) = \tilde{\mathcal{D}}^*(g). \tag{7.11}$$

The n-tuple of functions φ_i may be viewed as a vector φ in n-dimensional space with components φ_i, written as a column vector. The operator S defined by (7.8) transforms the vector φ into the vector φ' with components φ'_i given by (7.8).

How do the matrices $\mathcal{D}(g)$ transform when we go over from the representation φ_i to the representation φ'_i? The matrix element of the new representation is

$$\mathcal{D}'_{ij}(g) = \langle \varphi'_i \mathcal{D}(g)\, \varphi'_j \rangle.$$

Expressing φ' in terms of φ by (7.8) and using (7.9), we obtain

$$\mathcal{D}'_{ij}(g) = \sum_{kl} S^*_{ki} \mathcal{D}_{kl} S_{lj} = \sum_{kl} S^{-1}_{ik} \mathcal{D}_{kl} S_{lj} = (S^{-1} \mathcal{D} S)_{ij}$$

or

$$\mathcal{D}'(g) = S^{-1} \mathcal{D}(g)\, S, \tag{7.12}$$

giving the usual rule for transformation of matrices in quantum mechanics.

Representations which may be obtained from one another by a unitary transformation (7.12) are said to be equivalent. Representations $\mathcal{D}$ and $\mathcal{D}'$ with equal matrices $\mathcal{D}(g)$ and $\mathcal{D}'(g)$ will also be called equal.

An important property of the transformation (7.12) is that it preserves the trace of the matrix $\mathcal{D}(g)$, i.e., the sum of its diagonal elements. In fact, by (7.12),

$$\operatorname{Sp}\mathcal{D}' = \sum_i \mathcal{D}'_{ii} = \sum_{ikl} S^{-1}_{ik}\mathcal{D}_{kl}S_{li} = \sum_{lk} \mathcal{D}_{kl}\delta_{kl} = \sum_k \mathcal{D}_{kk} = \operatorname{Sp}\mathcal{D}. \tag{7.13}$$

The determinant of the matrix $\mathcal{D}(g)$ is also preserved under the transformation (7.12), since

$$|S^{-1}\mathcal{D}S| = |S^{-1}|\,|\mathcal{D}|\,|S| = |\mathcal{D}|.$$

The total number of matrices $\mathcal{D}(g)$ coincides with the number of elements in the group, h. However, some of these matrices may coincide. If all h matrices are different, the representation is said to be faithful. If several group elements correspond to the same matrix, the representation is unfaithful. In the latter case, the group $\mathcal{G}$ is homomorphic to the group $\mathcal{F}$ formed by those of the matrices which are in fact different. The kernel of the homomorphism is the set $\mathcal{E}$ of m (say) elements $e, e_2, \ldots, e_m$ which correspond to the identity I. These elements, as shown in §1, form an invariant subgroup of $\mathcal{G}$, and all the elements of the coset $g_k\mathcal{E}$, i.e., the elements $g_k e_i$ $(i = 1, 2, \ldots, m)$, $g_k \notin \mathcal{E}$, are associated with the same matrix $\mathcal{F}_k = \mathcal{D}(g_k)$. Consequently, the matrices $\mathcal{D}(g)$, though not a faithful representation of the group $\mathcal{G}$, always constitute a faithful representation of its factor group by $\mathcal{E}$. Thus the set of all representations of the group $\mathcal{G}$ exhausts the representations of all the factor groups of $\mathcal{G}$.

As mentioned above, the dimension of a representation is defined as the number of basis functions φ_i. However, it may turn out that a suitably chosen unitary transformation S divides the system of basis functions into two or more subsystems $\varphi^1, \varphi^2, \ldots$, in such a way that any symmetry transformation maps each of the functions $\varphi^\nu_i(g^{-1}x)$ onto a linear combination of the functions of the same subsystem:

$$\mathcal{D}(g)\,\varphi^\nu_i(x) = \varphi^\nu_i(g^{-1}x) = \sum_j \mathcal{D}^\nu_{ji}\varphi^\nu_j,$$

in other words, the linear space spanned by the functions decomposes into invariant subspaces. Consequently, the set of matrices $\mathcal{D}(g)$ for all the elements of the group is transformed by the unitary transformation (7.12) into a system of block-diagonal matrices of the form (say)

$$\mathcal{D}(g) = \begin{Vmatrix} \mathcal{D}_1(g) & 0 & 0 \\ 0 & \mathcal{D}_2(g) & 0 \\ 0 & 0 & \mathcal{D}_3(g) \end{Vmatrix}. \tag{7.14}$$

This means that each of the sets of matrices $\mathcal{D}_\nu(g)$ forms a representation of the group. The representation $\mathcal{D}$ is then said to be reducible. If there is no unitary transformation inducing further decomposition of the systems φ^ν into smaller subsystems with the above property, each representation $\mathcal{D}_\nu$ is said to be irreducible. The reduction of $\mathcal{D}$ to the form (7.14) is known as decomposition of the reducible representation $\mathcal{D}$ into irreducible representations $\mathcal{D}_\nu$ (its irreducible constituents).

In the general case, some of the representations $\mathcal{D}_\nu$ may be equivalent. These equivalent representations may always be reduced to equal representations by an appropriate unitary transformation.

Irreducible representations play a major role in the physical applications of group theory, since, as we shall show below, wave functions which transform according to the same irreducible representation correspond to the same energy eigenvalue. Thus, for example, the dimension of the irreducible representations directly determines the possible degeneracy of the terms.

In the following sections we shall discuss the properties of irreducible representations and show how the decomposition of a reducible representation into irreducible ones may be carried out in practice.

§8. IRREDUCIBLE REPRESENTATIONS. CHARACTERS

Matrices forming irreducible representations of a group have a number of important properties. These properties follow from the fundamental lemmas of Schur.

Consider two sets of square matrices $\mathcal{D}(g)$ and $\mathcal{D}'(g)$, both representations of a group $\mathcal{G}$. The orders of these matrices may be different. Let A be a rectangular matrix with as many rows as $\mathcal{D}$ and as many columns as $\mathcal{D}'$, such that for all $g \in \mathcal{G}$

$$\mathcal{D}(g)\,A = A\,\mathcal{D}'(g). \tag{8.1}$$

Schur's first lemma states that if representations $\mathcal{D}_\mu$ and $\mathcal{D}_\nu$ are equal, i.e., $\mu = \nu$ and $\mathcal{D}_\mu(g) = \mathcal{D}_\nu(g)$, then $A = cI$, i.e., any matrix A that commutes with every matrix of an irreducible representation $\mathcal{D}_\mu(g)$ is a multiple of the identity matrix:

$$\text{if } \mathcal{D}_\mu(g)\,A = A\,\mathcal{D}_\mu(g), \text{ where } g \in \mathcal{G}, \text{ then } A = cI. \tag{8.1a}$$

Here the matrices $\mathcal{D}_\mu(g)$ are assumed to be unitary.

To prove (8.1a), we take hermitian conjugates in (8.1); since $(AB)^+ = B^+A^+$, we obtain

$$A^+\mathcal{D}^+(g) = \mathcal{D}^+(g)\,A^+.$$

Multiplying the last equation on the left and the right by $\mathcal{D}(g)$ and using (7.11), we obtain

$$\mathcal{D}(g)\,A^+ = A^+\mathcal{D}(g).$$

Hence, if (8.1) holds for A, it is also true for A^+, and consequently also for the hermitian matrices

$$A' = \tfrac{1}{2}(A + A^+) \quad \text{and} \quad A'' = \tfrac{i}{2}(A - A^+).$$

Both hermitian and unitary matrices may be brought to diagonal form by a unitary transformation. If S is a transformation which diagonalizes A or A', it follows from (8.1) that

$$\bar{\mathcal{D}}(g)\,a = a\,\bar{\mathcal{D}}(g),$$

where $\bar{\mathcal{D}} = S^{-1}\mathcal{D}S$, and $a = S^{-1}AS$ is a diagonal matrix. We may write this as

$$\bar{\mathcal{D}}_{kl}(g)\,(a_{kk} - a_{ll}) = 0 \qquad (k, l = 1, 2, \ldots, h). \tag{8.1b}$$

There are two possibilities in regard to (8.1b). Either all the $a_{\mu\mu}$ are equal, so that the matrix is indeed a multiple of the identity matrix, or some of the elements, say a_{kk} $(k = 1, 2, \ldots, r)$, are different from other ones a_{ll} $(l = r+1, \ldots, h)$. In the latter case, by (8.1b), we have

$$\mathcal{D}_{kl}(g) = 0 \text{ where } k = 1, 2, \ldots, r, \; l = r+1, r+2, \ldots, h,$$

and this means that each matrix $\bar{\mathcal{D}}(g)$ is block-diagonal, as illustrated in (7.14), and each of the submatrices with elements $\bar{\mathcal{D}}_{kk'}(g)$ $(k, k' = 1, 2, \ldots, r)$ and $\bar{\mathcal{D}}_{ll'}(g)$ $(l, l' = r+1, \ldots, h)$ defines a representation of the group. Thus the representation $\mathcal{D}_\mu$ is reducible. But this contradicts our assumption, and so only the first possibility remains, i.e., $a = cI$. Consequently, the matrices $A' = SaS^{-1}$ and A'' are multiples of the identity, and therefore so is the original matrix $A = A' - iA''$.

Schur's second lemma states that if representations $\mathcal{D}$ and $\mathcal{D}'$ are irreducible and inequivalent, i.e., $\mathcal{D} = \mathcal{D}_\mu$, $\mathcal{D}' = \mathcal{D}_\nu$ and $\mu \neq \nu$, then the only matrix A satisfying condition (8.1) is the zero matrix, i.e., the matrix in which $A_{kl} = 0$ for all k and l:

$$\text{if } \mathcal{D}_\mu(g)\, A = A \mathcal{D}_\nu(g), \; g \in \mathfrak{G} \text{ and } \mu \neq \nu, \text{ then } A = 0. \tag{8.2}$$

On the other hand, if $A \neq 0$ for two representations $\mathcal{D}$ and $\mathcal{D}'$, then at least one of these representations is reducible, and $\mathcal{D}$ and $\mathcal{D}'$ must contain at least one common irreducible constituent.

We note that if $\mathcal{D}_\mu$ and $\mathcal{D}_\nu$ are equivalent representations, i.e., there is a unitary matrix S such that

$$\mathcal{D}_\nu(g) = S^{-1} \mathcal{D}_\mu(g)\, S,$$

then any matrix A satisfying (8.2) must be a multiple of the unitary transformation matrix, $A = cS$.

Let the matrices $\mathcal{D}_\mu(g)$ be of order h_1 and the matrices $\mathcal{D}_\nu(g)$ of order h_2, i.e., A has h_1 rows and h_2 columns. To fix ideas, assume that $h_2 \geqslant h_1$. To prove Schur's second lemma we go over to hermitian conjugates; using the fact that $\mathcal{D}^+(g) = \mathcal{D}^{-1}(g) = \mathcal{D}(g^{-1})$, we obtain

$$A^+ \mathcal{D}_\mu(g^{-1}) = \mathcal{D}_\nu(g^{-1})\, A^+.$$

Multiplying on the right by A and noting that by (8.2) $A\mathcal{D}_\nu(g^{-1}) = \mathcal{D}_\mu(g^{-1})\, A$, since $g^{-1} \in \mathfrak{G}$, we obtain

$$AA^+ \mathcal{D}_\mu(g^{-1}) = \mathcal{D}_\mu(g^{-1})\, AA^+, \quad g^{-1} \in \mathfrak{G}.$$

By Schur's first lemma, the square matrix AA^+ of order h_1 is a multiple of the identity, since it commutes with every matrix $\mathcal{D}_\mu(g)$:

$$AA^+ = cI$$

and so $\operatorname{Det} AA^+ = c^{h_1}$. If $c \neq 0$, then $\operatorname{Det} A \neq 0$.

If $h_1 = h_2$, so that A is a square matrix, the last condition implies that it has an inverse A^{-1}. Then multiplying (8.2) by A^{-1}, we obtain $A^{-1}\mathcal{D}_\mu(g)\, A = \mathcal{D}_\nu(g)$, so that the representations $\mathcal{D}_\mu$ and $\mathcal{D}_\nu$ are equivalent, contrary to hypothesis. Consequently, if $h_1 = h_2$ we have $c = 0$, i.e., $AA^+ = 0$ or

$$\sum_l A_{kl} A^+_{lk} = \sum_l A_{kl} A^*_{kl} = \sum_l |A_{kl}|^2 = 0,$$

which is possible only if all the matrix elements A_{kl} vanish, i.e., $A = 0$.

If $h_1 < h_2$, we complete A to a square matrix by adding $h_2 - h_1$ zero rows, to obtain a matrix $\bar{A}$ with determinant zero. On the other hand, $\bar{A}\bar{A}^+ = AA^+$, and so

$$\operatorname{Det} AA^+ = \operatorname{Det} \bar{A}\bar{A}^+ = \operatorname{Det} \bar{A} \operatorname{Det} \bar{A}^+ = 0,$$

and this means that if $h_1 < h_2$ then $c = 0$, i.e., $AA^+ = 0$, whence it follows as before that $A = 0$.

Using Schur's second lemma, we can prove the following orthogonality relation.

If $\mathcal{D}_\nu(g)$ and $\mathcal{D}_\mu(g)$ are inequivalent irreducible representations of the group $\mathcal{G}$, then the matrix elements $\mathcal{D}^\nu_{ij}(g)$ and $\mathcal{D}^\mu_{kl}(g)$, for arbitrary i, j, k, l, satisfy the orthogonality relation:

$$\sum_g \mathcal{D}^\mu_{ij}(g)\, \mathcal{D}^{\nu *}_{lk}(g) = 0 \qquad \text{if} \quad \mu \neq \nu. \tag{8.3}$$

To prove (8.3), we consider the matrix

$$A = \sum_g \mathcal{D}_\mu(g)\, B\, \mathcal{D}^{-1}_\nu(g), \tag{8.4}$$

where B is an arbitrary matrix. It is evident that the matrix A satisfies (8.2), since by (8.2)

$$\begin{aligned} \mathcal{D}_\mu(g')\, A &= \sum_g \mathcal{D}_\mu(g')\, \mathcal{D}_\mu(g)\, B \mathcal{D}^{-1}_\nu(g) = \\ &= \sum_g \mathcal{D}_\mu(g')\, \mathcal{D}_\mu(g)\, B \mathcal{D}^{-1}_\nu(g)\, \mathcal{D}^{-1}_\nu(g')\, \mathcal{D}_\nu(g') = \\ &= \sum_{g''} \mathcal{D}_\mu(g'')\, B \mathcal{D}^{-1}_\nu(g'')\, \mathcal{D}_\nu(g') = A \mathcal{D}_\nu(g'). \end{aligned} \tag{8.5}$$

Consequently, by Schur's second lemma, $A = 0$, i.e.,

$$\sum_g \sum_{k'l'} \mathcal{D}^\mu_{ik}(g)\, B_{k'l'} \mathcal{D}^{\nu -1}_{l'l}(g) = 0. \tag{8.6}$$

If we let B be a matrix whose only nonzero elements are $B_{k'l'} = \delta_{k'j}\delta_{l'k}$, it follows from (8.6) that

$$\sum_g \mathcal{D}^\mu_{ij}(g)\, \mathcal{D}^\nu_{k'l}(g^{-1}) = 0. \tag{8.7}$$

Equation (8.3) now follows from (8.7) and the unitarity condition (7.11).

Now consider the case that the representations μ and ν coincide. In proving (8.5) we imposed no conditions on the matrices $\mathcal{D}$, and it remains valid when $\mathcal{D}_\mu(g) = \mathcal{D}_\nu(g)$. In this case the matrix A satisfies condition (8.1), and so, by Schur's first lemma, $A = cI$, or

$$\sum_g \sum_{k'l'} \mathcal{D}^\mu_{ik'}(g)\, B_{k'l'} \mathcal{D}^{\mu -1}_{l'l}(g) = c\delta_{il}.$$

The value of the constant c depends on the choice of B. Letting $B_{k'l'} = \delta_{k'j}\delta_{l'k}$ as before and denoting $c = c_{jk}$, we get

$$\sum_g \mathcal{D}^\mu_{ij}(g)\, \mathcal{D}^\mu_{kl}(g^{-1}) = c_{jk}\delta_{il}.$$

To evaluate c_{jk}, we set $i = l$ and sum over i. Noting that

$$\sum_g \sum_i \mathcal{D}_{ij}(g)\, \mathcal{D}_{kl}(g^{-1}) = \sum_g \mathcal{D}_{kj}(g^{-1}g) = h\delta_{kj},$$

and $\sum_i \delta_{ii} = n_\mu$, where n_μ is the dimension of the irreducible representation $\mathcal{D}_\mu$,

we obtain $c_{jk} = (h/n_\mu)\,\delta_{jk}$, and consequently

$$\sum_g \mathcal{D}^\mu_{ij}(g)\,\mathcal{D}^\mu_{kl}(g^{-1}) = \frac{h}{n_\mu}\,\delta_{jk}\delta_{il}. \tag{8.8}$$

Using (7.11), we may rewrite this relation for unitary matrices as

$$\sum_g \mathcal{D}^\mu_{ij}(g)\,\mathcal{D}^{\mu*}_{lk}(g) = \frac{h}{n_\mu}\,\delta_{il}\delta_{jk}. \tag{8.9}$$

Equations (8.3) and (8.9) may be combined into a generalized orthogonality relation:

$$\sum_g \mathcal{D}^\mu_{ij}(g)\,\mathcal{D}^{\nu*}_{lk}(g) = \frac{h}{n_\mu}\,\delta_{\mu\nu}\delta_{il}\delta_{jk}. \tag{8.10}$$

The quantity

$$\mathcal{D}'_{pq} = \left(\frac{n_\mu}{h}\right)^{1/2} \mathcal{D}^\mu_{ij}(g_q), \tag{8.11}$$

where p stands for the triple μ, i, j, may be viewed as the q-th component of the p-th vector in h-dimensional space. Then (8.10) means that the scalar product of different vectors vanishes, i.e., vectors with different p's, i.e. different triples μ, i, j, are orthogonal and normalized. In fact, (8.10) is reminiscent of the familiar orthogonality relation for the unit vectors e^α in three-dimensional space:

$$(e^\alpha e^\beta) = \sum_{i=1}^{3} e^\alpha_i e^\beta_i = \delta_{\alpha\beta} \qquad (\alpha, \beta = 1, 2, 3).$$

The total number of orthogonal vectors cannot exceed the dimension h of the space. In the present case the number of vectors $\mathcal{D}_p = \mathcal{D}^\mu_{ij}$, for fixed μ is the square n_μ^2 of the dimension of the representation. Thus the total number of vectors, which equals $\sum_\mu n_\mu^2$, is at most h.

We shall show below that the system of all such vectors is complete in the h-dimensional g_q-space, i.e., their number equals the dimension of the space:

$$\sum_{\mu=1}^{N} n_\mu^2 = h. \tag{8.12}$$

Formula (8.12) is known as Burnside's theorem.

It can also be shown that n_μ always divides the order h of the group:

$$h/n_\mu = m \qquad (\mu = 1, 2, \ldots, N), \tag{8.13}$$

where m is an integer, and N the number of inequivalent irreducible representations.

It follows from (8.12) that the index p in (8.11) runs through h values, i.e., the matrix elements $\mathcal{D}'_{pq}$ form a square matrix $\mathcal{D}'$ of order h. The orthogonality condition (8.10) shows that this matrix has orthogonal rows, i.e., $\tilde{\mathcal{D}}'^{*}\mathcal{D}' = I$. By virtue of (7.9), this implies that $\mathcal{D}'$ is a unitary matrix and so, by (7.10), it also has orthogonal columns, i.e., $\mathcal{D}'^{*}\tilde{\mathcal{D}}' = I$ or, in the notation of (8.10),

$$\sum_\mu \sum_{ij} n_\mu \mathcal{D}^{\mu*}_{ij}(g)\,\mathcal{D}^\mu_{ij}(g') = h\delta_{gg'}. \tag{8.14}$$

Since the actual form of the representation matrices $\mathcal{D}(g)$ depends on the choice of basis functions and is changed by unitary transformations, it is particularly interesting to study the properties of the trace of the matrix $\mathcal{D}(g)$, which is invariant under unitary transformations and is thus the same for all equivalent representations. In group theory the trace is known as the character of g in the representation $\mathcal{D}$, denoted by $\chi(g)$:

$$\chi(g) = \sum_i \mathcal{D}_{ii}(g). \tag{8.15}$$

As we shall show below, the set of characters of all the elements completely determines an irreducible representation. The orthogonality relation (8.10) for elements implies an orthogonality relation for characters. To show this, we set $i = j$ and $k = l$ and sum over i and k:

$$\sum_g \chi_\mu^*(g)\chi_\nu(g) = h\delta_{\mu\nu}. \tag{8.16}$$

This relation implies that in inequivalent irreducible representations, the group elements cannot all have the same characters. It also enables one to check directly whether a given representation $\mathcal{D}$ is irreducible and to determine the irreducible representations contained in $\mathcal{D}$ and how many times they occur there.

By (8.16), for an irreducible representation,

$$\sum_g |\chi(g)|^2 = h. \tag{8.17}$$

If $\mathcal{D}$ is a reducible representation, it follows from (7.14) that each matrix $\mathcal{D}(g)$ may be reduced to block-diagonal form, each submatrix defining an irreducible representation. Consequently, the trace of the matrix $\mathcal{D}(g)$ of a reducible representation, which is invariant under the diagonalizing unitary transformation, is the sum of the traces of the submatrices, i.e., the sum of characters for all irreducible constituents of $\mathcal{D}$:

$$\chi(g) = \sum_\mu N_\mu \chi_\mu(g). \tag{8.18}$$

The coefficient N_μ indicates the number of times the irreducible representation with characters $\chi_\mu(g)$ occurs in $\mathcal{D}$. [This number is called the multiplicity of the irreducible representation.] Knowing $\chi(g)$, we can at once determine N_μ. To this end, multiply (8.18) by $\chi_\mu^*(g)$ and sum both sides over g. In view of (8.16), we obtain

$$N_\mu = \frac{1}{h}\sum \chi_\mu^*(g)\chi(g). \tag{8.19}$$

Formula (8.19) shows that in order to determine the number of irreducible constituents of a given reducible representation, we need only know their characters.

Multiplying equation (8.18) by its conjugate, summing over g and using (8.16), we obtain a relation similar to (8.17) but for reducible representations

$$\sum_g |\chi(g)|^2 = \sum_{\mu\nu} N_\mu N_\nu \sum_g \chi_\mu(g)\chi_\nu^*(g) = h\sum_{\mu\nu} N_\mu N_\nu \delta_{\mu\nu} = h\sum_\mu N_\mu^2. \tag{8.20}$$

It is clear that $\sum_g |\chi(g)|^2$ is always a multiple of h.

We now show that the characters $\chi(g)$ are actually functions of the conjugate class ρ, i.e., all elements g in the same class ρ have the same character χ_ρ.

By definition, g_1 and g_2 are in one class if there exists an element g_3 such that $g_1 = g_3 g_2 g_3^{-1}$. Consequently, by (7.5)

$$\mathcal{D}(g_1) = \mathcal{D}(g_3)\,\mathcal{D}(g_2)\,\mathcal{D}^{-1}(g_3).$$

By (7.13), this implies that $\chi(g_1) = \chi(g_2)$. In equations (8.16)–(8.20), therefore, instead of summing the characters over the group elements g, we may sum them over the classes ρ. Denoting the character of the elements of a class ρ in a representation μ by χ_ρ^μ, we may write the orthogonality relation (8.16) as

$$\sum_{\rho=1}^{N_\rho} h_\rho \chi_\rho^{\mu *} \chi_\rho^\nu = h\delta_{\mu\nu}. \tag{8.21}$$

Here h_ρ is the number of elements in the class ρ and N_ρ the number of classes in the group $\mathcal{G}$.

By (8.19), the number N_μ, which indicates how many times the representation μ occurs in a given representation with characters χ_ρ, is

$$N_\mu = \frac{1}{h}\sum_{\rho=1}^{N_\rho} h_\rho \chi_\rho^{\mu *} \chi_\rho. \tag{8.22}$$

We now use equation (8.14) to prove another orthogonality relation for characters. Set $g = g_1$, $g' = gg_2g^{-1}$ in (8.14) and sum both sides of (8.14) over g. By (7.11) and (8.10), we have

$$\frac{n_\mu}{h}\sum_g \mathcal{D}_{ij}^\mu(gg_2g^{-1}) = \sum_{lk}\mathcal{D}_{lk}^\mu(g_2)\frac{n_\mu}{h}\sum_g \mathcal{D}_{jr}^{\mu *}(g)\,\mathcal{D}_{il}^\mu(g) = \sum_{lk}\mathcal{D}_{lk}^\mu(g_2)\delta_{ij}\delta_{lk} = \chi_\mu(g_2)\delta_{ij},$$

and so the sum is

$$\sum_\mu \frac{n_\mu}{h}\sum_{ij}\sum_g \mathcal{D}_{ij}^{\mu *}(g_1)\mathcal{D}_{ij}^\mu(gg_2g^{-1}) = \sum_{\mu ij}\chi_\mu(g_2)\mathcal{D}_{ij}^{\mu *}(g_1)\delta_{ij} =$$
$$\sum_\mu \chi_\mu^*(g_1)\chi_\mu(g_2) = \sum_\mu \chi_\rho^{\mu *}\chi_\eta^\mu = \sum_g \delta_{g_1,\,gg_2g^{-1}},$$

where ρ is the class of g_1 and η that of g_2.

If g_1 and g_2 are in different classes, then for all g

$$g_1 \neq gg_2g^{-1} \quad \text{and} \quad \sum_g \delta_{g_1,\,gg_2g^{-1}} = 0.$$

If g_1 and g_2 are in the same class, it follows from (1.8) that g_1 occurs h/h_ρ times among the h elements gg_2g^{-1}, and so

$$\sum_g \delta_{g_1,\,gg_2g^{-1}} = \frac{h}{h_\rho}.$$

This means that

$$\sum_\mu \chi_\rho^{\mu *}\chi_\eta^\mu = \frac{h}{h_\rho}\delta_{\rho\eta}. \tag{8.23}$$

The first orthogonality relation (8.21) concerns characters in different irreducible representations and the summation extends over all classes; the second orthogonality relation (8.23) concerns characters of different classes and the summation extends over all irreducible representations. Equation (8.21) shows that the reduced characters

$$\chi'^\mu_\rho = (h_\rho/h)^{1/2}\chi_\rho^\mu \tag{8.24}$$

may be viewed as the ρ-th components of orthonormal vectors χ'_μ in the space of classes ρ, which has dimension N_ρ. The number of orthogonal vectors, which equals the number of irreducible representations N, is at most the dimension N_ρ of the space, $N \leqslant N_\rho$.

On the other hand, by (8.23) these same quantities $\chi'_{\rho,\mu}$ may be viewed as the μ-th components of orthonormal vectors χ'_ρ in the space of irreducible representations μ, which has dimension N. The number of orthogonal vectors which equals the number of classes N_ρ, is at most N, $N_\rho \leqslant N$. It follows that

$$N_\rho = N. \tag{8.25}$$

Consequently, the total number N of irreducible representations of a group $\mathcal{G}$ equals the number N_ρ of conjugate classes of the group.

Formulas (8.21) and (8.23) show that the matrix χ' is both row-orthogonal

$$\tilde{\chi}'^* \chi' = I,$$

and column-orthogonal

$$\chi'^* \tilde{\chi}' = I.$$

As shown above, this implies that χ' is a square matrix, i.e., $N = N_\rho$ * (see (8.25)).

To end this section, we consider the representations of the direct product $\mathcal{G}$ of two groups $\mathcal{G}_1$ and $\mathcal{G}_2$.

The elements of the group $\mathcal{G}$ are products of the form $g = g^{(1)}g^{(2)}(g^{(1)} \in \mathcal{G}_1, g^{(2)} \in \mathcal{G}_2)$. The order of the direct product is $h = h_1 h_2$, where h_1 and h_2 are the orders of $\mathcal{G}_1$ and $\mathcal{G}_2$, respectively.

If the μ-th irreducible representation of the group $\mathcal{G}_1$ has a basis φ^μ_i $(i = 1, 2, \ldots, n_\mu)$, and the ν-th representation of the group $\mathcal{G}_2$ a basis ψ^ν_j $(j = 1, 2, \ldots, n_\nu)$, then the functions $f^{\mu\nu}_{ij} = \varphi^\mu_i \psi^\nu_j$ may serve as a basis for the representations of the group $\mathcal{G}$. Then by (7.3) the elements of the matrices $\mathcal{D}(g^{(1)}g^{(2)})$, which form a representation of the group $\mathcal{G} = \mathcal{G}_1\mathcal{G}_2$, are

$$\mathcal{D}^{\mu\nu}_{ij,\,kl}(g^{(1)}g^{(2)}) = \mathcal{D}^\mu_{ik}(g^{(1)})\,\mathcal{D}^\nu_{jl}(g^{(2)}). \tag{8.26}$$

It is assumed here that the operation $g^{(1)}$ is not applied to the functions ψ of the group $\mathcal{G}_2$ and vice versa, so that the functions ψ and φ are defined in different spaces.

The resulting matrix $\mathcal{D}(g)$ is called the direct or Kronecker product of the matrices and denoted by $\mathcal{D}^{(1)} \times \mathcal{D}^{(2)}$ (not to be confused with the usual matrix product).

By (8.26) the character of an element in this representation is the product of the characters of the corresponding elements in the irreducible representations of $\mathcal{G}_1$ and $\mathcal{G}_2$:

$$\chi_{\mu\nu}(g) = \sum_{ij} \mathcal{D}^{\mu\nu}_{ij,\,ij}(g) = \sum_i \mathcal{D}^\mu_{ii}(g^{(1)}) \sum_j \mathcal{D}^\nu_{jj}(g^{(2)}) = \chi_\mu(g^{(1)})\chi_\nu(g^{(2)}). \tag{8.27}$$

* Formula (8.23) yields an immediate proof of Burnside's theorem (8.12). Indeed, let both ρ and η be the conjugate class of the identity element e, so that $h_\rho = 1$. Since $\chi_\mu(e) = n_\mu$, it follows from (8.23) that $\sum_\mu \eta_\mu \eta_\mu = h$, which is (8.12).

Note, however, that our proof of (8.23) is based on (8.14), which in turn was derived from (8.12). Although (8.23) may be proved without (8.14), the proof is more complicated. In the next section we shall therefore present an independent proof of Burnside's theorem.

The dimension of the representation, $n_{\mu\nu}$, is the product of the dimensions of the component representations, $n_\mu^{(1)} n_\nu^{(2)}$. The representations of the group $\mathcal{G}$ thus obtained are irreducible, for by (8.27) and (8.17)

$$\sum_g |\chi_{\mu\nu}(g)|^2 = \sum_{g^{(1)}} |\chi_\mu(g^{(1)})|^2 \sum_{g^{(2)}} |\chi_\nu(g^{(2)})|^2 = h_1 h_2 = h.$$

By (8.12), the sum of squared dimensions of all the representations is

$$\sum_{\mu\nu} n_{\mu\nu}^2 = \sum_{\mu\nu} n_\mu^2 n_\nu^2 = h_1 h_2 = h,$$

and so it follows via (8.17) that by multiplying together all pairs of irreducible representations of the groups $\mathcal{G}_1$ and $\mathcal{G}_2$ we obtain all the irreducible representations of the group $\mathcal{G}$.

§9. CONSTRUCTION OF BASIS FUNCTIONS OF IRREDUCIBLE REPRESENTATIONS. PRODUCTS OF REPRESENTATIONS

Once we know the matrices of the irreducible representations, we can construct basis functions which transform according to each of the representations. To this end, we choose an arbitrary function $\Phi_1(x)$. Successively applying all operations of the group $\mathcal{G}$,

$$g_1 = e,\ g_2,\ \ldots,\ g_h,$$

we obtain h functions

$$\Phi_i = \mathcal{D}(g_i)\Phi_1(x) = \Phi_1(g_i^{-1}x). \tag{9.1}$$

The function $\Phi(x)$ may be chosen so that all the functions Φ_i are linearly independent. The functions Φ_i are normalized to unity, provided Φ_1 is normalized. The operation g maps each of the h functions $\Phi_i(x)$ onto another function of the set:

$$\mathcal{D}(g)\Phi_i(x) = \mathcal{D}(g)\mathcal{D}(g_i)\Phi_1(x) = \Phi_1(g_i^{-1}g^{-1}x). \tag{9.2}$$

This representation, whose basis consists of h linearly independent functions Φ_i, is called the regular representation of the group.

The matrices of this representation are easily constructed via (9.2), using only the multiplication table of the group. Since $gg_i \neq g_i$, if $g \neq e$, it follows from (9.2) that the operator $\mathcal{D}(g)$ $(g \neq e)$ transforms each of the functions into another function of the set, not equal to Φ_i. Consequently, the matrix of the regular representation $\mathcal{D}(g)$, $g \neq e$, has zero diagonal elements, and the character is

$$\chi(g) = \begin{cases} h & \text{for } g = e, \\ 0 & \text{for } g \neq e. \end{cases} \tag{9.3}$$

In the general case, the regular representation is reducible. In order to determine the multiplicity of a given irreducible representation μ in the regular one, we use (8.19). By (8.19) and (9.3),

$$N_\mu = \frac{1}{h}\chi_\mu^*(e)\chi(e) = \chi_\mu^*(e) = n_\mu. \tag{9.4}$$

Consequently, the multiplicity of any irreducible representation μ in the regular representation is equal to its dimension.

Burnside's theorem follows directly from equation (9.4). In fact, by (9.4) all the basis functions fall into groups of n_μ functions which transform according to the irreducible representation μ, n_μ groups for each representation. Consequently, the total number of basis functions is $\sum_\mu n_\mu^2$. On the other hand, this is precisely the dimension of the regular representation, i.e., the order h of the group. Consequently, $\sum_\mu n_\mu^2 = h$.

Since the regular representation contains all the irreducible representations, we may use the functions Φ_i to construct h functions $\varphi_{mk}^\mu(x)$, forming a basis for each irreducible representation. Here μ indexes the irreducible representations, m ($m = 1, 2, \ldots, n_\mu$) indexes the equivalent μ-representations, and k ($k = 1, 2, \ldots, n_\mu$) indexes the basis functions of the appropriate representation.

We claim that the operator

$$P_{mk}^\mu = \frac{n_\mu}{h} \sum_g \mathcal{D}_{km}^{\mu *}(g)\, \mathcal{D}(g), \tag{9.5}$$

acting on any one of the functions Φ_i, yields the set of functions φ_{mk}^μ. To show this, we check that for fixed μ and m the partner-functions

$$\varphi_{mk}^\mu = P_{mk}^\mu \Phi_1 = \frac{n_\mu}{h} \sum_l \mathcal{D}_{km}^{\mu *}(g_l) \Phi_l \tag{9.6}$$

indeed transform according to the irreducible representation μ. By (9.5), (9.6), (7.4) and (1.2)

$$\begin{aligned} \mathcal{D}(g')\, \varphi_{mk}^\mu &= \frac{n_\mu}{h} \sum_g \mathcal{D}_{km}^{\mu *}(g)\, \mathcal{D}(g'g)\, \Phi_1 = \\ &= \frac{n_\mu}{h} \sum_{g''=g'g} \mathcal{D}_{km}^{\mu *}(g'^{-1}g'')\, \mathcal{D}(g'')\, \Phi_1 = \\ &= \frac{n_\mu}{h} \sum_l \mathcal{D}_{kl}^{\mu *}(g'^{-1}) \sum_{g''} \mathcal{D}_{lm}^{\mu *}(g'')\, \mathcal{D}(g'')\, \Phi_1 = \sum_l \mathcal{D}_{lk}^\mu(g')\, \varphi_{ml}^\mu. \end{aligned} \tag{9.7}$$

Using (8.10), one easily checks that any functions φ_{mk}^μ which form a basis for an irreducible unitary representation are orthogonal in all three indices.

Since the functions Φ_i are linearly independent, i.e., no linear combination of them can vanish, it follows from (9.6) that none of the functions φ_{mk}^μ vanishes and they are linearly independent. Therefore, applying the operators P_{mk}^μ to the functions $\Phi_i = \Phi_1(g_i^{-1}x)$, we obtain the functions $\varphi_{mk,i}^\mu = P_{mk}^\mu \Phi_i$, which represent a superposition of the functions $\varphi_{mk}^\mu = P_{mk}^\mu \Phi_1$ with the same μ and k but different m.

In the general case, however, there is no need to use (9.6) to determine all the functions φ_{mk}^μ. It is sufficient to pick one function for each representation μ, m, say φ_{ml}^μ. Applied to this function, the operator $\mathcal{D}(g)$ yields only functions of this representation, while the same operator applied to Φ_i produces the functions of all the representations. In practice, therefore, it is more convenient to obtain the other partner-functions φ_{mk}^μ by applying the operator P_{lk}^μ to φ_{ml}^μ. By (9.5), (9.7) and (8.10)

$$P^{\mu}_{lk}\varphi^{\mu}_{ml} = \frac{n_\mu}{h}\sum_g \mathcal{D}^{\mu*}_{kl}(g)\,\mathcal{D}(g)\,\varphi^{\mu}_{ml} = \frac{n_\mu}{h}\sum_{gn}\mathcal{D}^{\mu*}_{kl}(g)\,\mathcal{D}^{\mu}_{ln}(g)\,\varphi^{\mu}_{mn} = \sum_n \delta_{kn}\varphi^{\mu}_{mn} = \varphi^{\mu}_{mk}.$$

Consequently,

$$P^{\mu}_{lk}\varphi^{\mu}_{ml} = \varphi^{\mu}_{mk}. \tag{9.8}$$

For example, the operator P^{μ}_{mm} gives the m-th function of the representation μ, m:

$$\varphi^{\mu}_{mm} = P^{\mu}_{mm}\Phi_1 = \frac{n_\mu}{h}\sum_g \mathcal{D}^{\mu*}_{mm}(g)\,\mathcal{D}(g)\,\Phi_1, \tag{9.9}$$

whence the other functions of this representation follow:

$$\varphi^{\mu}_{mk} = P^{\mu}_{mk}\varphi^{\mu}_{mm}. \tag{9.10}$$

The above formulas (9.5)–(9.10) thus enable one to construct all the functions which transform according to any irreducible representation.

However, these equations are useless unless the matrices of the irreducible representations are available, and these are often quite difficult to determine. If only the characters of the representations are given, it follows from (9.9) that application of the operator

$$\mathcal{P}^{\mu} = \sum_m P^{\mu}_{mm} = \frac{n_\mu}{h}\sum_K \chi^{*}_{\mu}(g)\,\mathcal{D}(g) \tag{9.11}$$

to Φ_1 yields a set of functions

$$f^{\mu} = \sum_m \varphi^{\mu}_{mm} = \mathcal{P}^{\mu}\Phi_1, \tag{9.12}$$

which transform according to μ. Only one of the n_μ^2 linearly independent functions is obtained here.

Applying the operators $\mathcal{D}(g)$, $g \in \mathcal{G}$, to the function f^μ or, equivalently, applying the operator $\mathcal{P}^\mu$ to all the functions $\Phi_i = \mathcal{D}(g_i)\Phi_1$, we can obtain from this function f^μ another h functions, of which, however, only n_μ^2 are linearly independent: φ^{μ}_{mk} $(m = 1, 2, \ldots, n_\mu;\ k = 1, 2, \ldots, n_\mu)$, since

$$f^{\mu}(g^{-1}x) = \mathcal{D}(g)\,f^{\mu} = \sum_m \mathcal{D}(g)\,\varphi^{\mu}_{mm} = \sum_{mk}\mathcal{D}^{\mu}_{km}(g)\varphi^{\mu}_{mk}. \tag{9.13}$$

Of course, in order to select the n_μ^2 functions φ^{μ}_{mk} from these h functions $f^\mu(g^{-1}x)$ $(g = g_1, g_2, \ldots, g_h)$, we need all the matrices $\mathcal{D}^{\mu}_{km}(g)$. In simple cases, however, these functions may be selected quite easily and the use of characters shows that they transform according to the required representations.

The above expressions (9.5)–(9.13) are valid regardless of the choice of functions $\Phi_1(x)$. Therefore, using the operators (9.5), (9.9), or (9.11), which are called projection operators, we can determine all the basis functions of the irreducible representations that occur in the representation $\mathcal{D}$ generated by any function $\Phi(x)$.

If the set of functions $\Phi_i = \Phi(g_i^{-1}x)$ includes n' $(n' < h)$ linearly independent functions Φ_j, the representation in question is not regular, and some or all of the irreducible representations μ occur in $\mathcal{D}$ less than n_μ times, or even not at all. Thus some of the functions determined by the operators (9.5) or (9.11) are linearly dependent or zero. If the representation $\mathcal{D}$ does not contain the irreducible representation μ, then for any m and k all the functions φ^{μ}_{mk} and the functions f^μ determined by the operator (9.11) vanish.

If the matrices of the representation $\mathcal{D}(g)$ according to which the functions Φ_j transform are known, the projection operators (9.5) and (9.11) may be written in matrix form:

$$\varphi^{\mu}_{mk} = \sum_j P^{\mu}_{mk,\,j}\Phi_j, \text{ where } P^{\mu}_{mk,\,j} = \frac{n_\mu}{h}\sum_g \mathcal{D}^{\mu *}_{km}(g)\,\mathcal{D}_{jl}(g); \tag{9.14}$$

$$f^{\mu} = \sum_j \mathcal{P}^{\mu}_j \Phi_j, \text{ where } \mathcal{P}^{\mu}_j = \frac{n_\mu}{h}\sum_g \chi_\mu(g)\,\mathcal{D}_{jl}(g). \tag{9.14a}$$

A knowledge of the characters $\chi(g)$ of the representation $\mathcal{D}$ enables one at once, using (8.19) or (8.22), to evaluate the multiplicity of each irreducible representation μ in $\mathcal{D}$, and thus to find the total number $N_\mu n_\mu$ of linearly independent functions φ^{μ}_{mk} for given μ. The total number of linearly independent functions φ^{μ}_{mk} equals the dimension n' of the representation $\mathcal{D}$. Choosing the first $N_\mu n_\mu$ operators P^{μ}_{mk} $(m = 1, 2, \ldots, n_\mu)$ and using (9.14), we obtain the $n_\mu N_\mu$ functions φ^{μ}_{mk}. If some of these functions vanish or are linearly dependent, we must use additional operators P^{μ}_{mk} $(m = N_\mu + 1,\ N_\mu + 2, \ldots)$, until we obtain all the linearly independent functions.

Proceeding in this manner for every representation μ, we find n' linearly independent functions and determine the n' components of the operator $P^{\mu}_{mk,\,j}$, which selects n' functions φ^{μ}_{mk} from the n' functions Φ_j, to form bases of the irreducible representations.

These components of the operator form a square matrix $\boldsymbol{P}$ of order $n' - P_{jq}$, where q stands for the triple index μ, m, k $(q = 1, 2, \ldots, n')$. If these components are appropriately indexed, it follows from (7.12) that the matrix $\boldsymbol{P}$ transforms the matrix $\mathcal{D}$ into $\mathcal{D}' = \boldsymbol{P}^{-1}\mathcal{D}\boldsymbol{P}$, which is in block-diagonal form (7.14).

In practical construction of the basis functions it is often more convenient to begin with simple functions, such as the functions x, y, z, which form a basis for one or more irreducible representations, rather than from a general function $\Phi(x)$ generating the regular representation. The basis functions of the other representations may then be obtained from harmonic polynomials of higher degrees.

A similar problem often arises in other practical applications, when it is necessary to construct functions that transform according to irreducible representations as products of known functions f^{μ}_i $(i = 1, 2, \ldots, n_\mu)$ forming a basis for a representation $\mathcal{D}_\mu$ and functions φ^{ν}_k $(k = 1, 2, \ldots, n_\nu)$ forming a basis for a representation $\mathcal{D}_\nu$. The products $\psi_{ik} = f^{\mu}_i \varphi^{\nu}_k$ form a basis for a representation $\mathcal{D}_{\mu\nu}$ of dimension $n_\mu n_\nu$, which is called the direct product of the representations: $\mathcal{D}_{\mu\nu} = \mathcal{D}_\mu \mathcal{D}_\nu$.

The basis functions ψ_{ik} of this representation carry two indices in order to indicate their origin. Thus the matrix elements of the representation $\mathcal{D}_{\mu\nu}$ carry four indices: $\mathcal{D}^{\mu\nu}_{ik,\,jl}$. By (7.3)

$$\mathcal{D}(g)\psi_{ik} = \sum_{jl}\mathcal{D}^{\mu\nu}_{jl,\,ik}(g)\psi_{jl} = \mathcal{D}(g) f_i \varphi_k = \sum_{jl}\mathcal{D}^{\mu}_{jl}(g) f_j \mathcal{D}^{\nu}_{ik}(g)\varphi_l = \sum_{jl}\mathcal{D}^{\mu}_{jl}(g)\mathcal{D}^{\nu}_{ik}(g)\psi_{jl}.$$

Consequently, the matrices of the direct product $\mathcal{D}_{\mu\nu}$ are the direct (Kronecker) products of the matrices of the representations $\mathcal{D}_\mu$ and $\mathcal{D}_\nu$:

$$\mathcal{D}^{\mu\nu}_{ik,\,jl} = \mathcal{D}^{\mu}_{ij}\mathcal{D}^{\nu}_{kl}, \tag{9.15}$$

and the characters of the direct product are the products of the characters of the constituent representations. Indeed, by (9.15),

$$\chi_{\mu\nu}(g) = \sum_{ik} \mathcal{D}^{\mu\nu}_{ik,\,ik}(g) = \sum_{i} \mathcal{D}^{\mu}_{ii}(g) \sum_{k} \mathcal{D}^{\nu}_{kk}(g),$$

i.e.,

$$\chi_{\mu\nu}(g) = \chi_{\mu}(g)\,\chi_{\nu}(g). \tag{9.16}$$

In general, a direct product of irreducible representations may be reducible. The problem of decomposing a direct product of two or more representations into irreducible representations often arises in physical applications.

Equations (9.16) and (8.19) enable one directly to determine which irreducible representations occur in the direct product. If the functions f_i and φ_k transform according to the same representation, the character of the direct product is

$$\chi_{\mu\mu}(g) = (\chi_{\mu}(g))^2. \tag{9.17}$$

In this case one can use the n_μ^2 functions $\psi_{ik} = f_i\varphi_k$ to define the symmetrized and antisymmetrized functions ψ^s_{ik} and ψ^a_{ik}:

$$\psi^s_{ik} = f_i\varphi_k + f_k\varphi_i \qquad (i = 1, 2, \ldots, n_\mu;\ k = 1, 2, \ldots, i); \tag{9.18}$$

$$\psi^a_{ik} = f_i\varphi_k - f_k\varphi_i \qquad (i = 1, 2, \ldots, n_\mu;\ k = 1, 2, \ldots, i-1). \tag{9.19}$$

As we shall show below, these functions transform independently and form bases for the symmetrized product $[\mathcal{D}^2_\mu]$, whose characters are denoted by $[\chi^2_\mu(g)]$, and the antisymmetrized product $\{\mathcal{D}^2_\mu\}$, whose characters are denoted by $\{\chi^2_\mu(g)\}$, respectively.

Since $\psi^s_{ik} = \psi^s_{ki}$ and $\psi^a_{ik} = -\psi^a_{ki}$, the functions ψ^s_{ik} and ψ^s_{ki} should be treated as one function; the same holds for ψ^a_{ik} and ψ^a_{ki}. The values of the second index for the symmetrized functions should be confined to $k \leqslant i$, and for the antisymmetrized functions to $k < i$, since $\psi^a_{ii} = 0$.

The total number of symmetrized functions is

$$n^s_\mu = \sum_{i=1}^{n_\mu} i = \frac{1}{2}\, n_\mu (n_\mu + 1),$$

and the number of antisymmetrized functions

$$n^a_\mu = \sum_{i=1}^{n_\mu} (i-1) = \frac{1}{2}\, n_\mu (n_\mu - 1).$$

The total number of functions ψ^s_{ik} and ψ^a_{ik} is of course n^2_μ.

By (9.18) and (7.3),

$$\mathcal{D}(g)\,\psi^s_{ik} = \sum_{j=1}^{n_\mu} \sum_{l=1}^{n_\mu} \mathcal{D}_{jl}\mathcal{D}_{lk}\,(f_j\varphi_l + f_l\varphi_j).$$

Since the functions ψ^s_{jl}, $j \neq l$, appear in this sum twice, their coefficients must be combined:

$$\mathcal{D}(g)\,\psi^s_{ik} = \sum_{j=1}^{n_\mu} \left(\sum_{l=1}^{j-1} (\mathcal{D}_{jl}\mathcal{D}_{lk} + \mathcal{D}_{ll}\mathcal{D}_{lk})\,\psi^s_{jl} + \mathcal{D}_{jl}\mathcal{D}_{lk}\psi^s_{jj} \right).$$

Consequently, the matrix elements of the symmetrized product have the form

$$[\mathcal{D}^2_\mu]_{ik,\,jl} = (\mathcal{D}^\mu_{jl}\mathcal{D}^\mu_{ik} + \mathcal{D}^\mu_{il}\mathcal{D}^\mu_{jk})\left(1 - \tfrac{1}{2}\delta_{jl}\right). \tag{9.20}$$

Similarly, for the antisymmetrized product

$$\mathcal{D}(g)\,\psi^a_{ik} = \sum_{j=1}^{n_\mu}\sum_{l=1}^{n_\mu}\mathcal{D}_{jl}\mathcal{D}_{ik}(f_j\varphi_l - f_l\varphi_j) = \sum_{j=1}^{n_\mu}\sum_{l=1}^{j-1}(\mathcal{D}_{jl}\mathcal{D}_{ik} - \mathcal{D}_{il}\mathcal{D}_{jk})\,\psi^a_{jl},$$

i.e.,

$$\{\mathcal{D}^2_\mu\}_{ik,\,jl} = \mathcal{D}^\mu_{jl}\mathcal{D}^\mu_{ik} - \mathcal{D}^\mu_{il}\mathcal{D}^\mu_{jk}. \tag{9.21}$$

Thus the character of the symmetrized product is

$$[\chi^2_\mu(g)] = \sum_{i=1}^{n_\mu}\sum_{k=1}^{i}[\mathcal{D}^2_\mu(g)]_{ik,\,ik} = \sum_{i=1}^{n_\mu}\left(\sum_{k=1}^{i-1}\mathcal{D}^\mu_{il}(g)\,\mathcal{D}^\mu_{kk}(g) + \mathcal{D}^\mu_{kl}(g)\,\mathcal{D}^\mu_{ik}(g)\right) + \mathcal{D}^\mu_{il}(g)\,\mathcal{D}^\mu_{il}(g) =$$

$$= \tfrac{1}{2}\sum_{i=1}^{n_\mu}\sum_{k=1}^{n_\mu}\mathcal{D}^\mu_{il}(g)\,\mathcal{D}^\mu_{kk}(g) + \mathcal{D}^\mu_{kl}(g)\,\mathcal{D}^\mu_{ik}(g) = \tfrac{1}{2}\sum_{i=1}^{n_\mu}\left(\mathcal{D}^\mu_{il}(g)\sum_{k=1}^{n_\mu}\mathcal{D}^\mu_{kk}(g) + \mathcal{D}^\mu_{il}(g^2)\right),$$

whence

$$[\chi^2_\mu(g)] = \tfrac{1}{2}[(\chi_\mu(g))^2 + \chi_\mu(g^2)]. \tag{9.22}$$

Similarly, for the antisymmetrized product

$$\{\chi^2_\mu(g)\} = \tfrac{1}{2}[(\chi_\mu(g))^2 - \chi_\mu(g^2)]. \tag{9.23}$$

Thus, the direct product $\mathcal{D}_\mu \times \mathcal{D}_\mu$ of equal representations, whose characters are defined by (9.16) decomposes in the general case into two representations, the symmetrized and antisymmetrized products, whose characters are defined by (9.22) and (9.23), respectively. These representations may be reducible; the number of irreducible representations occurring in them may be determined with the aid of (8.19), (9.22), and (9.23).

The basis functions of the irreducible constituents of direct products, which are linear combinations of the products $f_i\varphi_i$, may be constructed with the help of the projection operator (9.14) and (9.14a), using expressions (9.15), (9.20), or (9.21) for the matrices of the appropriate products.

In certain applications, one is particularly interested in determining the number of times the identity representation [i.e., the (irreducible) one-dimensional representation defined by mapping each group element onto 1]* occurs in a given reducible representation, and in constructing basis functions which transform according to the identity representation. By the definition of the identity representation, these functions are invariant under all the symmetry operations of the group in question.

By (8.19), (9.5) and (9.14), the number of times the identity representation occurs in a representation with characters $\chi(g)$ is

$$N_0 = \frac{1}{h}\sum_g \chi(g), \tag{9.24}$$

* [The Russian term used here has been rendered "unit representation" in previous translations of the Russian literature (see, e.g., M.A.Naimark, Linear Representations of the Lorentz Group, New York, Pergamon Press, 1964, and the English translation of /I.7/). This is apparently in order to avoid confusion with (reducible) identity representations of dimension higher than one. Our usage follows W.Miller, Symmetry Groups and their Applications, New York, Academic Press, 1972, p. 78.– Trans. editor.]

and its basis functions of the representation are

$$\psi^0 = \frac{1}{h}\sum_g \mathcal{D}(g)\,\varphi_l = \frac{1}{h}\sum_g \sum_k \mathcal{D}_{kl}(g)\,\varphi_k, \tag{9.25}$$

where $\varphi_i(x)$ is any function appearing in a basis of the given reducible representation.

In particular, by (9.4) the regular representation contains the identity representation exactly once, and the invariant function ψ^0 is

$$\psi^0 = \frac{1}{h}\sum_g \mathcal{D}(g)\,\Phi_1(x) = \frac{1}{h}\sum_i \Phi_i(x). \tag{9.26}$$

We now consider a direct product $\mathcal{D}_\mu \times \mathcal{D}_\nu$. By (9.24) and (9.16), the product contains the identity representation if

$$N_0 = \frac{1}{h}\sum_g \chi_\mu(g)\,\chi_\nu(g) \neq 0.$$

On the other hand, by the orthogonality relation (8.16),

$$\frac{1}{h}\sum_g \chi_\mu^*(g)\,\chi_\nu(g) = \delta_{\mu\nu}.$$

We may treat χ_μ^* as the character of the representation $\mathcal{D}_\mu^*$, the complex conjugate of $\mathcal{D}_\mu$. We see from (7.3) that, if the matrices $\mathcal{D}(g)$ form an irreducible representation whose basis is the set of functions φ_i, the complex conjugate matrices $\mathcal{D}^*(g)$ also form an irreducible representation, whose basis is the set of functions φ_i^*.

Consequently, the identity representation occurs only in a direct product of mutually conjugate representations, $\chi_\mu^* = \chi^\nu$.

If the representation has real characters, $\chi_\mu^*(g) = \chi_\mu(g)$, the conjugate representations $\mathcal{D}$ and $\mathcal{D}^*$ are equivalent, i.e., $\mathcal{D}$ may be transformed into $\mathcal{D}^*$ by a unitary transformation (7.12). Under these conditions, if in addition the basis functions φ_i, and accordingly all the matrices $\mathcal{D}(g)$, can be made real by a unitary transformation, we shall say that the representation is real. If the character of the representation is real but its matrices $\mathcal{D}(g)$ are essentially complex, in the sense that no unitary transformation can make them real, we shall say that the representations $\mathcal{D}$ and $\mathcal{D}^*$ are complex equivalent. Representations $\mathcal{D}$ and $\mathcal{D}^*$ with complex characters are complex inequivalent.

Consequently, for complex inequivalent representations we can form an invariant function only from the product of basis functions φ_i and φ_i^* for the conjugate representations $\mathcal{D}$ and $\mathcal{D}^*$, and this function is unique. By (9.25), (9.15) and (8.9) the function is

$$\begin{aligned}\psi^0 = \frac{1}{h}\sum_g \mathcal{D}_{ik,\,ll}(g)\,\varphi_i^*\varphi_k = \frac{1}{h}\sum_g \sum_{ik} \mathcal{D}_{ll}^{\mu *}(g)\,\mathcal{D}_{kl}^{\mu}\varphi_i^*\varphi_k = \\ = \frac{1}{n_\mu}\sum_{ik}\delta_{ik}\delta_{ll}\varphi_i^*\varphi_k = \frac{1}{n_\mu}\sum_i \varphi_i^*\varphi_i.\end{aligned} \tag{9.27}$$

For equivalent representations, we may form an invariant function from the product of basis functions of one representation. This function coincides in form with (9.27), but now the functions φ_i^* depend linearly on φ_j via a unitary transformation T. Thus, for real representations with $\varphi_i^* = \varphi_i$,

$$\psi^0 = \frac{1}{n_\mu}\sum_i \varphi_i^2. \tag{9.28}$$

As we shall show below (see (18.27)), for real representations

$$\frac{1}{h}\sum_g \chi(g^2) = 1$$

and so, by (9.22) and (8.17),

$$\frac{1}{h}\sum_g [\chi_\mu^2(g)] = 1,$$

i.e., by (9.24), for real representations the symmetrized product, whose basis includes the functions φ_i^2, indeed contains the identity representation. By (18.27), for complex equivalent representations,

$$\frac{1}{h}\sum_g \chi(g^2) = -1,$$

so that, by (9.23) and (8.17),

$$\frac{1}{h}\sum_g \{\chi_\mu^2(g)\} = 1,$$

Thus, for complex equivalent representations, the identity representation whose basis is the function (9.27) occurs in the antisymmetrized product.

§10. REPRESENTATIONS OF THE FULL ROTATION GROUP

In this section we shall briefly discuss the representations of the full rotation group.

It can be shown that, as in the case of finite groups, every representation of the full rotation group is equivalent to a unitary representation. Since a rotation φ is defined by three parameters φ_x, φ_y, φ_z, each representation $\mathcal{D}(\varphi) = \mathcal{D}(\varphi_x, \varphi_y, \varphi_z)$ is also a function of these parameters.*

We shall show that all the matrices of any representation $\mathcal{D}(\varphi)$, where φ runs through all finite rotations, are completely determined by the matrices of the representation for infinitesimal rotations φ.

Expand $\mathcal{D}(\varphi_x, \varphi_y, \varphi_z)$ as a Taylor series in φ_i. Then, since $\mathcal{D}(0, 0, 0) = \mathcal{D}(0) = \tilde{I}$, it follows that up to second order terms in φ_i:

$$\mathcal{D}(\varphi_x, \varphi_y, \varphi_z) = I + i(A_x\varphi_x + A_y\varphi_y + A_z\varphi_z) = I + i(\mathbf{A}\boldsymbol{\varphi}), \tag{10.1}$$

where

$$A_x = \frac{1}{i}\frac{\partial \mathcal{D}}{\partial \varphi_x}\Big|_0, \quad A_y = \frac{1}{i}\frac{\partial \mathcal{D}}{\partial \varphi_y}\Big|_0, \quad A_z = \frac{1}{i}\frac{\partial \mathcal{D}}{\partial \varphi_z}\Big|_0 \tag{10.2}$$

are infinitesimal rotation matrices, i.e., matrices of the representation $\mathcal{D}$ for rotations through small angles about the x-, y- and z-axes, respectively.

Consider two rotations $s\varphi$ and $t\varphi$, where s and t are arbitrary numbers. The product of $s\varphi$ and $t\varphi$ is the rotation $(s+t)\varphi$. Consequently, the matrices

* By the derivative $\frac{\partial \mathcal{D}}{\partial \varphi_s}$ we mean the matrix $\left(\frac{\partial \mathcal{D}}{\partial \varphi_s}\right)_{ik} = \frac{\partial \mathcal{D}_{ik}}{\partial \varphi_s}$ whose elements are the derivatives of the elements of $\mathcal{D}$ with respect to φ_s.

of the representation $\mathcal{D}$ must satisfy the relation

$$\mathcal{D}((s+t)\varphi_x,\ (s+t)\varphi_y,\ (s+t)\varphi_z) = \mathcal{D}(s\varphi_x,\ s\varphi_y,\ s\varphi_z)\,\mathcal{D}(t\varphi_x,\ t\varphi_y,\ t\varphi_z).$$

Differentiating this equality with respect to s and setting $s=0$, we obtain a differential equation for the matrix $\mathcal{D}(t\varphi)$:

$$\frac{d}{ds}\mathcal{D}((s+t)\varphi)\Big|_{s=0} = \frac{d}{dt}\mathcal{D}(t\varphi) = \mathcal{D}(t\varphi)\frac{d\mathcal{D}}{ds}(s\varphi)\Big|_{s=0},$$

whence, by (10.2), it follows that

$$\frac{d}{dt}\mathcal{D}(t\varphi) = i\mathcal{D}(t\varphi)(A_x\varphi_x + A_y\varphi_y + A_z\varphi_z) = i\mathcal{D}(t\varphi)(A\varphi). \tag{10.3}$$

The matrices $\mathcal{D}(t\varphi)$ satisfy the boundary condition

$$\mathcal{D}(t\varphi)_{t=0} = \mathcal{D}(0) = I. \tag{10.4}$$

System (10.3) with boundary condition (10.4) has the solution

$$\mathcal{D}(t\varphi) = e^{it(A\varphi)} = e^{it(A_x\varphi_x + A_y\varphi_y + A_z\varphi_z)}, \tag{10.5}$$

and when $t=1$ we obtain an expression for $\mathcal{D}(\varphi)$ in terms of the infinitesimal rotation matrices A_x, A_y, A_z:

$$\mathcal{D}(\varphi) = e^{i(A_x\varphi_x + A_y\varphi_y + A_z\varphi_z)} = e^{i(A\varphi)}. \tag{10.6}$$

Thus, determination of the representation $\mathcal{D}(\varphi)$ reduces to determination of the matrices of an infinitesimal rotation A_x, A_y, A_z.

We now consider a few properties of infinitesimal rotation matrices. The matrices of the representation $\mathcal{D}$ for any rotations φ_1 and φ_2 satisfy the relation

$$\mathcal{D}(\varphi_1)\mathcal{D}(\varphi_2)\mathcal{D}^{-1}(\varphi_1) = \mathcal{D}(\varphi_1\varphi_2\varphi_1^{-1}). \tag{10.7}$$

It follows from (2.1) that $\varphi_1\varphi_2\varphi_1^{-1}$ is a rotation through φ_2 about the axis $\varphi_3 = \mathcal{R}(\varphi_1)\varphi_2$, which is the image of the axis φ_2 under the rotation φ_1. If φ_2 is an infinitesimal rotation, then $\varphi_1\varphi_2\varphi_1^{-1}$ is also an infinitesimal rotation. Using (10.1), we find from (10.7) that

$$\mathcal{D}(\varphi_1)(A\varphi_2)\mathcal{D}^{-1}(\varphi_1) = (A(\varphi_1\varphi_2\varphi_1^{-1})). \tag{10.8}$$

Formula (10.8) was obtained for small φ_2, but it can be shown to hold for arbitrary φ_2.

By (2.23), $\varphi_1\varphi_2\varphi_1^{-1} = \varphi_3 = \mathcal{R}(\varphi_1)\varphi_2$ or, in component notation, $(\varphi_3)_l = \sum_s \mathcal{R}_{ls}(\varphi_1)(\varphi_2)_s$, where $\mathcal{R}(\varphi_1)$ is the matrix of a transformation applied to vectors in a fixed coordinate system. Substituting these expressions into the right side of (10.8), we see that the matrix A with components A_x, A_y, A_z transforms in the same manner as a fixed vector x, y, z in a moving coordinate system:

$$\mathcal{D}(\varphi_1)A\mathcal{D}^{-1}(\varphi_1) = \mathcal{R}(\varphi_1^{-1})A \tag{10.9}$$

or

$$\mathcal{D}(\varphi_1)A_l\mathcal{D}^{-1}(\varphi_1) = \sum_s \mathcal{R}_{ls}(\varphi_1^{-1})A_s = \sum_s \mathcal{R}_{sl}(\varphi_1)A_s.$$

From (10.9) we can obtain commutation relations for the matrices A_x, A_y, A_z. Let φ_1 be a rotation about the x-axis through a small angle φ_x. According

to (4.2),

$$\mathscr{R}(\varphi_x)=\begin{Vmatrix} 1 & 0 & 0 \\ 0 & 1 & \varphi_x \\ 0 & -\varphi_x & 1 \end{Vmatrix}. \tag{10.10}$$

Setting $A = A_y$ in (10.9), we obtain

$$(1+i\varphi_x A_x)A_y(1-i\varphi_x A_x)=A_y+i\varphi_x(A_xA_y-A_yA_x)=A_y-\varphi_x A_z,$$

from which follows the commutation relation for A_x and A_y:

$$A_xA_y-A_yA_x=iA_z.$$

In a similar manner one obtains commutation relations for the other infinitesimal rotation matrices, similar in form to (4.5):

$$A_xA_y-A_yA_x=iA_z,\quad A_xA_z-A_zA_x=iA_y,\quad A_yA_z-A_zA_y=iA_x. \tag{10.11}$$

Formulas (10.11) were obtained using only properties of rotations and are therefore valid for infinitesimal rotation operators for all representations.

The unitarity condition for small rotations φ

$$\mathscr{D}(\varphi)\mathscr{D}^+(\varphi)=(1+i(A\varphi))(1-i(A^+\varphi))=I$$

implies

$$A=A^+, \tag{10.12}$$

i.e., the matrices A are hermitian. By virtue of condition (10.12), the representation $\mathscr{D}(\varphi)$ (10.6) is unitary for any finite angle φ.

Instead of the matrices A_x, A_y, A_z it is sometimes more convenient to introduce the matrices $A_3 = A_z$ and $A_\pm = A_x \pm iA_y$, which, according to (10.11), satisfy the following commutation relations:

$$\begin{gathered} A_+A_3-A_3A_+=-A_+,\quad A_-A_3-A_3A_-=A_-, \\ A_+A_--A_-A_+=2A_3. \end{gathered} \tag{10.13}$$

All infinitesimal rotation matrices, and consequently all different irreducible representations of the full rotation group, may be constructed effectively with the aid of the commutation relations (10.11) or (10.13). It can moreover be shown that every irreducible representation $\mathscr{D}_j$ of the full rotation group is characterized by an index j, which runs through all integer and half-integer values:

$$j=0,\quad 1/2,\quad 1,\quad 3/2,\quad 2,\ \ldots, \tag{10.14}$$

and is called the weight of the representation $\mathscr{D}_j$. The dimension of the representation $\mathscr{D}_j$ is $2j+1$. Thus, the full rotation group may have representations of all dimensions.

By (10.6), the representation $\mathscr{D}_j(\varphi)$ is fully determined by matrices A_x^j, A_y^j, A_z^j. As a basis of the representation $\mathscr{D}_j(\varphi)$ we take the eigenvectors Y_m^j of the matrix A_3^j, which satisfy the relations (see /I.7, I.8/)

$$\begin{aligned} A_3^jY_m^j &= mY_m^j, \\ A_+^jY_m^j &= \sqrt{(j+m+1)(j-m)}\,Y_{m+1}^j, \\ A_-^jY_m^j &= \sqrt{(j+m)(j-m+1)}\,Y_{m-1}^j, \end{aligned} \tag{10.15}$$

where m runs through the $2j+1$ values

$$m = -j,\ -j+1,\ -j+2,\ \ldots,\ j-1,\ j. \tag{10.16}$$

If j is an integer (half-integer), then m is also an integer (half-integer).

It follows from (10.15) that, relative to the basis we have chosen, the matrix elements of A_3^j, A_+^j, A_-^j are:

$$\begin{aligned} (A_3^j)_{m'm} &= m\delta_{mm'}, \\ (A_+^j)_{m'm} &= \sqrt{(j+m+1)(j-m)}\,\delta_{m+1,\,m'}, \\ (A_-^j)_{m'm} &= \sqrt{(j+m)(j-m+1)}\,\delta_{m-1,\,m'}. \end{aligned} \tag{10.17}$$

It is easily shown that

$$(A^2)_{mm'} = \left(A_x^{j^2} + A_y^{j^2} + A_z^{j^2}\right)_{mm'} = j(j+1)\,\delta_{mm'}. \tag{10.18}$$

Formulas (10.15) and (10.17) are valid for the special basis chosen above, which is known as a canonical basis. When one transforms to any other equivalent basis using linear combinations (7.8) of the functions Y_m^j, the infinitesimal rotation matrices A^j transform according to (7.12). The infinitesimal rotation matrices (10.17) completely determine the matrix of the representation $\mathcal{D}(\varphi)$ for arbitrary rotation angles φ, as shown by (10.6). Thus, the matrix $\mathcal{D}_j(\varphi)$ for a rotation about the z-axis through the angle φ is, by (10.6) and (10.17),

$$\mathcal{D}_j(\varphi) = \begin{Vmatrix} e^{ij\varphi} & 0 & 0 & \ldots & 0 \\ 0 & e^{i(j-1)\varphi} & 0 & \ldots & 0 \\ 0 & 0 & e^{i(j-2)\varphi} & \ldots & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & 0 & 0 & \ldots & e^{-ij\varphi} \end{Vmatrix}. \tag{10.19}$$

From (10.19) we easily obtain the character $\chi_j(\varphi)$ of the representation $\mathcal{D}_j$:

$$\chi_j(\varphi) = \sum_m \mathcal{D}_{j,\,mm}(\varphi) = \sum_{m=-j}^{m=j} e^{im\varphi} = \frac{\sin(j+1/2)\,\varphi}{\sin\frac{\varphi}{2}}. \tag{10.20}$$

The direct product of irreducible representations $\mathcal{D}_{j_1} \times \mathcal{D}_{j_2}$ is a $(2j_1+1)\times(2j_2+1)$-dimensional representation of the full rotation group. It is generally reducible. In fact, each irreducible representation with weight ranging from j_1+j_2 to $|j_1-j_2|$ occurs exactly once in $\mathcal{D}_{j_1}\times\mathcal{D}_{j_2}$:

$$\mathcal{D}_{j_1} \times \mathcal{D}_{j_2} = \sum_{\mu=|j_1-j_2|}^{j_1+j_2} \mathcal{D}_\mu. \tag{10.21}$$

Formula (10.21) is easily verified by observing that for small φ the character $\chi_j(\varphi) = 2j+1$ equals the dimension of the representation $\mathcal{D}_j$. Then, in view of the identity

$$(2j_1+1)(2j_2+1) = \sum_{\mu=|j_1-j_2|}^{j_1+j_2} (2\mu+1),$$

we obtain

$$\chi_{j_1\times j_2} = \sum_{\mu=|j_1-j_2|}^{j_1+j_2} \chi_\mu,$$

which is just (10.21).

It follows from (10.21) that the product of two representations with half-integer weights decomposes into representations with integer weights. The direct product $\mathcal{D}_{j_1} \times \mathcal{D}_{j_2}$ contains the identity representation if and only if $j_1 = j_2$.

Let us decompose the direct product $\mathcal{D}_j \times \mathcal{D}_j$ into the symmetrized and antisymmetrized products:

$$\mathcal{D}_j \times \mathcal{D}_j = [\mathcal{D}_j \times \mathcal{D}_j] + \{\mathcal{D}_j \times \mathcal{D}_j\}. \tag{10.22}$$

By (9.23), the character of the antisymmetrized product

$$\{\chi_j^2\} = \tfrac{1}{2}[\chi_j^2(\varphi) - \chi_j(2\varphi)]$$

is for small values of φ equal to $2j+1)j$. Hence we can show that the antisymmetrized product of $\mathcal{D}_j$ and $\mathcal{D}_j$ decomposes as follows:

$$\{\mathcal{D}_j \times \mathcal{D}_j\} = \begin{cases} \mathcal{D}_{2j-1} + \mathcal{D}_{2j-3} + \mathcal{D}_{2j-5} + \ldots + \mathcal{D}_1 & \text{for integer } j, \\ \mathcal{D}_{2j-1} + \mathcal{D}_{2j-3} + \mathcal{D}_{2j-5} + \ldots + \mathcal{D}_0 & \text{for half-integer } j. \end{cases} \tag{10.23}$$

For example, when j is an integer the sum of characters on the right of (10.23) is

$$\chi_{2j-1} + \chi_{2j-3} + \ldots + \chi_1 = 2(2j-1) + 1 + 2(2j-3) + 1 + \ldots + 1 = (2j+1)j,$$

which is $\{\chi_j^2\}$.

It follows from (10.21)–(10.23) that

$$[\mathcal{D}_j \times \mathcal{D}_j] = \begin{cases} \mathcal{D}_{2j} + \mathcal{D}_{2j-2} + \ldots + \mathcal{D}_0 & \text{for integer } j, \\ \mathcal{D}_{2j} + \mathcal{D}_{2j-2} + \ldots + \mathcal{D}_1 & \text{for half-integer } j. \end{cases} \tag{10.24}$$

Thus, the identity representation occurs in the symmetrized direct product of representations with integer weight and in the antisymmetrized product of representations with half-integer weight j.

The matrices of the representation $\mathcal{D}_j$ for integer j are single-valued functions of the rotation angle φ. As we see, for example, from (10.19), rotations φ and $\varphi + 2\pi$ are associated with the same matrix $\mathcal{D}_j$. Therefore, the basis functions Y_m^j with integer j may be constructed from single-valued functions of the coordinates, and the representation matrices $\boldsymbol{A}_x^j$, $\boldsymbol{A}_y^j$, $\boldsymbol{A}_z^j$ (integer j) are, as follows from (4.3), (4.5), (4.6) and (10.11), (10.6), (10.1), the matrices of the angular momentum operators L_x, L_y, L_z relative to this basis, in the representation for which L_z is diagonal.

If $j = 0$, any function $\mathcal{F}$ which depends only on the absolute value of the radius vector $\mathcal{F}(|\boldsymbol{x}|)$ generates a one-dimensional (scalar) representation of the full rotation group, since it obviously remains invariant under every space rotation.

If $j = 1$, the canonical basis Y_1^1, Y_{-1}^1, Y_0^1 for the representation $\mathcal{D}_1$ may be constructed as linear combinations of the three components x, y, z of the vector $\boldsymbol{x}$:

$$Y_0^1 = iz, \quad Y_1^1 = -i\frac{x+iy}{\sqrt{2}}, \quad Y_{-1}^1 = i\frac{x-iy}{\sqrt{2}}. \tag{10.25}$$

Using (10.21), we can successively construct basis functions for all the irreducible representations $\mathcal{D}_j$ with integer j, as products of different functions (10.25) corresponding to the vector representation $\mathcal{D}_1$.

Representations $\mathcal{D}_j$ with half-integer j form a special case, for, as is evident from (10.19), rotations φ and $\varphi+2\pi$ correspond to two matrices differing only in sign. Therefore, representations $\mathcal{D}_j$ with half-integer j are double-valued rather than single-valued functions and so, strictly speaking, are not representations of the full rotation group in the usual sense.

If we associate the two matrices $\pm\mathcal{D}_j(\varphi)$ with each rotation φ, each pair of matrices $\pm\mathcal{D}_j(\varphi)$ forms what is known as a "double-valued" representation of the full rotation group.

The non-uniqueness of representations $\mathcal{D}_j$ with half-integer weight j is due to the fact that the above representations $\mathcal{D}_j(\varphi)$ are in fact ordinary (single-valued) representations of the unitary group $\mathcal{U}$ (see §4), which is homomorphic to the full rotation group $\mathcal{K}$. If the representations of $\mathcal{U}$, which is known as the representation group for the full rotation group, are viewed as representations of the full rotation group, one obtains on the one hand the (single-valued) representations of the spherical group – the representations $\mathcal{D}_j$ with integer j, and on the other the double-valued representations $\mathcal{D}_j$ with half-integer j.

Let us consider the case $j=1/2$ in greater detail. From equation (10.17) we easily find the infinitesimal rotation matrices $A_x^{1/2}$, $A_y^{1/2}$, $A_z^{1/2}$ of the representation $\mathcal{D}_{1/2}$. Up to a factor $1/2$, these are simply the Pauli matrices introduced earlier:

$$A_x^{1/2}=\sigma_x/2,\quad A_y^{1/2}=\sigma_y/2,\quad A_z^{1/2}=\sigma_z/2, \tag{10.26}$$

so that the matrix of the representation $\mathcal{D}_{1/2}$ coincides with the matrix u of (4.12), which is an element of the group $\mathcal{U}$ and describes the motion of the $\xi\eta$-plane under a rotation of the sphere. The basis functions $Y_{1/2}^{1/2}$ and $Y_{-1/2}^{1/2}$ for the representation $\mathcal{D}_{1/2}$, which by (7.3) transform into each other under rotations:

$$\mathcal{D}(\varphi)\,Y_m^{1/2}=\sum_{m=-1/2}^{m=1/2}(\mathcal{D}_{1/2}(\varphi))_{m'm}\,Y_{m'}^{1/2}, \tag{10.27}$$

are called spinors of rank $1/2$, or simply spinors. They are not single-valued functions of the coordinates, and generate an ordinary representation of the group $\mathcal{U}$ and a double-valued representation of the full rotation group.

It follows from (10.21) that, using products of different numbers of spinors, we can construct representations of the full rotation group for any j. The product of an odd number of spinors decomposes into half-integer representations, and the product of an even number of spinors will yield representations of any dimension corresponding to integer weight.

Each element of the orthogonal group is the product of inversion and a rotation.

Since inversion commutes with every rotation, the total number of representations of the orthogonal group is twice the number of representations of the full rotation group, and each representations $\mathcal{D}_j$ with weight j may be either even or odd, according as the matrix $\mathcal{D}_j$ does or does not change sign under inversion.

Scalar quantities which transform according to the representation $\mathcal{D}_0$ under rotations and do not change sign under inversion are called pure scalars. A scalar that changes sign under inversion is called a pseudoscalar.

Quantities that transform according to the representation $\mathcal{D}_1$ and do not change sign under inversion are called pseudovectors.

§11. REPRESENTATIONS OF THE POINT GROUPS

In §3 we considered the various point groups and divided their elements into classes. Using the properties of irreducible representations, one can determine the characters of all irreducible representations of a point group without explicitly finding the representations themselves. As shown in §8, the number of irreducible representations is equal to the number of classes, their dimensions n_μ are divisors of the order h of the group, and the sum of squares of the dimensions of all the representations, $\sum_\mu n_\mu^2$, is equal to h. The set of irreducible representations always includes the (one-dimensional) identity representation (the representation in which the characters of all the elements equal unity). These requirements uniquely determine the dimensions of all the representations of any given point group, and the orthogonality and normalization conditions (8.21) and (8.23) uniquely determine their characters.

A useful fact here is that the characters of mutually inverse elements are related by

$$\chi(g^{-1}) = \chi^*(g), \tag{11.1}$$

as follows directly from the unitarity of the matrices (7.11). Therefore, if g and g^{-1} are in one class the characters of the class are real, while if they appear in different classes the characters of these classes are complex conjugates.

For many groups determination of the irreducible representations may be considerably simplified by using the theorem proved in §7 to the effect that the representations of a group contain the representations of all factor groups of the group relative to its invariant subgroups.

In determining representations of point groups, we restrict ourselves to groups containing twofold, threefold, fourfold, and sixfold rotation or improper rotation axes, since only such groups may be crystallographic point groups. All the [irreducible] representations of these groups are given in Table 11.1 at the end of this section. Following /I.7/, we denote one-dimensional representations in the table by the symbols A and B, depending on whether the representation is respectively invariant under rotation about the principal axis (the z-axis), i.e., $\chi(c_\varphi) = 1$, or noninvariant, $\chi(c_\varphi) \neq 1$. Two-dimensional representations are denoted by the symbol E, and three-dimensional representations by F. For direct products of the groups C_i or C_s with any group not containing a second order transformation, representations which are even relative to i or σ_h are provided with a plus sign, odd ones with a minus sign.

We now show how these representations and their characters are determined.

Cyclic groups C_n and S_n. Since these groups are abelian, the number of classes equals the number of elements, n, and all the representations are one-dimensional, i.e., the characters $\chi(g)$ coincide with the representation matrices $\mathcal{D}(g)$. Therefore, $\chi^n(c_n) = \chi(c_n^n) = \chi(e) = 1$, and for these groups

$$\chi(c_n^k) = e^{\frac{2\pi i M}{n} k}, \tag{11.2}$$

where M is an integer. Setting $M = 0, 1, 2, \ldots, n-1$, we obtain all n representations. Representations with $M = r$ and $M = h - r$ are complex conjugate pairs.

Similarly, for the groups S_{2n}, which are isomorphic to the groups C_{2n},

$$\chi(S_{2n}^k) = e^{\frac{\pi i M}{n} k}. \tag{11.3}$$

Groups C_s and $C_i = S_2$ are isomorphic to C_2, so that, like the latter, they have two one-dimensional representations. For direct products of two groups (the second group is usually C_i, C_s or C_2) the representations and their characters are determined (see (8.27)) by multiplying the characters of the factors, and the total number of representations is the product of the number of representations of the factors.

Thus, we may at once determine the characters for representations of $C_{nh} = C_n \times C_s$ and $S_{4p+2} = C_{2p+1} \times C_i$, $C_{4p+2} = C_{2p+1} \times C_2$, such as the groups $S_6 = C_3 \times C_i$, $C_6 = C_3 \times C_2$.

Since all the representations of the original groups are one-dimensional, these groups also have only one-dimensional representations.

Groups C_{2v} and $D_2 = V$ are isomorphic to the group $C_{2h} = C_2 \times C_s = C_2 \times C_i$ and have the same representations. Actually, these groups are also direct products $C_{2v} = C_s \times C_2'$, $D_2 = C_2 \times C_2'$. The axis c_2' in the group C_{2v}, as opposed to C_{2h}, lies in the plane σ, and the axes c_2 and c_2' in D_2 are perpendicular.

Group C_{3v}. As opposed to all the groups considered above, the group C_{3v} is noncommutative. It has six elements, distributed over three classes, and so there are three representations. We see at once from condition (8.12) that two of the representations are one-dimensional and one two-dimensional. By (11.1), all the representations are real, i.e., the characters in the one-dimensional representations may equal ± 1. It follows at once from the orthogonality condition for the characters of the one-dimensional representations A_1 and A_2 that, for A_2, $\chi(e) = \chi(c_3) = 1$, and $\chi(\sigma_v) = -1$. For the remaining two-dimensional representation E, $\chi(e) = 2$, and the column-orthogonality condition (8.23) at once gives $\chi(c_3) = -1$, $\chi(\sigma_v) = 0$.

Group D_3 is isomorphic to C_{3v} and has the same representations.

Group C_{4v} contains eight elements in five classes. Hence it has five representations, one of them two-dimensional, and all the representations are real. The row-orthogonality condition (8.21) implies that for the three nonidentity one-dimensional representations A_2, B_1 and B_2 the characters of two out of the three classes c_4, σ_v, σ_v' must be -1, while for the remaining classes, including one of these three, we have $\chi = 1$. This immediately yields the characters of all the one-dimensional representations.

Note that the factor group of the group C_{4v} relative to its invariant subgroup C_2, which consists of the elements e and c_2, contains four elements, the cosets eC_2, c_4C_2, σ_vC_2, $\sigma_v'C_2$. This group is isomorphic to C_{2v}. Thus the four one-dimensional representations of C_{4v} coincide with the representations of C_{2v}, and elements in the same coset have the same characters.

The characters of the two-dimensional representation E are determined at once from the column-orthogonality condition. Since the columns corresponding to the classes c_4, σ_v, σ_v' are orthogonal to the column of the class e without the last representation E, it follows that their characters in the representation E are $\chi = 0$, and the characters of the class c_2 are $\chi(c_2) = -\chi(e) = -2$.

Groups D_4 and D_{2d} are isomorphic to the group C_{4v}, and their representation coincide.

The characters of the representations of $D_{2h} = D_2 \times C_i$ and $D_{4h} = D_{2d} \times C_i$ are determined by multiplying through the characters of the appropriate groups.

In a similar manner we determine the characters of the representations of the group $D_{3d} = C_{3v} \times C_i$ and its isomorphic images $D_{3h} = D_3 \times C_s$, $C_{6v} = C_{3v} \times C_2$ and $D_6 = D_3 \times C_2$.

Knowing the characters of the group D_6, we can at once determine the characters of the representations of $D_{6h} = D_6 \times C_i = D_3 \times C_{2h}$.

Group T contains twelve elements in four classes, so that by (8.12) it has three one-dimensional representations and one three-dimensional representation. The subgroup D_2 of this group is invariant. The corresponding factor group contains three elements, the cosets eD_2, c_3D_2, $c_3^2D_2$, and is isomorphic to C_3. Thus the three one-dimensional representations of T coincide with the representations of C_3.

The characters of the classes e and c_2 in these representations coincide. The column-orthogonality condition at once yields the character of the three-dimensional representation F. Since the columns corresponding to the classes c_3 and c_3^2 are orthogonal to the column of the class e without this representation, it follows that their characters in the representation F are equal to $\chi = 0$, while the characters of the class c_2 are $\chi(c_2) = -\frac{1}{3}\chi(e) = -1$. Knowing the characters of the representations of the group T, we may at once determine the characters of the representations of $T_h = T \times C_i$, which has four even and four odd representations.

The characters of the representations of the group O are found in the same way as for the group T. The factor group of O by its invariant subgroup D_2, which includes the elements e and $3c_2$, contains six cosets, each having four elements: $eD_2 = D_2$, c_3D_2, $c_3'D_2$, u_2D_2, $u_2'D_2$, $u_2''D_2$. This group is isomorphic to D_3. Thus the characters of two one-dimensional representations and one two-dimensional representation of O coincide with the characters of the corresponding classes of the group D_3. The total number of elements in this group is 24, the number of classes 5. Consequently, the sum of squared dimensions of the remaining two representations is $24 - 6 = 18$, so that these representations are three-dimensional. By (11.1), the characters of all the representations are real.

Let us denote the characters of the classes c_3, c_2, u_2, c_4 in each of these representations by a_1, b_1, c_1, d_1 and a_2, b_2, c_2, d_2, respectively. The orthogonality condition for characters yields three equations, from which we get $a_i = 0$, $b_i = -1$, $c_i = -d_i$. Next we find from the orthogonality of the characters of both three-dimensional representations that $d_1d_2 = c_1c_2 = -1$, while the normalization condition (8.17) yields $d_1^2 = d_2^2 = 1$. Hence, for one of the representations $d_1 = -c_1 = 1$, and for the other $d_2 = -c_2 = -1$.

Thus, we have found the characters of all representations of the group O.

Group T_d, since it is isomorphic to O, also has five representations; the group $O_h = O \times C_i = T_d \times C_i$ has twice as many representations, whose characters are obtained by multiplying the characters of the representations of O or T_d by those of C_i. Accordingly, five of these representations are even and five odd.

We have thus determined the characters of the representations of all the crystallographic point groups, as listed in Table 11.1.

Tables 11.1 and 11.2 present basis functions for each representation, built up from the components of the polar vector $\boldsymbol{x}(x, y, z)$ or the axial vector $\boldsymbol{J}(J_x, J_y, J_z)$ and their products. In accordance with the rules described in §9, these functions may be constructed as follows.

First of all we determine the characters of a representation according to which the components of $\boldsymbol{x}$ or $\boldsymbol{J}$ transform, for each operation g appearing in the group. As shown in §10, the characters of these representations are

$$\chi(c_\varphi) = \frac{\sin(3\varphi/2)}{\sin(\varphi/2)}, \quad \chi(s_\varphi) = \mp\chi(c_\varphi), \qquad (11.4)$$
$$\chi(i) = \mp 3, \quad \chi(\sigma) = \mp\chi(c_2) = \pm 1.$$

The upper sign refers to the components of the polar vector (representation $\mathcal{D}_1^-$), the lower to those of the axial vector (representation $\mathcal{D}_1^+$). Evaluating the characters by (11.4) and using equation (8.19) or (8.22), we determine the irreducible constituents of the representation $\mathcal{D}_1^-$ or $\mathcal{D}_1^+$. We see that in the cubic groups T, T_h, T_d, O, O_h the representation $\mathcal{D}_1^-$ is irreducible and corresponds to the representation F, F^-, F_1 or F_1^-. In groups not containing transformations of the second kind, such as T and O, it is evident from (11.4) that the components of $\boldsymbol{x}$ and $\boldsymbol{J}$ transform according to the same representation; Tables 11.1 and 11.2 therefore list only functions based on the components x, y, z. In T_d the components J_i transform according to F_1; in O_h, as in all groups containing inversion, the components J_i transform according to even representations, i.e., according to F_1^+.

It is clear that the products J_iJ_k always transform like x_ix_k.

In all other groups (except T, T_h, T_d, O, O_h) the representations $\mathcal{D}_1^\pm$ are reducible. In C_{3v}, C_{4v}, C_{6v} and their isomorphic images, these representations decompose into one one-dimensional representation and one two-dimensional representation. If we take the direction of the principal axis as z, it is immediate that in all cases the z-component transforms according to the one-dimensional representation, and consequently x and y form a basis for the two-dimensional representation. The same applies to J_z and the pair J_x, J_y.

In the remaining groups, the representations $\mathcal{D}_1^\pm$ decompose into three one-dimensional representations, and the basis functions are at once determined with the aid of equation (9.11). Here it is convenient to use the basis (10.25):

$$Y_1^1 = -\frac{i}{\sqrt{2}}(x + iy), \quad Y_0^1 = iz, \quad Y_1^1 = \frac{i}{\sqrt{2}}(x - iy), \qquad (11.5)$$

in which (see (10.6) and (10.17)) the matrix $\mathcal{D}_1$ for rotation operations about the principal (z-)axis is diagonal:

$$\mathcal{D}^1_{mm'}(c_{z\varphi}) = e^{im\varphi}\delta_{mm'} \quad (m = 1, 0, -1), \qquad (11.6)$$
$$\mathcal{D}^1_{mm'}(i) = \mp\delta_{mm'}, \quad \mathcal{D}^1_{mm'}(\sigma_h) = \mp e^{i\pi m}\delta_{mm'}$$

(minus for $\mathcal{D}_1^-$, plus for $\mathcal{D}_1^+$).

For rotations through π about mutually perpendicular axes,

$$\mathcal{D}_1(u_{2x}) = \begin{Vmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{Vmatrix}, \quad \mathcal{D}_1(u_{2y}) = \begin{Vmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{Vmatrix}, \qquad (11.7)$$

and

$$\mathcal{D}_1(\sigma_v) = \mathcal{D}_1(u_{2x})\mathcal{D}_1(\sigma_h), \quad \mathcal{D}_1(\sigma_v') = \mathcal{D}_1(u_{2y})\mathcal{D}_1(\sigma_h).$$

After determining the representations that belong to the components x_i and J_i, we can at once find the representations according to which their products transform, using equations (9.16), (9.22), (9.23), (8.22). In so doing one should note that the antisymmetrized product $\{xy\}$ transforms like J_z, and so on. If the product of two representations is irreducible, the basis functions are determined at once; in particular, this is so whenever both representations are one-dimensional. In the remaining cases we may use formula (9.14a). No product of irreducible representations for point groups contains any irreducible representation more than once. Therefore, this formula, which involves only the characters $\chi_\mu(g)$, determines one of the functions, and the others are obtained by applying the operations $\mathcal{D}(g)$ to this function. The matrices $\mathcal{D}_{ij}(g)$ according to which the products $Y^l_m Y^l_{m'}$ transform (see (9.15), (9.20), or (9.21)) are determined by the direct product of the matrices (11.6) and (11.7). For example, for the function $Y^{l'}_m$:

$$\mathcal{D}_{mm'}(c_\varphi) = e^{2\pi i m\varphi}\delta_{mm'}. \tag{11.8}$$

For the group T_d, we find that $[F_1^2] = A_1 + E + F_1$. By (9.26), the invariant $x^2 + y^2 + z^2$ transforms according to A_1. It is easy to show that the symmetrized products $[xy]$, $[xz]$, $[yz]$ transform according to F_2. Consequently, the two remaining linearly independent functions, built up from x^2, y^2, z^2, transform according to E. These functions may be chosen as

$$R_1 = x^2 + \varepsilon_3 y^2 + \varepsilon_3^2 z^2, \quad R_2 = R_1^* = x^2 + \varepsilon_3^2 y^2 + \varepsilon_3 z^2, \tag{11.9}$$

where $\varepsilon_3 = e^{2\pi i/3}$.

With the basis functions determined, one can, if necessary, immediately construct the matrices of the corresponding representations. Of course, the matrices of the irreducible representations may be constructed by using the defining relations for point groups, (see §3), without specifying the basis functions in explicit form; this will be done for projective representations in §14.

Basis functions involving higher powers of the components x, y, z are constructed in a similar manner.

If the matrices of the representations are known, the construction of the basis functions may be based directly on the functions Y^l_m with sufficiently large j, forming a basis for the representation $\mathcal{D}_j$ of the rotation group. The matrices of these representations are given by equations (10.6) and (10.17). Since all the point groups are subgroups of the full orthogonal group, all their representations may be obtained from the representations of the latter. Using equation (8.19), one can determine the irreducible representations of point groups that occur in the representation $\mathcal{D}^\pm_l$, and find the functions themselves from equations (9.14).

TABLE 11.1. Character tables for the point groups

Group E

E	e
A	1

TABLE 11.1 (continued)

Groups C_2, C_i, C_s

C_2			e	c_2			
	C_i		e	i	C_2	C_i	C_s
		C_s	e	σ_h			
A	A^+	A^+	1	1	z	I_x, I_y, I_z	x, y
B	A^-	A^-	1	−1	x, y	x, y, z	z

Group C_3

C_3	e	c_3	c_3^2	
A	1	1	1	z
B_1	1	ε_3	ε_3^2	$x - iy$
B_2	1	ε_3^2	ε_3	$x + iy$

$\varepsilon_3 = e^{2\pi i/3}$

Groups C_4, S_4

C_4		e	c_4	c_2	c_4^3	C_4	S_4
	S_4	e	s_4	c_2	s_4^3		
A	A	1	1	1	1	z	I_z
B_1	B_1	1	−1	1	−1	$x^2 - y^2$	z
B_2	B_2	1	i	−1	$-i$	$x - iy$	$x - iy$, $I_x + iI_y$
B_3	B_3	1	$-i$	−1	i	$x + iy$	$x + iy$, $I_x - iI_y$

Groups D_3, C_{3v}

D_3		e	$2c_3$	$3u_2$	D_3	C_{3v}
	C_{3v}	e	$2c_3$	$3\sigma_v$		
A_1	A_1	1	1	1	$x^2 + y^2$, z^2	z
A_2	A_2	1	1	−1	z	I_z
E	E	2	−1	0	x, y	x, y, I_x, I_y

TABLE 11.1 (continued)

Groups D_4, C_{4v}, D_{2d}

D_4			e	c_2	$2c_4$	$2u_2$	$2u_2'$	D_4	C_{4v}	D_{2d}
	C_{4v}		e	c_2	$2c_4$	$2\sigma_v$	$2\sigma_v'$			
		D_{2d}	e	c_2	$2s_4$	$2u_2$	$2\sigma_d$			
A_1	A_1	A_1	1	1	1	1	1	z^2, x^2+y^2	z	z^2, x^2+y^2
A_2	A_2	A_2	1	1	1	−1	−1	z	J_z	J_z
B_1	B_1	B_1	1	1	−1	1	−1	x^2-y^2	x^2-y^2	x^2-y^2
B_2	B_2	B_2	1	1	−1	−1	1	xy	xy	xy, z
E	E	E	2	−2	0	0	0	x, y	x, y; J_x, J_y	x, y; J_x, J_y

Group T

T	e	$3c_2$	$4c_3$	$4c_3^2$	
A	1	1	1	1	$x^2+y^2+z^2$
B_1	1	1	ε_3	ε_3^2	$x^2+\varepsilon_3^2y^2+\varepsilon_3z^2$
B_2	1	1	ε_3^2	ε_3	$x^2+\varepsilon_3y^2+\varepsilon_3^2z^2$
F	3	−1	0	0	x, y, z

Groups T_d, O

T_d		e	$8c_3$	$3c_2$	$6\sigma_d$	$6s_4$	T_d	O
	O	e	$8c_3$	$3c_2$	$6u_2$	$6c_4$		
A_1	A_1	1	1	1	1	1	$x^2+y^2+z^2$	
A_2	A_2	1	1	1	−1	−1	$[J_xJ_yJ_z]$	xyz
E	E	2	−1	2	0	0	$x^2+\varepsilon_3y^2+\varepsilon_3^2z^2$, $x^2+\varepsilon_3^2y^2+\varepsilon_3z^2$ $J_x^2+\varepsilon_3^2J_y^2+\varepsilon_3J_z^2$, $J_x^2+\varepsilon_3J_y^2+\varepsilon_3^2J_z^2$	
F_1	F_1	3	0	−1	−1	1	J_x, J_y, J_z	x, y, z
F_2	F_2	3	0	−1	1	−1	x, y, z; xy, xz, yz; $[J_xJ_y]$, $[J_xJ_z]$, $[J_yJ_z]$	xy, xz, yz

Groups $D_2 = C_2 \times C_2'$, $C_{2h} = C_2 \times C_i$, $C_{2v} = C_2 \times C_s'$

D_2			e	c_{2z}	c_{2x}	c_{2y}	D_2	C_{2h}	C_{2v}
	C_{2h}		e	c_2	i	σ_h			
		C_{2v}	e	c_2	σ_v	σ_v'			
A_1	A^+	A^+	1	1	1	1	x^2, y^2, z^2	J_z	z
A_2	A^-	A^-	1	1	−1	−1	z	z	J_z
B_1	B^+	B^+	1	−1	1	−1	x	J_x, J_y	y; J_x
B_2	B^-	B^-	1	−1	−1	1	y	x, y	x; J_y

TABLE 11.1 (continued)

Groups $C_6 = C_3 \times C_2$, $C_{3h} = C_3 \times C_s$, $S_6 = C_3 \times C_i$

C_6			e	c_3	c_3^2	c_2	c_6^5	c_6	C_6	C_{3h}	S_6
	C_{3h}		e	c_3	c_2^2	σ_h	s_3	s_3^5			
		S_6	e	c_3	c_3^2	i	s_6^5	s_6			
A_1	A^+	A^+	1	1	1	1	1	1	z	J_z	J_z
A_2	A^-	A^-	1	1	1	−1	−1	−1	$(x \pm iy)^3$	z	z
B_1	B_1^+	B_1^+	1	ε_3	ε_3^2	1	ε_3	ε_3^2	$(x-iy)^3$	$x+iy$	J_x+iJ_y
B_2	B_1^-	B_1^-	1	ε_3	ε_3^2	−1	$-\varepsilon_3$	$-\varepsilon_3^2$	$x+iy$	J_x+iJ_y	$x+iy$
B_3	B_2^+	B_2^+	1	ε_3^2	ε_3	1	ε_3^2	ε_3	$(x+iy)^2$	$x-iy$	J_x-iJ_y
B_4	B_2^-	B_2^-	1	ε_3^2	ε_3	−1	$-\varepsilon_3^2$	$-\varepsilon_3$	$x-iy$	J_x-iJ_y	$x-iy$

Groups $D_6 = D_3 \times C_2$, $C_{6v} = C_{3v} \times C_2$, $D_{3h} = D_3 \times C_s$

D_6			e	$2c_3$	$3u_2$	c_2	$2c_6$	$3u_2'$	D_6	C_{6v}	D_{3h}
	C_{6v}		e	$2c_3$	$3\sigma_v$	c_2	$2c_6$	$2\sigma_v'$			
		D_{3h}	e	$2c_3$	$3u_2$	σ_h	$2s_3$	$3\sigma_v'$			
A_1	A_1	A_1^+	1	1	1	1	1	1	$x^2+y^2,\ z^2$	z	$x^2+y^2,\ z^2$
A_2	A_2	A_1^-	1	1	1	−1	−1	−1	$(x+iy)^3 + (x-iy)^3$	$(x+iy)^3 + (x-iy)^3$	$iz[(x+iy)^3 - (x-iy)^3]$
A_3	A_3	A_2^+	1	1	−1	1	1	−1	z	J_z	J_z
A_4	A_4	A_2^-	1	1	−1	−1	−1	1	$i[(x+iy)^3 - (x-iy)^3]$	$i[(x+iy)^3 - (x-iy)^3]$	z
E_1	E_1	E^+	2	−1	0	2	−1	0	$(x+iy)^2,$ $(x-iy)^2$	$(x+iy)^2,$ $(x-iy)^2$	$x,\ y$
E_2	E_2	E^-	2	−1	0	−2	1	0	$x,\ y$	$x,\ y,\ J_x,\ J_y$	$J_x,\ J_y$

For the remaining eight groups
$C_{4h} = C_4 \times C_i$, $C_{6h} = C_6 \times C_i$, $D_{2h} = D_2 \times C_i$, $D_{3d} = D_3 \times C_i$
$D_{4h} = D_4 \times C_i$, $D_{6h} = D_6 \times C_i$, $T_h = T \times C_i$, $O_h = O \times C_i = T_d \times C_i$
each representation of the original group $\mathcal{D}$ is associated with two representations $\mathcal{D}^{\pm}$ with characters $\chi(ig) = \pm\chi(g)$, belonging to even and odd functions of the coordinates, respectively. All the functions $\varphi(J)$ transform according to even representations.

TABLE 11.2. Basis functions for the groups T_d, O, O_h

Representations			Basis functions	
T_d	O	O_h	$\varphi(x)$	$\varphi(J)$
A_1	A_1	A_1^+	$x^2+y^2+z^2,\ x^4+y^4+z^4$	
A_2	A_2	A_2^+	$x^4(y^2-z^2)+y^4(z^2-x^2)+z^4(x^2-y^2)$	$[J_xJ_yJ_z]$
E	E	E^+	$x^2+\varepsilon_3y^2+\varepsilon_3^2z^2,$ $x^2+\varepsilon_3^2y^2+\varepsilon_3z^2,$ $x^4+\varepsilon_3y^4+\varepsilon_3^2z^4,$ $x^4+\varepsilon_3^2y^4+\varepsilon_3z^4$	$J_x^2+\varepsilon_3J_y^2+\varepsilon_3^2J_z^2,$ $J_x^2+\varepsilon_3^2J_y^2+\varepsilon_3J_z^2$
F_1	F_1	F_1^+	$xy(x^2-y^2),\ xz(x^2-z^2),$ $yz(y^2-z^2)$	$J_x,\ J_y,\ J_z;\ J_x^3,\ J_y^3,\ J_z^3$
F_2	F_2	F_2^+	$xy,\ xz,\ yz;\ xyz^2,\ xzy^2,\ yzx^2;$ $zx^2y^2,\ xy^2z^2,\ yx^2z^2$	$[J_xJ_y],\ [J_xJ_z],\ [J_yJ_z];$ $V_x=\left[J_x\left(J_y^2-J_z^2\right)\right],$ $V_y,\ V_z$
A_1	A_2	A_1^-	xyz	
A_2	A_1	A_2^-	$xyz\,[x^4(y^2-z^2)+y^4(z^2-x^2)+z^4(x^2-y^2)]$	
E	E	E^-	$xyz\left(x^2+\varepsilon_3y^2+\varepsilon_3^2z^2\right),$ $xyz\left(x^2+\varepsilon_3^2y^2+\varepsilon_3z^2\right)$	
F_1	F_2	F_1^-	$x(y^2-z^2),\ y(z^2-x^2),\ z(x^2-y^2);$ $x^3(y^2-z^2),\ y^3(z^2-x^2),$ $z^3(x^2-y^2)$	
F_2	F_1	F_2^-	$x,\ y,\ z;\ x^3,\ y^3,\ z^3;\ x^5,\ y^5,\ z^5$	

TABLE 11.3. Multiplication table for T_d and O

	A_1	A_2	E	F_1	F_2
A_1	A_1	A_2	E	F_1	F_2
A_2	A_2	A_1	E	F_2	F_1
E	E	E	A_1+A_2+E	F_1+F_2	F_1+F_2
F_1	F_1	F_2	F_1+F_2	$A_1+E+F_1+F_2$	$A_2+E+F_1+F_2$
F_2	F_2	F_1	F_1+F_2	$A_2+E+F_1+F_2$	$A_1+E+F_1+F_2$

§12. REPRESENTATIONS OF SPACE GROUPS. BRILLOUIN ZONE. LITTLE GROUP

In order to determine the irreducible representations of a space group, we first find the representations of its translation subgroup, which, as shown in §6, is an abelian invariant subgroup of the space group.

Representations of the Translation Group

Since the translation group is abelian, all its representations are one-dimensional.

Let $\varphi(\boldsymbol{x})$ be a function realizing an irreducible unitary representation of a translation group with generators $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$. Translation by the vectors $\boldsymbol{a}_1$, $\boldsymbol{a}_2$, $\boldsymbol{a}_3$ multiplies the function φ by factors λ_1, λ_2, λ_3. (Unitarity implies that the absolute value of each λ is unity).

$$\begin{gathered}(e\,|\,\boldsymbol{a}_1)\,\varphi = \varphi\left(t_{\boldsymbol{a}_1}^{-1}\boldsymbol{x}\right) = \varphi(\boldsymbol{x}-\boldsymbol{a}) = \lambda_1\varphi(\boldsymbol{x}),\\ t_{\boldsymbol{a}_2}\varphi(\boldsymbol{x}) = \lambda_2\varphi(\boldsymbol{x}),\quad t_{\boldsymbol{a}_3}\varphi(\boldsymbol{x}) = \lambda_3\varphi(\boldsymbol{x}).\end{gathered} \tag{12.1}$$

A function $\varphi(\boldsymbol{x})$ which forms a basis of an irreducible unitary representation of the translation group will be denoted by $\varphi_{\lambda_1\lambda_2\lambda_3}$.

It follows from (12.1) that for the general element $\boldsymbol{a}$ of the translation group,

$$\boldsymbol{a} = m_1\boldsymbol{a}_1 + m_2\boldsymbol{a}_2 + m_3\boldsymbol{a}_3,$$

$\varphi_{\lambda_1\lambda_2\lambda_3}$ transforms in the following manner:

$$(e\,|\,\boldsymbol{a})\,\varphi_{\lambda_1\lambda_2\lambda_3}(\boldsymbol{x}) = \varphi_{\lambda_1\lambda_2\lambda_3}(\boldsymbol{x}-\boldsymbol{a}) = \lambda_1^{m_1}\lambda_2^{m_2}\lambda_3^{m_3}\varphi_{\lambda_1\lambda_2\lambda_3}(\boldsymbol{x}). \tag{12.2}$$

Thus the three numbers λ_1, λ_2, λ_3 completely determine an irreducible representation of the translation group.

Instead of λ_1, λ_2, λ_3 it is convenient to introduce a single vector $\boldsymbol{k}$, defined by

$$\lambda_1 = e^{-i\boldsymbol{k}\boldsymbol{a}_1},\quad \lambda_2 = e^{-i\boldsymbol{k}\boldsymbol{a}_2},\quad \lambda_3 = e^{-i\boldsymbol{k}\boldsymbol{a}_3}. \tag{12.3}$$

However, the vector $\boldsymbol{k}$ is not uniquely determined by λ_1, λ_2, λ_3. To clarify this ambiguity, we define vectors $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\boldsymbol{b}_3$ by

$$\boldsymbol{b}_1 = \frac{2\pi}{\Omega_0}[\boldsymbol{a}_2\times\boldsymbol{a}_3],\quad \boldsymbol{b}_2 = \frac{2\pi}{\Omega_0}[\boldsymbol{a}_3\times\boldsymbol{a}_1],\quad \boldsymbol{b}_3 = \frac{2\pi}{\Omega_0}[\boldsymbol{a}_1\times\boldsymbol{a}_2], \tag{12.4}$$

where $\Omega_0 = (\boldsymbol{a}_1[\boldsymbol{a}_2\times\boldsymbol{a}_3])$ is the volume of a primitive cell. We see from (12.4) that the vectors $\boldsymbol{b}_i$ are orthogonal to the vectors $\boldsymbol{a}_j$:

$$\boldsymbol{b}_i\boldsymbol{a}_j = 2\pi\delta_{ij} \qquad (i,\ j = 1,\ 2,\ 3) \tag{12.5}$$

and therefore satisfy the equations

$$e^{i\boldsymbol{b}_i\boldsymbol{a}_j} = 1. \tag{12.6}$$

Taking $\boldsymbol{b}_1$, $\boldsymbol{b}_2$, $\boldsymbol{b}_3$ as a basis, we can construct vectors

$$\boldsymbol{b} = n_1\boldsymbol{b}_1 + n_2\boldsymbol{b}_2 + n_3\boldsymbol{b}_3, \tag{12.7}$$

where n_1, n_2, n_3 are arbitrary integers (positive, negative or zero). The endpoints of these vectors form a lattice, called the reciprocal lattice with

respect to the Bravais lattice defined by the vectors a_1, a_2, a_3. If the vectors a_1, a_2, a_3 have the dimensions of length, the reciprocal lattice vectors b have the dimensions of inverse length (dimensions of a wave vector).

It follows from (12.6) that equalities (12.3) determine the vector k up to an arbitrary reciprocal lattice vector (12.7).

We now describe some properties of the reciprocal lattice. Using the definition of the vectors b (or the relations (12.5)), we can show that the symmetry point group of the reciprocal lattice coincides with the symmetry group of the Bravais lattice. However, the type of reciprocal Bravais lattice is generally not the same as that of the Bravais lattice.

Using the definition of reciprocal lattice vectors, we can establish the correspondence shown in Table 21.1 between the types of Bravais and reciprocal lattices.

The volume of the primitive cell of the reciprocal lattice is readily seen from (12.5) to be $(2\pi)^3/\Omega_0$.

Thus, each irreducible representation of the translation group is characterized by a vector k such that

$$t_a\varphi_k = (e\,|\,a)\,\varphi_k = \varphi_k(x-a) = e^{-ika}\,\varphi_k(x). \tag{12.8}$$

Since k is determined only up to an arbitrary reciprocal lattice vector, two vectors k and k' will be called equivalent, $k \equiv k'$, if they differ by a reciprocal lattice vector.

TABLE 12.1

System	Lattice type	Reciprocal lattice type
Triclinic	Primitive	Primitive
Monoclinic	Primitive	Primitive
	Base-centered	Base-centered
Orthorhombic	Primitive	Primitive
	Base-centered	Base-centered
	Body-centered	Face-centered
	Face-centered	Body-centered
Tetragonal	Primitive	Primitive
	Body-centered	Body-centered
Rhombohedral	Primitive	Primitive
Hexagonal	Primitive	Primitive
Cubic	Primitive	Primitive
	Body-centered	Face-centered
	Face-centered	Body-centered

Brillouin Zone

The domain of definition of the vector k may be taken as the primitive cell of the reciprocal lattice. However, this is not always convenient, since the choice of the primitive cell is quite arbitrary and, moreover, in the general case the primitive cell is not invariant under transformations from

the symmetry group of the reciprocal lattice. The volume of the invariant Bravais parallelepiped (or Bravais prism, for the hexagonal system) generally exceeds that of the primitive cell.

We can construct a primitive cell which on the one hand is invariant under the transformations in the group $\mathcal{H}$, and on the other has volume equal to the volume of the primitive cell. As before, the Bravais lattice may be obtained by unlimited repetition of cells. In the Bravais lattice this cell is known as the symmetrized Wigner-Seitz cell; in the reciprocal lattice it is called the first Brillouin zone or simply the Brillouin zone. The Brillouin zone is not a parallelepiped, but rather (in the general case) a certain polyhedron. The first Brillouin zone is usually taken as the domain of definition of the vector $\boldsymbol{k}$.

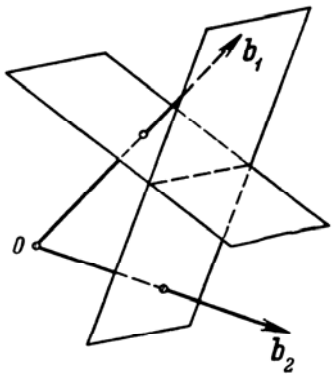


FIGURE 17. Construction of Brillouin zone.

The method for constructing the Brillouin zone is as follows. Choose an arbitrary reciprocal lattice point O as the origin. The Brillouin zone is the set of all points whose distance from the zero point O is less than or equal to its distance from any other point of the reciprocal lattice. To construct the Brillouin zone, join the point O to the various reciprocal lattice points determined by the vectors $\boldsymbol{b}$ (12.7), and construct planes perpendicular to $\boldsymbol{b}$ which lie equidistant between O and the corresponding point (Figure 17). The polyhedron bounded by these planes is the Brillouin zone.

The system of planes bounding the Brillouin zone, and the cell itself, are invariant under the symmetry group of the Bravais lattice. In particular, the point O is a center of symmetry for the cell. Its volume is equal to that of the primitive cell.

The equation for a vector $\boldsymbol{x}$ lying on a plane perpendicular to $\boldsymbol{b}$ at a distance $b/2$ from the origin is

$$\boldsymbol{x}\boldsymbol{b} = b^2/2. \tag{12.9}$$

By varying the vector $\boldsymbol{b}$ in (12.9), we easily obtain analytical expressions for the planes bounding the Brillouin zone in cartesian coordinates.

It follows from this construction of the symmetrized cell that inside the Brillouin zone there are no pairs of equivalent vectors $\boldsymbol{k}$. If the vector $\boldsymbol{k}$

lies on the boundary of the Brillouin zone, however, there is always at least one equivalent vector $\boldsymbol{k}'$ on boundary of the Brillouin zone.

Let us consider the form of the Brillouin zone in our hierarchy of crystal systems.

In the cubic system there are three possible types of systems: primitive Γ_c, face-centered Γ_c^f, body-centered Γ_c^v.

The Brillouin zone for the primitive cubic lattice is a cube (Figure 18, a). It is clearly formed by intersecting planes perpendicular to the edges of the cube forming the primitive cell. The Brillouin zone for the face-centered cubic lattice* is shown in Figure 18, c. Formed by intersecting twelve planes perpendicular to the six twofold axes, it is a dodecahedron, all of whose faces are rhombuses. The threefold and fourfold axes intersect the symmetrized cell at its vertices.

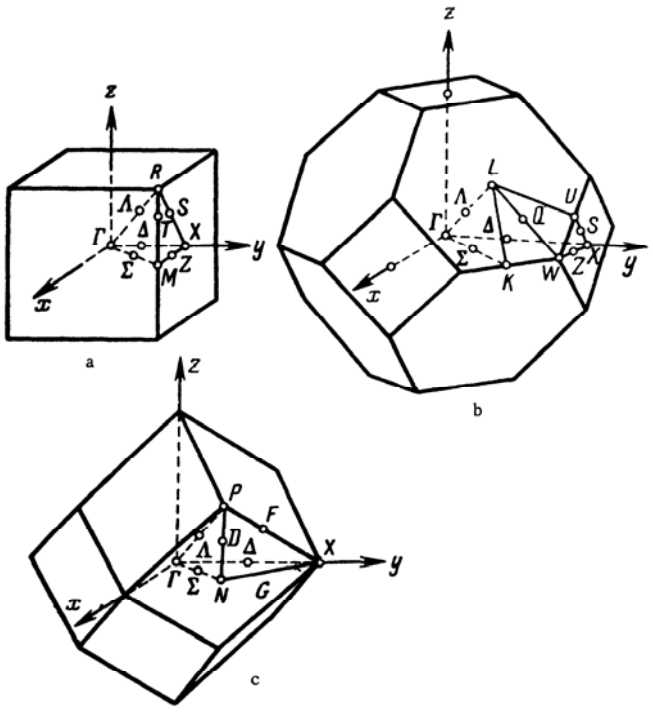


FIGURE 18. Brillouin zone for cubic lattices:

a) simple cubic lattice; b) body-centered reciprocal lattice; c) face-centered reciprocal lattice.

In the case of the body-centered lattice, the symmetrized cell is formed by intersecting six planes perpendicular to the three fourfold axes and eight planes perpendicular to the four threefold axes. It is a tetradecahedron, six

* In order to avoid misunderstandings, we stress that all references are to the type of the reciprocal lattice. The correspondence between the original and reciprocal lattices was given above in Table 12.1.

faces of which are squares and eight regular hexagons. The fourfold axes pass through the centers of the square faces, the threefold axes through the centers of the hexagonal faces (Figure 18, b).

In the tetragonal system there are two types of lattices: primitive Γ_q and body-centered Γ_q^v.

The Brillouin zone for the primitive lattice Γ_q has the same form as the primitive cell — a rectangular prism (Figure 19, a). It may be obtained from the Brillouin zone for a primitive cubic lattice by stretching (or compressing) along a fourfold axis.

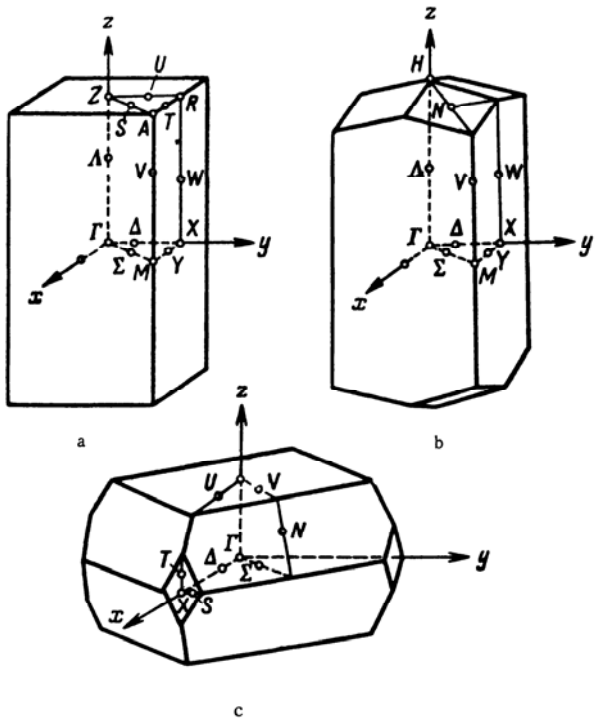


FIGURE 19. Brillouin zone for tetragonal lattices:

a) primitive lattice; b) body-centered, height greater than diagonal of the square; c) body-centered, height less than diagonal of the square.

For the body-centered lattice, there are two possible types of symmetrized cell, depending on the relation between the edges a and c of the Bravais parallelepiped in the reciprocal lattice, since the system of planes bounding the symmetrized cell will differ according as $c > \sqrt{2}\,a$ or $c < \sqrt{2}\,a$. The Brillouin zone for $c > \sqrt{2}\,a$ is depicted in Figure 19, b, and for $c < \sqrt{2}\,a$ in Figure 19, c. The situation becomes clearer if we recall that according to Figure 16 the lattice Γ_q^v may be obtained by continuously deforming the lattices Γ_c^v and Γ_c^f.

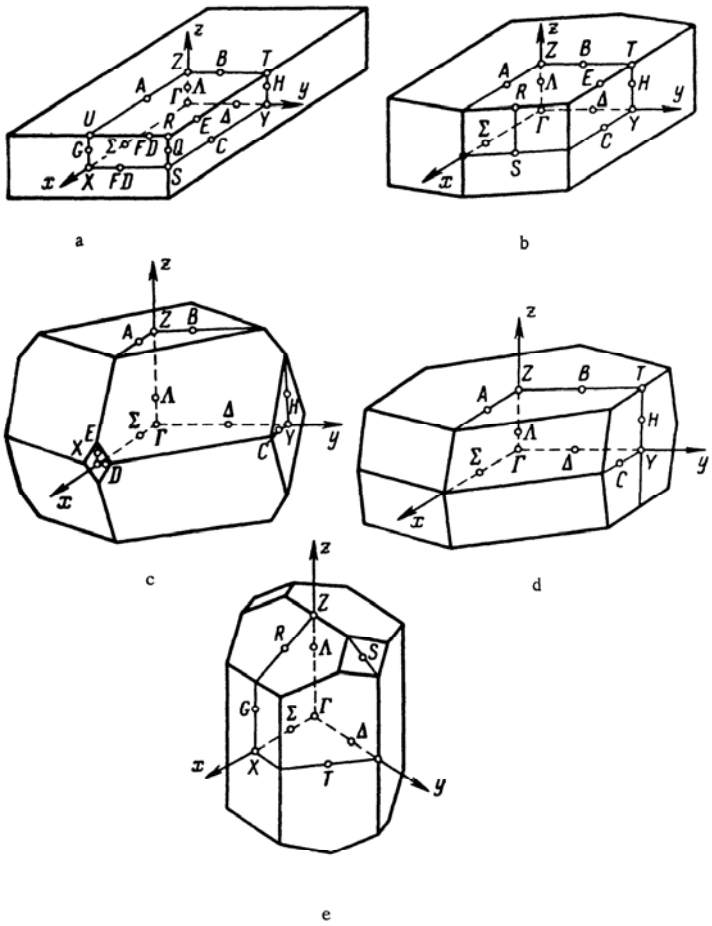


FIGURE 20. Brillouin zone for orthorhombic lattices:

a) primitive; b) base-centered; c) body-centered, height greater than diagonal of rectangular base; d) body-centered, height less than diagonal of base; e) face-centered lattice.

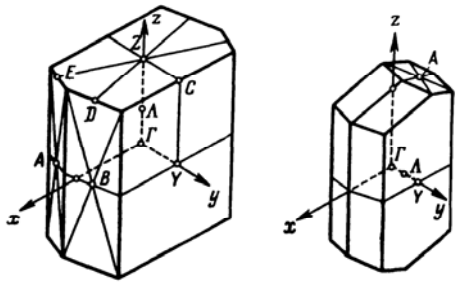
In the first case a small deformation will keep $c < \sqrt{2}\,a$ (since in a cubic lattice $c = a$) and the symmetrized cell in Figure 19, c is obtained from the symmetrized cell for Γ_c^v by stretching (or compressing) along a fourfold axis

The Γ_c^f lattice is equivalent to a body-centered lattice of the tetragonal system when $c = \sqrt{2}\,a$. If we dilate this lattice along a fourfold axis, c becomes greater than $\sqrt{2}\,a$. Consequently, the symmetrized cell for Γ_q^v in this case (Figure 19, b) is obtained from the Brillouin zone of the Γ_c^f lattice (Figure 18) by dilation along a fourfold axis.

In the orthorhombic system there are four possible types: Γ_0, Γ_0^b, Γ_0^f, Γ_0^v. The Brillouin zone for the primitive lattice is a right parallelepiped with rectangular faces (Figure 20, a). The Brillouin zone for the base-centered lattice, shown in Figure 20, b, is a hexagonal prism. For the body-centered lattice there are three types of Brillouin zone, depending on the relation

between the parameters. Figures 20, c and d show two types of Brillouin zone for the body-centered lattice; Figure 20, e shows the symmetrized cell for the Γ_0^I lattice.

In the monoclinic system there are two possible types of Bravais lattice: primitive Γ_m and base-centered Γ_m^b. The Bravais parallelepiped in the monoclinic system is determined by four parameters: the angle α between the edges of the base and the lengths of the edges. Therefore, the shape of the symmetrized cells will depend on the relations between these parameters.



a b

FIGURE 21. Brillouin zone for monoclinic lattices:

a) primitive; b) base-centered.

The Brillouin zone for the primitive lattice Γ_m is shown in Figure 21, a. Depending on the parameters characterizing the primitive cell, five types of Brillouin zone may occur for the Γ_m^b lattice; one of them is shown in Figure 21, b.

In the triclinic system we have only the primitive Bravais lattice Γ_t. However, depending on the form of the primitive cell there are three types of Brillouin zone.

In the hexagonal system there is one type of lattice and one type of Brillouin zone, shown in Figure 22.

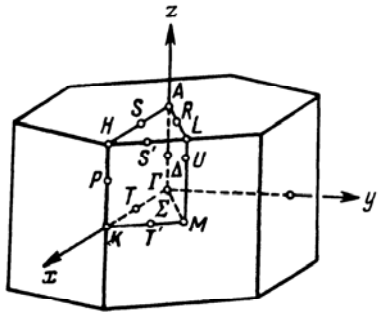


FIGURE 22. Brillouin zone for hexagonal lattice.

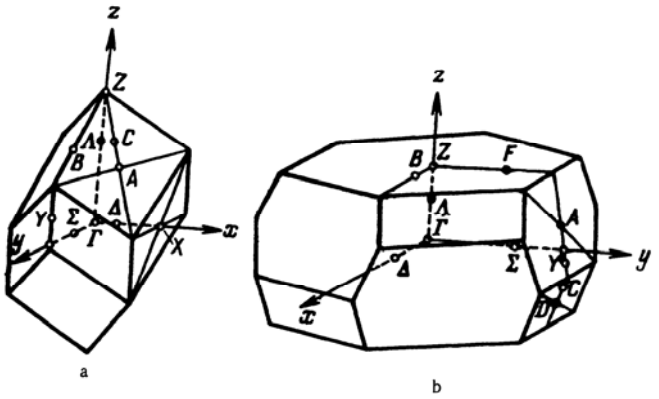


FIGURE 23. Brillouin zone for rhombohedral lattices. Three translation vectors of equal length lie on the surface of a cone about the threefold axis:

a) height of cone greater than $\sqrt{2}r$, where r is the radius of the base; b) height of cone less than $\sqrt{2}r$.

In the rhombohedral system there is only one type of Bravais lattice but, depending on the degree of elongation of its primitive cell (rhombohedron), there are two possible types of Brillouin zone, obtained by dilating the Brillouin zone for the face-centered and body-centered cubic lattices of Figures 18, b and c. These lattices are shown in Figure 23.

Thus, there are altogether twenty four types of Brillouin zone in the fourteen Bravais lattices. These symmetrized cells are discussed in greater detail in /I.10, I.14/.

Construction of Representations of a Space Group

We now show how to construct the representations of a space group on the assumption that the representations of its translation subgroup are known. This procedure for constructing the representations of a group based on those of an (abelian) invariant subgroup dates back to Frobenius /I.11/.

Consider some s-dimensional representation $\mathcal{D}(g)$ of the space group, its basis consisting of s functions $\varphi^{(1)}, \varphi^{(2)}, \ldots, \varphi^{(s)}$. If $s > 1$, the representation $\mathcal{D}$ is reducible as a representation of the translation subgroup.

Choose the basis $\varphi^{(i)}$ in such a way that each function $\varphi^{(i)}$ belongs to an irreducible representation of the translation subgroup, i.e., choose the functions φ_{k_i} (12.8) as $\varphi^{(i)}$. Relative to this basis, the matrix

$$\mathcal{D}(t_a) = \mathcal{D}(e|a)$$

is diagonal and has the form

$$\mathcal{D}(e|a) = \begin{Vmatrix} e^{-ik_1 a} & 0 & \ldots & 0 \\ 0 & e^{-ik_2 a} & \ldots & 0 \\ \ldots & \ldots & \ldots & \ldots \\ 0 & 0 & \ldots & e^{-ik_s a} \end{Vmatrix}. \qquad (12.10)$$

In the general case some of the s vectors $\boldsymbol{k}_i$ may be identical. We define the star of the representation $\mathcal{D}$ to be the set of all distinct vectors $\boldsymbol{k}_1, \boldsymbol{k}_2, \ldots, \boldsymbol{k}_n$ $(n \leqslant s)$ (equivalent vectors, i.e., vectors differing by a reciprocal lattice vector, are also treated here as equal).

We claim that the star of a representation is invariant with respect to the group G, i.e., if $\boldsymbol{k}$ is a vector in the star, then any vector $\boldsymbol{k}' = g\boldsymbol{k} = r\boldsymbol{k}$ is also in the star.

For the proof, consider the function $(r|\alpha)\varphi_{\boldsymbol{k}}$, where α is the nonprimitive translation corresponding to the "rotational" element r, and find its transformation law under the primitive translations $\boldsymbol{a}$:

$$(e|\boldsymbol{a})(r|\alpha)\varphi_{\boldsymbol{k}} = (r|\alpha)(e|r^{-1}\boldsymbol{a})\varphi_{\boldsymbol{k}} = (r|\alpha)e^{-i\boldsymbol{k}r^{-1}\boldsymbol{a}}\varphi_{\boldsymbol{k}} = e^{-ir\boldsymbol{k}\boldsymbol{a}}(r|\alpha)\varphi_{\boldsymbol{k}}. \qquad (12.11)$$

Thus, the function $(r|\alpha)\varphi_{\boldsymbol{k}}$, which belongs to the space spanned by the functions $\varphi_{\boldsymbol{k}_i}$, is an eigenfunction of the translation operators $t_{\boldsymbol{a}}$, corresponding to the wave vector $\boldsymbol{k}' = g\boldsymbol{k} = r\boldsymbol{k}$ (for any element $g = (r|\alpha + \boldsymbol{a})$, $g\boldsymbol{k}$ will always denote the vector $\boldsymbol{k}' = r\boldsymbol{k}$). Since the set of vectors $\boldsymbol{k}_i$ $(i = 1, 2, \ldots, n)$ for functions transforming according to the representation $\mathcal{D}$ coincides with the whole set of vectors $\boldsymbol{k}$, it follows that for every $g \in G$ the vector $r\boldsymbol{k}$ is one of the $\boldsymbol{k}_i$ $(i = 1, \ldots, n)$.

Now take any vector $\boldsymbol{k}_1$ in the star of the representation, and consider all possible vectors $r\boldsymbol{k}_1$. They are all elements of the star, but some of them may be identical. There are two possibilities.

1) The set of vectors $r\boldsymbol{k}_1$ exhausts the whole star of the representation $\mathcal{D}$. The star is then said to be irreducible. Clearly, every irreducible star is completely determined by specifying any of its vectors $\boldsymbol{k}_1$, and the remaining vectors are obtained by applying the operations g in the space group G. An irreducible star may thus be characterized by a single vector $\boldsymbol{k}_1$, and we shall denote it by $\{\boldsymbol{k}_1\}$.

2) It may turn out, however, that the set $g\boldsymbol{k}_1$ does not exhaust the whole star, in which case the star is said to be reducible. Any reducible star may be decomposed into irreducible stars, in the following manner.

Since the vectors $g\boldsymbol{k}_1$ do not exhaust the whole star, there is some vector $\boldsymbol{k}_2$ in the star not belonging to the irreducible star $\{\boldsymbol{k}_1\}$; constructing all possible vectors $g\boldsymbol{k}_2$, form the irreducible star $\{\boldsymbol{k}_2\}$. These stars are disjoint, since otherwise, for some r_1 and r_2, we would have $r_1\boldsymbol{k}_1 = r_2\boldsymbol{k}_2$, or $r_2^{-1}r_1\boldsymbol{k}_1 = \boldsymbol{k}_2$, contradicting the assumption that $\boldsymbol{k}_2 \notin \{\boldsymbol{k}_1\}$. If union of $\{\boldsymbol{k}_1\}$ and $\{\boldsymbol{k}_2\}$ is not the entire star of the representation $\mathcal{D}$, we can choose a vector $\boldsymbol{k}_3$, $\boldsymbol{k}_3 \notin \{\boldsymbol{k}_1\}$, $\boldsymbol{k}_3 \notin \{\boldsymbol{k}_2\}$, and construct the irreducible star $\{\boldsymbol{k}_3\}$. Continuing this process until the star of the representation $\mathcal{D}$ is exhausted, we thus decompose it into irreducible stars.

In what follows, irreducible stars will be essential for our study of irreducible representations of space groups: we shall now show that every irreducible representation has an irreducible star. (Note that the converse is false, since at the center of the Brillouin zone, $\boldsymbol{k} = 0$, any representation, reducible or not, corresponds to the irreducible star consisting of the single vector $\boldsymbol{k} = 0$.)

Suppose that the star of the representation $\mathcal{D}$ consists of two irreducible stars $\{\boldsymbol{k}_1\}$ and $\{\boldsymbol{k}_2\}$ and accordingly the space of the representation $\mathcal{D}$ decomposes into two subspaces L_1 and L_2. It is not difficult to see that each of these subspaces is invariant under the group G, since any function $g\varphi_{\boldsymbol{k}}$, $\boldsymbol{k} \in \{\boldsymbol{k}_1\}$,

is characterized by the wave vector $\boldsymbol{k}' = g\boldsymbol{k} \in \{\boldsymbol{k}_1\}$ and thus belongs to the subspace L_1. Similarly, for all $g \in G$ the functions $g\varphi_{\tilde{\boldsymbol{k}}}, \boldsymbol{k} \in \{\boldsymbol{k}_2\}$, belong to the subspace L_2. But since there are two invariant subspaces of basis functions, the representation $\mathfrak{D}$ is reducible. Thus, an irreducible representation cannot have a reducible star.

Little Group; Little Representations

The group of the wave vector $G_{\boldsymbol{k}}$ [or the little group] is the subgroup of the space group all of whose elements h either leave the vector $\boldsymbol{k}$ unchanged or map it onto an equivalent vector, i.e., for any $h \in G_{\boldsymbol{k}}$

$$h\boldsymbol{k} = \boldsymbol{k} \quad \text{or} \quad h\boldsymbol{k} \equiv \boldsymbol{k}. \tag{12.12}$$

Since there is no pair of equivalent vectors inside the Brillouin zone, the group $G_{\boldsymbol{k}}$ for points inside the Brillouin zone can contain only those elements which leave $\boldsymbol{k}$ unchanged. If $\boldsymbol{k}$ lies on the boundary of the Brillouin zone, $G_{\boldsymbol{k}}$ will also contain elements which map $\boldsymbol{k}$ onto an equivalent vector.

Like the space group, the little group $G_{\boldsymbol{k}}$ contains an invariant translation subgroup. The corresponding factor group is isomorphic to the crystallographic point group $F_{\boldsymbol{k}}$, which includes all the "rotational" elements $r \in F_{\boldsymbol{k}}$ which either leave $\boldsymbol{k}$ unchanged or map it onto an equivalent vector. The group $F_{\boldsymbol{k}}$ is determined by the vector $\boldsymbol{k}$ and is a subgroup of the crystallographic point group F characterizing the crystal class. In the special case $\boldsymbol{k} = 0$ we have $F_{\boldsymbol{k}} = F$, and of course $G_{\boldsymbol{k}} = G$.

Let us partition the crystallographic point group F into its cosets relative to the subgroup $F_{\boldsymbol{k}}$:

$$F = F_{\boldsymbol{k}} + \{r_2 F_{\boldsymbol{k}}\} + \{r_3 F_{\boldsymbol{k}}\} + \ \dots \ + \{r_n F_{\boldsymbol{k}}\}, \tag{12.13}$$

where $r_2, r_3, \dots, r_n \in F$, but $r_2 \notin F_{\boldsymbol{k}}$, $r_3 \notin F_{\boldsymbol{k}}$, $\{r_2 F_{\boldsymbol{k}}\}$, etc.

Let $\boldsymbol{k}$ be any vector which defines an irreducible star $\{\boldsymbol{k}\}$ and construct the vectors

$$\boldsymbol{k}_1 = \boldsymbol{k}, \quad \boldsymbol{k}_2 = r_2\boldsymbol{k}, \quad \boldsymbol{k}_3 = r_3\boldsymbol{k}, \ \dots, \ \boldsymbol{k}_n = r_n\boldsymbol{k}. \tag{12.14}$$

These vectors also define the star of $\boldsymbol{k}$. In fact, none of them are equal, since it would follow from $\boldsymbol{k}_i = \boldsymbol{k}_j$ that $r_i = r_j r$, $r \in F_{\boldsymbol{k}}$, i.e., $r_i \in \{r_j F_{\boldsymbol{k}}\}$, contrary to the basic properties of cosets. On the other hand, for any vector $r_i r\boldsymbol{k}$, $r \in F_{\boldsymbol{k}}$, we have $r_i r\boldsymbol{k} = r_i\boldsymbol{k} = \boldsymbol{k}_i$.

Since the cosets (12.13) exhaust the whole group F, the vectors $r_i\boldsymbol{k}$ also yield all the "points" of the star $\{\boldsymbol{k}\}$. If the little group $G_{\boldsymbol{k}}(h)$ is known for one of the points of the star, we easily construct the little group for any $\boldsymbol{k}_i$ in $\{\boldsymbol{k}\}$. This group $G_{\boldsymbol{k}_i}(h_i)$ consists of all elements

$$h_i = g_i h g_i^{-1}, \tag{12.15}$$

where $h \in G_{\boldsymbol{k}}$, $g_i = (r_i | \alpha_i + \boldsymbol{a})$, and r_i is determined from (12.13). In fact, $h_i\boldsymbol{k}_i = g_i h g_i^{-1}\boldsymbol{k}_i = \boldsymbol{k}_i$.

$G_{\boldsymbol{k}_i}(h_i)$ is isomorphic to $G_{\boldsymbol{k}}$.

The number of points of the star, i.e., distinct vectors $\boldsymbol{k}_i$ (12.14) forming the star $\{\boldsymbol{k}\}$, equals the number of cosets (12.13), which is by definition the

index of the subgroup $F_{\boldsymbol{k}}$ in F. Thus, the order f of the group F, the order l of the subgroup $F_{\boldsymbol{k}}$ and the number n of points in the star $\{\boldsymbol{k}\}$ satisfy the relation

$$f = ln. \tag{12.16}$$

If the little group coincides with the group G, the star consists of one point; if $G_{\boldsymbol{k}}$ is the translation subgroup, the number of points in the star $\{\boldsymbol{k}\}$ is the order of the group F.

We now show that any representation $\mathscr{D}^{\boldsymbol{k}}$ of the little group, also called a little representation, uniquely determines a representation $\mathscr{D}$ of the space group with irreducible star $\{\boldsymbol{k}\}$. Let $\mathscr{D}^{\boldsymbol{k}}$ be an m-dimensional representation of the little group $G_{\boldsymbol{k}}$, with basis functions

$$\varphi_{\boldsymbol{k}}^{(1)},\ \varphi_{\boldsymbol{k}}^{(2)},\ \ldots,\ \varphi_{\boldsymbol{k}}^{(m)}, \tag{12.17}$$

which transform under $h \in G_{\boldsymbol{k}}$ according to

$$h\varphi_{\boldsymbol{k}}^{(t)} = \sum_q \mathscr{D}_{qt}^{\boldsymbol{k}}(h)\,\varphi_{\boldsymbol{k}}^{(q)} \qquad (q,\ t = 1,\ 2,\ \ldots,\ m), \tag{12.18}$$

where $\mathscr{D}_{qt}^{\boldsymbol{k}}(h)$ are the matrix elements of $\mathscr{D}^{\boldsymbol{k}}$.

Along with the functions (12.17) we construct another $n-1$ m-tuples of functions

$$\begin{gathered}\varphi_{\boldsymbol{k}_i}^{(1)} = g_i\varphi_{\boldsymbol{k}}^{(1)},\quad \varphi_{\boldsymbol{k}_i}^{(2)} = g_i\varphi_{\boldsymbol{k}}^{(2)},\ \ldots,\ \varphi_{\boldsymbol{k}_i}^{(m)} = g_i\varphi_{\boldsymbol{k}}^{(m)};\quad g_i = (r_i \mid \boldsymbol{\alpha}_i)\\ (i = 2,\ 3,\ \ldots,\ n).\end{gathered} \tag{12.19}$$

The element g_i may be any representative of the coset $\{r_iF_{\boldsymbol{k}}\}$. To fix the choice of the basis functions (12.19) once and for all, we choose the elements $g_i = (r_i|\boldsymbol{\alpha}_i)$ of (12.13) as representatives. The linear space spanned by the functions

$$\varphi_{\boldsymbol{k}_i}^{(t)} \equiv \varphi_i^{(t)} \qquad (t = 1,\ 2,\ \ldots,\ m;\ i = 1,\ 2,\ \ldots,\ n)$$

forms the basis of a certain representation $\mathscr{D}$ with irreducible star $\{\boldsymbol{k}\}$.

Let us express the matrix elements of this representation in terms of those of $\mathscr{D}^{\boldsymbol{k}}(h)$, $h \in G_{\boldsymbol{k}}$. Take some element $g \in G$, and suppose that g maps $\boldsymbol{k}_i$ onto a (generally different) vector $\boldsymbol{k}_j$:

$$g\boldsymbol{k}_i = \boldsymbol{k}_j. \tag{12.20}$$

Consider the element

$$h = g_j^{-1}gg_i, \tag{12.21}$$

where g_j and g_i are the fixed elements chosen above, which map $\boldsymbol{k}$ onto $\boldsymbol{k}_j$ and $\boldsymbol{k}_i$, respectively:

$$g_i\boldsymbol{k} = \boldsymbol{k}_i,\quad g_j\boldsymbol{k} = \boldsymbol{k}_j.$$

It is easy to see that $h \in G_{\boldsymbol{k}}$, since, by (12.21), $h\boldsymbol{k} = g_j^{-1}gg_i\boldsymbol{k} = \boldsymbol{k}$. Apply g to $\varphi_{\boldsymbol{k}_i}^{(p)}$; by (12.19) and (12.18), we obtain

$$g\varphi_{\boldsymbol{k}_i}^{(p)} = g_jhg_i^{-1}\varphi_{\boldsymbol{k}_i}^{(p)} = g_jh\varphi_{\boldsymbol{k}}^{(p)} = g_j\sum_q \mathscr{D}_{qp}^{\boldsymbol{k}}(h)\,\varphi_{\boldsymbol{k}}^{(q)} = \sum_q \mathscr{D}_{qp}^{\boldsymbol{k}}(h)\,\varphi_{\boldsymbol{k}_j}^{(q)}. \tag{12.22}$$

Here h depends on i and j, by (12.21). Equation (12.22) yields the matrix elements of the representation $\mathscr{D}_{ji}^{qp}(g)$:

$$\mathscr{D}_{ji}^{qp}(g) = \mathscr{D}_{qp}^{\boldsymbol{k}}\left(g_j^{-1}gg_i\right). \tag{12.23}$$

In particular, by (12.23) the representations $\mathcal{D}(h_i)$ of the little group with elements $h_i \in G_{k_i}$ as in (12.15) are related to the representations $\mathcal{D}(h)$ of G_k by

$$\mathcal{D}^{pq}_{ii}(h_i) = \mathcal{D}^{k_i}_{pq}(h_i) = \mathcal{D}^{k}_{pq}\left(g_i^{-1} h_i g_i\right) \tag{12.24}$$

or

$$\mathcal{D}^{k_i}\left(g_i h g_i^{-1}\right) = \mathcal{D}^{k}(h).$$

The representation $\mathcal{D}^{k_i}$ to which the functions φ_{k_i} belong is usually not equivalent to $\mathcal{D}^{k}$; indeed the equality

$$\mathcal{D}^{k}(g_i^{-1} g g_i) = \mathcal{D}^{k}(g_i^{-1})\,\mathcal{D}^{k}(g)\,\mathcal{D}^{k}(g_i)$$

does not hold for arbitrary g, since the matrix $\mathcal{D}^{k}$ is defined only for elements $h \in G_k$, and g and g_i need not be elements of G_k.

Thus, equations (12.23) and (12.24) define a representation of the entire space group in terms of irreducible representations $\mathcal{D}^{k}$ of the little group.

If $\mathcal{D}^{k}$ is an irreducible representation, the corresponding representation of the space group will also be irreducible. If $\mathcal{D}^{k}$ is a unitary representation, the total representation $\mathcal{D}$ defined by equations (12.22) is also unitary.

The dimension N of an irreducible representation of the space group is obviously the product of the dimension s_k of the little representation $\mathcal{D}^{k}$ and the number of different points n in the star $\{k\}$:

$$N = s_k n. \tag{12.25}$$

In the general case of an arbitrary interior point of the Brillouin zone, where the little group is the translation subgroup, the dimension of the representation of the space group is equal to the number of points, i.e., to the order f of the crystallographic point group F.

To summarize: in order to determine the irreducible representations of the space group, we need only find the irreducible representations of the little group G_k. These representations are determined by specifying the wave vector k and the specific irreducible representation of G_k.

Representations of the Little Group G_k

The infinite group G_k has an abelian invariant subgroup, viz. its translation subgroup, and the corresponding factor group is isomorphic to the point group F_k.

Let us establish the connection between a representation $\mathcal{D}^{k}(h)$ of the little group and the representations of its factor group F_k. As noted above, every element $h \in G_k$ has the form

$$h = (r \mid a + \alpha) = (r \mid \beta), \quad \beta = a + \alpha,$$

where a is translation by the period of the Bravais lattice, r a "rotational" element, $r \in F_k$, and α the nonprimitive translation vector corresponding to the rotational element r. With each little representation $\mathcal{D}^{k}(h)$ we associate a matrix $\mathcal{D}(r)$:

$$\mathcal{D}(r) = e^{ik\beta}\mathcal{D}^{k}(h), \quad h = (r \mid \beta), \quad \beta = a + \alpha. \tag{12.26}$$

Although each rotational element r corresponds to an infinite number of elements h in the group G_k, differing by primitive translations, the matrix $\mathcal{D}(r)$ in (12.26) depends only on the rotational element r, since for any little representation $\mathcal{D}^k$, by (12.10),

$$\mathcal{D}^k(ht_a) = e^{-ika}\mathcal{D}^k(h). \tag{12.27}$$

We now establish a multiplication rule for the matrices $\mathcal{D}(r)$. Let

$$h_1 = (r_1|\beta_1), \quad \beta_1 = a_1 + \alpha_1, \quad h_2 = (r_2|\beta_2), \quad \beta_2 = a_2 + \alpha_2$$

and

$$\mathcal{D}(r_1) = e^{ik\beta_1}\mathcal{D}^k(h_1), \quad \mathcal{D}(r_2) = e^{ik\beta_2}\mathcal{D}^k(h_2).$$

Consider the product

$$\mathcal{D}(r_1)\mathcal{D}(r_2) = e^{ik(\beta_1+\beta_2)}\mathcal{D}^k(h_1h_2).$$

By (2.22a),

$$h_1h_2 = (r_1|\beta_1)(r_2|\beta_2) = (r_1r_2|\beta_1 + r_1\beta_2),$$

and so

$$\mathcal{D}^k(h_1h_2) = e^{-ik(\beta_1+r_1\beta_2)}\mathcal{D}(r_1r_2).$$

Consequently,

$$\mathcal{D}(r_1)\mathcal{D}(r_2) = \omega(r_1, r_2)\mathcal{D}(r_1r_2), \tag{12.28}$$

where

$$\omega(r_1, r_2) = e^{i\left(k - r_1^{-1}k\right)a_2} = e^{ib_1a_2}. \tag{12.29}$$

Since $b_1 \equiv k - r_1^{-1}k$ is a reciprocal lattice vector or zero, it follows that $e^{ib_1a_2} = 1$.

The appearance of the factor $\omega(r_1, r_2)$ in the multiplication law (12.28) shows that the matrices $\mathcal{D}(r)$ do not form a representation of the group F_k in the usual sense, and therefore the representations $\mathcal{D}^k(h)$ of the little group generally do not define an ordinary representation of the point group F_k. However, if $\omega(r_1, r_2) = 1$ for all $r_1, r_2 \in F_k$, then, as follows from (12.28), the matrices $\mathcal{D}(r)$ define a representation of F_k, and then equations (12.26) at once determine a representation $\mathcal{D}^k$ of the little group, given a representation of the point group. This occurs, in particular, in two very important cases:

1) the point k is inside the Brillouin zone, when $k - r^{-1}k = 0$ for all r;

2) the little group G_k does not contain nontrivial screw axes and glide planes.

If there are nontrivial screw axes or glide planes in the little group and k lies on the boundary of the Brillouin zone, the representations of the little group cannot be determined unless we construct matrices $\mathcal{D}(r)$ satisfying (12.28). The following section is devoted to this question.

§13. PROJECTIVE REPRESENTATIONS

A representation such that

$$\mathcal{D}(r_1)\mathcal{D}(r_2) = \omega(r_1, r_2)\mathcal{D}(r_1r_2), \quad \text{where} \quad |\omega(r_1, r_2)| = 1, \tag{13.1}$$

is called a projective representation or ray representation belonging to the factor system $\omega(r_1, r_2)$.*

Projective representations play an important role in applications of group theory to quantum mechanics.

A factor system is specified by h^2 coefficients $\omega(r_1, r_2)$, where h is the order of the point group $\mathcal{G}$. These coefficients cannot be arbitrary, since the associative law of group multiplication $r_1(r_2r_3) = (r_1r_2)r_3$ and equation (13.1) imply that

$$\mathcal{D}(r_1)\mathcal{D}(r_2)\mathcal{D}(r_3) = \mathcal{D}(r_1)\mathcal{D}(r_2r_3)\omega(r_2, r_3) = \\ = \mathcal{D}(r_1r_2r_3)\omega(r_1, r_2r_3)\omega(r_2, r_3) = \mathcal{D}(r_1r_2r_3)\omega(r_1r_2, r_3)\omega(r_1, r_2),$$

whence it follows that the factor system $\omega(r_1, r_2)$ must satisfy the following identities for any r_1, r_2, r_3:

$$\omega(r_1, r_2r_3)\omega(r_2, r_3) = \omega(r_1r_2, r_3)\omega(r_1, r_2). \tag{13.2}$$

It can be shown that conditions (13.2) are not only necessary but also sufficient: any set of numbers $\omega(r_1, r_2)$ satisfying (13.2) may be a factor system for the group.

However, conditions (13.2) do not define a factor system uniquely. In fact, if $\mathcal{D}(r)$ is a projective representation belonging to the factor system $\omega(r_1, r_2)$, then any other representation

$$\mathcal{D}'(r) = \frac{\mathcal{D}(r)}{u(r)}, \tag{13.3}$$

where $u(r)$ is an arbitrary single-valued function on the group $\mathcal{G}$, $|u(r)| = 1$, also defines a projective representation of the group $\mathcal{G}$, but with a different factor system $\omega'(r_1, r_2)$:

$$\mathcal{D}'(r_1)\mathcal{D}'(r_2) = \omega'(r_1, r_2)\mathcal{D}'(r_1r_2), \tag{13.4}$$

where

$$\omega'(r_1, r_2) = \frac{\omega(r_1, r_2)u(r_1r_2)}{u(r_1)u(r_2)}.$$

It is easy to prove that the new factor system $\omega'(r_1, r_2)$ also satisfies relations (13.2).

Thus, given any factor system, we can use (13.4) to obtain infinitely many new factor systems, corresponding to different choices of the function $u(r)$. Factor systems and representations satisfying (13.2) are said to be projectively equivalent or p-equivalent. The set of all p-equivalent factor systems is called a class of factor systems.

Note that two different p-equivalent representations may belong to the same factor system. For this to occur it is necessary that $u(r_1)u(r_2) = u(r_1r_2)$, i.e., the function $u(r)$ defines some (ordinary) one-dimensional representation of the group $\mathcal{G}$. In the general case, p-equivalent factor systems do not coincide. However, conditions (13.4) do not exhaust all possible factor systems for the group $\mathcal{G}$, since there may exist factor systems which cannot be

* Projective representations were first introduced by Schur, who developed a general theory of projective representations and worked out methods for constructing projective representations of finite groups /4.1/. The connection between projective representations and representations of space groups was demonstrated by Kovalev and Lyubarskii. Lyubarskii /I.3/ uses the terms loaded representation and load for projective representation and factor system $\omega(r_1, r_2)$, respectively.

reduced to one another by transformation (13.4), i.e., the group may have several classes of factor systems.

Thus, if $\omega(r_1, r_2)$ and $\omega'(r_1, r_2)$ are two factor systems such that for some pair of commuting elements a and b

$$\frac{\omega'(a, b)}{\omega'(b, a)} \neq \frac{\omega(a, b)}{\omega(b, a)},$$

these factor systems belong to different classes, since the transformation (13.4) leaves the quotient $\omega(a, b)/\omega(b, a)$ unchanged when a and b commute.

As the results of §14 will show, the converse is also true for all point groups: if

$$\frac{\omega'(a, b)}{\omega'(b, a)} = \frac{\omega(a, b)}{\omega(b, a)},$$

for every pair of commuting elements a and b, then the factor systems ω and ω' are p-equivalent. In particular, any factor system such that $\omega(a, b) = \omega(b, a)$ is p-equivalent to the identity factor system, $\omega(r_1, r_2) = 1$.

If we have the projective representations $\mathcal{D}(r)$ belonging to one factor-system $\omega(r_1, r_2)$, we can use (13.3) to find the projective representations belonging to all other factor systems $\omega'(r_1, r_2)$ of the same class. It is therefore sufficient to find the projective representations for one factor system in each class. Although the total number of possible factor systems is infinite, it can be shown that for a finite group the number of classes of factor systems is finite /I.5, 4.1/.

For every group there is a class K_0 containing a factor system all of whose coefficients are equal to unity, $\omega(r_1, r_2) = 1$. By (13.4), this class also contains any other factor system for which

$$\omega(r_1, r_2) = \frac{u(r_1)\, u(r_2)}{u(r_1 r_2)}.$$

The class K_0 with $\omega(r_1, r_2) = 1$ corresponds to the usual representations of the group $\mathcal{G}$, which in this context are called vector representations. The other representations of the class K_0 with $\omega(r_1, r_2) \neq 1$ are projectively equivalent to vector representations.

Suppose there are m classes of factor systems $K_0, K_1, \ldots, K_{m-1}$ for some group $\mathcal{G}$. Consider two classes K_p and K_q with factor systems $\omega^p(r_1, r_2)$ and $\omega^q(r_1, r_2)$ and construct the factor system

$$\omega^R(r_1, r_2) = \omega^p(r_1, r_2)\, \omega^q(r_1, r_2),$$

which is a factor system of some classes K_R. The class K_R containing $\omega^R(r_1, r_2)$ is fully determined by the classes K_p and K_q containing the factor systems ω^p and ω^q, since it follows from (13.4) that the product of factor systems p-equivalent to ω^p and ω^q is again a factor system p-equivalent to ω^R. Thus we can define multiplication of classes by

$$K_R = K_p K_q.$$

The set of classes $K_0, K_1, \ldots, K_{m-1}$ forms a group with respect to this multiplication, with the class K_0 serving as the identity element. This group is abelian, since the definition of multiplication implies $K_p K_q = K_q K_p$. It is called the multiplicator of the group $\mathcal{G}$. The order of the multiplicator is equal to the number of classes of factor systems. If the multiplicator of a group consists only of the single element K_0, the group may have only vector

representations. The number of classes of factor systems and the structure of the multiplicator are determined by the structure of the group $\mathcal{G}$.

We now consider the properties of projective representations. We first note that, as in the case of vector representations, the matrices $\mathcal{D}$ of projective representations of finite groups may always be chosen as unitary.

Two projective representations $\mathcal{D}(r)$ and $\mathcal{D}'(r)$ are said to be equivalent if there exists a unitary matrix S such that for all $r \in \mathcal{G}$

$$\mathcal{D}(r) = S\mathcal{D}'(r)S^{-1}. \tag{13.5}$$

In order to distinguish between p-equivalent representations (13.3) and equivalent representations (13.5), we shall call the latter unitarily equivalent.

Unitarily equivalent representations belong to the same factor system, since

$$\mathcal{D}'(r_1)\mathcal{D}'(r_2) = S^{-1}\mathcal{D}(r_1)\mathcal{D}(r_2)S = \omega(r_1, r_2)\mathcal{D}'(r_1r_2). \tag{13.6}$$

We saw above that p-equivalent representations may belong to the same factor system in a special case, but such projective representations are generally not unitarily equivalent.

A projective representation $\mathcal{D}$ is said to be irreducible if there exists a matrix S such that for all representation matrices $\mathcal{D}(r)$ the equivalent matrix $\mathcal{D}'(r)$ (see (13.5)) decomposes into invariant submatrices of lower order.

An essential feature of projective representations is that if a group $\mathcal{G}$ has several classes of factor systems, then only the class K_0 may correspond to one-dimensional representations (e.g., the identity representation) and there will be no one-dimensional representations for classes $K_p \neq K_0$. To prove this, suppose that $\mathcal{D}_0(r)$ is a one-dimensional representation,

$$\mathcal{D}_0(r_1)\mathcal{D}_0(r_2) = \omega^p(r_1, r_2)\mathcal{D}_0(r_1r_2), \tag{13.7}$$

belonging to a factor system $\omega^p(r_1, r_2)$ in the class K_p. Letting $u(r)$ be the representation $\mathcal{D}_0(r)$ itself, we see from (13.4) and (13.7) that the factor system $\omega^p(r_1, r_2)$ is p-equivalent to the factor system $\omega'^p(r_1, r_2) = 1$, i.e., $\omega^p(r_1, r_2)$ is in the class K_0. Thus classes $K_p \neq K_0$ cannot correspond to one-dimensional representations.

The number of classes of factor systems and the structure of the multiplicator depend on the properties of the group $\mathcal{G}$. Schur /4.1/ described a general method to construct all projective representations of a finite group, reducing the problem to finding the vector (usual) representations of a certain expanded group $\mathcal{G}'$. To construct the group $\mathcal{G}'$ we must first find the multiplicator of the group $\mathcal{G}$.

Let $\mathcal{G}$ be defined by generators $a, b, c, \ldots$, satisfying the ν relations

$$a^{n_i}b^{l_i}c^{p_i}\ldots = e \qquad (i = 1, 2, \ldots, \nu), \tag{13.8}$$

where n_i, l_i, p_i are integers. Let $A = \mathcal{D}(a), B = \mathcal{D}(b), C = \mathcal{D}(c)$, etc., be the matrices of an irreducible representation $\mathcal{D}$ of $\mathcal{G}$ for the generators $a, b, c, \ldots$

If $\mathcal{D}$ is a vector representation of $\mathcal{G}$, the matrices $A, B, C, \ldots$ satisfy the same relations as the generators:

$$A^{n_i}B^{l_i}C^{p_i}\ldots = I \qquad (i = 1, 2, \ldots, \nu). \tag{13.9}$$

In the case of projective representations, however, we have additional numerical factors α_i ($|\alpha_i| = 1$), determined by the coefficients of the factor system, and conditions (13.9) become*

$$\alpha_i A^{n_i} B^{l_i} C^{p_i} \ldots = I, \tag{13.10}$$

where

$$\alpha_i^{-1} = \{\omega(a^{n_i}, b^{l_i}c^{p_i} \ldots)\,\omega(b^{l_i}, c^{p_i} \ldots) \ldots\}\,\omega_{an_i}\omega_{bl_i}\omega_{cp_i} \ldots, \tag{13.11}$$

$$\begin{aligned} \omega_{an_i} &= \omega(a, a)\,\omega(a, a^2) \ldots \omega(a, a^{n_i-1}), \\ \omega_{bl_i} &= \omega(b, b)\,\omega(b, b^2) \ldots \omega(b, b^{l_i-1}) \end{aligned} \tag{13.12}$$

and so on. Going over to the p-equivalent representations

$$A' = \frac{A}{u(a)}, \quad B' = \frac{B}{u(b)}, \quad C' = \frac{C}{u(c)}, \ldots, \tag{13.13}$$

we obtain

$$\alpha_i' A'^{n_i} B'^{l_i} C'^{p_i} \ldots = I, \tag{13.14}$$

where

$$\alpha_i' = \alpha_i u^{n_i}(a)\,u^{l_i}(b)\,u^{p_i}(c) \ldots \tag{13.15}$$

If a suitable choice of the functions $u(a)$, $u(b)$ $u(c)$, ... will reduce (13.14) to (13.9), i.e., make all the α_i' equal to unity, the projective representations of $\mathfrak{G}$ are equivalent to its vector representations. In the general case, however, the coefficients α_i' cannot all be normalized to unity by any choice of the functions u, so that (13.14) will always involve a certain minimal number of independent coefficients α_i'. Let this number be $\nu' \leqslant \nu$. In the sequel we shall assume that conditions (13.14) contain only such independent parameters α_i'.

Conditions (13.14) yield equations for the possible values of the coefficients α_i'. By varying the functions $u(a)$, $u(b)$, $u(c)$, ... we can simplify these equations. As we shall see from the results of §14, for all 32 point groups appearing in the space groups these equations may be expressed in the form

$$\alpha_i'^{\,2} = 1 \qquad (i = 1, 2, \ldots, \nu'). \tag{13.16}$$

Equations (13.16) yield all possible p-inequivalent values for the coefficients α_i', including, of course, the values $\alpha_i' = 1$ for vector representations. Each set of solutions α_i' of equations (13.16) defines a class of factor systems, since it follows from the definition of α_i' that all p-equivalent factor systems are characterized by the same set of values α_i'. In the case of the point groups, for which $\alpha_i' = \pm 1$, the number of classes (order of the multiplicator) is $2^{\nu'}$.

If two solutions α_i' (1) and α_i' (2) correspond to classes of factor systems K_1 and K_2, the solution α_i' (3) $= \alpha_i'$ (1) α_i' (2) corresponds to the class $K_3 = K_1K_2$. Setting up all possible products of admissible solutions α_i', we obtain the multiplication law for classes of factor systems, in other words, the structure

* From now on we shall assume that $\omega(e, e) = 1$ for every factor system. This can always be achieved by putting $u(e) = \omega(e, e)$, for $\mathfrak{D}(e) = I$. It is clear from (12.29) that for space groups the condition $\omega(e, e) = 1$ is fulfilled identically, as follows from the definition of a factor system. This condition and identity (13.2) imply that $\omega(e, r) = \omega(r, e) = 1$ for all r. For space groups this also follows from (12.29).

of the multiplicator. Note that the admissible solutions α_i' form a representation of the multiplicator. This method will be used in §14 to construct multiplicators for all the 32 crystallographic point groups.

We shall now view the α_i' not as numerical coefficients but as abstract elements α_i which commute with each other and satisfy the equations

$$\alpha_i^2 = e, \quad \alpha_i\alpha_j = \alpha_j\alpha_i \qquad (i, j = 1, 2, \ldots, \nu'). \tag{13.17}$$

Conditions (13.17) define a group H with generators α_i. This group contains $2^{\nu'}$ elements h of the form

$$h = \prod_{i=1, 2, \ldots, \nu'} \alpha_i^{p_i} \qquad (p_i = 0, 1). \tag{13.18}$$

The group H whose elements are $h_1 = e, h_2, \ldots, h_m$ $(m = 2^{\nu'})$ is isomorphic to the multiplicator.

Now let $\mathcal{G}'$ be a group on generators $a, b, c, \ldots, \alpha_i$, defined by relations analogous to (13.14). The generators α_i of the group H commute with all elements of the group $\mathcal{G}$. Thus $\mathcal{G}'$ is defined by the relations

$$\begin{gathered} \alpha_i a^{n_i} b^{l_i} c^{p_i} = e, \quad \alpha_i^2 = e, \quad a\alpha_i = \alpha_i a, \quad b\alpha_i = \alpha_i b, \\ c\alpha_i = \alpha_i c, \ \ldots, \ \alpha_i\alpha_j = \alpha_j\alpha_i. \end{gathered} \tag{13.19}$$

Each element g' of $\mathcal{G}'$ has the form $g' = hr$, where $h \in H$, $r \in \mathcal{G}$. If two elements r_1 and r_2 have a product r_3 in the group G, $r_1 r_2 = r_3$, their product in the group $\mathcal{G}$ will generally involve in addition an element h of H, depending on the elements r_1 and r_2 and denoted by h_{12}:

$$r_1 r_2 = h_{12} r_3. \tag{13.20}$$

H is the center of $\mathcal{G}'$, since by the construction of $\mathcal{G}'$ all its elements commute with the elements of H. Partition $\mathcal{G}'$ into its cosets S_i relative to the subgroup H:*

$$S_0 = \{H\}, \quad S_1 = \{r_1 H\}, \quad S_2 = \{r_2 H\}, \ \ldots, \ S_k = \{r_k H\}, \tag{13.21}$$

where $r_i \in \mathcal{G}$. The factor group by H, i.e., the group with elements S_0, S_1, ..., S_k, is isomorphic to $\mathcal{G}$.

Indeed, we establish a one–one correspondence between the elements S_i of the factor group and the elements r_i of $\mathcal{G}$ in the following manner:

$$S_i \longleftrightarrow r_i. \tag{13.22}$$

Then, if $S_i \longleftrightarrow r_i$ and $S_j \longleftrightarrow r_j$, we have $S_i S_j \longleftrightarrow r_i r_j$, since the product $S_i S_j$ is the set of all possible elements $r_i r_j h$, i.e., the set $\{r_i r_j H\}$, to which corresponds the element $r_i r_j$. It follows that $\mathcal{G}'$ is homomorphic to $\mathcal{G}$, and the kernel of the homomorphism, the subgroup H, is isomorphic to the multiplicator.

The resulting group $\mathcal{G}'$ of order mk is called the representation group of $\mathcal{G}$. We shall now show that all projective representations of $\mathcal{G}$ may be obtained from vector representations of $\mathcal{G}'$.

Let $\mathcal{D}_\mu$ be any vector representation of $\mathcal{G}'$. Let $r_1, r_2 \in \mathcal{G}$. Their product in $\mathcal{G}'$, as noted above, generally involves an element $h_{12} \in H$ (13.20). Since $\mathcal{D}_\mu$ is a vector representation, it follows from (13.20) that

$$\mathcal{D}_\mu(r_1)\,\mathcal{D}_\mu(r_2) = \mathcal{D}_\mu(h_{12} r_3) = \mathcal{D}_\mu(h_{12})\,\mathcal{D}_\mu(r_3). \tag{13.23}$$

* [The center of a group is always an invariant subgroup. — Trans. editor.]

Since h_{12} commutes with all elements of $\mathcal{G}'$, $\mathcal{D}_\mu(h_{12})$ commutes with all matrices $\mathcal{D}_\mu(g')$, $g' \in \mathcal{G}'$. Thus, by Schur's first lemma (equation (8.1a)), $\mathcal{D}_\mu(h_{12})$ is a multiple of the identity matrix,

$$\mathcal{D}_\mu(h_{12}) = \omega_{12}^\mu I, \tag{13.24}$$

and (13.23) becomes

$$\mathcal{D}_\mu(r_1)\,\mathcal{D}_\mu(r_2) = \omega_{12}^\mu\,\mathcal{D}_\mu(r_3) = \omega_{12}^\mu\,\mathcal{D}_\mu(r_1 r_2). \tag{13.25}$$

Now consider the set of matrices $\mathcal{D}_\mu(r)$ for elements $r \in \mathcal{G}$ only. These matrices satisfy the multiplication law (13.25), so they define a projective representation of $\mathcal{G}$ in which the numbers ω_{12}^μ of (13.24) serve as the factor system $\omega(r_1, r_2)$. The defining relations for $\mathcal{G}'$ (13.19) imply similar relations for the matrix elements of the representation $\mathcal{D}_\mu(r)$:

$$\mathcal{D}_\mu(a_i)\,\mathcal{D}_\mu(a^{n_i})\,\mathcal{D}_\mu(b^{l_i})\,\mathcal{D}_\mu(c^{p_i})\ldots = \alpha_i'^{\mu}\,(\mathcal{D}_\mu(a))^{n_i}(\mathcal{D}_\mu(b))^{l_i}(\mathcal{D}_\mu(c))^{p_i}\ldots = I, \tag{13.26}$$

since by (13.24) we have $\mathcal{D}_\mu(a_i) = \alpha_i'^{\mu} I$, where $\alpha_i'^{\mu}$ is a number ($(\alpha_i'^{\mu})^2 = 1$). Conditions (13 26) are precisely conditions (13.14) for the matrix elements of projective representations. Therefore, every projective representation thus obtained belongs to some class of factor systems for the group $\mathcal{G}$.

We claim that the set of all irreducible representations $\mathcal{D}_\mu$ of the group $\mathcal{G}'$ yields projective representations belonging to all classes of factor systems.

Indeed, any irreducible representation $\mathcal{D}_\mu$ of $\mathcal{G}'$ clearly defines a certain (generally reducible) representation of its abelian subgroup H, and the numbers ω^μ of (13.24) define irreducible representations of H. Since the set of all irreducible representations $\mathcal{D}_\mu$ yields all the irreducible representations of H, the values of the coefficients ω and, in particular, the values of the coefficients α_i', exhaust all possible values of the matrix elements of representations of H. Since the generators a_i of H satisfy equations (13.17), the set of all values of $\mathcal{D}_\mu(a_i)$ coincides with the set of all solutions of equations (13.16); thus these are precisely all possible values of the coefficients in (13.14), which determine the class of factor systems. Thus the projective representations obtained from a full set of representations of $\mathcal{G}'$ include representations belonging to all the classes of factor systems for the group $\mathcal{G}$.

As noted above, for space groups we have $\alpha_i' = \pm 1$, and by (13.18) the possible values of ω_{12} are also ± 1. Consequently, for space groups each class contains a factor system all of whose coefficients $\omega(r_1, r_2)$ are equal to ± 1.

It is easy to see that if two representations $\mathcal{D}_\mu$ of the representation group $\mathcal{G}'$ are irreducible and inequivalent, then the corresponding projective representations are also irreducible and (unitarily) inequivalent. The converse is also true: given any irreducible projective representation of the group $\mathcal{G}$, we can construct an irreducible vector representation of the group $\mathcal{G}'$. Thus the full set of inequivalent irreducible representations of the representation group $\mathcal{G}'$ yields all unitarily inequivalent irreducible projective representations of the group $\mathcal{G}$, belonging to all possible classes of factor systems.

Thus determination of all irreducible projective representations of a finite group $\mathcal{G}$ reduces to the problem of finding the usual representations

of the representation group $\mathcal{G}'$. The solution of the latter problem is known in principle, though in general it is quite laborious.*

We now consider the orthogonality relations for projective representations belonging to one factor system; these will follow from the orthogonality relations for representations of $\mathcal{G}'$.

Any irreducible representations $\mathcal{D}_\mu$ and $\mathcal{D}_{\mu'}$ of $\mathcal{G}'$ satisfy the orthogonality relation (8.10):

$$\sum_{g' \in \mathcal{G}'} \mathcal{D}^{\mu}_{ik}(g')\, \mathcal{D}^{*\mu'}_{jl}(g') = \frac{m\hbar}{n_\mu} \delta_{ij}\delta_{kl}\delta_{\mu\mu'}, \tag{13.27}$$

where n_μ is the dimension of the representation $\mathcal{D}_\mu$. Each element of $\mathcal{G}'$ has the form $g' = hr$, so that instead of summing over $g' \in \mathcal{G}'$ in (13.27) we can sum over $r \in \mathcal{G}$ and $h \in H$. We then obtain from (13.27)

$$\sum_{g' \in \mathcal{G}'} \mathcal{D}^{\mu}_{ik}(g')\, \mathcal{D}^{*\mu'}_{jl}(g') = \sum_{h \in H} \omega^{\mu}_{h} \omega^{*\mu'}_{h} \sum_{r \in \mathcal{G}} \mathcal{D}^{\mu}_{ik}(r)\, \mathcal{D}^{*\mu'}_{jl}(r), \tag{13.28}$$

where ω^{μ}_{h} is defined by (13.23), (13.24).

The representations $\mathcal{D}_\mu$ and $\mathcal{D}_{\mu'}$ may lead to either identical or different factor systems. Let μ and μ' be representations which lead to the same factor system; then

$$\sum_h \omega^{\mu}_{h}\, \omega^{*\mu'}_{h} = \sum_h |\omega^{\mu}_{h}|^2 = m,$$

and (13.28) yields an orthogonality relation for projective representations belonging to the factor system in question:

$$\sum_r \mathcal{D}^{\mu}_{ik}(r)\, \mathcal{D}^{*\mu'}_{jl}(r) = \frac{h}{n_\mu} \delta_{ij}\delta_{kl}\delta_{\mu\mu'}, \tag{13.29}$$

which is reminiscent of the corresponding orthogonality condition for vector representations. In (13.29) the indices μ and μ' denote distinct irreducible projective representations belonging to the same factor system. If μ and μ' are such that $\mathcal{D}_\mu$ and $\mathcal{D}_{\mu'}$ define projective representations belonging to different factor systems, we have from (8.10) that

$$\sum_h \omega^{\mu}_{h}\, \omega^{*\mu'}_{h} = 0, \tag{13.30}$$

since ω^{μ}_{h} and $\omega^{\mu'}_{h}$ form different one-dimensional representations of the group H, and in this case (13.29) holds identically.

In order to obtain the second orthogonality relation for the projective representations, we use the relations (8.14) for representations of $\mathcal{G}'$, for elements g'_1 and g'_2:

$$\sum_{\mu jl} n_\mu \mathcal{D}^{\mu}_{jl}(g'_1)\, \mathcal{D}^{*\mu}_{jl}(g'_2) = m\hbar\delta_{g'_1 g'_2}.$$

* If the functions $u(a)$ in (13.15) are not optimally chosen, so that the number of elements of the group H defined by relations (13.17) exceeds the number of elements of the multiplicator, the group $\mathcal{G}''$ defined by relations (13.19) will also have a larger number of elements than the representation group. Clearly, every vector representation of the group $\mathcal{G}''$, which is known as the covering group of $\mathcal{G}$, also determines projective representations of $\mathcal{G}$. However, if the covering group does not coincide with the representation group, some of these representations will be projectively equivalent.

Set $g_1' = hr_1$ and $g_2' = r_2$, where $r_1, r_2 \in \mathcal{G}$, $h \in H$. Then

$$\sum_{\mu jl} n_\mu \mathcal{D}^\mu_{jl}(r_1 h)\, \mathcal{D}^{*\mu}_{jl}(r_2) = \sum_{\mu jl} n_\mu \omega^\mu_h \mathcal{D}^\mu_{jl}(r_1)\, \mathcal{D}^{*\mu}_{jl}(r_2) = m\hbar\, \delta_{he}\delta_{r_1 r_2}. \tag{13.31}$$

Multiplying both sides of (13.31) by $\omega^{*\mu'}_h$ and summing over $h \in H$, we obtain

$$\sum_{\mu} \sum_{h \in H} \omega^\mu_h \omega^{*\mu'}_h \sum_{jl} n_\mu \mathcal{D}^\mu_{jl}(r_1)\, \mathcal{D}^{*\mu}_{jl}(r_2) = m\hbar\delta_{r_1 r_2}\omega^{*\mu'}_e = m\hbar\delta_{r_1 r_2}, \tag{13.32}$$

since it follows from (13.23) and (13.24) that $\omega^{\mu'}_e = 1$. Since ω^μ_h and $\omega^{\mu'}_h$ define a certain irreducible representation of the group H, it follows via (13.30) that the sum

$$\sum_{h \in H} \omega^\mu_h \omega^{*\mu'}_h$$

fails to vanish only if the representations ω^μ_h and $\omega^{\mu'}_h$ of H induced by the representation $\mathcal{D}^\mu$ and $\mathcal{D}^{\mu'}$ of $\mathcal{G}'$ are unitarily equivalent, i.e., if ω^μ_h and $\omega^{\mu'}_h$ form the same factor system. If this is so,

$$\sum_{h \in H} \omega^\mu_h \omega^{*\mu'}_h = m.$$

On the left of (13.31), therefore, we need only sum over representations μ belonging to the same factor system as μ', and (13.32) yields the second orthogonality relation for projective representations belonging to the same factor system:

$$\sum_{\mu jl} n_\mu \mathcal{D}^\mu_{jl}(r_1)\, \mathcal{D}^{*\mu}_{jl}(r_2) = \hbar\delta_{r_1 r_2}. \tag{13.33}$$

It follows from the first orthogonality relation (13.29) for projective representations that the vectors $\mathcal{D}^\mu_{ik}\sqrt{n_\mu/\hbar}$ form an orthonormal system in the $\hbar$-dimensional space spanned by the elements of the group $\mathcal{G}$. Since the number $\sum_\mu n^2_\mu$ of these vectors is at most the dimension $\hbar$ of the space, we have

$$\sum_\mu n^2_\mu \leqslant \hbar.$$

On the other hand, the second orthogonality relation (13.33) implies that the vectors $\mathcal{D}^\mu_{jl}(r)\sqrt{n_\mu/\hbar}$, $r \in \mathcal{G}$, with components μ, j, l form an orthonormal system in a space of dimension $\sum_\mu n^2_\mu$; hence the inequality

$$\hbar \leqslant \sum_\mu n^2_\mu.$$

Consequently, Burnside's theorem is also valid for projective representations belonging to the same factor system:

$$\sum_\mu n^2_\mu = \hbar. \tag{13.34}$$

The character of a projective representation $\mathcal{D}_\mu$ is defined as in the case of vector representations as the trace of the matrices of $\mathcal{D}_\mu$:

$$\chi_\mu(r) = \mathrm{Tr}\,\mathcal{D}_\mu(r) = \sum_t \mathcal{D}^\mu_{tt}(r), \tag{13.35}$$

and is the same for all unitarily equivalent representations.

The orthogonality relations for projective representations imply an orthogonality condition for the characters of irreducible projective representations:

$$\sum_{r \in \mathcal{G}} \chi_\mu^*(r)\,\chi_{\mu'}(r) = h\delta_{\mu\mu'}. \tag{13.36}$$

Relations (13.36) enable us to decompose any reducible projective representation into irreducible representations belonging to the same factor system as the original one:

$$\mathcal{D} = \sum_\mu a_\mu \mathcal{D}_\mu, \tag{13.37}$$

where, as in (8.19), the coefficients a_μ are given by

$$a_\mu = \frac{1}{h}\sum_r \chi(r)\,\chi_\mu^*(r), \tag{13.38}$$

and $\chi(r)$ is the character of the representation $\mathcal{D}$.

The characters of projective representations are not functions of the conjugate classes of the group $\mathcal{G}$. They are indeed functions of conjugate classes in the group $\mathcal{G}'$, but the distribution of elements over classes in the groups $\mathcal{G}$ and $\mathcal{G}'$ is generally different, for elements which are conjugates in $\mathcal{G}$ need not be conjugates in $\mathcal{G}'$.

It is easy to show directly that

$$\chi(r_1 r_2 r_1^{-1}) = \frac{\omega(r_1^{-1}, r_1)}{\omega(r_1, r_2 r_1^{-1})\,\omega(r_2, r_1^{-1})}\,\chi(r_2) \tag{13.39}$$

and in the general case $\chi(r_1 r_2 r_1^{-1}) \neq \chi(r_2)$. Thus the second orthogonality relation (8.23) fails to hold for projective representations, and the number of projective representations for all classes of factor systems other than K_0 is less than the number of conjugate classes in $\mathcal{G}$.

We note one property of the characters of projective representations. If the factor system is not symmetric for some pair of commuting elements r_1, $r_2 \in \mathcal{G}$, i.e., $\frac{\omega(r_1, r_2)}{\omega(r_2, r_1)} = \alpha \neq 1$, $r_1 r_2 = r_2 r_1$, then the characters of these elements in all p-equivalent representations vanish:

$$\chi(r_1) = \chi(r_2) = 0.$$

Indeed, it follows from the condition $\mathcal{D}(r_1)\mathcal{D}(r_2) = \alpha\mathcal{D}(r_2)\mathcal{D}(r_1)$ that $\mathcal{D}^{-1}(r_2)\mathcal{D}(r_1)\mathcal{D}(r_2) = \alpha\mathcal{D}(r_1)$, whence $(\alpha - 1)\chi(r_1) = 0$, and if $\alpha \neq 1$ we have $\chi(r_1) = 0$. The proof that $\chi(r_2) = 0$ is similar.

Consider the product of two projective representations $\mathcal{D} = \mathcal{D}_1 \times \mathcal{D}_2$ belonging to factor systems $\omega^p(r_1, r_2)$, $\omega^q(r_1, r_2)$ in classes K_p and K_q, respectively. The product of the representations belongs to the factor system $\omega^R(r_1, r_2)$, the product of the original factor systems:

$$\omega^R(r_1, r_2) = \omega^p(r_1, r_2)\,\omega^q(r_1, r_2); \tag{13.40}$$

this factor system is in the class $K_R = K_p K_q$. A product of irreducible projective representations is in general reducible and may be decomposed as in (13.37) and (13.38) into irreducible representations belonging to class K_R.

§14. PROJECTIVE REPRESENTATIONS OF POINT GROUPS

In §12 we showed that determination of the irreducible representations of a space group G which have an irreducible star $\{\boldsymbol{k}\}$ reduces to finding the projective representations of point group $F_{\boldsymbol{k}}$ which is a subgroup of the little group G_k. The group $F_{\boldsymbol{k}}$ may be any subgroup of the crystallographic point group F characterizing the crystal class of the crystal lattice. The totality of all subgroups of the 32 crystallographic point groups consists of the 32 groups themselves; thus, in order to find the irreducible representations of all 230 space groups all we need to know is the projective representations of the 32 point groups described in §6.

To determine the classes of factor systems and the projective representations of the point groups we use the method of the preceding section.

We first consider cyclic groups of order n, i.e. groups with one generator a and defining relation

$$a^n = e. \tag{14.1}$$

Let $\mathcal{D}(a) = \boldsymbol{A}$ be the matrix of an irreducible projective representation corresponding to the element a. Then, by (14.1) and (13.11),

$$\boldsymbol{A}^n = \omega_{an}\boldsymbol{I}, \tag{14.2}$$

where

$$\omega_{an} = \omega(a, a)\,\omega(a, a^2)\,\ldots\,\omega(a, a^{n-1}). \tag{14.3}$$

Set

$$\boldsymbol{A}' = \mathcal{D}'(a) = \omega_{an}^{-1/n}\boldsymbol{A}. \tag{14.4}$$

Then (14.2) becomes

$$\boldsymbol{A}'^n = \boldsymbol{I}. \tag{14.5}$$

Hence all the projective representations of cyclic groups are p-equivalent to vector representations. The multiplicator of a cyclic group consists of one element, the class K_0. Since all vector representation of cyclic groups are one-dimensional, all projective representations of cyclic groups are also one-dimensional.

It is easy to see that the function $u(a^k)$ converting a factor system $\omega(a^k, a^p)$ into the identity factor system via (13.4) has the form

$$u(a^k) = \frac{\omega_{an}^{k/n}}{\omega_{ak}}. \tag{14.6}$$

The matrices $\mathcal{D}(a^k)$ are then related to the matrices $\mathcal{D}'(a^k) = (\mathcal{D}'(a))^k = \boldsymbol{A}'^k$, which define vector representations of cyclic groups, by (13.3):

$$\mathcal{D}(a^k) = \boldsymbol{A}'^k\,u(a^k). \tag{14.7}$$

Indeed, it follows from (13.4) and (14.6) that

$$\omega'(a, a^k) = \frac{u(a^{k+1})\,\omega(a, a^k)}{u(a)\,u(a^k)} = 1.$$

Hence $\mathcal{D}'(a^k) = \mathcal{D}'(a)\,\mathcal{D}'(a^{k-1}) = \ldots = \mathcal{D}'^k(a)$. This means that $\omega'(a^k, a^p) = 1$ for all k and p.

Of the 32 point groups cited in § 6, ten groups, e, S_2, C_s, C_2, S_4, C_4, C_3, S_6, C_6, C_{3h}, are cyclic; therefore, whenever the crystallographic point group is one of these, (14.7) defines all the projective representations belonging to the factor system in question.

Now consider a group with two commuting generators a and b of order n and m, respectively, and defining relations

$$a^n = e, \quad b^m = e, \quad ab = ba. \tag{14.8}$$

Examples of these groups are the groups C_{nh} ($a = c_n$, $b = \sigma_h$, $m = 2$).

Let $\boldsymbol{A}' = \mathfrak{D}(a)$ and $\boldsymbol{B}' = \mathfrak{D}(b)$ be matrices of a projective representation for the elements a and b; by (13.14) and (14.8),

$$\boldsymbol{A}'^n = \omega_{an}\boldsymbol{I}, \quad \boldsymbol{B}'^m = \omega_{bm}\boldsymbol{I}, \quad \boldsymbol{A}'\boldsymbol{B}' = \boldsymbol{B}'\boldsymbol{A}'\alpha, \tag{14.9}$$

$$\alpha = \frac{\omega(a, b)}{\omega(b, a)}. \tag{14.10}$$

We set $\boldsymbol{A} = \omega_{an}^{-1/n}\boldsymbol{A}'$ and $\boldsymbol{B} = \omega_{bm}^{-1/m}\boldsymbol{B}'$; then, by (14.9),

$$\boldsymbol{A}^n = \boldsymbol{I}, \quad \boldsymbol{B}^m = \boldsymbol{I}, \quad \boldsymbol{AB} = \boldsymbol{BA}\alpha. \tag{14.11}$$

To determine the possible values of the constant α, multiply both sides of the last equality by $\boldsymbol{A}$; using the commutation relation (14.11) for $\boldsymbol{A}$ and $\boldsymbol{B}$, we obtain $\boldsymbol{A}^2\boldsymbol{B} = \alpha^2\boldsymbol{B}\boldsymbol{A}^2$. Repeating this procedure n times and remembering that $\boldsymbol{A}^n = \boldsymbol{I}$, we obtain

$$\alpha^n = 1. \tag{14.12}$$

Multiplying (14.11) by $\boldsymbol{B}$ m times, we see similarly that

$$\alpha^m = 1. \tag{14.13}$$

Let d be the greatest common divisor of n and m; then equations (14.12) and (14.13) may be combined:

$$\alpha^d = 1. \tag{14.14}$$

If n and m are relatively prime, then $d = 1$ and $\alpha = 1$. Hence it follows that for the groups C_{nh} with odd n all projective representations are p-equivalent to vector representations. This also follows from the fact that, as shown in § 3, these groups are cyclic with generator $a = c_{2n}i$.

When n is even, i.e., for the point groups $C_{2p,h}$ (C_{2h}, C_{4h}, C_{6h}), we have $d = 2$ and therefore, by (14.14),

$$\alpha^2 = 1, \text{ i.e., } \alpha = \pm 1. \tag{14.15}$$

For these groups, then, there are two classes of factor systems, K_0 and K_1, corresponding to $\alpha = 1$ and $\alpha = -1$. The class K_0, as usual, corresponds to the vector representations. Since the groups (14.8) are abelian, all their vector representations are one-dimensional, and consequently so are the projective representations belonging to class K_0. The matrices $\boldsymbol{A}'$ and $\boldsymbol{B}'$ of a representation belonging to class K_1 ($\alpha = -1$) anticommute, and therefore none of the projective representations of class K_1 is one-dimensional. This agrees with the general theory of § 13.

In order to construct the representation group with defining relations (13.19), we adjoin to the elements a and b a new second order element α which commutes with a and b. By (13.19), (14.11), (14.15) the representation group is defined by the relations

$$a^n = e, \quad b^m = e, \quad \alpha^2 = e, \quad ab = \alpha ba, \quad \alpha b = b\alpha, \quad \alpha a = a\alpha. \tag{14.16}$$

Using (13.24) and (14.16), we easily obtain the factor system $\omega'(a^k, b^p)$ for the projective representations of the group (14.8) induced by vector representations of the group (14.16). If $r_1 = a^k b^p$, $r_2 = a^{k'} b^{p'}$, then, using (14.16), we obtain

$$r_1 r_2 = a^k b^p a^{k'} b^{p'} = \alpha^{k'p} a^{k+k'} b^{p+p'}, \text{ i.e., } h_{12} = \alpha^{k'p},$$

and (13.20) and (13.25) imply that

$$\omega'(a^k b^p, a^{k'} b^{p'}) = \alpha^{k'p}, \qquad \text{where} \quad \alpha = \pm 1. \tag{14.17}$$

Below we shall obtain all the unitarily inequivalent projective representations of the group (14.8) that belong to the factor system (14.17).

Certain questions arise in practical applications: how can we classify a given factor system as belonging to a particular class according to its form? How should we choose the functions u in order to convert a given factor system via (13.4) to the standard form (14.17) corresponding to its class?

The answer to the first question is given by equation (14.10). If $\frac{\omega(a, b)}{\omega(b, a)} = 1$ for a given factor system, it belongs to class K_0; if $\frac{\omega(a, b)}{\omega(b, a)} = -1$, it belongs to class K_1.

We define $u(a^q b^p)$ by

$$u(a^q b^p) = u(b^p a^q) = \frac{u(a^q)\, u(b^p)}{\omega(a^q, b^p)}, \tag{14.18}$$

where $u(a^q)$ and $u(b^p)$ are defined as in (14.6):

$$u(a^q) = \frac{\omega_{an}^{q/n}}{\omega_{aq}}, \quad u(b^p) = \frac{\omega_{bm}^{p/m}}{\omega_{bp}}. \tag{14.19}$$

Substituting (14.18) into (13.4), we obtain $\omega'(a^k, b^p) = 1$, whence

$$\omega'(a^k b^p, a^{k'} b^{p'}) = \frac{\mathcal{D}'(a^k b^p)\, \mathcal{D}'(a^{k'} b^{p'})}{\mathcal{D}'(a^{k+k'} b^{p+p'})} = \frac{\mathcal{D}'^{k}(a)\, \mathcal{D}'^{p}(b)\, \mathcal{D}'^{k'}(a)\, \mathcal{D}'^{p'}(b)}{\mathcal{D}'^{k+k'}(a)\, \mathcal{D}'^{p+p'}(b)} = \alpha^{pk'}, \tag{14.20}$$

i.e., ω' is indeed the standard factor system (14.17).

Thus, if all the unitarily inequivalent irreducible representations that belong to the factor system (14.17) are known, we can construct all the irreducible representations for an arbitrary factor system by (13.3) and (14.18), (14.19).

Since in all groups the class K_0 corresponds to the usual representations, we shall confine ourselves below to projective representations belonging to the other classes of factor systems.

Since the groups C_{2v} and D_2 are isomorphic to C_{2h}, the results obtained for C_{2h} are also applicable to the former groups. By Burnside's theorem, the class K_1 for the four-group C_{2h} corresponds to one two-dimensional representation. Since the matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ anticommute when $\alpha = -1$, and $\boldsymbol{A}^2 = \boldsymbol{B}^2 = \boldsymbol{I}$, they may be chosen as any two of the three Pauli matrices σ_x, σ_y, σ_z. The representation matrices for the group C_{2h} are shown in Table 14.2 at the end of the section.

The representation for an arbitrary element $a^q b^p$ of the group C_{nh} is

$$\mathcal{D}(a^q b^p) = \mathcal{D}(b^p a^q) = \boldsymbol{A}^q \boldsymbol{B}^p = \alpha^{pq} \boldsymbol{B}^p \boldsymbol{A}^q. \tag{14.21}$$

By (13.4) the matrices of a representation of the group C_{nh} belonging to a given factor system $\omega(r_1, r_2)$ are

$$\mathcal{D}(a^q b^p) = u(a^q b^p) A^q B^p, \tag{14.22}$$

where $u(a^k b^p)$ is defined by (14.18) and (14.19).

There are eight elements in the group C_{4h}; therefore, by Burnside's theorem (13.34), it has two two-dimensional representations, belonging to class K_1.

For one of these representations, we can take the matrices of the representation of the group C_{2h} as the matrices.

To find the matrices of the second irreducible representation of C_{4h} in class K_1, we make the following observation. If instead of the matrix A for C_{nh} we consider $A'' = \varepsilon_n^q A$ ($\varepsilon_n = e^{2\pi i/n}$, $q = 0, 1, 2, \ldots, n-1$), the matrices A'' will also satisfy relations (14.11). In the general case, however, not all the matrices $\varepsilon_n^q A$ and A are unitarily nonequivalent. Indeed, the matrices A and $\varepsilon_n^q A$ are unitarily inequivalent for $q = 1, 2, \ldots, (n/2) - 1$ and even n, since otherwise there would exist a matrix S such that $SAS^{-1} = \varepsilon_n^q A$. Squaring this equality and remembering that $A^2 = I$, we see that $\varepsilon_n^{2q} = 1$, but this contradicts the choice of $q < n/2$. Each of the remaining matrices $A\varepsilon_n^q$ ($q = n/2, \ldots, n-1$) is unitarily equivalent to one of the matrices $A\varepsilon_n^q$ ($q = 0, 1, \ldots, (n/2) - 1$). Thus, for example, A is unitarily equivalent to the matrix $-A = A\varepsilon_n^{n/2}$, as can be checked directly by setting $S = \sigma_x$.

Thus the other unitarily inequivalent representation of the group C_{4h} in class K_1 may be obtained by multiplying the matrices A of the representation of the group C_{2h} by $\varepsilon_4 = i$.

There are twelve elements in the group C_{6h}, so by Burnside's theorem there are three two-dimensional representations in class K_1; these are presented in Table 14.2 at the end of the section.

Group D_n. The groups D_n and the isomorphic groups C_{nv} are also defined by two generators: $a = c_n$; $b = u_2$ for D_n, $b = \sigma_v$ for C_{nv}. The defining relations (3.4) are:

$$a^n = e, \quad b^2 = e, \quad ba = a^{n-1}b.$$

Let

$$A' = \frac{\mathcal{D}(a)}{\omega_{an}^{1/n}}, \quad B' = \frac{\mathcal{D}(b)}{\omega^{1/2}(b, b)}.$$

Then the matrices A' and B' satisfy the relations

$$A'^n = I, \quad B'^2 = I, \quad B'A' = \alpha' A'^{n-1} B', \tag{14.23}$$

where

$$\alpha' = \frac{\omega(b, a)\,\omega(a^{n-1}, a)}{\omega_{an}^{2/n}\,\omega(a^{n-1}, b)}. \tag{14.24}$$

In order to determine the possible values of the constant α', multiply the last equation in (14.23) by A' and use (14.23); this gives

$$B'A'^2 = \alpha'^2 A'^{2(n-1)} B'.$$

Repeating this procedure n times, we find that

$$\alpha'^n = 1, \tag{14.25}$$

i.e.,

$$\alpha' = \varepsilon_n^m \qquad (m = 0, 1, 2, \ldots, n-1). \tag{14.26}$$

However, not all the possible values of α' in (14.26) correspond to different classes of factor systems. Indeed, set $A = A'\varepsilon_n^{-q}$, where q is some integer. With this choice of the matrices A, they again satisfy relations (14.23), with α' replaced by

$$\alpha = \varepsilon_n^{-2q}\alpha' = \varepsilon_n^{m-2q}.$$

If n is odd, $n = 2p + 1$, we can always choose q so that $\alpha = 1$. Indeed, if m is even, $\alpha = 1$ for $q = m/2$, and if m is odd, $\alpha = 1$ for $q = (m-n)/2$. Therefore, when n is odd there is only one class, K_0, and all representations are p-equivalent to vector representations. In particular, all the projective representations of D_3 and C_{3v} are p-equivalent to vector representations.

For even n, there are two classes, K_0 and K_1. Indeed, if m in (14.26) is even, the choice of $q = m/2$ gives $\alpha = 1$ and the factor system is p-equivalent to the identity factor system, thus belonging to class K_0. If m is odd, no choice of q will make α equal to 1, and in this case the factor system is in class K_1. Consequently, all factor systems with odd $m = 1, 3, \ldots, n-1$ are equivalent to each other and p-equivalent to the factor system with $\alpha = \varepsilon_n$.

Thus, the groups D_n with even n have two possible classes of factor systems, K_0 and K_1. It is easily verified that multiplication of classes satisfies the relations

$$K_0^2 = K_0, \quad K_0K_1 = K_1, \quad K_1^2 = K_0.$$

To construct the representation group, we distinguish two possibilities for even n: a) $n/2$ is odd, b) $n/2$ is even.

If $n/2$ is odd, we can always make $\alpha = \pm 1$ by appropriate choice of q. In fact, if m is even we get $\alpha = 1$ for $q = m/2$. If m is odd, the choice $q = \left(m + \frac{n}{2}\right)/2$, gives $\alpha = \varepsilon_n^{n/2} = -1$. Therefore, if $n/2$ is odd, α takes the values ± 1, corresponding to classes K_0 and K_1.

Viewing α now as a new second order element, $\alpha^2 = e$, we can construct the representation group for the groups D_n in the case of odd $n/2$ using the results of the preceding section. The representation group is defined by the relations

$$a^n = e, \quad b^2 = e, \quad \alpha^2 = e, \quad ba = \alpha a^{n-1}b, \quad \alpha a = a\alpha, \quad \alpha b = b\alpha. \tag{14.27}$$

It is easy to see that any factor system for the group (14.27) has the form

$$\omega'(a^k b^p, a^{k_1}b^{p_1}) = \alpha^{k_1 p}, \tag{14.28}$$

where $\alpha = \pm 1$. Here $p, p_1 = 0, 1$; $k, k_1 = 0, 1, \ldots, n-1$.

If $n/2$ is even and m is odd, we cannot make α' equal ± 1 by any choice of q without altering relations (14.23). Set

$$A' = \varepsilon_{2n}^{(n/2)+m}A = +\, i\alpha'^{1/2}A, \tag{14.29}$$

where m is determined from (14.26). Then the third relation of (14.23) becomes

$$BA = \alpha' A^{(n-1)}B\varepsilon_{2n}^{(n-1)\left(m+\frac{n}{2}\right)-\frac{n}{2}-m} = A^{n-1}B.$$

With this choice of A, however, the first relation of (14.23) is changed:

$$A^n = (-1)^{-m-(n/2)} I = (-1)^{-m} I = \alpha I,$$

where $\alpha = \pm 1$, depending on the parity of m. Therefore, in the case of even $n/2$ relations (14.23) for the matrices A (14.29) and B become

$$A^n = \alpha I, \quad B^2 = I, \quad BA = A^{n-1}B; \tag{14.30}$$

here $\alpha = 1$ for the class K_0 and $\alpha = -1$ for the class K_1. Using (14.30), we readily construct the representation group for groups D_n with even $n/2$. It is defined by the relations

$$a^n = \alpha, \quad b^2 = e, \quad ba = a^{n-1}b, \quad \alpha a = a\alpha, \quad b\alpha = \alpha b, \quad \alpha^2 = e. \tag{14.31}$$

The group (14.31) leads to the factor system

$$\omega'(a^k b^p, a^{k'} b^{p'}) = \alpha^{\left[\frac{k+k'(1-2p+pn)}{n}\right]}, \tag{14.32}$$

where $[l/n]$ denotes the integral part of l/n.

In § 13 we noted that if $\frac{\omega(r_1, r_2)}{\omega(r_2, r_1)} \neq 1$ for some pair of commuting elements r_1 and r_2, the factor system ω cannot belong to class K_0. In groups D_n with even n, the two mutually perpendicular twofold axes $c_2 = a^{n/2}$ and $u_2 = b$ commute:

$$a^{n/2} b = b a^{n/2}.$$

Hence the matrices of the projective representation $\mathfrak{D}(a^{n/2})$ and $\mathfrak{D}(b)$ satisfy the relation

$$\mathfrak{D}(a^{n/2})\,\mathfrak{D}(b) = \mathfrak{D}(b)\,\mathfrak{D}(a^{n/2})\,\frac{\omega(b, a^{n/2})}{\omega(a^{n/2}, b)}.$$

As for the group C_{2h}, this readily implies

$$\frac{\omega(b, a^{n/2})}{\omega(a^{n/2}, b)} = \pm 1. \tag{14.32a}$$

Moreover, if this quotient is $+1$, the factor system belongs to class K_0; if it is -1, the factor system belongs to class K_1.

In fact, as shown in § 13, the quotient (14.32a) is the same for all p-equivalent factor systems and thus equals $\frac{\omega'(b, a^{n/2})}{\omega'(a^{n/2}, b)}$, where ω' is the standard factor system. Our assertion may now be proved directly from (14.28) or (14.32) for the standard factor system. Therefore, the value of the quotient (14.32a) is a convenient criterion for classification of a given factor system.

For any group D_n with even n, there exists a single-valued function $u(a^k b^p)$ $(k = 0, 1, \ldots, n-1;\ p = 0, 1)$, defined on the elements $a^k b^p$ of D_n, which converts any given factor system $\omega(a^k b^p, a^{k'} b^{p'})$ to standard form (14.28) or (14.32):

$$u(a^k b^p) = \frac{u(a^k)\,u(b^p)}{\omega(a^k, b^p)}, \qquad u(a^k) = \frac{\omega_{an}^{k/n}}{\omega_{ak}}\,\varepsilon^k, \quad u(b^p) = \omega^{p/2}(b, b). \tag{14.33}$$

For even m, $\varepsilon = \alpha'^{1/2} = \varepsilon_n^{m/2}$. For odd m, $\varepsilon = +i\alpha'^{1/2} = i\varepsilon_n^{m/2}$.

For example, let us show that if both m and $n/2$ are even, then

$$\omega'(a^{k'}, a^k) = \frac{\omega(a^{k'}, a^k)\, u(a^{k+k'})}{u(a^k)\, u(a^{k'})} = \alpha^{\left[\frac{k+k'}{n}\right]}.$$

We first note that although $k, k' \leqslant n-1$, their sum $k+k'$ may exceed n. Let $\{k+k'\}$ denote the difference between $k+k'$ and $\left[\frac{k+k'}{n}\right]n$:

$$k+k' = \{k+k'\} + \left[\frac{k+k'}{n}\right]n.$$

Since u is a single-valued function on the group, $u(a^{k+k'}) = u(a^{\{k+k'\}})$. Therefore,

$$\omega'(a^{k'}, a^k) = \frac{\omega(a^{k'}, a^k)\, e^{\{k+k'\}}\omega_{an}^{\frac{\{k+k'\}}{n}}}{e^{k+k'}\omega_{an}^{\frac{k+k'}{n}}} \frac{\omega_{ak}\omega_{ak'}}{\omega_{a\{k+k'\}}} = e^{-n\left[\frac{k+k'}{n}\right]}\omega_{an}^{-\left[\frac{k'+k}{n}\right]n}\omega(a^{k'}, a^k)\frac{\omega_{ak'}\omega_{ak}}{\omega_{a\{k+k'\}}}.$$

But

$$\omega_{an}^{-\left[\frac{k'+k}{n}\right]n}\frac{\omega_{ak}\omega_{ak'}\omega(a^{k'}, a^k)}{\omega_{a\{k+k'\}}} = \omega_{an}^{-\left[\frac{k'+k}{n}\right]n}\frac{\mathcal{D}^{k'}(a)\,\mathcal{D}^{k}(a)}{\mathcal{D}(a^{k'})\,\mathcal{D}(a^k)}\frac{\mathcal{D}(a^{\{k'+k\}})}{\mathcal{D}^{\{k+k'\}}(a)}\omega(a^{k'}, a^k) =$$

$$= \omega_{an}^{-\left[\frac{k+k'}{n}\right]n}\mathcal{D}^{\left[\frac{k'+k}{n}\right]n}(a) = 1,$$

because $\mathcal{D}^n(a) = \omega_{an}I$. Since $e_m^n = (-1)^m = \alpha$, we have

$$\omega(a^{k'}, a^k) = \alpha^{\left[\frac{k+k'}{n}\right]},$$

which coincides with (14.32) for $p = p' = 0$.

One proves similarly that $u(a^k b^p)$ (14.33) converts any factor system to the form (14.32) for p, $p' \neq 0$.

Consider the projective representations of the groups D_4 and D_6 that belong to the factor systems (14.32) and (14.28). Since C_{4v}, D_{2d} are isomorphic to D_4, while C_{6v}, D_{3h}, D_{3d} are isomorphic to D_6, the projective representations of the groups D_4 and D_6 coincide with the projective representations of the groups C_{4v}, D_{2d} and C_{6v}, D_{3h}, D_{3d}, respectively.

D_4 has eight elements, and so it has two two-dimensional projective representations belonging to class K_1. D_6 contains twelve elements and so has three two-dimensional representations of class K_1. The projective representations of D_4 and D_6 are given in Table 14.2.

Groups D_{nh}. We shall confine ourselves to the case of even n, since as shown in §3, for odd n the group D_{nh} is isomorphic to D_{2n}. Recall that D_{nh} is obtained from D_n by adjoining a reflection plane $\sigma_h = c$. This plane is perpendicular to the n-fold axis and commutes with the other elements of D_{nh}. The groups D_{nh} are defined by relations (3.5):

$$a^n = e, \quad b^2 = e, \quad ba = a^{n-1}b, \quad c^2 = e, \quad ac = ca, \quad bc = cb. \tag{14.34}$$

Let $\mathcal{D}(a) = A'$, $\mathcal{D}(b) = B'$, $\mathcal{D}(c) = C'$ be matrices of an irreducible projective representation of D_{nh}. We introduce the matrices

$$A = \frac{A'}{\omega_{an}^{1/n}}, \quad B = \frac{B'}{\omega^{1/2}(b, b)}, \quad C = \frac{C'}{\omega^{1/2}(c, c)}.$$

Then the defining relations for D_{nh} yield the following relations for the matrices A, B, C:

$$A^n = I, \quad B^2 = I, \quad C^2 = I, \quad BA = \alpha A^{n-1}B, \quad AC = \beta CA, \quad BC = \gamma CB, \tag{14.35}$$

where

$$\beta = \frac{\omega(a, c)}{\omega(c, a)}, \quad \gamma = \frac{\omega(b, c)}{\omega(c, b)}, \tag{14.36}$$

and α is defined by equation (14.24).

If $n/2$ is odd then α in (14.35) takes the values ± 1. If $n/2$ is even then, as in the groups D_n with even $n/2$, (14.35) may be brought to the form

$$A^n = \alpha I, \quad B^2 = C^2 = I, \quad BA = A^{n-1}B, \quad AC = \beta CA, \quad BC = \gamma CB, \tag{14.37}$$

where $\alpha = \pm 1$.

As in the case of the groups C_{nh}, it is easy to see that

$$\beta^2 = \gamma^2 = 1, \text{ i.e., } \beta = \pm 1, \quad \gamma = \pm 1. \tag{14.38}$$

Therefore, groups D_{nh} with even n have $2^3 = 8$ classes of factor systems, depending on the possible values ± 1 of α, β, γ:

$$K_0(1, 1, 1), \quad K_1(-1, 1, 1), \quad K_2(1, 1, -1), \quad K_3(1, -1, 1),$$
$$K_4(1, -1, -1) = K_2K_3, \quad K_5(-1, -1, -1) = K_1K_2K_3 = K_1K_4,$$
$$K_6(-1, -1, 1) = K_1K_3, \quad K_7(-1, 1, -1) = K_2K_1.$$

This readily gives the multiplication table for classes of factor systems, i.e. the multiplication table of the multiplicator. It is sufficient to form the products of the corresponding constants α, β, γ and check the class to which the products $\alpha_3 = \alpha_1\alpha_2$, $\beta_3 = \beta_1\beta_2$, $\gamma_3 = \gamma_1\gamma_2$ belong.

To construct the representation group for D_{nh}, we introduce new second order elements α, β, γ, which commute with each other and with the other elements of the group D_{nh}. As in the case of the groups D_n, the representation group has different defining relations for odd and even $n/2$.

For odd $n/2$, the representation group for D_{nh} is defined by the relations

$$\begin{aligned} &a^n = e, \quad b^2 = e, \quad c^2 = e, \quad \alpha^2 = e, \quad \beta^2 = e, \quad \gamma = e, \quad ba = \alpha a^{n-1}b, \\ &\alpha a = a\alpha, \quad b\alpha = \alpha b, \quad c\alpha = \alpha c, \quad ac = \beta ca, \quad bc = \gamma cb, \\ &a\gamma = \gamma a, \quad a\beta = \beta a, \quad b\gamma = \gamma b, \quad c\gamma = \gamma c, \quad a\beta = \beta a, \\ &b\beta = \beta b, \quad c\beta = \beta c, \quad \alpha\beta = \beta\alpha, \quad \alpha\gamma = \gamma\alpha, \quad \beta\gamma = \gamma\beta, \end{aligned} \tag{14.39}$$

and for even $n/2$ by the relations

$$\begin{aligned} &a^n = \alpha, \quad b^2 = c^2 = \alpha^2 = \beta^2 = \gamma^2 = e, \\ &ba = a^{n-1}b, \quad \alpha a = a\alpha, \quad b\alpha = \alpha b, \quad c\alpha = \alpha c, \quad ac = \beta ca, \\ &bc = \gamma cb, \quad a\beta = \beta a, \quad b\beta = \beta b, \quad c\beta = \beta c, \quad a\gamma = \gamma a, \\ &b\gamma = \gamma b, \quad c\gamma = \gamma c, \quad \alpha\beta = \beta\alpha, \quad \alpha\gamma = \gamma\alpha, \quad \beta\gamma = \gamma\beta. \end{aligned} \tag{14.40}$$

The defining relations (14.39) and (14.40) easily yield expressions for the factor system $\omega'(a^k b^p c^q, a^{k'} b^{p'} c^{q'})$ ($k, k' = 0, 1, 2, \ldots, n-1$; $p, p', q, q' = 0, 1$) corresponding to the groups (14.39) and (14.40).

For odd $n/2$, the factor system ω' is

$$\omega'(a^k b^p c^q, a^{k'} b^{p'} c^{q'}) = \alpha^{pk'} \beta^{qk'} \gamma^{qp'}, \tag{14.41}$$

and for even $n/2$,

$$\omega'(a^k b^p c^q, a^{k'} b^{p'} c^{q'}) = \alpha^{\left[\frac{k+k'(1-2p+pn)}{n}\right]} \beta^{qk'} \gamma^{qp'}. \tag{14.42}$$

Any given factor system may easily be assigned to one of the eight classes of factor systems for D_{nh}, depending on the value of the quotients of the coefficients for commuting elements:

$$\frac{\omega(a^{n/2}, b)}{\omega(b, a^{n/2})}, \quad \frac{\omega(a, c)}{\omega(c, a)}, \quad \frac{\omega(b, c)}{\omega(c, b)}.$$

If we choose the function $u(a^k b^p c^q)$ to be

$$u(a^k b^p c^q) = \frac{u(a^k)\,\omega^{p/2}(b, b)\,\omega^{q/2}(c, c)}{\omega(a^k, b^p c^q)\,\omega(b^p, c^q)}, \tag{14.43}$$

where $u(a^k)$ is defined by (14.33), it is easily seen that any given factor system $\omega(a^k b^p c^q, a^{k'} b^{p'} c^{q'})$ may be reduced to the form (14.41) or (14.42), for which we present all the projective representations below.

D_{2h} has eight elements, and each class (except K_0) contains two two-dimensional representations.

The relations between the matrices $\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{C}$ for the group D_{2h} $(n = 2)$ differ only by permutations of the numbers α, β, γ. Thus the representations corresponding to classes obtained by permuting the numbers α, β, γ may be obtained from the representations for one class by the appropriate permutations of the representation matrices. For example, the representations for classes K_3 and K_2, as well as K_4 and K_7, may be obtained from the representations for classes K_1 and K_6 by permuting the representation matrices $\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$.

There are sixteen elements in the group D_{4h}, so that by Burnside's theorem there may be either four two-dimensional projective representations or one four-dimensional projective representation. Each of the classes K_1, K_2, K_3, K_4, K_7 contains four two-dimensional representations, while each of K_5 and K_6 contains one four-dimensional representation.

There are 24 elements in the group D_{6h}, so it may have either six two-dimensional representations, or one four-dimensional and two two-dimensional representations. Both these cases occur, the latter in classes K_3, K_4, K_5, K_6.

The matrices of the projective representations for the generators of the groups D_{nh} are given in Table 14.2. These matrices completely determine all the projective representations of the groups D_{nh} belonging to the factor systems (14.41) and (14.42), since the representation matrix for an arbitrary element $a^k b^p c^q$ $(k = 0, 1, \ldots, n-1;\ p, q = 0, 1)$ is

$$\mathcal{D}'(a^k b^p c^q) = \boldsymbol{A}^k \boldsymbol{B}^p \boldsymbol{C}^q. \tag{14.44}$$

By (13.3), the representation $\mathcal{D}(a^k b^p c^q)$ belonging to a given factor system is

$$\mathcal{D}(a^k b^p c^q) = \boldsymbol{A}^k \boldsymbol{B}^p \boldsymbol{C}^q\, u(a^k b^p c^q), \tag{14.45}$$

where $u(a^k b^p c^q)$ is given by (14.43).

Group T. This group has two generators $a = c_2$, $b = c_3$, and defining relations (3.7):

$$a^2 = e, \quad b^3 = e, \quad bab = ab^2a. \tag{14.46}$$

The remaining elements are expressed in terms of the generators as in (3.8).

The defining relations (14.46) imply relations for the matrices of the projective representations,

$$\boldsymbol{A}' = \frac{\mathcal{D}(a)}{\omega^{1/2}(a, a)} \quad \text{and} \quad \boldsymbol{B}' = \frac{\mathcal{D}(b)}{\omega_{b3}^{1/3}},$$

namely,

$$\boldsymbol{A}'^2 = \boldsymbol{I}, \quad \boldsymbol{B}'^3 = \boldsymbol{I}, \quad \boldsymbol{B}'\boldsymbol{A}'\boldsymbol{B}' = \alpha'\boldsymbol{A}'\boldsymbol{B}'^2\boldsymbol{A}', \tag{14.47}$$

where

$$\alpha' = \frac{\omega^{1/2}(a, a)\,\omega(b, ab)\,\omega(a, b)}{\omega(a, b^2a)\,\omega(b^2, a)\,\omega(b, b)}. \tag{14.48}$$

From (14.47) we have $\boldsymbol{B}'\boldsymbol{A}'\boldsymbol{B}'^2 = \alpha'\boldsymbol{A}'\boldsymbol{B}'\boldsymbol{B}'\boldsymbol{A}'\boldsymbol{B}' = \alpha'^2\boldsymbol{A}'\boldsymbol{B}'\boldsymbol{A}'\boldsymbol{B}'^2\boldsymbol{A}' = \alpha'^3\boldsymbol{B}'^2\boldsymbol{A}'\boldsymbol{B}'\boldsymbol{A}' = \alpha'^4\boldsymbol{B}'\boldsymbol{A}'\boldsymbol{B}'^2$, whence it follows that $\alpha'^4 = 1$ and so

$$\alpha' = \varepsilon_4^m \qquad (m = 0, 1, 2, 3). \tag{14.49}$$

If m is even ($m = 0, 2$), we can always make $\alpha' = 1$ by suitable choice of the sign of $\boldsymbol{A}$. The representation is then p-equivalent to a vector representation. If m is odd ($m = 1, 3$), then, as in the case of the groups D_n for even $n/2$, the substitution $\boldsymbol{A} = \alpha'\boldsymbol{A}'$ brings (14.47) to the form

$$\boldsymbol{A}^2 = \alpha\boldsymbol{I}, \quad \boldsymbol{B}^3 = \boldsymbol{I}, \quad \boldsymbol{BAB} = \boldsymbol{AB}^2\boldsymbol{A}, \quad \alpha = \pm 1. \tag{14.50}$$

Therefore there are two possible classes of factor systems for the group T, K_0 and K_1, corresponding to $\alpha = \pm 1$.

The representation group for T is defined by the relations

$$a^2 = \mathfrak{a}, \quad b^3 = e, \quad \mathfrak{a}^2 = e, \quad bab = ab^2a, \quad a\mathfrak{a} = \mathfrak{a}a, \quad b\mathfrak{a} = \mathfrak{a}b. \tag{14.51}$$

The factor system $\omega'(r_1, r_2)$, $r_1, r_2 \in T$, for the group T that corresponds to the representation group (14.51) is constructed using (13.23) and (13.24), as follows. Each element r of T is a product of powers of the generators. The product r_1r_2 is also an element of the group T, and therefore, with the aid of the relations (3.7), it can be converted into one of the elements (3.8). However, in the representation group this may involve the appearance of the additional factor $\mathfrak{a}$. If it appears, we have $\omega'(r_1, r_2) = -1$; for K_1 otherwise $\omega'(r_1, r_2) = 1$. For example, to evaluate $\omega(c_2, c_2')$ we consider the product c_2c_2' and obtain $c_2c_2' = abab^2 = a^2b^2ab = \mathfrak{a}b^2ab$, so that $\omega'(c_2, c_2') = -1$. But $\omega'(c_2', c_2) = 1$, since $c_2'c_2 = bab^2a = b^2ab$.

The group T has three two-dimensional representations defined by the matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ given in Table 14.2. Equations (14.48) and (14.49) enable us to determine the class of any given factor system according to its coefficients. In practice, however, it is more convenient to consider the quotients of the coefficients for commuting elements. In T, any two rotations about a twofold axis, such as c_2 and c_2', commute. The matrix elements of projective representations satisfy the equality

$$\boldsymbol{ABAB}^2 = \beta\boldsymbol{BAB}^2\boldsymbol{A},$$

where

$$\beta = \frac{\omega(c_2', c_2)}{\omega(c_2, c_2')}. \tag{14.52}$$

It follows from (14.50) that $\beta = \alpha$, and thus $\beta = 1$ or -1 for classes K_0 and K_1, respectively. Since (14.52) is the same for all p-equivalent factor systems, we easily classify a given factor system as being in class K_0 or K_1, depending on the value of (14.52) for any pair of twofold axes.

By (3.8), any element of T may be written

$$a^k b^p a^{k'} b^{p'}, \ (k, k' = 0, 1; \ p, p' = 0, 1, 2).$$

The function $u(a^k b^p a^{k'} b^{p'})$ which reduces a given factor system ω to standard form ω' is

$$u(a^k b^p a^{k'} b^{p'}) = \tilde{u}(a^k)\,\tilde{u}(a^{k'})\,u(b^p)\,u(b^{p'})\frac{\omega'(a^k, b^p a^{k'} b^{p'})\,\omega'(b^p, a^{k'} b^{p'})\,\omega'(a^{k'}, b^{p'})}{\omega(a^k, b^p a^{k'} b^{p'})\,\omega(b^p, a^{k'} b^{p'})\,\omega(a^{k'}, b^{p'})} =$$

$$= \frac{\tilde{u}(a^k)\,\tilde{u}(a^{k'})\,u(b^p)\,u(b^{p'})}{\omega(a^k, b^p a^{k'} b^{p'})\,\omega(b^p, a^{k'} b^{p'})\,\omega(a^{k'}, b^{p'})}, \tag{14.53}$$

since by construction of the standard factor system

$$\omega'(a^k, b^p a^{k'} b^{p'}) = \omega'(b^p, a^{k'} b^{p'}) = \omega'(a^{k'}, b^{p'}) = 1.$$

The functions $\tilde{u}(a^k)$ and $u(b^p)$ are defined by the coefficients of the factor system:

$$\tilde{u}(a) = \frac{\omega^{1/2}(a, a)}{\alpha'}, \quad u(b^p) = \frac{\omega_{b3}^{p/3}}{\omega_{bp}}, \tag{14.54}$$

where α' is defined by (14.49). Using (14.53), we easily find explicit expres sions for the functions u in terms of the coefficients of the factor system. These are given in Table 14.1.

TABLE 14.1

	u		u
e	1	ab	$\frac{\omega^{1/2}(a, a)}{\alpha'}\frac{\omega_{b3}^{1/3}}{\omega(a, b)}$
a	$\frac{\omega^{1/2}(a, a)}{\alpha'}$	ba	$\frac{\omega^{1/2}(a, a)}{\alpha'}\frac{\omega_{b3}^{1/3}}{\omega(b, a)}$
bab^2	$\frac{\omega^{1/2}(a, a)}{\alpha'}\frac{\omega(b, b^2)}{\omega(b, ab^2)\,\omega(a, b^2)}$	b^2	$\frac{\omega_{b3}^{2/3}}{\omega(b, b)}$
b^2ab	$\frac{\omega^{1/2}(a, a)}{\alpha'}\frac{\omega(b, b^2)}{\omega(b^2, ab)\,\omega(a, b)}$	ab^2a	$\frac{\omega(a, a)}{\alpha'^2}\frac{\omega_{b3}^{2/3}}{\omega(b, b)\,\omega(a, b^2a)\,\omega(b^2, a)}$
b	$\omega_{b3}^{1/3}$	b^2a	$\frac{\omega^{1/2}(a, a)\,\omega_{b3}^{2/3}}{\alpha'\omega(b, b)\,\omega(b^2, a)}$
aba	$\frac{\omega(a, a)}{\alpha'^2}\frac{\omega_{b3}^{1/3}}{\omega(a, ba)\,\omega(b, a)}$	ab^2	$\frac{\omega^{1/2}(a, a)}{\alpha'}\frac{\omega_{b3}^{2/3}}{\omega(b, b)}\frac{1}{\omega(a, b^2)}$

Group T_h. This group is the direct product of T and inversion: $T_h = T \times \times C_i$. It is defined by two generators $a = c_2$, $s_6 = s$, where s_6 is an improper rotation, satisfying the relations (3.9):

$$a^2 = e, \quad s^6 = e, \quad sas = as^2a.$$

Here $c_3 = s_6^2$.

The 24 elements of T_h comprise the twelve elements of T and the products of these elements with inversion $i = s_6^3$.

Set

$$A' = \frac{\mathfrak{D}(a)}{\omega^{1/2}(a, a)}, \quad B = \frac{\mathfrak{D}(s)}{\omega_{s6}^{1/6}}; \tag{14.55}$$

using the defining relations, we obtain

$$A'^2 = I, \quad B^6 = I, \quad BA'B = \alpha' A' B^2 A', \tag{14.56}$$

$$\alpha' = \frac{\omega(s, as)\,\omega(a, s)\,\omega^{1/2}(a, a)}{\omega(a, s^2a)\,\omega(s^2, a)\,\omega(s, s)}. \tag{14.57}$$

Reasoning as in the case of T, we can find that $\alpha'^4 = 1$, i.e.,

$$\alpha' = e_4^m. \tag{14.58}$$

Here again the factor system belongs to class K_0 if $m = 0, 2$, to class K_1 if $m = 1, 3$.

Setting $A = \alpha' A'$, we reduce relations (14.56) to a form similar to (14.50):

$$A^2 = \alpha I, \quad B^6 = I, \quad BAB = AB^2A, \quad \alpha = \pm 1. \tag{14.59}$$

The representation group for T_h contains 48 elements; it is defined by the relations

$$a^2 = \alpha, \quad s^6 = e, \quad \alpha^2 = e, \quad sas = as^2a, \quad a\alpha = \alpha a, \quad s\alpha = \alpha s. \tag{14.60}$$

From (14.60) we easily see that the standard factor system ω'_{T_h} for T_h is related to the factor system ω'_T for T by

$$\omega'_{T_h}(r_1, r_2) = \omega'_{T_h}(r_1, ir_2) = \omega'_{T_h}(ir_1, r_2) = \omega'_{T_h}(ir_1, ir_2) = \omega'_T(r_1, r_2), \tag{14.61}$$

where r_1 and r_2 are any elements of T, and i is inversion s^3.

Formula (14.53) readily yields a function u which reduces any given factor system to the form (14.61). For the elements of T_h which are also T, the function u is defined in Table 14.1, with b replaced by s^2. For the remaining elements of the group T_h, which are products of the elements r of T and inversion i, we have

$$u(ri) = \frac{u(r)\,\omega^{1/2}(i, i)}{\omega(r, i)},$$

where $u(r)$ is given in Table 14.1.

There are six two-dimensional representations of the group T_h in class K_1. Three of these are representations of T, and the others are obtained from them by multiplying B by the factor $\varepsilon_6 = e^{\pi i/3}$. They are given in Table 14.2.

Group O. The octahedral group O and the isomorphic group T_d are defined by two generators. The generators of O are $a = c_4$ and $b = c_3$, satisfying the relations (3.10):

$$a^4 = e, \quad b^3 = e, \quad aba = b^2.$$

Let

$$A' = \frac{\mathfrak{D}(a)}{\omega_{a4}^{1/4}}, \quad B' = \frac{\mathfrak{D}(b)}{\omega_{b3}^{1/3}},$$

where $\mathfrak{D}(a)$ and $\mathfrak{D}(b)$ are matrices of a projective representation for a and b.

Then the defining relations yield

$$A'^4 = I, \quad B'^3 = I, \quad A'B'A' = \alpha' B'^2, \tag{14.62}$$

where

$$\alpha' = \frac{\omega_{b3}^{1/3}\omega(a, ba)\,\omega(b, a)}{\omega_{a4}^{1/2}\,\omega(b, b)}. \tag{14.63}$$

Equations (14.62) imply the equality $B'A'^2B' = \alpha'^3 A'^2 B'^2 A'^2$, analogous to the third equality in (14.56); therefore,

$$\alpha'^{12} = 1, \text{ i.e., } \alpha' = \varepsilon_{12}^m \qquad (m = 0, 1, 2, \ldots, 11). \tag{14.64}$$

We now introduce new matrices A and B by

$$A = A'\varepsilon_8^q, \qquad B = \varepsilon_3^p B';$$

then relations (14.62) become

$$A^4 = \alpha I, \quad B^3 = I, \quad ABA = \alpha'' B^2, \quad \alpha = (-1)^q, \tag{14.65}$$

where

$$\alpha'' = \alpha' \varepsilon_8^{2q}\varepsilon_3^p = \varepsilon_{12}^m \varepsilon_3^p \varepsilon_4^q.$$

Since $\varepsilon_{12} = \varepsilon_3\varepsilon_4^3$, the expression for α'' may be put in the form

$$\alpha'' = \varepsilon_3^{m+p}\varepsilon_4^{3m+q}. \tag{14.66}$$

It is clear from (14.66) that the choice of $p = -m$ and $q = -3m$, makes α'' equal to 1. Moreover, if m is even then $\alpha = (-1)^{-m} = 1$, and all the projective representations are p-equivalent to vector representations. But if m is odd we have $\alpha = -1$, $A^4 = -I$, and the factor system belongs to class K_1. Thus there are two classes of factor systems for the group $O(T_d)$, K_0 and K_1, corresponding to $\alpha = \pm 1$ (even or odd m in equation (14.64)).

As in the case of T, here again the membership of a given factor system in K_0 or K_1 is conveniently determined by quotients of its coefficients for the pair of commuting elements c_4^2 and $c_4'^2$, since it follows from (14.65) that this quotient is $\alpha'^6 = \pm 1$ for classes K_0 and K_1, respectively.

The representation group for the octahedral group is defined by the relations

$$a^4 = \alpha, \quad \alpha^2 = e, \quad b^3 = e, \quad aba = b^2, \quad \alpha a = a\alpha, \quad \alpha b = b\alpha. \tag{14.67}$$

For the group O, the class K_1 contains two two-dimensional representations and one four-dimensional representation. They are given in Table 14.2

Using equation (14.53), we easily find the function $u(r)$ reducing a factor system ω of $O(T_d)$ to the standard factor system ω' defined by relations (14.67). For an arbitrary element $a^k b^p a^{k'} b^{p'}$ of the group $O(T_d)$,

$$u(a^k b^p a^{k'} b^{p'}) = \frac{u(a^k)\,u(a^{k'})\,u(b^p)\,u(b^{p'})}{\omega(a^k, b^p a^{k'} b^{p'})\,\omega(b^p, a^{k'} b^{p'})\,\omega(a^{k'}, b^{p'})}, \tag{14.68}$$

where

$$u(a^k) = \frac{\varepsilon_8^{3mk}\,\omega_{a4}^{k/4}}{\omega_{ak}}, \qquad u(b^p) = \frac{\omega_{b3}^{p/3}\,\varepsilon_3^{-pm}}{\omega_{bp}}; \tag{14.69}$$

m is defined by (14.64).

Group O_h. This group is the direct product of O (or T_d) and inversion i. It is defined by two generators $a = c_4$, $s = s_6$, satisfying the relations (3.13):

$$a^4 = e, \quad s^6 = e, \quad sa^3s = a, \quad as^3 = s^3a. \tag{14.70}$$

O_h contains 48 elements, half of which are the elements of O, the others their products by inversion $i = s_6^3$.

From (14.70) we obtain relations for the matrices

$$A' = \frac{\mathcal{D}(a)}{\omega_{a4}^{1/4}} \quad \text{and} \quad B' = \frac{\mathcal{D}(s)}{\omega_{s6}^{1/6}},$$

namely,

$$A'^4 = I, \quad B'^6 = I, \quad B'A'^3B' = \alpha' A, \quad A'B'^3 = \beta B'^3 A', \tag{14.71}$$

where

$$\alpha' = \frac{\omega(s, a^3s)\,\omega(a^3, s)\,\omega_{s3}}{\omega_{a4}^{1/2}\,\omega_{s6}^{1/3}}, \qquad \beta = \frac{\omega(a, s^3)}{\omega(s^3, a)}. \tag{14.72}$$

It follows from (14.71) that $\beta^2 = 1$, or $\beta = \pm 1$.

To determine the possible values of α', we observe that the third relation in (14.71) may be brought to the form $B'^3A'^3B'A'^3 = \alpha' B'^2$. Using the last relation in (14.71), we obtain $B'^4 = A'B'^2A'\alpha'\beta$, which is similar to the corresponding relation for O. This implies that

$$(\alpha'\beta)^{12} = \alpha'^{12} = 1, \quad \text{i.e.,} \quad \alpha = \varepsilon_{12}^m.$$

Introducing the matrices $A = A'e_8^q$, $B = B'e_6^p$, we obtain the relations

$$A^4 = \alpha I, \quad B^6 = I, \quad BA^3B = \alpha'' A, \quad AB = \beta BA, \tag{14.73}$$

where

$$\alpha = (-1)^q, \qquad \alpha'' = \alpha' e_4^q e_3^p = \varepsilon_3^{m+p} e_4^{3m+q}.$$

Setting $p = -m$, $q = -3m$, we find that $\alpha'' = 1$, and relations (14.73) become

$$\begin{gathered} A^4 = \alpha I, \quad B^6 = I, \quad BA^3B = A, \quad AB^3 = \beta B^3 A, \\ \alpha = (-1)^m = \pm 1, \quad \beta = \pm 1. \end{gathered} \tag{14.74}$$

As in the case of O, if m is even then $\alpha = 1$, and if it is odd, $\alpha = -1$.

Thus the group O_h has four classes of factor systems, corresponding to the possible values of α and β:

$$K_0(1, 1), \quad K_1(-1, 1), \quad K_2(1, -1) \quad K_3(-1, -1) = K_1K_2.$$

The representation group for O_h is defined by four generators a, s, α, β and relations

$$\begin{gathered} a^4 = \alpha, \quad s^6 = e, \quad \alpha^2 = e, \quad \beta^2 = e, \quad sa^3s = a, \quad as^3 = \beta s^3 a, \\ \alpha\beta = \beta\alpha, \ \alpha a = a\alpha, \ \alpha s = s\alpha, \ \beta a = a\beta, \quad \beta s = s\beta. \end{gathered} \tag{14.75}$$

Half of the elements of O_h are elements of O, and the others are their products by inversion $i = s_6^3$, which commutes with all the elements. However, it is clear from (14.75) that in the representation group inversion does not commute with a. Thus the factor system ω'_{O_h} for O_h, which corresponds to (14.75), depends on the specific choice of the elements of O_h. To fix ideas,

we shall write the elements of O_h as r or $ri = rs^3$, where r is an element of O. Then it is easy to show that a factor system for O_h is related to a factor system for O by

$$\begin{aligned} &\omega'_{O_h}(r_1, r_2) = \omega'_O(r_1, r_2), \quad \omega'_{O_h}(r_1, r_2 i) = \omega'_O(r_1, r_2), \\ &\omega'_{O_h}(r_1 i, r_2) = \omega'_{O_h}(r_1 i, r_2 i) = \beta^{\mu}\, \omega'_O(r_1, r_2), \end{aligned} \tag{14.76}$$

where the number μ indicates how many times inversion i and the fourfold axis $c_1 = a$ must be permuted to obtain $r_2 i$ from ir_2.

The function $u(r)$ $(r \in O_h)$ reducing any factor system ω for O_h to the standard factor system (14.76) has the form (14.68), with

$$u(a^k) = \frac{\varepsilon^{3mk}\, \omega_{a4}^{k/4}}{\omega_{ak}}, \qquad u(s^p) = \frac{\omega_{s6}^{p/6}\, \varepsilon_6^{pm}}{\omega_{sp}}. \tag{14.77}$$

The following remark is important here. The function $u(r)$ should be single-valued, so that $u(ri) = u(ir)$. However, the right-hand side of equality (14.68) depends on the order of the factors and, in particular, may differ for ri and ir. In order to eliminate this ambiguity, we shall consistently write inversion to the right of the rotation in the right-hand side of equality (14.68): ri. With this choice, $u(r)$ indeed reduces any given factor system to standard form (14.76). For example,

$$\omega'(a, s^3) = \frac{\omega(a, s^3)\, u(as^3)}{u(a)\, u(s^3)} = \frac{\omega(a, s^3)}{\omega(a, s^3)} \frac{u(a)\, u(s^3)}{u(a)\, u(s^3)} = 1,$$

but

$$\omega'(s^3, a) = \frac{\omega(s^3, a)}{\omega(a, s^3)} \frac{u(a)\, u(s^3)}{u(s^3)\, u(a)} = \beta$$

in accordance with (14.76).

The group O_h has four two-dimensional and two four-dimensional representations in class K_1, three four-dimensional representations in class K_3, one six-dimensional and three two-dimensional representations in class K_2. These representations are defined by the representation matrices $\boldsymbol{A}$ and $\boldsymbol{B}$ for the generators, satisfying relations (14.74); they are presented in Table 14.2.

We have thus constructed the projective representations of all the point groups, with a view to constructing the representations of the space groups. The corresponding matrices for the generators of the 32 point groups are presented in Table 14.2. Two-dimensional representations are denoted by the symbol $P_n^{(m)}$. The superscript m specifies the class of factor systems, the subscript n indexes the representation. Four-dimensional representations are denoted by $Q_n^{(m)}$, six-dimensional ones by $R_n^{(m)}$.

The characters of the irreducible projective representations are presented in Table 14.3.

These tables make it possible to find the representations of any space group

By the results of §§12, 13 and 14, the procedure for determining the representations of a space group with star $\{\boldsymbol{k}\}$ is as follows.

1) Select the vector $\boldsymbol{k}$ and determine the crystallographic point group $F_{\boldsymbol{k}}$ whose elements leave $\boldsymbol{k}$ invariant up to addition of a reciprocal lattice vector (see (12.12)).

2) Using formula (12.29), find the factor system $\omega(r_1, r_2)$, $r_1, r_2 \in F_{\boldsymbol{k}}$, corresponding to the selected point $\boldsymbol{k}$.

TABLE 14.2. Projective representations of the point groups

Group	Class	Representation	A	B	Relations
C_{2h} (C_{2v}, D_2)	K_1	$P^{(1)}$	σ_z	σ_x	$A^2 = B^2 = I$, $AB = -BA$
C_{4h}	K_1	$P_1^{(1)}$	σ_z	σ_x	$A^4 = B^2 = I$, $AB = -BA$
		$P_2^{(1)}$	$i\sigma_z$	σ_x	
C_{6h}	K_1	$P_1^{(1)}$	σ_z	σ_x	$A^6 = B^2 = I$, $AB = -BA$
		$P_2^{(1)}$	$\varepsilon_6\sigma_z$	σ_x	$\varepsilon_6 = e^{\pi i/3} = \frac{1+i\sqrt{3}}{2}$
		$P_3^{(1)}$	$\varepsilon_3\sigma_z$	σ_x	
D_4 (C_{4v}, D_{2d})	K_1	$P_1^{(1)}$	$\begin{Vmatrix} \varepsilon_8^3 & 0 \\ 0 & \varepsilon_8 \end{Vmatrix}$	σ_x	$A^4 = -I$, $B^2 = I$
		$P_2^{(1)}$	$\begin{Vmatrix} \varepsilon_8^{-1} & 0 \\ 0 & \varepsilon_8^{-3} \end{Vmatrix}$	σ_x	$BA = A^3B$, $\varepsilon_8 = e^{\pi i/4} = \frac{1+i}{\sqrt{2}}$
D_6 (C_{6v}, D_{3h}, D_{3d})	K_1	$P_1^{(1)}$	$-\sigma_z$	σ_x	$A^6 = I$, $B^2 = I$
		$P_2^{(1)}$	$\begin{Vmatrix} \varepsilon_6^2 & 0 \\ 0 & \varepsilon_6 \end{Vmatrix}$	σ_x	$BA = -A^5B$
		$P_3^{(1)}$	$\begin{Vmatrix} \varepsilon_6^4 & 0 \\ 0 & \varepsilon_6^5 \end{Vmatrix}$	σ_x	$\varepsilon_6 = e^{\pi i/3} = \frac{1+i\sqrt{3}}{2}$

Group	Class	Representation	A	B	C	Relations
D_{2h}	K_1	$P_1^{(1)}$	σ_z	σ_x	I	$A^2 = B^2 = C^2 = I$ $AB = -BA$ $AC = CA$ $BC = CB$
		$P_2^{(1)}$	σ_z	σ_x	$-I$	
	K_5	$P_1^{(5)}$	σ_z	σ_x	$-\sigma_y$	$A^2 = B^2 = C^2 = I$ $AB = -BA$ $AC = -CA$ $BC = -CB$
		$P_2^{(5)}$	$-\sigma_z$	σ_x	$-\sigma_y$	
	K_6	$P_1^{(6)}$	σ_z	σ_x	σ_x	$A^2 = B^2 = C^2 = I$ $AB = -BA$ $AC = -CA$ $BC = CB$
		$P_2^{(6)}$	σ_z	σ_x	$-\sigma_x$	

TABLE 14.2 (continued)

Group	Class	Representation	A	B	C	Relations
D_{4h}	K_1	$P_1^{(1)}$	$\varepsilon_8 \begin{Vmatrix} i & 0 \\ 0 & 1 \end{Vmatrix}$	σ_x	I	$A^4 = -I$ $B^2 = C^2 = I$
		$P_2^{(1)}$	$-\varepsilon_8 \begin{Vmatrix} i & 0 \\ 0 & 1 \end{Vmatrix}$	σ_x	I	$BA = A^3B$
		$P_3^{(1)}$	$\varepsilon_8 \begin{Vmatrix} i & 0 \\ 0 & 1 \end{Vmatrix}$	σ_x	$-I$	$AC = CA$
		$P_4^{(1)}$	$-\varepsilon_8 \begin{Vmatrix} i & 0 \\ 0 & 1 \end{Vmatrix}$	σ_x	$-I$	$BC = CB$
	K_2	$P_1^{(2)}$	I	σ_z	σ_y	$A^4 = B^2 = C^2 = I$
		$P_2^{(2)}$	$i\sigma_z$	σ_x	σ_z	$BA = A^3B$
		$P_3^{(2)}$	$-I$	σ_z	σ_y	$AC = CA$
		$P_4^{(2)}$	$i\sigma_z$	σ_x	$-\sigma_z$	$BC = -CB$
	K_3	$P_1^{(3)}$	σ_z	I	σ_y	$A^4 = B^2 = C^2 = I$
		$P_2^{(3)}$	$i\sigma_z$	σ_x	σ_x	$BA = A^3B$
		$P_3^{(3)}$	σ_z	$-I$	σ_y	$AC = -CA$
		$P_4^{(3)}$	$i\sigma_z$	$-\sigma_x$	σ_x	$BC = CB$
	K_4	$P_1^{(4)}$	σ_z	σ_z	σ_x	$A^4 = B^2 = C^2 = I$
		$P_2^{(4)}$	$i\sigma_z$	$-\sigma_x$	σ_y	$BA = A^3B$
		$P_3^{(4)}$	σ_z	$-\sigma_z$	σ_x	$AC = -CA$
		$P_4^{(4)}$	$i\sigma_z$	σ_x	σ_y	$BC = -CB$
	K_5	$Q^{(5)}$	$\frac{1}{\sqrt{2}} \begin{Vmatrix} -i & -1 & 0 & 0 \\ -1 & -i & 0 & 0 \\ 0 & 0 & i & 1 \\ 0 & 0 & 1 & i \end{Vmatrix}$	$\begin{Vmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{Vmatrix}$	$\begin{Vmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{Vmatrix}$	$A^4 = -I$ $B^2 = I$ $C^2 = I$ $BA = A^3B$ $AC = -CA$ $BC = -CB$
	K_6	$Q^{(6)}$	$\frac{1}{\sqrt{2}} \begin{Vmatrix} -i & -1 & 0 & 0 \\ -1 & -i & 0 & 0 \\ 0 & 0 & i & 1 \\ 0 & 0 & 1 & i \end{Vmatrix}$	$\begin{Vmatrix} 0 & i & 0 & 0 \\ -i & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & -i & 0 \end{Vmatrix}$	$\begin{Vmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{Vmatrix}$	$A^4 = -I$ $B^2 = I$ $C^2 = I$ $BA = A^3B$ $AC = -CA$ $BC = CB$

TABLE 14.2 (continued)

Group	Class	Representation	A	B	C	Relations
D_{4h}	K_7	$P_1^{(7)}$	$\varepsilon_8 \begin{Vmatrix} i & 0 \\ 0 & 1 \end{Vmatrix}$	σ_x	σ_z	$A^4 = -I,\ B^2 = I$
		$P_2^{(7)}$	$-\varepsilon_8 \begin{Vmatrix} i & 0 \\ 0 & 1 \end{Vmatrix}$	σ_x	σ_z	$C^2 = I,\ BA = A^3B$
		$P_3^{(7)}$	$\varepsilon_8 \begin{Vmatrix} i & 0 \\ 0 & 1 \end{Vmatrix}$	σ_x	$-\sigma_z$	$AC = CA,\ BC = -CB$
		$P_4^{(7)}$	$-\varepsilon_8 \begin{Vmatrix} i & 0 \\ 0 & 1 \end{Vmatrix}$.	σ_x	$-\sigma_z$	
D_{6h}	K_1	$P_1^{(1)}$	$\begin{Vmatrix} -\varepsilon_6^{-1} & 0 \\ 0 & \varepsilon_6 \end{Vmatrix}$	σ_y	I	$A^6 = I,\ B^2 = I$
		$P_2^{(1)}$	$\begin{Vmatrix} -\varepsilon_6 & 0 \\ 0 & \varepsilon_6^{-1} \end{Vmatrix}$	σ_y	I	$C^2 = I,\ BA = -A^5B$
		$P_3^{(1)}$	$-\sigma_z$	σ_y	I	$AC = CA$
		$P_4^{(1)}$	$\begin{Vmatrix} -\varepsilon_6^{-1} & 0 \\ 0 & \varepsilon_6 \end{Vmatrix}$	σ_y	$-I$	$BC = CB$
		$P_5^{(1)}$	$\begin{Vmatrix} -\varepsilon_6 & 0 \\ 0 & \varepsilon_6^{-1} \end{Vmatrix}$	σ_y	$-I$	$\varepsilon_6 = e^{\pi i/3} = \dfrac{1 + i\sqrt{3}}{2}$
		$P_6^{(1)}$	$-\sigma_z$	σ_y	$-I$	
	K_2	$P_1^{(2)}$	I	σ_z	σ_x	$A^6 = I,\ B^2 = I$
		$P_2^{(2)}$	$\begin{Vmatrix} \varepsilon_6 & 0 \\ 0 & \varepsilon_6^{-1} \end{Vmatrix}$	σ_x	$-\sigma_z$	$C^2 = I,\ BA = A^5B$
		$P_3^{(2)}$	$-\begin{Vmatrix} \varepsilon_6 & 0 \\ 0 & \varepsilon_6^{-1} \end{Vmatrix}$	σ_x	$-\sigma_z$	$AC = CA$
		$P_4^{(2)}$	$-I$	σ_z	σ_x	$BC = -CB$
		$P_5^{(2)}$	$\begin{Vmatrix} \varepsilon_6 & 0 \\ 0 & \varepsilon_6^{-1} \end{Vmatrix}$	σ_x	σ_z	
		$P_6^{(2)}$	$-\begin{Vmatrix} \varepsilon_6^{-1} & 0 \\ 0 & \varepsilon_6 \end{Vmatrix}$	σ_x	$-\sigma_z$	

TABLE 14.2 (continued)

Group	Class	Representation	A	B	C	Relations
D_{6h}	K_3	$P_1^{(3)}$	σ_z	I	$-\sigma_y$	$A^6 = I$ $B^2 = I$
		$P_2^{(3)}$	σ_z	$-I$	$-\sigma_y$	$C^2 = I$ $BA = A^5B$
		$Q^{(3)}$	$\begin{Vmatrix} -\varepsilon_6 & 0 & 0 & 0 \\ 0 & -\varepsilon_6^{-1} & 0 & 0 \\ 0 & 0 & \varepsilon_6 & 0 \\ 0 & 0 & 0 & \varepsilon_6^{-1} \end{Vmatrix}$	$\begin{Vmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{Vmatrix}$	$\begin{Vmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \\ -i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{Vmatrix}$	$AC = -CA$ $BC = CB$
	K_4	$P_1^{(4)}$	σ_z	σ_z	σ_y	$A^6 = I$ $B^2 = I$
		$P_2^{(4)}$	σ_z	$-\sigma_z$	σ_y	$C^2 = I$ $BA = A^5B$
		$Q^{(4)}$	$\begin{Vmatrix} -\varepsilon_6 & 0 & 0 & 0 \\ 0 & -\varepsilon_6^{-1} & 0 & 0 \\ 0 & 0 & \varepsilon_6 & 0 \\ 0 & 0 & 0 & \varepsilon_6^{-1} \end{Vmatrix}$	$\begin{Vmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{Vmatrix}$	$\begin{Vmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & i \\ -i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{Vmatrix}$	$AC = -CA$ $BC = -CB$
	K_5	$P_1^{(5)}$	σ_z	σ_x	σ_y	$A^6 = I$ $B^2 = I$
		$P_2^{(5)}$	σ_z	σ_x	$-\sigma_y$	$C^2 = I$ $BA = -A^5B$
		$Q^{(5)}$	$\begin{Vmatrix} \varepsilon_6 & 0 & 0 & 0 \\ 0 & -\varepsilon_6^{-1} & 0 & 0 \\ 0 & 0 & -\varepsilon_6 & 0 \\ 0 & 0 & 0 & \varepsilon_6^{-1} \end{Vmatrix}$	$\begin{Vmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{Vmatrix}$	$\begin{Vmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{Vmatrix}$	$AC = -CA$ $BC = -CB$
	K_6	$P_1^{(6)}$	σ_z	σ_x	σ_x	$A^6 = I$ $B^2 = I$
		$P_2^{(6)}$	σ_z	σ_x	$-\sigma_x$	$C^2 = I$ $BA = -A^5B$
		$Q^{(6)}$	$\begin{Vmatrix} \varepsilon_6 & 0 & 0 & 0 \\ 0 & -\varepsilon_6^{-1} & 0 & 0 \\ 0 & 0 & -\varepsilon_6 & 0 \\ 0 & 0 & 0 & \varepsilon_6^{-1} \end{Vmatrix}$	$\begin{Vmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{Vmatrix}$	$\begin{Vmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{Vmatrix}$	$AC = -CA$ $BC = CB$

TABLE 14.2 (continued)

Group	Class	Representation	A	B	C	Relations
D_{6h}	K_7	$P_1^{(7)}$	$\begin{Vmatrix} -\varepsilon_6^{-1} & 0 \\ 0 & \varepsilon_6 \end{Vmatrix}$	σ_y	σ_z	$A^6 = I,\ B^2 = I$
		$P_2^{(7)}$	$\begin{Vmatrix} \varepsilon_6 & 0 \\ 0 & -\varepsilon_6^{-1} \end{Vmatrix}$	σ_y	σ_z	$C^2 = I,\ BA = -A^5B$
		$P_3^{(7)}$	σ_z	σ_y	σ_z	$AC = CA$
		$P_4^{(7)}$	$\begin{Vmatrix} -\varepsilon_6^{-1} & 0 \\ 0 & \varepsilon_6 \end{Vmatrix}$	σ_y	$-\sigma_z$	$BC = -CB$
		$P_5^{(7)}$	$\begin{Vmatrix} \varepsilon_6 & 0 \\ 0 & -\varepsilon_6^{-1} \end{Vmatrix}$	σ_y	$-\sigma_z$	$\varepsilon_6 = e^{\pi i/3} = \dfrac{1+i\sqrt{3}}{2}$
		$P_6^{(7)}$	σ_z	σ_y	$-\sigma_z$	

Group	Class	Representation	A	B	Relations
T	K_1	$P_1^{(1)}$	$i\sigma_x$	$(1/\sqrt{2})\, e^{3\pi i/4}\,\delta$	$A^2 = -I$
		$P_2^{(1)}$	$i\sigma_x$	$-(1/\sqrt{2})\, e^{5\pi i/12}\delta$	$B^3 = I$
		$P_3^{(1)}$	$i\sigma_x$	$(1/\sqrt{2})\, e^{\pi i/12}\,\delta$	$BAB = AB^2A$
					$\delta = \begin{Vmatrix} 1 & 1 \\ -i & i \end{Vmatrix}$
T_h	K_1	$P_1^{(1)}$	$i\sigma_x$	$(1/\sqrt{2})\, e^{3\pi i/4}\,\delta$	
		$P_2^{(1)}$	$i\sigma_x$	$-(1/\sqrt{2})\, e^{5\pi i/12}\,\delta$	$A^2 = -I$
		$P_3^{(1)}$	$i\sigma_x$	$(1/\sqrt{2})\, e^{\pi i/12}\,\delta$	$B^6 = I$
		$P_4^{(1)}$	$i\sigma_x$	$-(1/\sqrt{2})\, e^{\pi i/12}\,\delta$	$BAB = AB^2A$
		$P_5^{(1)}$	$i\sigma_x$	$-(1/\sqrt{2})\, e^{3\pi i/4}\,\delta$	$\delta = \begin{Vmatrix} 1 & 1 \\ -i & i \end{Vmatrix}$
		$P_6^{(1)}$	$i\sigma_x$	$(1/\sqrt{2})\, e^{5\pi i/12}\,\delta$	
$O\,(T_d)$	K_1	$P_1^{(1)}$	$\varepsilon_8 \begin{Vmatrix} i & 0 \\ 0 & 1 \end{Vmatrix}$	$\dfrac{1}{\sqrt{2}}\, e^{-3i\pi/4}\,\delta$	$A^4 = -I,$ $B^3 = I$
		$P_2^{(1)}$	$-\varepsilon_8 \begin{Vmatrix} i & 0 \\ 0 & 1 \end{Vmatrix}$	$\dfrac{1}{\sqrt{2}}\, e^{-3i\pi/4}\,\delta$	$ABA = B^2$
		$Q^{(1)}$	$\varepsilon_8^3 \begin{Vmatrix} 0 & 0 & -\beta_1 & 0 \\ 0 & 0 & 0 & i\beta_1 \\ -\beta_2 & 0 & 0 & 0 \\ 0 & i\beta_2 & 0 & 0 \end{Vmatrix}$	$\dfrac{1}{\sqrt{2}}\, e^{-\pi i/12} \begin{Vmatrix} \delta & 0 \\ 0 & \varepsilon_3\delta \end{Vmatrix}$	$\beta_1 = e^{5\pi i/6}$ $\beta_2 = e^{i\pi/6} = -\dfrac{1}{\beta_1}$ $\delta = \begin{Vmatrix} 1 & 1 \\ i & -i \end{Vmatrix}$

TABLE 14.2 (continued)

Group	Class	Representation	A	B	Relations
O_h	K_1	$P_1^{(1)}$	ρ	δ	$A^4 = -I,\ B^6 = I$
		$P_2^{(1)}$	$-\rho$	δ	$BA^3B = A,\ AB^3 = B^3A$
		$P_3^{(1)}$	ρ	$-\delta$	$\rho = \frac{1}{\sqrt{3}} \begin{Vmatrix} \sqrt{2} & i\varepsilon^2 & 1 \\ -1 & -i\sqrt{2}\,\varepsilon & \end{Vmatrix}$
		$P_4^{(1)}$	$-\rho$	$-\delta$	$\delta = \begin{Vmatrix} \varepsilon^2 & 0 \\ 0 & \varepsilon \end{Vmatrix}$
		$Q_1^{(1)}$	$\begin{Vmatrix} 0 & \tau \\ \theta & 0 \end{Vmatrix}$	$\begin{Vmatrix} 1 & 0 & 0 & 0 \\ 0 & \varepsilon^2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \varepsilon \end{Vmatrix}$	$\tau = \frac{1}{\sqrt{3}} \begin{Vmatrix} 1 & -\sqrt{2}\,\varepsilon^2 \\ \sqrt{2}\,\varepsilon & 1 \end{Vmatrix}$
		$Q_2^{(1)}$	$\begin{Vmatrix} 0 & \tau \\ \theta & 0 \end{Vmatrix}$	$-\begin{Vmatrix} 1 & 0 & 0 & 0 \\ 0 & \varepsilon^2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & \varepsilon \end{Vmatrix}$	$\theta = -\frac{1}{\sqrt{3}} \begin{Vmatrix} 1 & \sqrt{2}\,\varepsilon \\ -\sqrt{2}\,\varepsilon^2 & 1 \end{Vmatrix} = -\tilde{\tau}$ $\varepsilon = \varepsilon_3$

K_2	$P_1^{(2)}$	$i\sigma_z$	σ_x	$A^4 = I,\ B^6 = I$
	$P_2^{(2)}$	$i\sigma_x$	$\begin{Vmatrix} \varepsilon & 0 \\ 0 & -\varepsilon^2 \end{Vmatrix}$	$BA^3B = A$
	$P_3^{(2)}$	$i\sigma_x$	$-\begin{Vmatrix} \varepsilon & 0 \\ 0 & -\varepsilon^2 \end{Vmatrix}$	$AB^3 = -B^3A$
	$R^{(2)}$	$\begin{Vmatrix} 0 & i & 0 & 0 & 0 & 0 \\ -i & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & i \end{Vmatrix}$	$\begin{Vmatrix} 0 & 0 & 0 & 0 & i & 0 \\ 0 & 0 & 0 & 0 & 0 & i \\ 0 & 0 & 0 & i & 0 & 0 \\ 0 & -i & 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 & 0 & 0 \\ -i & 0 & 0 & 0 & 0 & 0 \end{Vmatrix}$	$\varepsilon = \varepsilon_3$
K_3	$Q_1^{(3)}$	$\begin{Vmatrix} \rho & 0 \\ 0 & -\rho \end{Vmatrix}$	$\frac{\varepsilon_3}{\sqrt{2}}\begin{Vmatrix} 0 & -\delta \\ \delta & 0 \end{Vmatrix}$	$A^4 = -I,\ B^6 = I$ $BA^3B = A,\ AB^3 = -B^3A$
	$Q_2^{(3)}$	$\begin{Vmatrix} 0 & \rho \\ \rho & 0 \end{Vmatrix}$	$\frac{1}{\sqrt{2}}e^{\pi i/12}\begin{Vmatrix} \varepsilon_6\delta & 0 \\ 0 & \delta \end{Vmatrix}$	$\rho = \begin{Vmatrix} \varepsilon_8^3 & 0 \\ 0 & \varepsilon_8 \end{Vmatrix}$
	$Q_3^{(3)}$	$\begin{Vmatrix} 0 & \rho \\ \rho & 0 \end{Vmatrix}$	$-\frac{1}{\sqrt{2}}e^{\pi i/12}\begin{Vmatrix} \varepsilon_6\delta & 0 \\ 0 & \delta \end{Vmatrix}$	$\delta = \begin{Vmatrix} 1 & 1 \\ -i & i \end{Vmatrix}$

TABLE 14.3. Character tables for the point groups

C_{2h}			C_{2v}			D_2	$a^2=e,\ b^2=e,\ ab=ba$ $A^2=I,\ B^2=I,\ AB=\alpha BA$ $\alpha=\pm$
$a=c_2,\ b=i$ (or σ_h)			$a=c_2,\ b=\sigma_v$			$a=c_2,\ b=u_2$	
	e	a	b	ab	α		
$P^{(1)}$	2	0	0	0	-1		

C_{4h}										$a^4=e,\ b^2=e,\ ab=ba$ $A^4=I,\ B^2=I,\ AB=\alpha BA$ $\alpha=\pm 1$
$a=c_4,\ b=i$ (or σ_h)										
	e	a	a^2	a^3	b	ab	a^2b	a^3b	α	
$P_1^{(1)}$	2	0	2	0	0	0	0	0	-1	
$P_1^{(2)}$	2	0	-2	0	0	0	0	0		

C_{6h}													$a^6=e,\ b^2=e,\ ab=ba$ $A^6=I,\ B^2=I,\ AB=\alpha BA$ $\varepsilon_6=e^{\pi i/3},\ \alpha=\pm 1$
$a=c_6,\ b=i$ (or σ_h)													
	e	a	a^2	a^3	a^4	a^5	b	ab	a^2b	a^3b	a^4b	a^5b	α
$P_1^{(1)}$	2	0	2	0	2	0	0	0	0	0	0	0	
$P_2^{(1)}$	2	0	$2\varepsilon_6^2$	0	$2\varepsilon_6^4$	0	0	0	0	0	0	0	-1
$P_3^{(1)}$	2	0	$2\varepsilon_6^4$	0	$2\varepsilon_6^2$	0	0	0	0	0	0	0	

C_{4v}			D_4		D_{2d}		$a^4=e,\ b^2=e,\ ba=a^3b$ $A^4=\alpha I,\ B^2=I,\ BA=A^3B$ $\alpha=\pm 1$
$a=c_4,\ b=\sigma_v$			$a=c_4,\ b=u_2$		$a=s_4,\ b=u_2$		
	e	$a,\ a^3$	a^2	$b,\ a^2b$	$ab,\ a^3b$	α	
$P_1^{(1)}$	2	$\sqrt{2}i$	0	0	0	-1	
$P_2^{(1)}$	2	$-\sqrt{2}i$	0	0	0		

TABLE 14.3 (continued)

D_6	C_{6v}	D_{3d}	D_{3h}	$a^6=e,\ b^2=e,\ ba=a^5b$
$a=c_6,\ b=u_2$	$a=c_6,\ b=\sigma_v$	$a=s_6,\ b=u_2$	$a=s_6,\ b=u_2$	$A^6=I,\ B^2=I,\ BA=\alpha A^5B$ $\alpha=\pm 1$

	e	a	$a^2,\ a^4$	a^3	$b,\ a^2b,\ a^4b$	$ab,\ a^3b,\ a^5b$	α
$P_1^{(1)}$	2	0	2	0	0	0	
$P_2^{(1)}$	2	$i\sqrt{3}$	-1	$-i\sqrt{3}$	0	0	-1
$P_3^{(1)}$	2	$-i\sqrt{3}$	-1	$i\sqrt{3}$	0	0	

D_{2h}	$a^2=b^2=c^2=e,\ ba=ab,\ cb=bc,\ ac=ca$
$a=c_2,\ b=u_2,\ c=i$ (or σ_h)	$A^2=B^2=C^2=I,\ BA=\alpha AB,\ CB=\gamma BC,\ AC=\beta CA$ $\alpha,\ \beta,\ \gamma=\pm 1$

Class		e	a	b	c	ab	bc	ca	abc
K_1	$P_1^{(1)}$	2	0	0	2	0	0	0	0
$\alpha=-1,\beta=\gamma=1$	$P_2^{(1)}$	2	0	0	-2	0	0	0	0
K_2	$P_1^{(2)}$	2	0	2	0	0	0	0	0
$\alpha=\beta=1,\gamma=-1$	$P_2^{(2)}$	2	0	-2	0	0	0	0	0
K_3	$P_1^{(3)}$	2	2	0	0	0	0	0	0
$\alpha=\gamma=1,\beta=-1$	$P_2^{(3)}$	2	-2	0	0	0	0	0	0
K_4	$P_1^{(4)}$	2	0	0	0	2	0	0	0
$\beta=\gamma=-1,\alpha=1$	$P_2^{(4)}$	2	0	0	0	-2	0	0	0
K_5	$P_1^{(5)}$	2	0	0	0	0	0	0	2
$\alpha=\beta=\gamma=-1$	$P_2^{(5)}$	2	0	0	0	0	0	0	-2
K_6	$P_1^{(6)}$	2	0	0	0	0	2	0	0
$\alpha=\beta=-1,\gamma=1$	$P_2^{(6)}$	2	0	0	0	0	-2	0	0
K_7	$P_1^{(7)}$	2	0	0	0	0	0	2	0
$\alpha=\gamma=-1,\beta=1$	$P_2^{(7)}$	2	0	0	0	0	0	-2	0

Table 14.3 (continued)

D_{4h}		$a^4=e,\ b^2=e,\ ba=a^3b$
$a=c_4,\ b=u_2,\ c=i$ (or σ_h)		$A^4=\alpha I,\ BA=A^3B,\ B^2=C^2=I,\ AC=\beta CA,\ BC=\gamma CB$ $\alpha,\ \beta,\ \gamma=\pm 1$

Class		e	a	a^2	a^3	b	ab	a^2b	a^3b	c	ac	a^2c	a^3c	bc	abc	a^2bc	a^3bc
K_1 $\beta=\gamma=1$ $\alpha=-1$	$P_1^{(1)}$	2	$\sqrt{2}i$	0	$\sqrt{2}i$	0	0	0	0	2	$\sqrt{2}i$	0	$\sqrt{2}i$	0	0	0	0
	$P_2^{(1)}$	2	$-\sqrt{2}i$	0	$-\sqrt{2}i$	0	0	0	0	2	$-\sqrt{2}i$	0	$-\sqrt{2}i$	0	0	0	0
	$P_3^{(1)}$	2	$\sqrt{2}i$	0	$\sqrt{2}i$	0	0	0	0	−2	$-\sqrt{2}i$	0	$-\sqrt{2}i$	0	0	0	0
	$P_4^{(1)}$	2	$-\sqrt{2}i$	0	$-\sqrt{2}i$	0	0	0	0	−2	$\sqrt{2}i$	0	$\sqrt{2}i$	0	0	0	0
K_2 $\alpha=\beta=1$ $\gamma=-1$	$P_1^{(2)}$	2	2	2	2	0	0	0	0	0	0	0	0	0	0	0	0
	$P_2^{(2)}$	2	0	−2	0	0	0	0	0	0	$2i$	0	$-2i$	0	0	0	0
	$P_3^{(2)}$	2	−2	2	−2	0	0	0	0	0	0	0	0	0	0	0	0
	$P_4^{(2)}$	2	0	−2	0	0	0	0	0	0	$-2i$	0	$2i$	0	0	0	0
K_3 $\alpha=\gamma=1$ $\beta=-1$	$P_1^{(3)}$	2	0	2	0	2	0	2	0	0	0	0	0	0	0	0	0
	$P_2^{(3)}$	2	0	−2	0	0	0	0	0	0	0	0	0	2	0	−2	0
	$P_3^{(3)}$	2	0	2	0	−2	0	−2	0	0	0	0	0	0	0	0	0
	$P_4^{(3)}$	2	0	−2	0	0	0	0	0	0	0	0	0	−2	0	2	0
K_4 $\beta=\gamma=$ $=-1$ $\alpha=1$	$P_1^{(4)}$	2	0	2	0	0	2	0	2	0	0	0	0	0	0	0	0
	$P_2^{(4)}$	2	0	−2	0	0	0	0	0	0	0	0	0	0	2	0	−2
	$P_3^{(4)}$	2	0	2	0	0	−2	0	−2	0	0	0	0	0	0	0	0
	$P_4^{(4)}$	2	0	−2	0	0	0	0	0	0	0	0	0	0	−2	0	2
K_5 $\alpha=\beta=$ $=\gamma=-1$	$Q^{(5)}$	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
K_6 $\alpha=\beta=$ $=-1$ $\gamma=1$	$Q^{(6)}$	4	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
K_7 $\alpha=\gamma=$ $=-1$ $\beta=1$	$P_1^{(7)}$	2	$\sqrt{2}i$	0	$\sqrt{2}i$	0	0	0	0	0	$-\sqrt{2}$	$-2i$	$\sqrt{2}$	0	0	0	0
	$P_2^{(7)}$	2	$-\sqrt{2}i$	0	$-\sqrt{2}i$	0	0	0	0	0	$\sqrt{2}$	$-2i$	$-\sqrt{2}$	0	0	0	0
	$P_3^{(7)}$	2	$\sqrt{2}i$	0	$\sqrt{2}i$	0	0	0	0	0	$\sqrt{2}$	$2i$	$-\sqrt{2}$	0	0	0	0
	$P_4^{(7)}$	2	$-\sqrt{2}i$	0	$-\sqrt{2}i$	0	0	0	0	0	$-\sqrt{2}$	$2i$	$\sqrt{2}$	0	0	0	0

Table 14.3 (continued)

D_{6h} $a=c_6,\ b=u_2,\ c=i\ (\text{or}\ \sigma_h)$		$a^6=b^2=c^3=e,\ ba=a^5b,\ ca=ac,\ cb=bc$ $A^6=B^2=C^2=I,\ BA=\alpha A^5B,\ CA=\beta AC,\ CB=\gamma BC$ $\alpha,\ \beta,\ \gamma=\pm 1$														
Class		e	a	a^2 a^4	a^3	a^5	b a^2b a^4b	ab a^3b a^5b	c	ac	a^2c	a^3c	a^4c	a^5c	bc a^2bc a^4bc	abc a^3bc a^5bc
K_1 $\beta=\gamma=1$ $\alpha=-1$	$P_1^{(1)}$	2	$i\sqrt{3}$	−1	0	$-i\sqrt{3}$	0	0	2	$i\sqrt{3}$	−1	0	−1	$-i\sqrt{3}$	0	0
	$P_2^{(1)}$	2	$-i\sqrt{3}$	−1	0	$i\sqrt{3}$	0	0	2	$-i\sqrt{3}$	−1	0	−1	$i\sqrt{3}$	0	0
	$P_3^{(1)}$	2	0	2	0	0	0	0	2	0	2	0	2	0	0	0
	$P_4^{(1)}$	2	$i\sqrt{3}$	−1	0	$-i\sqrt{3}$	0	0	−2	$-i\sqrt{3}$	1	0	1	$i\sqrt{3}$	0	0
	$P_5^{(1)}$	2	$-i\sqrt{3}$	−1	0	$i\sqrt{3}$	0	0	−2	$i\sqrt{3}$	1	0	1	$-i\sqrt{3}$	0	0
	$P_6^{(1)}$	2	0	2	0	0	0	0	−2	0	−2	0	−2	0	0	0
K_2 $\alpha=\beta=1$ $\gamma=-1$	$P_1^{(2)}$	2	2	2	2	2	0	0	0	0	0	0	0	0	0	0
	$P_2^{(2)}$	2	1	−1	−2	1	0	0	0	$-i\sqrt{3}$	$-i\sqrt{3}$	0	$i\sqrt{3}$	$i\sqrt{3}$	0	0
	$P_3^{(2)}$	2	−1	−1	2	−1	0	0	0	$i\sqrt{3}$	$-i\sqrt{3}$	0	$i\sqrt{3}$	$-i\sqrt{3}$	0	0
	$P_4^{(2)}$	2	−2	2	−2	−2	0	0	0	0	0	0	0	0	0	0
	$P_5^{(2)}$	2	1	−1	−2	1	0	0	0	$i\sqrt{3}$	$i\sqrt{3}$	0	$-i\sqrt{3}$	$-i\sqrt{3}$	0	0
	$P_6^{(2)}$	2	−1	−1	2	−1	0	0	0	$-i\sqrt{3}$	$i\sqrt{3}$	0	$-i\sqrt{3}$	$i\sqrt{3}$	0	0
K_3 $\alpha=\gamma=1$ $\beta=-1$	$P_1^{(3)}$	2	0	2	0	0	2	0	0	0	0	0	0	0	0	0
	$P_2^{(3)}$	2	0	2	0	0	−2	0	0	0	0	0	0	0	0	0
	$Q^{(3)}$	4	0	−2	0	0	0	0	0	0	0	0	0	0	0	0
K_4 $\beta=\gamma=$ $=-1$ $\alpha=1$	$P_1^{(4)}$	2	0	2	0	0	0	2	0	0	0	0	0	0	0	0
	$P_2^{(4)}$	2	0	2	0	0	0	−2	0	0	0	0	0	0	0	0
	$Q^{(4)}$	4	0	−2	0	0	0	0	0	0	0	0	0	0	0	0
K_5 $\alpha=\beta=$ $=\gamma=-1$	$P_1^{(5)}$	2	0	2	0	0	0	0	0	0	0	0	0	0	0	$2i$
	$P_2^{(5)}$	2	0	2	0	0	0	0	0	0	0	0	0	0	0	$-2i$
	$Q^{(5)}$	4	0	−2	0	0	0	0	0	0	0	0	0	0	0	0
K_6 $\alpha=\beta=$ $=-1$ $\gamma=1$	$P_1^{(6)}$	2	0	2	0	0	0	0	0	0	0	0	0	0	2	0
	$P_2^{(6)}$	2	0	2	0	0	0	0	0	0	0	0	0	0	−2	0
	$Q^{(6)}$	4	0	−2	0	0	0	0	0	0	0	0	0	0	0	0
K_7 $\alpha=\gamma=$ $=-1$ $\beta=1$	$P_1^{(7)}$	2	$i\sqrt{3}$	−1	0	$-i\sqrt{3}$	0	0	0	−1	$-i\sqrt{3}$	2	$i\sqrt{3}$	−1	0	0
	$P_2^{(7)}$	2	$-i\sqrt{3}$	−1	0	$i\sqrt{3}$	0	0	0	−1	$i\sqrt{3}$	2	$-i\sqrt{3}$	−1	0	0
	$P_3^{(7)}$	2	0	2	0	0	0	0	0	2	0	2	0	2	0	0
	$P_4^{(7)}$	2	$i\sqrt{3}$	−1	0	$-i\sqrt{3}$	0	0	0	1	$i\sqrt{3}$	−2	$-i\sqrt{3}$	1	0	0
	$P_5^{(7)}$	2	$-i\sqrt{3}$	−1	0	$i\sqrt{3}$	0	0	0	1	$-i\sqrt{3}$	−2	$i\sqrt{3}$	1	0	0
	$P_6^{(7)}$	2	0	2	0	0	0	0	0	−2	0	−2	0	−2	0	0

TABLE 14.3 (continued)

T	$a^2 = e,\quad b^3 = e,\quad bab = ab^2a$ $\boldsymbol{A^2 = -I,\ B^3 = I,\ BAB = AB^2A}$ $\varepsilon_3 = e^{2\pi i/3}$
$a = c_2,\ b = c_3$	

	e	$a,\ bab^2,\ b^2ab$	$b,\ ba,\ ab$	aba	$bab,\ b^2a,\ ab^2$	b^2
$P_1^{(1)}$	2	0	-1	1	1	-1
$P_2^{(1)}$	2	0	$-\varepsilon_3$	ε_3	ε_3^2	$-\varepsilon_3^2$
$P_3^{(1)}$	2	0	$-\varepsilon_3^2$	ε_3^2	ε_3	$-\varepsilon_3$

T_h	$a^2 = e,\quad s^6 = e,\quad sas = as^2a$ $\boldsymbol{A^2 = -I,\ S^6 = I,\ SAS = AS^2A}$
$a = c_2,\ s = s_6$	

	e	s^3	a sas^2 s^2as	s^2a s^4as^3 s^2as^4	s sa as	s^4 s^4a as	asa	as^4a	sas s^2a as^2	sas^4 s^3a as^5	s^2	s^5
$P_1^{(1)}$	2	2	0	0	-1	-1	1	1	1	1	-1	-1
$P_2^{(1)}$	2	2	0	0	$-\varepsilon_3$	$-\varepsilon_3$	ε_3	ε_3	ε_3^2	ε_3^2	$-\varepsilon_3^2$	$-\varepsilon_3^2$
$P_3^{(1)}$	2	2	0	0	$-\varepsilon_3^2$	$-\varepsilon_3^2$	ε_3^2	ε_3^2	ε_3	ε_3	$-\varepsilon_3$	$-\varepsilon_3$
$P_4^{(1)}$	2	-2	0	0	ε_3^2	$-\varepsilon_3^2$	$-\varepsilon_3^2$	ε_3^2	ε_3	$-\varepsilon_3$	$-\varepsilon_3$	ε_3
$P_5^{(1)}$	2	-2	0	0	1	-1	-1	1	1	-1	-1	1
$P_6^{(1)}$	2	-2	0	0	ε_3	$-\varepsilon_3$	$-\varepsilon_3$	ε_3	ε_3^2	$-\varepsilon_3^2$	$-\varepsilon_3^2$	ε_3^2

O	T_d	$a^4 = e,\ b^3 = e,\ aba = b^2$ $\boldsymbol{A^4 = -I,\ B^3 = I,\ ABA = B^2}$
$a = c_4,\ b = c_3$	$a = s_4,\ b = c_3$	

	e	a bab^2 b^2ab	a^2 ba^2b^2 b^2a^2b	a^3 b^2a ab^2	ab b^2ab^2 ba^2b^2a	ba a^2ba^3 a^3ba^2	$b,\ b^2$ a^2b b^2a	$a^2b^2,\ b^2a^2$ $a^2b^2a^2$ a^2ba^2
$P_1^{(1)}$	2	$\sqrt{2}\,i$	0	$-\sqrt{2}\,i$	0	0	-1	1
$P_2^{(1)}$	2	$-\sqrt{2}\,i$	0	$\sqrt{2}\,i$	0	0	-1	1
$Q^{(1)}$	4	0	0	0	0	0	1	-1

TABLE 14.3 (continued)

O_h* ($a = c_4$, $b = s_6$)			$a^4 = e$, $b^6 = e$, $ba^3b = a$, $ab^3 = b^3a$; $A^4 = \alpha I$, $B^6 = I$, $BA^3B = A$, $AB^3 = \beta B^3A$; $\alpha = \pm 1$, $\beta = \pm 1$									
Class		e	a b^3ab^4 b^4ab^3 a^3 b^4a ab^4	b^3 b^4 ab^3a^3 $a^3b^3a^3$ a^3b^3a $a^3b^4a^3$ a^3b^3 b^3a^3	a^3 $b^3a^3b^4$ $a^3b^4a^3$	ab^3 b^3a b^4ab^4 $a^3b^3a^3$ $a^3b^3a^3$ $b^3a^3b^4a$	b^3	ab^3 b^3ab b^4ab^3 a^3b^3 b^4ab^3 ab	b b^4 $ab^3a^3b^3$ $a^3b^3ab^3$ a^3b^3 b^3a^3 a^3ba^3 $a^3b^3a^3$	a^3b^3 b^3a^3b ba^3b^3	ab^3 b^3ab^3 b^4ab a^3bab^3 $a^3b^3a^3$ $b^3a^3b^4ab^3$
K_1 $\alpha=-1$ $\beta=1$	$P_1^{(1)}$	2	$\sqrt{2}$	-1	0	0	2	$\sqrt{2}$	-1	0	0
	$P_2^{(1)}$	2	$-\sqrt{2}$	-1	0	0	2	$-\sqrt{2}$	-1	0	0
	$P_3^{(1)}$	2	$\sqrt{2}$	-1	0	0	-2	$-\sqrt{2}$	1	0	0
	$P_4^{(1)}$	2	$-\sqrt{2}$	-1	0	0	-2	$\sqrt{2}$	1	0	0
	$Q_1^{(1)}$	4	0	1	0	0	4	0	1	0	0
	$Q_2^{(1)}$	4	0	1	0	0	-4	0	-1	0	0
K_2 $\alpha=1$ $\beta=-1$	$P_1^{(2)}$	2	0	2	-2	0	0	0	0	0	0
	$P_2^{(2)}$	2	0	-1	-2	0	0	0	$i\sqrt{3}$	0	0
	$P_3^{(2)}$	2	0	-1	-2	0	0	0	$-i\sqrt{3}$	0	0
	$R^{(2)}$	6	0	0	2	0	0	0	0	0	0
K_3 $\alpha=-1$ $\beta=-1$	$Q_1^{(3)}$	4	0	-2	0	0	0	0	0	0	0
	$Q_2^{(3)}$	4	0	1	0	0	0	0	$i\sqrt{3}$	0	0
	$Q_3^{(3)}$	4	0	1	0	0	0	0	$-i\sqrt{3}$	0	0

* To simplify the notation, inversion b^3 is expressed in terms of even powers of a, since $a^3b^3 = b^3a^3$ both in O_h and in the representation group (14.75). For example, $a^3b^3a^3b^3 = a^3b^6a^3$.

3) Determine the class of the factor system, using the appropriate formulas of §14 for the group F_k. Knowledge of the class enables one immediately to determine the dimensions of the representations of the little group. If the factor system obtained is not in the standard form corresponding to the group F_k, use the formulas of §14 to find a function $u(r)$ which reduces the factor system to standard form via (13.4).

4) The representation $\mathcal{D}^k(h)$ of the little group for the element $h = (r|a + \alpha)$ is determined from the formula

$$\mathcal{D}^k(h) = e^{ik(a+\alpha)}\, u(r)\, \mathcal{D}(r),$$

where $\mathcal{D}(r)$ is a projective representation belonging to the standard factor system. If the element $r = a^m b^n c^p \ldots$, where a, b, c, ... are the generators of F_k, then $\mathcal{D}(r) = A^m B^n C^p \ldots$, where A, B, C, ... are the matrices of the projective representation belonging to the standard factor system; these matrices may be found in Table 14.2.*

5) The total representation $\mathcal{D}^{(k)}$ of the space group is determined in terms of the representation of the little group, using formula (12.23).

* Care should be taken here that the order of the generators $a^m b^n c^p \ldots$ in the expression for r coincide with the definition of r as given in the character tables for projective representations (Table 14.3).

Chapter III

SYMMETRY IN QUANTUM MECHANICS

The first chapters of this book presented the elements of symmetry theory and representation theory. We now proceed to a discussion of the physical consequences of symmetry in quantum mechanics and vibration theory. Both determination of the allowed energies and eigenfunctions in quantum mechanics and determination of vibrational frequencies and the corresponding displacement vectors are essentially problems of determining the eigenvalues and eigenfunctions of a suitable operator. The general nature of the spectrum of an operator is largely conditioned by its symmetry. This is the reason for the wide use of group theory in quantum mechanics and vibration theory.

Symmetry theory provides a description, independent of the specific type of interaction, of the important features of electronic and vibrational spectra of atoms, molecules and crystals, the systematics of terms and the possible types of degeneracy, the positions of extremum points for spectra in crystals and the shape of the spectrum near these points, selection rules for various transitions, the change in the spectra in external fields which break the symmetry, and so on.

In §15 we dwell on the first of these questions.

§15. IRREDUCIBLE REPRESENTATIONS AND CLASSIFICATION OF TERMS. NORMAL MODES. PERTURBATION THEORY

The steady state of an electron in an external field is described by the Schrödinger equation

$$\mathscr{H}(\boldsymbol{x})\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x})\right)\psi = E\psi. \tag{15.1}$$

Since the kinetic energy operator

$$T = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)$$

is invariant under any operation of the space groups, i.e., under rotations and translations, the symmetry of the Hamiltonian $\mathscr{H}(\boldsymbol{x})$ is determined by the symmetry of the potential $V(\boldsymbol{x})$. For example, the potential $V(\boldsymbol{x})$ for an electron in an ideal crystal is invariant under any transformation in the appropriate space group. For an electron located at an impurity center in the

lattice, $V(\boldsymbol{x})$ is invariant under the point group defined by the crystal symmetry and the position of the impurity center in the lattice. Hence, under all operations g in the symmetry group $\mathcal{G}$ of the Hamiltonian

$$\mathcal{H}(g^{-1}\boldsymbol{x}) = \mathcal{H}(\boldsymbol{x}) \tag{15.2}$$

or

$$\mathcal{D}(g)\mathcal{H}(\boldsymbol{x})\psi(\boldsymbol{x}) = \mathcal{H}(g^{-1}\boldsymbol{x})\psi(g^{-1}\boldsymbol{x}) = \mathcal{H}(\boldsymbol{x})\mathcal{D}(g)\psi(\boldsymbol{x}).$$

Therefore, invariance of $\mathcal{H}$ under the operation g implies that the operators $\mathcal{H}$ and $\mathcal{D}(g)$ commute:

$$\mathcal{D}(g)\mathcal{H} = \mathcal{H}\mathcal{D}(g). \tag{15.3}$$

In the new coordinate system $\boldsymbol{x}' = g^{-1}\boldsymbol{x}$, the Schrödinger equation (15.1) becomes

$$\mathcal{H}(\boldsymbol{x})\psi(g^{-1}\boldsymbol{x}) = E\psi(g^{-1}\boldsymbol{x}). \tag{15.4}$$

Equations (15.1) and (15.2) show that the functions $\psi(\boldsymbol{x})$ and $\psi(g^{-1}\boldsymbol{x})$ belong to the same energy eigenvalue E. Applying all the transformations g in the group, we thus obtain h functions $\psi(g^{-1}\boldsymbol{x})$, of which in general only a certain subset $\psi_j(\boldsymbol{x})$ are linearly independent, and all the others may be expressed in terms of them. Thus any function obtained by applying $\mathcal{D}(g)$ to a function ψ_j is a linear combination of these functions:

$$\mathcal{D}(g)\psi_l = \psi_l(g^{-1}\boldsymbol{x}) = \sum_i \mathcal{D}_{il}\psi_i(\boldsymbol{x}). \tag{15.5}$$

Equation (15.5) shows that the system of eigenfunctions of the operator $\mathcal{H}$ belonging to one eigenvalue forms a basis for a representation $\mathcal{D}$ of the symmetry group $\mathcal{G}$ of the Hamiltonian.

The representation $\mathcal{D}$ may be reducible or irreducible. Since the action of all the operators $g \in \mathcal{G}$ on any of the functions ψ_j yields all the functions on an irreducible representation, it follows that in any case all the functions of an irreducible representation correspond to the same energy.

On the other hand, coincidence of eigenvalues for several independent systems of functions, each forming a basis for a different representation, may occur only accidentally. As a rule one has a different energy eigenvalue for each irreducible representation. Therefore, the possible degeneracy of each term is determined by the dimension of the corresponding irreducible representation, and the solution set of the Schrödinger equation will contain terms of all multiplicites permitted by this condition. For this reason the state of an electron is frequently characterized by the index of the corresponding irreducible representation. Of course, this does not mean that only one term can correspond to each representation. On the contrary, as a rule one has a whole set of terms corresponding to each.

In some cases, however, additional symmetry conditions, unrelated to spatial symmetry, lead to coincidence of the energies of several irreducible representations. This additional degeneracy, as will be shown below, may be caused by invariance of the equations of motion under time reversal. In special cases the symmetry group of the Hamiltonian $\mathcal{H} = T + V$ may possess higher symmetry than the potential V; this is another source of additional degeneracy. This is the case for the Coulomb potential $V = -c/x$, and also for the harmonic oscillator, with $V = -cx^2$.

Vibrational Spectra of Molecules and Crystals

Representation theory makes it possible similarly to classify the vibrational spectra of molecules and crystals. As we know, in classical theory the vibrational frequencies ω and displacement vectors $\boldsymbol{u}(l)$ of a system consisting of N_a atoms l are defined by the system of equations /9.1, 9.2/

$$M_l \ddot{u}_i(l) = -M_l \omega^2 u_i(l) = -\sum_{l'=1}^{N_a} \sum_{i'=1}^{3} \Phi_{ii'}(l, l')\, u_{i'}(l'), \tag{15.6}$$

where M_l is the mass of the atom and $\Phi_{ii'}(l, l') = \Phi_{i'i}(l', l)$ are force constants, i.e., the second derivatives of the potential energy with respect to the displacements $u_i(l)$, $u_{i'}(l')$. Equation (15.6) can be rewritten as

$$\sum_{l'i'} (D_{ii'}(l, l') - \omega^2 \delta_{ll'} \delta_{ii'})\, u_{i'}(l') \sqrt{M_l} = 0. \tag{15.6a}$$

Here $\boldsymbol{D}$ is the dynamical matrix, whose elements are

$$D_{ii'}(l, l') = D_{i'i}(l', l) = \frac{\Phi_{ii'}(l, l')}{\sqrt{M_l M_{l'}}}. \tag{15.6b}$$

We now transform from the $3N_a$ variables $\frac{1}{2}\sqrt{M_l/M}\, u_i(l)$ to the variables

$$a_\alpha = \frac{1}{2} \sum_{li} B_{li}^{\alpha *} u_i(l) \sqrt{\frac{M_l}{M}}, \quad \text{where} \quad M = \sum_l M_l, \tag{15.7}$$

letting $\boldsymbol{B}$ be a matrix diagonalizing the dynamical matrix $\boldsymbol{D}$: $\boldsymbol{B}^{-1}\boldsymbol{D}\boldsymbol{B} = \Omega$, where Ω is a diagonal matrix with elements $\Omega_\alpha = \omega_\alpha^2$:

$$\sum_{lil'i'} B_{li}^{*\alpha} D_{ii'}(l, l')\, B_{l'i'}^{\alpha'} = \omega_\alpha^2 \delta_{\alpha\alpha'}, \tag{15.8}$$

and the natural frequencies ω_α^2 are the roots of the secular equation

$$| D_{ii'}(l, l') - \omega^2 \delta_{ii'} \delta_{ll'} | = 0. \tag{15.8a}$$

In principle, some of the eigenvalues may be degenerate, several functions a_α corresponding to one frequency ω_α. The matrix $\boldsymbol{B}$ is unitary, $\boldsymbol{B}\tilde{\boldsymbol{B}}^* = \boldsymbol{I}$ and $\tilde{\boldsymbol{B}}^*\boldsymbol{B} = \boldsymbol{I}$, or

$$\sum_{li} B_{li}^{\alpha} B_{li}^{\beta *} = \delta_{\alpha\beta}, \tag{15.9a}$$

$$\sum_{\alpha} B_{li}^{\alpha *} B_{l'i'}^{\alpha} = \delta_{ll'} \delta_{ii'}, \tag{15.9b}$$

so that the eigenvectors B_{li}^{α} are orthonormal. It can also be shown that $\tilde{\boldsymbol{B}}^{\alpha}\boldsymbol{B}^{\beta} = 0$ if $\omega_\alpha \neq \omega_\beta$, or, in coordinate notation,*

$$\sum_{li} B_{li}^{\alpha} B_{li}^{\beta} = 0 \quad \text{if} \quad \omega_\alpha \neq \omega_\beta. \tag{15.9c}$$

It follows from (15.8) that in the new variables the system of equations (15.6) splits into $3N_a$ independent equations

$$(\omega_\alpha^2 - \omega^2)\, a_\alpha = 0. \tag{15.10}$$

* The eigenvectors $\boldsymbol{B}^{\beta}$ belonging to frequency ω_β satisfy equation (15.11b): $\boldsymbol{D}\boldsymbol{B}^{\beta} = \Omega_\beta \boldsymbol{B}^{\beta}$. Multiply this equation on the right by $\tilde{\boldsymbol{B}}^{\alpha}$, and the transposed equation $\tilde{\boldsymbol{B}}^{\alpha}\tilde{\boldsymbol{D}} = \Omega_\alpha \tilde{\boldsymbol{B}}^{\alpha}$ on the left by $\boldsymbol{B}^{\beta}$, and add. Since $\tilde{\boldsymbol{D}} = \boldsymbol{D}$ (15.6b), we obtain, by (15.9b): $(\Omega_\alpha - \Omega_\beta)\, \tilde{\boldsymbol{B}}^{\alpha}\boldsymbol{B}^{\beta} = 0$.

Applying the inverse transformation to (15.7) and using (15.9), we express u_l in terms of a_α:

$$u_l(l) = 2\sqrt{\frac{M}{M_l}} \sum_\alpha B^\alpha_{ll}\, a_\alpha. \tag{15.11}$$

The vectors $u^\alpha(l)$ defined by the relations

$$u^\alpha_l(l) = 2\sqrt{\frac{M}{M_l}}\, B^\alpha_{ll}\, a_\alpha \tag{15.11a}$$

are the eigenfunctions of equations (15.7) for $\omega = \omega_\alpha$ and are called normal modes. They show how the atom l is displaced when vibrating in mode a_α. In order to find the elements B^α_{ll} in explicit form, we must find the natural frequencies and solve the system of equations $\boldsymbol{DB} = \boldsymbol{B\Omega}$, which in terms of the elements is

$$\sum_{l'i'} D_{ii'}(ll')\, B^\alpha_{l'i'} = \omega^2_\alpha\, B^\alpha_{ll}. \tag{15.11b}$$

In a crystal, each atom l may be characterized by two indices: the number f of the cell and the number $\varkappa$ of the atom in the cell. These indices have the property that the force constants $\Phi_{ii'}(f\varkappa, f'\varkappa')$ possess translational symmetry, i.e., depend only on the difference $f - f'$. Therefore, the eigenvectors $\boldsymbol{B}^\alpha_l$ can be chosen as

$$\boldsymbol{B}^{\nu q}_{f\varkappa} = \sqrt{\frac{M_\varkappa}{M_0 N}}\, e^\nu_\varkappa(q)\, e^{iq x^\varkappa_f}, \tag{15.12}$$

where ν is the number of the spectrum branch and q the wave vector; N is the number of cells, $M_0 = \sum_\varkappa M_\varkappa$ the cell mass, and $M = M_0 N = \rho\mathcal{V}^\circ$, where ρ is the density and $\mathcal{V}^\circ$ the volume of the crystal. The matrix $\boldsymbol{B}$ defined in (15.12) enables one to go over from the $3Nn_a$ functions $u_{f\varkappa,l}$ to the $3Nn_a$ functions $a_{q\nu}$ introduced below (equation (15.16)), where n_a is the number of atoms in a primitive cell. Here q takes N different values, ν varies from 1 to $3n_a$, and for each q the matrix e with elements $e^\nu_{\varkappa l}(q)$ is the matrix of transformation from the $3n_a$ functions $u_{\varkappa l}(q)$ to the $3n_a$ functions $a_{q\nu}$. The matrix e diagonalizes the matrix D' whose elements are

$$D'_{ii'\varkappa\varkappa'}(q) = \frac{\sqrt{M_\varkappa M_{\varkappa'}}}{M} D_{ii'\varkappa\varkappa'}(q), \tag{15.13}$$

where

$$D_{ii'\varkappa\varkappa'}(q) = \frac{1}{N} \sum_{ff'} D_{ii'ff'\varkappa\varkappa'}\, e^{-iq\left(x^\varkappa_f - x^{\varkappa'}_{f'}\right)}. \tag{15.13a}$$

In fact, substituting (15.12) into (15.8) and summing over f and f', we obtain the system of equations:

$$\sum_{i\varkappa i'\varkappa'} \frac{\sqrt{M_\varkappa M_{\varkappa'}}}{M_0}\, e^{\nu*}_{\varkappa l}\, D_{ii'\varkappa\varkappa'}(q)\, e^{\nu'}_{\varkappa' i'}(q) = \omega^2_{q\nu}\delta_{\nu\nu'}. \tag{15.13b}$$

By (15.9), polarization vectors belonging to different branches or to different atoms in the cell are orthogonal:

$$\sum_{\varkappa l} M_\varkappa e^\nu_{\varkappa l}(q)\, e^{\nu'*}_{\varkappa l}(q) = M_0\delta_{\nu\nu'}, \tag{15.14a}$$

$$\sum_{\nu} \sqrt{M_\varkappa M_{\varkappa'}}\, e^{\nu}_{\varkappa l}(q)\, e^{\nu *}_{\varkappa' l'}(q) = M_0 \delta_{\varkappa\varkappa'}\delta_{ll'}, \tag{15.14b}$$

$$\sum_{\varkappa l} M_\varkappa e^{\nu}_{\varkappa l}(q)\, e^{\nu'}_{\varkappa l}(q) = 0 \quad \text{if} \quad \omega_{q\nu} \neq \omega_{q\nu'}. \tag{15.14c}$$

By (15.11b), in order to determine the elements $e^{\nu}_{\varkappa l}$ directly we must solve the system of equations

$$\sum_{\varkappa' l'} \left(D_{ll'\varkappa\varkappa'}(q) - \omega^2_{q\nu}\delta_{\varkappa\varkappa'}\delta_{ll'}\right) e^{\nu}_{\varkappa' l'} \sqrt{M_{\varkappa'}} = 0, \tag{15.15}$$

where the matrix $D_{ll'\varkappa\varkappa'}(q)$ is defined by equation (15.13a), and the $\omega_{q\nu}$ are the roots of the secular equation

$$\left| D_{ll'\varkappa\varkappa'}(q) - \omega^2_{q\nu}\delta_{\varkappa\varkappa'}\delta_{ll'} \right| = 0, \tag{15.15a}$$

which determines the vibrational spectrum of the crystal, i.e., the function $\omega_\nu(q)$ for each branch ν of the spectrum, just as the solution of the Schrödinger equation (15.1) determines the electronic spectrum $E(k)$ for each band in an ideal crystal lattice.

The total number of branches is $3n_a$, i.e., thrice the number of atoms in the primitive cell. The three branches for which $\omega_\nu(q) \to 0$ as $q \to 0$ are called acoustical, and the other $3(n_a - 1)$ are called optical.

By (15.11a) and (15.12), the displacement of an atom f, $\varkappa$ vibrating in mode $a_{q\nu}$ is

$$u^{q\nu}_{f\varkappa, l} = 2a_{q\nu} e^{\nu}_{\varkappa l}(q)\, e^{iqx^{\varkappa}_f}. \tag{15.16}$$

An arbitrary displacement $u_{f\varkappa, l}$ can be expanded in terms of normal modes $u^{q\nu}_{f\varkappa, l}$. By (15.7) and (15.11),

$$u_{f\varkappa} = \sum_{q\nu} u^{q\nu}_{f\varkappa} = 2\sum_{q\nu} a_{q\nu} e^{\nu}_{\varkappa}(q)\, e^{iqx^{\varkappa}_f} = \sum_{q\nu} a_{q\nu} e^{\nu}_{\varkappa}(q)\, e^{iqx^{\varkappa}_f} + \dot{a}_{q\nu} e^{\nu *}_{\varkappa}(q)\, e^{-iqx^{\varkappa}_f}. \tag{15.12a}$$

If this equation is multiplied by $e^{-iq'x^{\varkappa}_f}$ and the right-hand and left-hand sides summed over f, the result is

$$u_\varkappa(q) = 2\sum_{\nu} e^{\nu}_{\varkappa}(q)\, a_{q\nu}, \tag{15.16a}$$

where

$$u_\varkappa(q) = \frac{1}{N}\sum_{f} u_{f\varkappa} e^{-iqx^{\varkappa}_f}. \tag{15.16b}$$

In the quantum mechanical description of the motion of the atoms in a molecule or crystal, the classical equation of motion (15.6) is replaced by the Schrödinger equation with the operator

$$\mathcal{H} = \sum_{kll'} \frac{p^2_l(k)}{2M_k}\delta_{kl}\delta_{ll'} + \frac{1}{2}\Phi_{ll'}(k, l')\, u_l(k)\, u_{l'}(l'), \tag{15.17}$$

where

$$p_l(k) = -i\hbar \frac{\partial}{\partial u_l(k)}.$$

We have

$$\{p_l(k)\, u_{l'}(l')\} = -i\hbar\delta_{lk}\delta_{ll'}. \tag{15.17a}$$

In order to diagonalize the Hamiltonian (15.16), we introduce operators b_α and b_α^+:

$$b_\alpha = \frac{1}{\sqrt{2\hbar}} \sum_{kl} B_{kl}^{\alpha *} \left(\sqrt{M_k \omega_\alpha}\, u_l(k) + \frac{i}{\sqrt{M_k \omega_\alpha}}\, p_l(k) \right), \tag{15.18a}$$

$$b_\alpha^+ = \frac{1}{\sqrt{2\hbar}} \sum_{kl} B_{kl}^{\alpha} \left(\sqrt{M_k \omega_\alpha}\, u_l(k) - \frac{i}{\sqrt{M_k \omega_\alpha}}\, p_l(k) \right). \tag{15.18b}$$

By (15.17a),

$$\{ b_\alpha b_\alpha^+ \} = \delta_{\alpha\beta}. \tag{15.19}$$

In order to express $u(k)$ in terms of these operators, we multiply (15.18a) by $B_{lf}^{\alpha} (\hbar/2M_l\omega_\alpha)^{1/2}$ and (15.18b) by $B_{lf}^{\alpha *} (\hbar/2M_l\omega_\alpha)^{1/2}$, add, and sum over α, using (15.11a). We obtain*

$$u_l = \sum_\alpha \left(\frac{\hbar}{2M_l\omega_\alpha} \right)^{1/2} (b_\alpha B_l^\alpha + b_\alpha^+ B_l^{\alpha *}). \tag{15.20a}$$

Similarly, multiplying (15.18a) by $B_{lf}^{\alpha} (\hbar M_l \omega_\alpha/2)^{1/2}$ and (15.18b) by $B_{lf}^{\alpha *} (\hbar M_l \omega_\alpha/2)^{1/2}$, subtracting, and summing over α, we obtain

$$p_l = -i \sum_\alpha \left(\frac{\hbar M_l \omega_\alpha}{2} \right)^{1/2} (b_\alpha B_l^\alpha - b_\alpha^+ B_l^{\alpha *}). \tag{15.20b}$$

If we now substitute (15.20a) and (15.20b) into (15.17) and sum over k and l, noting (15.15), (15.8), and (15.19), we see that the Hamiltonian $\mathcal{H}$ splits into the sum of independent Hamiltonians $\mathcal{H}_\alpha$:

$$\mathcal{H} = \sum_\alpha \mathcal{H}_\alpha = \sum_\alpha \hbar\omega_\alpha \left(b_\alpha^+ b_\alpha + \frac{1}{2} \right). \tag{15.21}$$

Each of these Hamiltonians is the Hamiltonian of a harmonic oscillator. b^+ is the "creation operator" and b the "destruction operator" of a phonon:

$$b\phi_n^\alpha = \sqrt{n_\alpha}\, \phi_{n-1}^\alpha, \quad b^+ \phi_n^\alpha = \sqrt{n_\alpha + 1}\, \phi_{n+1}^\alpha. \tag{15.22}$$

Here ϕ_n^α is the eigenfunction of the harmonic oscillator corresponding to the quantum state n.

Hence $b^+ b\phi_n = n\phi_n$, and consequently the eigenvalues of (15.21) are

$$E_n^\alpha = \hbar\omega_\alpha \left(n_\alpha + \frac{1}{2} \right). \tag{15.23}$$

In thermal equilibrium at a given temperature T, the average number of phonons for a given normal mode at frequency ω_α is

$$\bar{n}_\alpha = \frac{\sum_n n \exp(-E_n^\alpha/kT)}{\sum_n \exp(-E_n^\alpha/kT)} = \frac{1}{\exp(\hbar\omega_\alpha/kT) - 1}. \tag{15.24}$$

If $kT \gg \hbar\omega_\alpha$, then $n_\alpha = kT/\hbar\omega_\alpha$.

In a crystal, where B_{fx}^α can be expressed in the form (15.12), the displacement u_{fx} may be expanded in plane waves:

$$u_{fx} = \sum_{q\nu} a_{q\nu}\, e_x^\nu(q)\, e^{-iqx_f^x} + a_{q\nu}^+ e_x^{\nu *}(q)\, e^{iqx_f^x}. \tag{15.25}$$

* Here one uses the fact that $S \sum_\alpha \omega_\alpha^{-1} (B_{kl}^{\alpha *} B_{ll}^{\alpha} - B_{kl}^{\alpha} B_{ll}^{\alpha *}) = 0$. Indeed, $S^* = -S$, but since the displacement u_l and the derivative $\frac{\partial}{\partial u_l} = \frac{i}{\hbar} p_l$ are real it follows that $S^* = S$. Hence $S = 0$.

Substituting (15.12) into (15.20a) and comparing the result with (15.25), we establish the relationship between the operators a and b:

$$a_{q\nu}=\left(\frac{\hbar}{2\rho\omega_{q\nu}\mathcal{V}}\right)^{1/2}b_{q\nu},\quad a_{q\nu}^{+}=\left(\frac{\hbar}{2\rho\omega_{q\nu}\mathcal{V}}\right)^{1/2}b_{q\nu}^{+}. \tag{15.26}$$

Hence, by (15.22), the matrix elements of the operator a are

$$\langle n'\,|\,a_{q\nu}\,|\,n\rangle=\left(\frac{\hbar n_{q\nu}}{2\rho\omega_{q\nu}\mathcal{V}}\right)^{1/2}\delta_{n',\,n-1}, \tag{15.26a}$$

$$\langle n'\,|\,a_{q\nu}^{+}\,|\,n\rangle=\left(\frac{\hbar\,(n_{q\nu}+1)}{2\rho\omega_{q\nu}\mathcal{V}}\right)^{1/2}\delta_{n',\,n+1}. \tag{15.26b}$$

Group theory makes it possible to determine the irreducible representations according to which the normal modes a_l or $a_{q\nu}$ in the crystal transform; moreover, once the matrices of these representations are known one can use projection operators to find the matrices $\boldsymbol{B}$ or $\boldsymbol{e}$, respectively, of transformation from the reducible basis $u_i(l)$ or $u_{\varkappa i}(\boldsymbol{q})$ to the irreducible basis a_l or $a_{q\nu}$.

Since the force constants $\Phi_{ll'}(l, l')$, which are the coefficients of the expansion of the potential energy of the molecule or crystal in terms of small displacements $u_i(l)$ from the equilibrium position, are determined by the undisplaced coordinates of the atoms, they remain invariant under all the symmetry operations corresponding to the space group (for a crystal) or the point group (for a molecule); moreover, it is readily seen that the elements of the matrix $\boldsymbol{D}$, as defined by (15.13), are invariant under all the operations in the little group G_q. Exactly as in the case of the eigenfunctions of the Schrödinger equation, all the linear combinations of $u_i(l)$ or $u_{\varkappa i}(\boldsymbol{q})$ forming a basis of the same irreducible representation, i.e., transforming into one another under an operation of the symmetry group, correspond to the same vibration frequency ω_α. Consequently, these linear combinations are precisely the normal modes.

To determine according to which representations the functions a_l or $a_{q\nu}$ transform, it is necessary to find the matrices of the vibrational representation $\mathcal{D}_u(g)$, according to which the components $u_i(l)$ or $u_{\varkappa i}(\boldsymbol{q})$ transform, and then to expand $\mathcal{D}_u(g)$ in terms of the irreducible representations of the appropriate group.

We shall now find these matrices $\mathcal{D}_u(g)$ and also the characters $\chi_u(g)$ of the vibrational representations.

We first consider an N-atomic molecule. Applying a transformation g^{-1} from the symmetry group of the molecule transforms the $3N$ displacement components $u_i(l)$ into one another according to the equation

$$g^{-1}u_i(l)=\sum_{i=1}^{3}\sum_{l'=1}^{N}\mathcal{D}_{il',\,il}(g)\,u_{i'}(l'), \tag{15.27}$$

where

$$\mathcal{D}_{il',\,il}(g)=\mathcal{R}_{i'i}(g)\,\delta_{l',\,g^{-1}l}.$$

Here $\mathcal{R}(g)$ is the transformation matrix of the vector components (see (2.29)) and $g^{-1}l$ is the index of the atom into which atom l is transformed by g^{-1}. Note our use of the fact that a transformation g of the coordinate system corresponds to a transformation g^{-1} of the molecule, i.e., in accordance with

the customary definition the transformation matrix $\mathcal{D}(g)$ corresponds to the operation $g^{-1}u_i(l)$. The matrices $\mathcal{D}_{l'l', ll'}(g)$ form a $3N$-dimensional representation $\mathcal{D}_u$. By (15.27), the character of this representation is

$$\chi_u(g) = \sum_{lil'l'} \mathcal{D}_{l'l', ll'}(g)\,\delta_{ll'}\delta_{ll'} = n_g\chi_l(g), \tag{15.27a}$$

where n_g is the number of atoms which remain fixed under the transformation g. When $\mathcal{D}_u$ is expanded in terms of the irreducible representations corresponding to the normal modes of the molecule, one must eliminate the three normal coordinates

$$\bar{u}_i = \frac{1}{\sum_l M_l}\sum_l M_l u_i(l),$$

describing the motion of the center of gravity, which transform like the components of a polar vector, and the three normal coordinates

$$\Omega_i = \frac{1}{\sum_l M_l}\sum_l M_l [x_l u(l)]_i$$

(x_l is the radius-vector from the center of gravity to the atom l), describing the rotation of the molecule as a whole, which transform like the components of an axial vector, since neither of these types of motion is a vibration.* Since the character $\chi_l(g)$ of the representation according to which the components of the vector transform is (see (10.20))

$$\chi_l(c_\varphi) = 1 + 2\cos\varphi, \quad \chi_l(s_\varphi) = -\chi_l(c_{\varphi+\pi}) = -1 + 2\cos\varphi,$$

it follows that the character of the representation $\mathcal{D}_u$ according to which the normal modes of the molecule transform, after the six components mentioned above have been excluded, is

$$\chi_u(c_\varphi) = (1 + 2\cos\varphi)(n_g - 2), \quad \chi_u(s_\varphi) = (-1 + 2\cos\varphi)\,n_g. \tag{15.27b}$$

The transformation s_φ clearly leaves only one atom fixed. This atom is located at the intersection of the rotation axis and the reflection plane or at the inversion center, i.e., n_g is 0 or 1 (except for the operation $\sigma_h = s_{2\pi}$).

We now determine the transformation law of the components $u_\varkappa(q)$; by (15.16b), these are related to the displacement $u_{f\varkappa}$ by

$$u_\varkappa(q) = \frac{1}{N}\sum_f e^{-iqx_f^\varkappa} u_{f\varkappa}.$$

The operation $g^{-1} = (r\,|\,\tau)^{-1}$ transforms the components $u_{f\varkappa l}$ as in formula (15.27) and $u_{\varkappa l}(q)$ becomes

$$g^{-1}u_{\varkappa l}(q) = \frac{1}{N}\sum_{ff'} e^{-iqx_f^\varkappa}\sum_{l'\varkappa'} \mathcal{R}_{l'l}(g)\,u_{f'\varkappa'l'}\,\delta_{g\varkappa',\varkappa}\delta_{gf',f} =$$
$$= \frac{1}{N}\sum_{f'f\varkappa'l'} e^{-iqx_{f'}^{\varkappa'}} u_{f'\varkappa'l'}\mathcal{R}_{l'l}(g)\,e^{iq\left(x_{f'}^{\varkappa'} - x_f^\varkappa\right)}\delta_{g\varkappa',\varkappa}\delta_{gf',f}.$$

Here $u_{f'\varkappa'}$ is the displacement of atom $f'\varkappa'$, which is the image of atom $f\varkappa$ under the transformation $g^{-1} = (r\,|\,\tau)^{-1}$. The difference between the coordinates of $f'\varkappa'$ and $f\varkappa$ is

$$x_{f'}^{\varkappa'} - x_f^\varkappa = r^{-1}x_f - x_f + r^{-1}(x_\varkappa - \tau) - x_\varkappa.$$

* Except in the case of linear molecules, for which only two rotational degrees of freedom need be excluded.

Here $\boldsymbol{x}_f = \boldsymbol{x}_f^l$, $\boldsymbol{x}_\varkappa = \boldsymbol{x}_f^\varkappa - \boldsymbol{x}_f^l$, and moreover

$$\boldsymbol{q}(r^{-1}\boldsymbol{x}_f - \boldsymbol{x}_f) = \boldsymbol{x}_f(r\boldsymbol{q} - \boldsymbol{q}) = 2\pi m,$$

since $\boldsymbol{x}_f$ is a vector of the original lattice and, by (12.12), if $g \in G_{\boldsymbol{q}}$ then $r\boldsymbol{q} - \boldsymbol{q}$ is either zero or a vector of the reciprocal lattice. Thus the factor $\exp\{i\boldsymbol{q}(\boldsymbol{x}_{f'}^{\varkappa'} - \boldsymbol{x}_f^\varkappa)\}$ equals $\exp\{i\boldsymbol{q}(r^{-1}(\boldsymbol{x}_\varkappa - \boldsymbol{\tau}) - \boldsymbol{x}_\varkappa)\}$ and does not depend on f. Consequently,

$$g^{-1}u_{\varkappa l}(\boldsymbol{q}) = \sum_{\varkappa' l'} \mathscr{D}^u_{\varkappa' l', \varkappa l}(g)\, u_{\varkappa' l'}(\boldsymbol{q}),$$

where

$$\mathscr{D}^u_{\varkappa' l', \varkappa l}(g) = \mathscr{R}_{l' l}(g) \exp\{i\boldsymbol{q}(r^{-1}(\boldsymbol{x}_\varkappa - \boldsymbol{\tau}) - \boldsymbol{x}_\varkappa)\}\, \delta_{g\varkappa', \varkappa}. \tag{15.28}$$

Hence we see that the character of the representation $\mathscr{D}_u$ equals

$$\chi_u(g) = \chi_l(g) \sum_\varkappa \exp\{i\boldsymbol{q}(r^{-1}(\boldsymbol{x}_\varkappa - \boldsymbol{\tau}) - \boldsymbol{x}_\varkappa)\}\, \delta_{\varkappa, g\varkappa}, \tag{15.28a}$$

whence

$$\chi_u(c_\varphi | \boldsymbol{\tau}) = (1 + 2\cos\varphi) \sum_\varkappa \exp\{i\boldsymbol{q}(c_\varphi^{-1}(\boldsymbol{x}_\varkappa - \boldsymbol{\tau}) - \boldsymbol{x}_\varkappa)\}\delta_{\varkappa, c_\varphi\varkappa}, \tag{15.28b}$$

$$\chi_u(s_\varphi | \boldsymbol{\tau}) = (-1 + 2\cos\varphi) \sum_\varkappa \exp\{i\boldsymbol{q}(s_\varphi^{-1}(\boldsymbol{x}_\varkappa - \boldsymbol{\tau}) - \boldsymbol{x}_\varkappa)\}\delta_{\varkappa, s_\varphi\varkappa}. \tag{15.28c}$$

In these formulas, $\delta_{\varkappa, g\varkappa} = 1$ if the operation g moves atom $\varkappa$ to an equivalent position, i.e., $r^{-1}(\boldsymbol{x}_\varkappa - \boldsymbol{\tau}) - \boldsymbol{x}_\varkappa$ is zero or a lattice vector, and $\delta_{\varkappa, g\varkappa} = 0$ if the atom is moved to an inequivalent position. For points such that $r\boldsymbol{q} = \boldsymbol{q}$, in particular, for all points inside the Brillouin zone

$$\boldsymbol{q}[r^{-1}(\boldsymbol{x}_\varkappa - \boldsymbol{\tau}) - \boldsymbol{x}_\varkappa] = (r\boldsymbol{q} - \boldsymbol{q})\boldsymbol{x}_\varkappa - r\boldsymbol{q}\boldsymbol{\tau} = -\boldsymbol{q}\boldsymbol{\tau}$$

and so

$$\mathscr{D}_u(g) = \mathscr{R}(g)\, e^{-i\boldsymbol{q}\boldsymbol{\tau}} n_g, \tag{15.29}$$

where $n_g = \sum_\varkappa \delta_{\varkappa, g\varkappa}$ is the number of atoms that remain fixed under g. The character of the corresponding projective representation is $\chi_u(r) = \chi_l(r) n_g$, an equation similar to (15.27a). (In (15.29) the little group plays the role of the symmetry group of the molecule.) For lattices which do not contain identical atoms in the primitive cell, if $r\boldsymbol{q} = \boldsymbol{q}$,

$$\mathscr{D}_u(r) = \mathscr{R}(r)\, n_a, \tag{15.29a}$$

where n_a is the number of atoms in the primitive cell, so that the projective representation $\mathscr{D}_u$ is p-equivalent to a vector representation and contains only the representations occurring in $\mathscr{R}$, each n_a times.

We shall use these formulas in §23 to determine the representations corresponding to normal modes at different points of the Brillouin zone, for certain cubic and hexagonal crystals.

Splitting of Terms Due to a Perturbation

Thanks to representation theory, one can not only classify the terms, establish their degree of degeneracy and determine the basis functions, but

Degenerate Perturbation Theory

In perturbation theory the Hamiltonian $\mathcal{H}$ is expressed as the sum of two parts: a Hamiltonian $\mathcal{H}_0$ with known eigenvalues E_n^0 and eigenfunctions φ_n, and $\mathcal{H}'$, which is treated as a perturbation. The wave function ψ is sought in the form of a series:

$$\psi = \sum_n c_n \varphi_n. \tag{15.30}$$

Substituting (15.30) into (15.1), multiplying by $\varphi_{n'}^*$ and integrating with respect to all the variables x, we obtain a system of equations defining the coefficients c_n for a given eigenvalue E, which may be written in matrix form as

$$\| \mathcal{H}_0 - IE + \mathcal{H}' \| \| c \| = 0, \tag{15.31}$$

where $\|c\|$ is a column matrix with elements $c_{nn'} = c_n \delta_{n'1}$, $\mathcal{H}_0$ is a diagonal matrix,

$$\mathcal{H}_{0nn'} = E_n^0 \delta_{nn'}, \tag{15.31a}$$

and $\mathcal{H}'$ is the perturbation matrix:

$$\mathcal{H}'_{n'n} = \langle \varphi_{n'} | \mathcal{H}' | \varphi_n \rangle = \int \varphi_n^* \mathcal{H}' \varphi_n \, dx. \tag{15.31b}$$

The eigenvalues E are the zeros of the determinant

$$| \mathcal{H}_0 - IE + \mathcal{H}' | = 0. \tag{15.32}$$

In effect, determination of the eigenfunctions (15.30) and eigenvalues E means that one goes over to a representation in which the matrix $\mathcal{H}_0 + \mathcal{H}'$ is diagonal. The problem is usually solved by the method of successive approximations. The corrections to the energy E_m^0 are determined from (15.32), and the corrections to the wave function φ_m of a given state m, i.e., the coefficient $c_n(E_m)$, from (15.31).

If this state m is not degenerate, i.e., there is only one state with energy E_m^0, then the expression for the corresponding corrections can at once be obtained in series form.

If there are, however, several states $\varphi_m, \varphi_{m'}, \ldots$ with energy E_m^0, it is customary first to determine the true functions and eigenvalues in the zeroth approximation, i.e., all the matrix elements $\mathcal{H}'_{nn'}$ in (15.31) and (15.32) are assumed to vanish except the elements $\mathcal{H}'_{mm'}$, between the functions $\varphi_m, \varphi_{m'}, \ldots$, corresponding to the given energy, and then corrections due to higher order terms are found.

However, this method is not always convenient, since even in the zeroth approximation accurate evaluation of the zeros of the determinant (15.32) is not always possible. The problem may be reformulated to yield at once a system of equations (15.31) for the relevant N states $m, m', \ldots, m^{(N)}$, allowing for the contribution of all the other states $s, s', s'', \ldots$ in the required approximation of perturbation theory. As will be shown below, this is the procedure in construction of the Hamiltonian in the effective mass approximation for degenerate bands or for several close-lying bands.

To solve the problem we introduce a unitary matrix S which "partially" diagonalizes the Hamiltonian (15.31), in the sense that the matrix

$$\overline{\mathcal{H}} = e^{-S} \mathcal{H} e^{S} \tag{15.33}$$

also determine how the terms split when a perturbation is applied. Suppose the Hamiltonian $\mathscr{H}$ may be divided into two parts $\mathscr{H} = \mathscr{H}_0 + \mathscr{H}_1$, where the symmetry group of $\mathscr{H}_0$ is $\mathscr{G}_0$, and that of $\mathscr{H}_1$ is a subgroup $\mathscr{G}_1$ of $\mathscr{G}_0$. Then a knowledge of the characters of the irreducible representations of these groups is sufficient to determine how the terms of the operator $\mathscr{H}_0$ split into terms of the operator $\mathscr{H}$. The degeneracy of term of $\mathscr{H}_0$ depends on the dimension of the irreducible representations of $\mathscr{G}_0$. If the splitting of terms of $\mathscr{H}_0$ due to the perturbation $\mathscr{H}_1$ is small compared with the distance between the terms of the unperturbed Hamiltonian $\mathscr{H}_0$, i.e., each term of $\mathscr{H}$ is produced by splitting of only one of the terms of $\mathscr{H}_0$ and there is no intersection of terms, the nature of the splitting is determined by expanding every irreducible representation of the group $\mathscr{G}_0$, which may become reducible in $\mathscr{G}_1$, in terms of irreducible representations $\mathscr{G}_1$. If the representation is also irreducible in $\mathscr{G}_1$, then the corresponding term does not split but is only shifted. If it becomes reducible, the term splits, and the number of new terms is the number of irreducible representations of $\mathscr{G}_1$ occurring in the given representation $\mathscr{D}$ of $\mathscr{G}_0$.

For actual performance of such calculations, one must evaluate the characters of the representation $\mathscr{D}(g)$ for the elements g appearing in the group $\mathscr{G}_1$ and then, using the equations of §8, expand the representation in terms of the irreducible representations of $\mathscr{G}_1$.

If the operator $\mathscr{H}$ is the sum of several parts, $\mathscr{H}_0, \mathscr{H}_1, \mathscr{H}_2, \ldots$, each being treated as a perturbation of that preceding it, application of the method described above reveals the progressive nature of the splitting of terms. For example, if an atom possessing some definite symmetry is placed in a crystal lattice, its terms are split by the crystal field, whose symmetry depends on the symmetry of the crystal and the position of the impurity atom Perturbation of the lattice due to an internal strain or the appearance of other foreign atoms at neighboring sites can bring about further splitting of the terms, and the new terms in turn will split when the crystal is placed in a magnetic field.

The eigenfunctions of an unperturbed atom with given orbital angular momentum l are $(2l+1)$-fold degenerate and transform according to the appropriate representations of the full spherical group, whose characters are given by equation (10.20). Since the maximum degeneracy of the levels in a crystal field with the highest cubic symmetry is 3 (with allowance for spin, as we shall show below, the maximum degeneracy is 4), then all levels with $l \geqslant 2$ always split in the crystal field; on the other hand, it is easily shown that the levels with $l = 3/2$ and $l = 1$ do not split in a cubic field but do split when the symmetry is lowered. For example, the fivefold degenerate atomic term $\mathscr{D}_2$, corresponding to $l = 2$ in a cubic field with T_d (or O) symmetry, splits into two terms corresponding to the representations E and F_1. If the crystal is dilated along the principal z-axis, its symmetry is lowered to D_{2d} (or D_4, respectively); the representation E then splits into two one-dimensional representations A_1 and B_1, and the representation F_1 into the one-dimensional representation B_2 and the two-dimensional representation E.

It must be noted that representation theory tells us whether or not term splitting occurs, but not the order of perturbation theory in which it takes place. The answer to this question is provided by perturbation theory.

does not contain "off-diagonal" elements $\overline{\mathcal{H}}_{ml}$ between the N given states and the other states $l, l', \ldots$. The transformation (15.33) corresponds to transition from a representation c to the representation $\bar{c}$ defined by

$$\bar{c} = e^{-S}c. \tag{15.33a}$$

Since $\overline{\mathcal{H}}$ has no "off-diagonal" elements, the equations $\|\overline{\mathcal{H}} - EI\|\|c\| = 0$ fall into two independent systems: one for the N states $m, m', \ldots, m^{(N)}$ and another for the other states $l, l', \ldots$; the basis of the first system comprises the functions

$$\bar{\varphi}_m = \sum_l (e^{-S})_{lm}\varphi_l. \tag{15.34}$$

If we could determine the matrix S exactly, the problem would thereby be solved. Except in the simplest cases, however, the problem must be solved by expanding e^S in series

$$e^S = 1 + S + \frac{1}{2}S^2 + \frac{1}{3!}S^3 + \ldots$$

and determining the matrix S by successive approximations. Since the transformation (15.33) is unitary, this matrix must be antihermitian, i.e.

$$S^+ = \tilde{S}^* = -S.$$

Substituting the series expansion of $e^{\pm S}$ into (15.22), we obtain

$$\overline{\mathcal{H}} = \sum_{n=0}^{\infty}\frac{1}{n!}\{\mathcal{H}S\}^{(n)} = \sum_{n=0}^{\infty}\{\mathcal{H}^0S\}^{(n)} + \sum_{n=0}^{\infty}\{\mathcal{H}_2S\}^{(n)}. \tag{15.35}$$

Here

$$\{\mathcal{H}S\}^{(0)} = \mathcal{H}, \quad \{\mathcal{H}S\}^{(1)} = \{\mathcal{H}S\}, \quad \{\mathcal{H}S\}^{(2)} = \{\{\mathcal{H}S\}S\}, \ldots$$

We have thus expressed the matrix $\mathcal{H}$ as the sum of a diagonal matrix $\mathcal{H}^0 = \mathcal{H}_0 + \mathcal{H}_1$ which has no off-diagonal elements $\mathcal{H}_{ml}$, and a nondiagonal matrix $\mathcal{H}_2$ which does not contain the elements $\mathcal{H}_{m'm}$ and $\mathcal{H}_{l'l}$, simultaneously expressing $\mathcal{H}'$ as the sum of a diagonal part $\mathcal{H}_1$ and a nondiagonal part $\mathcal{H}_2$. Since the matrix S defined by this condition is also nondiagonal, the diagonal part of the matrix $\overline{\mathcal{H}}_d$ must contain the commutators $\{\mathcal{H}^0S\}^{(n)}$ involving even powers of S and the commutators $\{\mathcal{H}_2S\}^{(n)}$ with odd powers of S. Conversely, the nondiagonal part must contain the commutators $\{\mathcal{H}^0S\}^{(n)}$ with odd powers of S and $\{\mathcal{H}_2S\}^{(n)}$ with even powers of S. In other words,

$$\overline{\mathcal{H}}_d = \sum_{t=0}^{\infty}\frac{1}{(2t)!}\{\mathcal{H}^0S\}^{(2t)} + \sum_{t=0}^{\infty}\frac{1}{(2t+1)!}\{\mathcal{H}_2S\}^{(2t+1)}. \tag{15.36}$$

The matrix S is defined by the condition that its nondiagonal part vanishes:

$$\overline{\mathcal{H}}_{nd} = \sum_{t=0}^{\infty}\frac{1}{(2t+1)!}\{\mathcal{H}^0S\}^{(2t+1)} + \sum_{t=0}^{\infty}\frac{1}{(2t)!}\{\mathcal{H}_2S\}^{(2t)} = 0. \tag{15.37}$$

Using successive approximations, one can eliminate the terms $\{\mathcal{H}^0S\}^{(2t+1)}$ with $t \neq 0$ from this equality. To this end, we substitute the expression for $\{\mathcal{H}^0S\}$ (see (15.37)),

$$\{\mathcal{H}^0S\} = -\sum_{t=1}^{\infty}\frac{1}{(2t+1)!}\{\mathcal{H}^0S\}^{(2t+1)} - \sum_{t=0}^{\infty}\frac{1}{(2t)!}\{\mathcal{H}_2S\}^{(2t)},$$

into all the terms $\{\mathcal{H}^0 S\}^{(2t+1)}$ with $t \geqslant 1$. The result is

$$\overline{\mathcal{H}}_{nd} = \{\mathcal{H}^0 S\} + \sum_{t=2}^{\infty} b_t \{\mathcal{H}^0 S\}^{(2t+1)} + \sum_{t=0}^{\infty} c_t \{\mathcal{H}_2 S\}^{(2t)}, \tag{15.38}$$

where

$$b_t = -\sum_{r=1}^{r=t-1} [(2r+1)!\,(2(t-r)+1)!]^{-1} =$$

$$= -\frac{1}{[2(r+1)]!} \sum_{r=1}^{r=t-1} C_{2(t+1)}^{2r+1} = -\frac{4}{[2(r+1)]!} [2^{2t-1} - t - 1], \tag{15.38a}$$

$$c_t = \frac{1}{(2t)!} - \sum_{r=1}^{r=t} [(2r+1)!\,(2(t-r))!]^{-1} =$$

$$= \frac{1}{(2t)!} - \frac{1}{(2t+1)!} \sum_{r=1}^{t} C_{2t+1}^{2r+1} = -\frac{2}{(2t+1)!} [2^{2t-1} - 2t - 1]. \tag{15.38b}$$

Here we have used a standard identity for the binomial coefficients $C_t^r = t!/r!\,(t-r)!$:

$$\sum_{r=0}^{2r \leqslant t} C_t^{2r} = \sum_{r=0}^{2r+1 \leqslant t} C_t^{2r+1} = 2^{t-1}.$$

Apart from $\{\mathcal{H}^0 S\}$, equation (15.38) involves the terms $\{\mathcal{H}^0 S\}^{(n)}$ with $n \geqslant 3$. Expressing $\{\mathcal{H}^0 S\}$ through the other terms and substituting into $\{\mathcal{H}^0 S\}^{(2t+1)}$ ($t \geqslant 2$), we obtain an equation containing $\{\mathcal{H}^0 S\}^{(n)}$ with $n \geqslant 9$:

$$\overline{\mathcal{H}}_{nd} = \{\mathcal{H}^0 S\} + \sum_{t=4}^{\infty} \delta_t \{\mathcal{H}^0 S\}^{(2t+1)} + \sum_{t=0}^{\infty} \gamma_t \{\mathcal{H}_2 S\}^{(2t)} = 0. \tag{15.39}$$

Here

$$\delta_t = \sum_{r=2}^{r=t-2} b_r b_{t-r}, \qquad \gamma_t = c_t - \sum_{r=2}^{r=t} b_r c_{t-r}. \tag{15.39a}$$

Consequently, up to eighth order, we have

$$\{\mathcal{H}^0 S\} \approx -\sum_{t=0}^{t=3} \gamma_t \{\mathcal{H}_2 S\}^{(2t)} - \{\mathcal{H}_1 S\}. \tag{15.40}$$

Substituting (15.40) into (15.36), we find that, up to ninth order,

$$\overline{\mathcal{H}}_d \approx \mathcal{H}_0 + \mathcal{H}_1 + \sum_{t=0}^{t=3} \xi_t \{\mathcal{H}_2 S\}^{t(2t+1)}, \tag{15.41}$$

where

$$\xi_t = \frac{1}{(2t+1)!} - \sum_{r=0}^{r=t} \frac{\gamma_r}{[2(t-r+1)]!}. \tag{15.41a}$$

The first few coefficients γ_t and ξ_t in (15.40) and (15.41) are:

$$\begin{aligned} &\gamma_0 = 1, \quad \gamma_1 = \frac{1}{3}, \quad \gamma_2 = -\frac{1}{45}, \quad \gamma_3 = \frac{32}{3 \cdot 7!}; \\ &\xi_0 = \frac{1}{2}, \quad \xi_1 = -\frac{1}{4}, \quad \xi_2 = \frac{1}{2 \cdot 5!}, \quad \xi_3 = \frac{17}{8!}. \end{aligned} \tag{15.42}$$

Equation (15.39) may be solved by successive approximations, setting

$$S = S_1 + S_2 + S_3 + \ldots,$$

where S_1 is of first order in $\mathcal{H}'$, S_2 of second order, etc. Retaining successively first, second, etc. order terms in (15.41), we obtain

$$\begin{aligned} &\{\mathcal{H}_0 S_1\} = -\mathcal{H}_2, \\ &\{\mathcal{H}_0 S_2\} = -\{\mathcal{H}_1 S_1\}, \\ &\{\mathcal{H}_0 S_3\} = -\{\mathcal{H}_1 S_2\} - \tfrac{1}{3}\{\{\mathcal{H}_2 S_1\} S_1\}, \\ &\{\mathcal{H}_0 S_4\} = -\{\mathcal{H}_1 S_3\} - \tfrac{1}{3}\{\{\mathcal{H}_2 S_2\} S_1\} - \tfrac{1}{3}\{\{\mathcal{H}_2 S_1\} S_2\}, \end{aligned} \tag{15.43}$$

and so on.

By (15.31a), $\{\mathcal{H}_0 S\}_{ml} = (E_m^0 - E_l^0) S_{ml}$, and so it follows from these equations that

$$\begin{aligned} S_{1ml} &= -\frac{\mathcal{H}'_{ml}}{E_m - E_l}, \\ S_{2ml} &= \sum_{m'} \frac{\mathcal{H}'_{mm'}\mathcal{H}'_{m'l}}{(E_m^0 - E_l^0)(E_{m'}^0 - E_l^0)} - \sum_{l'} \frac{\mathcal{H}'_{ml'}\mathcal{H}'_{l'l}}{(E_m^0 - E_l^0)(E_m^0 - E_{l'}^0)}, \end{aligned} \tag{15.44}$$

and so on.

The derivation of these formulas uses the fact that the only nonzero matrix elements of the operator $\mathcal{H}_1$ are the diagonal matrix elements $\mathcal{H}_{1mm'} = \mathcal{H}'_{mm'}$ and $\mathcal{H}_{1ll'} = \mathcal{H}'_{ll'}$; similarly, for the operator $\mathcal{H}_2$ only the off-diagonal elements $\mathcal{H}_{2ml} = \mathcal{H}'_{ml}$ are nonzero.

Evaluation of S yields the operator $\overline{\mathcal{H}}$, which may be written (see (15.41) and (15.42))

$$\overline{\mathcal{H}} = \mathcal{H}_0 + \mathcal{H}_1 + \tfrac{1}{2}\{\mathcal{H}_2 S_1\} + \tfrac{1}{2}\{\mathcal{H}_2 S_2\} + \tfrac{1}{2}\{\mathcal{H}_2 S_3\} - \tfrac{1}{24}\{\{\mathcal{H}_2 S_1\} S_1\} S_1\} - \ldots \tag{15.45}$$

Substituting the values of S_{1ml} and S_{2ml} from (15.44), we find the matrix elements $\overline{\mathcal{H}}_{mm'}$ up to third order terms:

$$\begin{aligned} \overline{\mathcal{H}}_{mm'} = \mathcal{H}_{mm'} &- \frac{1}{2}\sum_s \left(\frac{1}{E_s^0 - E_m^0} + \frac{1}{E_s^0 - E_{m'}^0}\right)\mathcal{H}'_{ms}\mathcal{H}'_{sm'} - \\ &- \frac{1}{2}\sum_{sm''}\left(\frac{\mathcal{H}'_{ms}\mathcal{H}'_{sm''}\mathcal{H}'_{m''m}}{(E_s^0 - E_{m''}^0)(E_s^0 - E_{m'}^0)} + \frac{\mathcal{H}'_{mm''}\mathcal{H}'_{m''s}\mathcal{H}'_{sm'}}{(E_s^0 - E_{m''}^0)(E_s^0 - E_m^0)}\right) + \\ &+ \frac{1}{2}\sum_{ss'} \mathcal{H}'_{ms}\mathcal{H}'_{ss'}\mathcal{H}'_{s'm'}\left(\frac{1}{(E_s^0 - E_m^0)(E_{s'}^0 - E_m^0)} + \frac{1}{(E_s^0 - E_{m'}^0)(E_{s'}^0 - E_{m'}^0)}\right), \end{aligned} \tag{15.46}$$

where

$$\mathcal{H}_{mm'} = E_m^0 \delta_{mm'} + \mathcal{H}'_{mm'}.$$

For the sake of generality, we have not assumed here that all these states have the same energy. If degeneracy occurs, i.e., $E_m^0 = E_{m'}^0 = E_{m''}^0 = \ldots$, then

$$\begin{aligned} \overline{\mathcal{H}}_{mm'} = \mathcal{H}_{mm'} &- \sum_s \frac{\mathcal{H}'_{ms}\mathcal{H}'_{sm'}}{E_s^0 - E_m^0} - \\ &- \frac{1}{2}\sum_{m''s} \frac{\mathcal{H}'_{ms}\mathcal{H}'_{sm''}\mathcal{H}'_{m''m'} + \mathcal{H}'_{mm''}\mathcal{H}'_{m''s}\mathcal{H}'_{sm'}}{(E_s^0 - E_m^0)^2} + \sum_{ss'} \frac{\mathcal{H}'_{ms}\mathcal{H}'_{ss'}\mathcal{H}'_{s'm'}}{(E_s^0 - E_m^0)(E_{s'}^0 - E_m^0)}. \end{aligned} \tag{15.47}$$

In particular, for a nondegenerate state one obtains the usual equation for the energy correction:

$$E_m^{(3)} = E_m^0 + \mathcal{H}'_{mm} - \sum_s \frac{|\mathcal{H}'_{ms}|^2}{E_s^0 - E_m^0} - \mathcal{H}'_{mm} \sum_s \frac{\mathcal{H}'_{ms}\mathcal{H}'_{sm}}{(E_s^0 - E_m^0)^2} + \sum_{ss'} \frac{\mathcal{H}'_{ms}\mathcal{H}'_{ss'}\mathcal{H}'_{s'm}}{(E_s^0 - E_m^0)(E_{s'}^0 - E_m^0)}. \quad (15.48)$$

If one is considering only two states with energies E_1^0 and E_2^0, each of which may be degenerate, equation (15.47) becomes

$$\overline{\mathcal{H}}_{mm'} = \mathcal{H}_{mm'} - \frac{1}{\Delta} \sum_s \mathcal{H}'_{ms}\mathcal{H}'_{sm'} + \ldots, \quad (15.49)$$

where $\Delta = E_2^0 - E_1^0$. This equation can be rewritten in matrix form. If the matrix $\mathcal{H}$ is written

$$\mathcal{H} = \begin{Vmatrix} \mathcal{H}_{11} & \mathcal{H}_{12} \\ \mathcal{H}_{21} & \mathcal{H}_{22} \end{Vmatrix},$$

where $\mathcal{H}_{11}$ and $\mathcal{H}_{22}$ are diagonal matrices with matrix elements $\mathcal{H}_{mm'}$ and $\mathcal{H}_{ss'}$, respectively, $\mathcal{H}_{12}$ and $\mathcal{H}_{21} = \mathcal{H}_{12}^+$ are nondiagonal matrices with matrix elements $\mathcal{H}_{ms}$, then (15.49) is rewritten as*

$$\overline{\mathcal{H}}_{11} = \mathcal{H}_{11} - \frac{1}{\Delta} \mathcal{H}_{12}\mathcal{H}_{12}^+ + \ldots \quad (15.49a)$$

Formulas (15.35) and (15.44) also enable one immediately to express the matrix elements of any operator F relative to the new basis (15.33) in terms of the corresponding elements relative to the basis φ_n:

$$\overline{F} = e^S F e^{-S} = F + \{FS\} + \frac{1}{2}\{\{FS\}\ S\} + \frac{1}{6}\{\{\{FS\}S\}S\} + \ldots, \quad (15.50)$$

whence we obtain, for example, in the second approximation

$$\overline{F}_{mm'} = F_{mm'} - \sum_s \frac{\mathcal{H}'_{ms}F_{sm'}}{E_s^0 - E_m^0} + \frac{\mathcal{H}'_{sm'}F_{ms}}{E_s^0 - E_{m'}^0}. \quad (15.51)$$

The summation in (15.51) extends, as in (15.46)–(15.48), over all states $s \neq m, m', \ldots, m^{(N)}$. Of course, some of these states can be degenerate.

It will be shown below that symmetry theory makes it possible, when only the symmetry of the operators $\mathcal{H}_0$, $\mathcal{H}'$ and F is known, to determine the number of linearly independent matrix elements and establish a relation between the linearly dependent elements. All one needs, then, to determine in which order of perturbation theory the splitting occurs, is the representation according to which the functions φ_m of the unperturbed Hamiltonian transform One is thus provided with a qualitative estimate of the amount of splitting; it

* This formula is readily derived from the equations $(\mathcal{H} - E)\psi = 0$, regarded as a system of two matrix equations

$$(\mathcal{H}_{11} - E)\psi_1 + \mathcal{H}_{12}\psi_2 = 0, \quad \mathcal{H}_{21}\psi_1 + (\mathcal{H}_{22} - E)\psi_2 = 0.$$

Multiplying the second equation by $(\mathcal{H}_{22} - E)^{-1}$, we express ψ_2 in terms of ψ_1. Then, substituting this expression into the first equation, we obtain

$$(\overline{\mathcal{H}}_{11} - E)\psi_1 = (\mathcal{H}_{11} - \mathcal{H}_{12}(\mathcal{H}_{22} - E)^{-1}\mathcal{H}_{21} - E)\psi_1 = 0.$$

The general equation (15.47) provides a practical means of determining the matrix $(\mathcal{H}_{22} - E)^{-1}$. In the first approximation,

$$(\mathcal{H}_{22} - E)^{-1} = (E_2^0 - E_1^0)^{-1}.$$

is also possible to ascertain which of the elements $\mathcal{H}'_{nn'}$ do not vanish and how elements with different n and n' are related to each other. Of course, the general picture of the splitting, which depends on the selection rules for the matrix elements $\overline{\mathcal{H}}_{mm'}$, agrees with that furnished by general representation theory, provided that all the necessary orders of perturbation theory have been taken into consideration. Thus comparison of the two methods provides an immediate indication of when one must resort to higher orders of perturbation theory.

§16. SPINOR REPRESENTATIONS

In discussing representations of point groups and space groups, we have as yet made no allowance for electron spin.

The Schrödinger-Pauli equation, incorporating the first nonvanishing relativistic terms, is

$$\mathcal{H}\psi = \left\{ \frac{P^2}{2m} + V(\boldsymbol{x}) + \frac{\hbar}{4m^2c^2}(\sigma[\nabla V \boldsymbol{P}]) - \frac{i\hbar}{4m^2c^2}(\nabla V \boldsymbol{P}) - \frac{P^4}{8m^3c^2} \right\} \psi = i\hbar \frac{\partial \psi}{\partial t}, \qquad (16.1)$$

where $\boldsymbol{P} = -i\hbar\nabla$ and σ_i are the Pauli matrices (see (4.13)).

Equation (16.1) is the matrix notation of a system of two equations for the two spinor components ψ_1 and ψ_2. In matrix notation, the function ψ_j is written as a column vector:

$$\psi_j = \begin{Vmatrix} \psi_{j1} \\ \psi_{j2} \end{Vmatrix}.$$

Here the indices 1 and 2 refer to the two spin states of the electron, where the projection of the spin on the z-axis is $+1/2$ and $-1/2$, respectively.*

In order to determine how the wave functions ψ_j transform under the operations g in the symmetry group of the Hamiltonian (16.1), one must remember that the coordinate transformations do not only affect the arguments of the functions $\psi_{j1}(\boldsymbol{x})$ and $\psi_{j2}(\boldsymbol{x})$, but also transform the spinor components into one another, since only transformations with this property preserve the Hamiltonian in (16.1). It follows from equations (10.6) and (10.26) that, under a clockwise rotation through an angle θ about an axis z' directed along the unit vector $\boldsymbol{e}$ with projections $e_x = \sin\theta\sin\varphi$, $e_y = \sin\theta\cos\varphi$, $e_z = \cos\theta$ in the polar coordinate system, the spinors with spin 1/2 transform according to the matrix

$$\mathcal{D}_{1/2}(c_\theta) = e^{i(\sigma\boldsymbol{e})\theta/2} = \boldsymbol{I}\cos\frac{\theta}{2} + i(\sigma\boldsymbol{e})\sin\frac{\theta}{2}. \qquad (16.2)$$

Therefore, under an operation g, the wave function $\psi_j(\boldsymbol{x})$ becomes

$$\psi'_j = \mathcal{D}(g)\psi_j = \mathcal{D}_{1/2}(g)\psi_j(g^{-1}\boldsymbol{x}) \qquad (16.3)$$

* Since the operations of the space groups – inversion, rotation, translation, and also time reversal – do not cause mixing of the "electron" and "positron" components of the four-component wave function, which is a solution of the Dirac equation, and moreover each pair of components transforms independently, none of the consequences of symmetry theory depends on whether the starting point is the exact Dirac equation or the approximate Schrödinger-Pauli equation (16.1), whose eigenfunction has two components.

or in matrix notation

$$\begin{Vmatrix} \psi'_{j1} \\ \psi'_{j2} \end{Vmatrix} = \begin{Vmatrix} \alpha & \beta \\ -\beta & \alpha^* \end{Vmatrix} \begin{Vmatrix} \psi_{j1}(g^{-1}x) \\ \psi_{j2}(g^{-1}x) \end{Vmatrix}, \tag{16.4}$$

where α and β are matrix elements of the matrix $\mathcal{D}^{1/2}(g)$ defined by equation (16.2).

All the symmetry operations g which leave the potential $V(x)$ invariant produce a wave function $\mathcal{D}(g)\psi_j$ which is a combination of linearly independent functions $\psi_j(x)$ belonging to the same energy:

$$\mathcal{D}(g)\psi_j = \sum_i \mathcal{D}_{ij}(g)\psi_i. \tag{16.5}$$

The set of matrices $\mathcal{D}(g)$ forms a representation of the group $\mathcal{G}$, called a spinor representation. Like the usual representations, spinor representations may be reducible or irreducible, and any reducible representation may be decomposed into irreducible representations as indicated above. Just as in the case of the usual representations, functions belonging to the same energy form the basis of an irreducible representation, except in cases where the invariance of equation (16.1) under time reversal results in additional degeneracy or if accidental degeneracy occurs. When transformed by g, each coordinate function ψ_{jk} also becomes a linear combination of the others:

$$\mathcal{D}(g)\psi_{jk} = \psi_{jk}(g^{-1}x) = \sum_{il} \mathcal{D}'_{il,\,jk}\psi_{il}(x). \tag{16.6}$$

The representation $\mathcal{D}'(g)$ formed by these matrices is generally reducible Given the matrices $\mathcal{D}^{1/2}(g)$ and $\mathcal{D}(g)$ one can determine the matrix $\mathcal{D}'(g)$. To do this, compare the l-th rows of the function ψ'_j as given by the matrix equations (16.5) and (16.3):

$$\sum_i \mathcal{D}_{ij}(g)\psi_{il}(x) = \sum_m \mathcal{D}^{1/2}_{ml}(g)\psi_{jm}(g^{-1}x).$$

Multiply this equation by $\mathcal{D}^{-1}_{lk}$ and sum over l. Then, using the relation $\sum_l \mathcal{D}^{1/2}_{ml}\mathcal{D}^{-1}_{lk} = \delta_{mk}$, we obtain

$$\psi_{jk}(g^{-1}x) = \sum_{il} \tilde{\mathcal{D}}^{-1}_{lk}(g)\mathcal{D}_{ij}(g)\psi_{il}(x). \tag{16.7}$$

Comparing (16.7) and (16.6), we see that

$$\mathcal{D}'_{il,\,jk}(g) = \tilde{\mathcal{D}}^{*}_{lk}(g)\mathcal{D}_{ij}(g) \tag{16.8}$$

or

$$\mathcal{D}' = \tilde{\mathcal{D}}^{*}_{1/2} \times \mathcal{D}. \tag{16.8a}$$

At this point one should ask in what cases allowance for spin in symmetry theory implies new physical phenomena. It can be seen from equation (16.1) that the only term that mixes wave functions ψ_{jk} with different spin indices k is the so-called spin-orbit coupling

$$\mathcal{H}_{so} = \frac{\hbar}{4m^2c^2}(\sigma[\nabla V \boldsymbol{P}]), \tag{16.9}$$

which describes the interaction between the spin and orbital angular momenta in atoms. If this term is negligible, the matrix equation (16.1) splits into two identical equations for the functions ψ_{j1} and ψ_{j2}, and so these functions

may also be identified. Thus, when spin-orbit coupling is neglected the eigenfunctions of equation (16.1) correspond to values $1/2$ and $-1/2$ of σ_z; each of them is the product of the coordinate function $\psi(r)$ and one of the spin functions

$$\alpha = \begin{vmatrix} 1 \\ 0 \end{vmatrix} \quad \text{and} \quad \beta = \begin{vmatrix} 0 \\ 1 \end{vmatrix}.$$

The functions $\psi(r)\alpha$, $\psi(r)\beta$ transform according to the representation $\mathcal{D}$, which is the direct product of the representation $\mathcal{D}_\mu$ according to which the coordinate function $\psi(r)$ transforms, and the representation $\mathcal{D}_{1/2}$, defined by equation (16.2), according to which the spin functions transform. If the operator in question does not explicitly affect the spin functions, all selection rules etc. depend only on the representations according to which the coordinate functions transform, since all the transitions are spin-conserving and allowance for spin only doubles the number of electrons in each state.

Allowance for spin-orbit coupling may partially remove degeneracy, i.e., it may cause splitting of terms corresponding to the set of functions $\alpha\psi(r)$, $\beta\psi(r)$. This kind of splitting occurs when the representation $\mathcal{D} = \mathcal{D}_\mu \times \mathcal{D}_{1/2}$ according to which these functions transform is reducible. These functions no longer correspond to a definite value of the spin projection, but are produced by superposition of states with σ_z equal to $+1/2$ and $-1/2$.

If spin-orbit coupling is neglected, all these representations correspond to the same energy. On the other hand, when allowance is made for spin-orbit coupling there is a specific eigenvalue E for each irreducible representation occurring in the direct product $\mathcal{D}_\mu \times \mathcal{D}_{1/2}$.

Thus, group theory makes it possible, irrespective of the specific form of $\mathcal{H}_{so}$, to determine immediately whether a given term splits when allowance is made for spin-orbit coupling and to establish the nature of the splitting. In fact, we need only check what irreducible representations occur in the product $\mathcal{D}_\mu \times \mathcal{D}_{1/2}$. Although in atoms spin-orbit splitting is usually small relative to the distance between terms, in crystals it usually exceeds the thermal energy of the electron or the Fermi energy, if the degeneracy is not too strong. In some crystals spin-orbit splitting is comparable with the band gap or the separation between bands produced by splitting of one atomic term by the crystal field.

In all these cases the shape of the electronic spectrum and other properties are determined precisely by the spinor representations.

Construction of Spinor Representations

As we see from (16.2), spinors have the special property that the matrices $\mathcal{D}(c_\theta)$ and $\mathcal{D}(c_{\theta+2\pi})$ corresponding to rotations about an arbitrary z'-axis through angles θ and $\theta + 2\pi$ differ in sign:

$$\mathcal{D}(c_{\theta+2\pi}) = -\mathcal{D}(c_\theta), \tag{16.10}$$

while

$$\mathcal{D}(c_{2\pi}) = -\mathcal{D}(c_{4\pi}) = -\mathcal{D}(e) = -I. \tag{16.11}$$

For the coordinate functions, these two rotations are equivalent, and so the relationships (16.10) and (16.11) must hold for any spinor functions. The matrices $\mathcal{D}(i)$ for these functions have the same form as for the usual functions, i.e., depending on their parity,

$$\mathcal{D}(i) = \pm \mathcal{D}(e) = \pm I. \tag{16.12}$$

An improper rotation through an angle θ may be represented as the product of inversion and rotation through the angle $\theta' = \theta + \pi$ if $\theta < \pi$ or $\theta' = \theta - \pi$ if $\theta \geqslant \pi$ (this assures that $\theta' < 2\pi$). Thus (16.10) remains valid for improper rotations. In particular, the operation σ_h, which may be treated as an improper rotation through $\theta = 2\pi$, is $\sigma_h = ic_2$. Therefore,

$$\mathcal{D}(\sigma_h^2) = \mathcal{D}(c_2^2 i^2) = \mathcal{D}(c_2^2) = -I. \tag{16.13}$$

Relationships (16.10) – (16.13) show that the spinor representations of point groups are projective rather than vector representations, i.e., their matrices satisfy the relationship

$$\mathcal{D}(r_1)\,\mathcal{D}(r_2) = \omega_2(r_1, r_2)\,\mathcal{D}(r_1 r_2). \tag{16.14}$$

Any product of operations $r_1 r_2$ can be expressed as a rotation about some z' axis through the angle θ or as rotation and inversion. By (16.10), (16.11), the factor system $\omega_2(r_1, r_2)$ is then defined by

$$\omega_2(r_1, r_2) = \begin{cases} 1 & \text{if} \quad \theta < 2\pi, \\ -1 & \text{if} \quad 4\pi > \theta > 2\pi, \end{cases} \tag{16.15}$$

where rotation through $-\theta$ coincides with rotation through $4\pi - \theta$, since $\mathcal{D}(c_{-\theta})\,\mathcal{D}(c_\theta) = \mathcal{D}(c_{4\pi})$. Formula (16.15) immediately yields $\omega_2(r_1, r_2)$ if r_1 and r_2 are rotations about the same axis (or rotations plus inversion). If the axes are different, it is convenient to use the defining relations to determine $\omega_2(r_1, r_2)$.

For example, in the group C_{3v}, rotations through the angle π about the axes u_2' and u_2'' obtained from u_2 by rotations through $2\pi/3$ and $4\pi/3$, respectively, are expressed as $u_2' = c_3 u_2 c_3^{-1}$ and $u_2'' = c_3^2 u_2 c_3^{-2}$. Since $u_2 c_3 u_2^{-1} = c_3^{-1}$, it follows that $u_2' = c_3^2 u_2$ and $u_2'' = c_3^4 u_2$. Consequently, the operation $c_3 u_2$ differs from u_2'' by a rotation through 2π, i.e., $\omega_2(c_3, u_2) = -1$, whereas $\omega_2(c_3^2, u_2) = 1$. Similarly, according to the usual rules, $u_2' u_2$ and $u_2'' u_2'$ are the rotation c_3^2, and $u_2'' u_2$ is the rotation c_3. It follows from the defining relations that $u_2' u_2 = c_3^2 u_2^2$, $u_2'' u_2' = c_3^2 u_2^2$, $u_2'' u_2 = c_3^4 u_2^2$. This means that $\omega_2(u_2', u_2) = \omega_2(u_2'', u_2') = -1$, $\omega_2(u_2'', u_2) = 1$.

Spinor representations may be viewed as vector representations of the double group, which includes an element Qg for each element g; here Q is a rotation through 2π, which commutes with every element g; for spinor representations $\mathcal{D}(Q) = -\mathcal{D}(e)$, but for vector representations $\mathcal{D}(Q) = \mathcal{D}(e)$.

This method of determining the spinor representations, proposed by Bethe, is essentially equivalent to construction of the covering group corresponding to the factor system (16.15). In the general case, this group is a subgroup of the [universal] covering group introduced in §13, since it contains projective representations for only one class – that containing the given factor system. Thus Bethe's method is a variant of Schur's general method for constructing projective representations.

The techniques of §12 reduce spinor representations of space groups to projective representations of the corresponding point group. When this is

done, the factor system $\omega(a, b)$ will be the product of a factor system $\omega_1(a, b)$ defined by equation (i.e., by the properties of the space group) and a factor system $\omega_2(a, b)$ defined by equation (16.15) (i.e., by the properties of the spinors):

$$\omega(a, b) = \omega_1(a, b)\,\omega_2(a, b). \tag{16.16}$$

Using the formulas of §14, we shall determine below the classes containing the factor systems $\omega_2(a, b)$ for all the point groups. A knowledge of the classes $K^{(1)}$ and $K^{(2)}$ of the factor systems ω_1 and ω_2 immediately yields the class $K = K^{(1)}K^{(2)}$ of the factor system ω, since the multiplication of classes is governed by the multiplication table of the multiplicator group. In fact, as shown in §13, it is sufficient to multiply the coefficients $\alpha_i^{(1)}$ and $\alpha_i^{(2)}$ corresponding to the classes $K^{(1)}$ and $K^{(2)}$, as given in Table 14.2 (pp. 113–118). The values of $\alpha_i = \alpha_i^{(1)}\alpha_i^{(2)}$ then determine the class K.

Since all the projective representations of the point groups were found in §14, the spinor representations of a given space group must coincide (up to p-equivalence) with one of the types of projective representations or with the vector representations of the point groups.* To determine the spinor representations of the space groups, one uses (12.29) and (16.15) to construct the factor system, determines its class and, using the tables of the corresponding projective representations, employs the p-equivalence transformations given in §14 to go over from the standard factor system to a factor system with the structure described above.

Thus, the only departure from the construction of vector representations of these groups is the need to incorporate (16.15) in construction of the factor system (16.16). We shall therefore describe the determination of the factor system (16.15) in greater detail and construct the spinor representations of the point groups (see the next subsection).

According to (13.4), the standard factor system used in the construction of Table 14.2 yields the present system when the matrix $\mathcal{D}(r)$ corresponding to the standard system is multiplied by a certain function $u(r)$:

$$\mathcal{D}'(r) = \mathcal{D}(r)\,u(r). \tag{16.17}$$

Table 16.2 (p. 150) gives the values of $u(r)$ for all elements of the point groups such that the factor system (16.15) corresponds to the class K_0. The spinor representations for the remaining groups correspond to the class K_1 in Table 14.2. The characters of these representations are obtained by multiplying the characters of the representations $\chi(r)$ which correspond to these classes by $u(r)$.

We now show how to determine the classes of the factor systems (16.15) and the functions $u(r)$ for specific groups.

Spinor Representations of Point Groups

If all the projective representations of a group are p-equivalent to vector representations, the spinor representations are of course also p-equivalent

* There is therefore no need to construct in addition projective representations of the double point groups, as in references /11.2, 11.3/.

to vector representations; the characters of the latter may be found in Table 11.1 (pp. 71–74). The cyclic groups C_n are of this type, and by (14.6) u may be written

$$u(c_n^k) = \frac{\omega_{c_n n}^{k/n}}{\omega_{c_n k}} = e^{\frac{i\pi M}{n}k}, \tag{16.18}$$

where M is any odd integer, which may be chosen in the most convenient manner. Equation (16.18) follows from the fact that by (16.15)

$$\omega(c_n^k, c_n) = \begin{cases} 1 & \text{for } k < n-1, \\ -1 & \text{for } k = n-1 \end{cases} \tag{16.19}$$

so that

$$\omega_{c_n k} = \omega(c_n, c_n)\,\omega(c_n^2, c_n) \ldots \omega(c_n, c_n^{k-1}) = \begin{cases} 1 & \text{for } k < n, \\ -1 & \text{for } k = n. \end{cases} \tag{16.20}$$

By equation (16.13), $\omega(\sigma_h, \sigma_h) = -1$. Therefore for the group C_s, just as for C_2

$$u(\sigma_h) = e^{\pi i/2} = i, \quad u(c_2) = i. \tag{16.21}$$

Now, for spinor representations, just as for vector representations, $\mathfrak{D}(i) = \pm \mathfrak{D}(e)$; thus

$$\omega(a, b) = \omega(b, a) = 1, \quad \text{if} \quad a = i \quad \text{and/or} \quad b = i. \tag{16.22}$$

Therefore, for the group C_i

$$u(i) = 1. \tag{16.23}$$

For the groups $C_{2h} = C_2 \times C_i$, $C_{4h} = C_4 \times C_i$, $C_{6h} = C_6 \times C_i$, $S_6 = C_3 \times C_i$, the spinor representations are also p-equivalent to vector representations, as follows from (14.10) and (16.22), and by virtue of (16.12) the spinor representations of these groups are the products of the spinor representations of groups C_n and C_i, as was the case for vector representations. For these groups, therefore, and in fact for any group $G \times C_i$, we have

$$u(ai) = u(a), \tag{16.24}$$

where a is any element of C_n for which $u(r)$ is defined by (16.18).

In particular, for the groups C_3 and $S_6 = C_3 \times C_i$, we set $M = 3$ in (16.18), obtaining

$$u(c_3) = u(s_6^5) = -1, \quad u(c_3^2) = u(s_6) = 1. \tag{16.25}$$

For the groups C_6 and $C_{6h} = C_6 \times C_i$ it is again convenient to set $M = 3$ in (16.18). This also applies to the cyclic group D_{3h}, whose generator a may be expressed as $a = c_6 i = c_3^2 \sigma_h$. Then, by (16.18) and (16.24),

$$u(\sigma_h) = -i, \; u(c_3\sigma_h) = u(c_3^2\sigma_h) = i, \; u(c_3) = -1, \; u(c_3^2) = 1. \tag{16.26}$$

The only groups now remaining all of whose projective representations are in class K_0 are S_4, D_3 and C_{3v}. By (16.15) and (14.3), for S_4 we have

$$\omega(s_4, s_4) = \omega(s_4, s_4^2) = \omega(s_4, s_4^3) = -1,$$

i.e.,

$$\omega_{s_4 2} = \omega_{s_4 4} = -1, \quad \omega_{s_4 3} = 1$$

and, consequently, by (14.6),

$$u(s_4^k) = -(-1)^k e^{\frac{\pi i}{4}k} = e^{\pi i\left(1-\frac{3}{4}k\right)}. \tag{16.27}$$

The spinor representations of the isomorphic groups D_n and C_{nv} have the same factor systems $\omega(a, b)$, where $a = c_n^k$, and $b = u_2$ or $b = \sigma_v = iu_2$ respectively. Thus the spinor representations of these groups coincide.

By (14.45), the values of the coefficients $u(c_3^k)$ for D_3 and C_{3v} are defined by (16.25). As indicated above, $\omega(c_3, u) = -1$ and $\omega(c_3^2, u) = 1$. Therefore, by (14.45) and (16.21),

$$u(u_2') = u(c_3^2)\,u(u_2) = i, \quad u(u_2'') = -u(c_3)\,u(u_2) = i. \tag{16.28}$$

Consequently, for all three elements u_2 or σ_v, the function u is defined by (16.21).

For the remaining groups, C_{nv} and D_n, the spinor representations belong to class K_1, since for these groups it follows from (16.15) that the quotient

$$\frac{\omega(c_n^{n/2}, u_2)}{\omega(u_2, c_n^{n/2})} \quad \text{or} \quad \frac{\omega(c_n^{n/2}, \sigma_v)}{\omega(\sigma_v, c_n^{n/2})}$$

equals -1. Indeed, if $u_2 c_n^{n/2}$ is rotation through the angle 2π about an axis perpendicular to c_n and u_2, then $c_n^{n/2}u_2$ is rotation through the angle -2π.

For the groups C_{2v} and D_2, one sees from (14.45) that $u(a)$ and $u(b)$ are given by equations (16.21). Here $a = c_2$, and $b = u_2$ or $b = \sigma_v$; $u(ab) = u(a)u(b) = -1$, since $\omega(a, b) = 1$.

For all elements $a^k b$ of the groups C_{4v} and D_4, specifically, u_2, $u_2' = c_4 u_2$, $u_2'' = c_4 u_2 c_4^{-1} = c_4^2 u_2$, and $u_2''' = c_4 u_2' c_4^{-1} = c_4^3 u_2$, as for all the elements σ_v, we have $\omega(a^k, b) = 1$ and $\omega(b, a) = -1$, since $u_2 c_4 = c_4^{-1} u_2$. Therefore, by (14.24), (14.33) and (14.47), $\alpha' = \dfrac{\omega(u_2, c_4)\,\omega(c_4^3, c_4)}{\omega_{c_4}^{1/2}\omega(c_4^3, u_2)} = -1$, whence

$$u(c_4^k) = e^{\frac{\pi i}{2}k},$$

$$u(c_4^k u_2) = u(c_4^k)\,u(u_2) = e^{\frac{\pi i}{2}(k+1)} \qquad u(c_4^k\sigma_v) = e^{\frac{\pi i}{2}(k+1)}. \tag{16.29}$$

For the isomorphic group D_{2d}, it follows from (14.24), (14.33) and (16.26) that

$$u(s_4^k) = -(-1)^k e^{\frac{\pi i}{2}k} = e^{\pi i\left(1-\frac{k}{2}\right)}, \quad u(s_4^k u_2) = e^{-\frac{\pi i}{2}(k+1)}, \tag{16.30}$$

since for all elements $a^k b$, specifically, u_2, $u_2' = s_4 u_2 s_4^{-1} = s_4^2 u_2$, $\sigma_v = s_4 u_2$, $\sigma_v' = s_4 u_2'' = s_4^3 u_2$, we again have $\omega(a^k, b) = 1$ and $\omega(b, a) = -1$.

From (16.25) we see that the spinor representations of the group $D_{3d} = D_3 \times C_i$, like those of D_3, belong to class K_0, i.e., are p-equivalent to vector representations; $u(c_3^k)$ and $u(c_3^k\sigma_v)$ are defined by (16.25), (16.28), and for the other elements equation (16.24) is valid.

For the group D_{3h}, as for C_{2v}, we have $\omega(\sigma_v, \sigma_h) = -\omega(\sigma_h, \sigma_v)$, thus the spinor representations belong to class K_1, as is the case for the isomorphic groups C_{6v} and D_6. By (14.45) $u(a^k)$, $a = c_6 i$ or c_6, is defined by (16.18). For all the other elements, $c_6^k u_2$, $c_6^k\sigma_v$ or $ic_6^k u_2$, it is easy to show that $\omega(c_6^k, u_2) = \omega(c_6^k, \sigma_v) = 1$;

consequently,

$$u(c_6^k) = u(ic_6^k) = e^{\frac{\pi i}{2}k}, \quad u(c_6^k u_2) = u(c_6^k \sigma_v) = u(ic_6^k u_2) = e^{\frac{\pi i}{2}(k+1)}. \tag{16.31}$$

As for the groups $D_{2h} = D_2 \times C_i$, $D_{4h} = D_4 \times C_i$ and $D_{6h} = D_6 \times C_i$, it follows from (16.24) that the factors $u(a)$ and $u(ai)$ have the same values as for the groups D_2, D_4 and D_6, respectively.

From condition (16.22) it follows at once that the factor system (16.15) corresponds to the class K_1 of these groups, since in these representations $ai = ia$ for any element a. For the groups T, T_h, T_d, O and O_h, the spinor representations are again p-equivalent to the projective representations in class K_1, since they all contain perpendicular twofold axes with $\omega(a, b) = -\omega(b, a)$.

The function $u(r)$ for T and O is defined by (14.53), (14.54) and (14.68), (14.69); its values for T may be found in Table 14.1 (p. 108). For T_d the values of $u(r)$ are the same as for O, since the factor systems (16.15) are the same. For the groups $T_h = T \times C_i$ and $O_h = O \times C_i$, it follows from (16.24) that the values of $u(r)$ and $u(ir)$ coincide with the values of $u(r)$ for the same elements of groups T and O, respectively, and this at once determines the appropriate class of factor systems.

If the characters of the irreducible spinor representations are known, the formulas of §8 enable one directly to ascertain the irreducible constituents of any product $\mathcal{D} \times \mathcal{D}_{1/2}$, where $\mathcal{D}$ is any vector representation of the point group; here one uses the fact that by (10.20) and (16.12) the characters of the representation $\mathcal{D}_{1/2}^{+}$ are given by

$$\chi(c_\varphi) = 2\cos\frac{\varphi}{2}, \quad \chi(s_\varphi) = \chi(ic_{\varphi+\pi}) = -2\sin\frac{\varphi}{2}. \tag{16.32}$$

The basis functions of any spinor representation may be built up from the basis functions of a representation $\mathcal{D} \times \mathcal{D}_{1/2}$ containing the given representation. For this purpose one expands the system of functions $\psi_i\alpha$ and $\psi_i\beta$, where ψ_i are basis functions for $\mathcal{D}$, in terms of irreducible representations. The required basis functions may also be derived from basis functions for the representations of the full spherical group with half-integer j, expanding the latter in terms of the irreducible representations of the point group in question. If $j = 3/2$ and the canonical basis is used,

$$Y_{1/2}^{3/2} = -\frac{i}{\sqrt{2}}(x + iy)\alpha, \qquad Y_{1/2}^{1/2} = \frac{i}{\sqrt{6}}[(x + iy)\beta - 2z\alpha],$$

$$Y_{-1/2}^{3/2} = \frac{i}{\sqrt{2}}(x - iy)\beta, \qquad Y_{-1/2}^{1/2} = -\frac{i}{\sqrt{6}}[(x - iy)\alpha + 2z\beta].$$

Table 16.1 gives the characters of the spinor representations for point groups possessing projective representations not equivalent to vector representations, for which the spinor representations do not belong to the class K_0; basis functions are also listed. Table 16.2 indicates the representations according to which the spinor functions transform, for groups such that these representations are p-equivalent to vector representations, and the values of the products $\mathcal{D} \times \mathcal{D}_{1/2}$ are given for these groups. Groups which are products of these groups and C_i preserve the same multiplication rules, since $\mathcal{D}_{1/2}$ is even. In such cases the representations $\mathcal{D}_i'$ according to which the spinor functions transform are p-equivalent to appropriate vector representations $\mathcal{D}_i$ and differ from them by the factor $u(r)$ presented in the text and in Table 16.2.

TABLE 16.1. Character tables for spinor representations

Groups D_2, C_{2v}

D_2	e	c_{2z}	c_{2x}	c_{2y}	Basis functions	Multiplication table			
C_{2v}	e	c_2	σ_v	σ'_v	D_2, C_{2v}	A_1	A_2	B_1	B_2
E'	2	0	0	0	α, β	E'	E'	E'	E'

Groups D_4, C_{4v}, D_{2d}

D_4	e	c_2	c_4	c_4^3	$2u_2$	$2u'_2$	Basis functions		Multiplication table
C_{4v}	e	c_2	c_4	c_4^3	$2\sigma_v$	$2\sigma'_v$	D_4, C_{4v}	D_{2d}	
D_{2d}	e	c_2	s_4	s_4^3	$2u_2$	$2\sigma_d$			A_1 A_2 B_1 B_2 E
E'_1	2	0	$\sqrt{2}$	$-\sqrt{2}$	0	0	α, β	$(x+iy)\alpha$, $(x-iy)\beta$	E'_1 E'_1 E'_2 E'_2 $E'_1+E'_2$
E'_2	2	0	$-\sqrt{2}$	$\sqrt{2}$	0	0	$(x+iy)\alpha$, $(x-iy)\beta$	α, β	E'_2 E'_2 E'_1 E_1 $E'_1+E'_2$

Groups D_6, C_{6v}, D_{3h}

D_6	e	c_2	c_3	c_3^2	c_6	c_6^5	$3u_2$	$3u'_2$	Basis functions	
C_{6v}	e	c_2	c_3	c_3^2	c_6	c_6^5	$3\sigma_v$	$3\sigma'_v$	D_6, C_{6v}	D_{3h}
D_{3h}	e	σ_h	c_3	c_3^2	s_6	s_6^5	$3u_2$	$3\sigma'_v$		
E'_1	2	0	1	-1	$\sqrt{3}$	$-\sqrt{3}$	0	0	α, β	$(x-iy)\alpha$, $(x+iy)\beta$
E'_2	2	0	1	-1	$-\sqrt{3}$	$\sqrt{3}$	0	0	$(x+iy)^3\alpha$, $(x-iy)^3\beta$	α, β
E'_3	2	0	-2	2	0	0	0	0	$(x+iy)\alpha$, $(x-iy)\beta$	$(x+iy)\alpha$, $(x-iy)\beta$

Multiplication table

	A_1 A_1^+	A_2 A_1^-	A_3 A_2^+	A_4 A_2^-	E_1 E^+	E_2 E^-
E'_1	E'_1	E'_1	E'_2	E'_2	$E'_2+E'_3$	$E'_1+E'_3$
E'_2	E'_2	E'_2	E'_1	E'_1	$E'_1+E'_3$	$E'_2+E'_3$
E'_3	E'_3	E'_3	E'_3	E'_3	$E'_1+E'_2$	$E'_1+E'_2$

TABLE 16.1 (continued)

Group T

T	e	$4c_3$	$4c_3^2$	$3c_2$	Basis functions
E_1'	2	1	-1	0	$\alpha,\ \beta$
E_2'	2	ε_3	$-\varepsilon_3^2$	0	$\frac{1}{\sqrt{2}}\left(Y^{3/2}_{-1/2}-iY^{3/2}_{3/2}\right),\ \frac{1}{\sqrt{2}}\left(Y^{3/2}_{1/2}-iY^{3/2}_{-3/2}\right)$
E_3'	2	ε_3^2	$-\varepsilon_3$	0	$\frac{1}{\sqrt{2}}\left(Y^{3/2}_{1/2}+iY^{3/2}_{-3/2}\right),\ \frac{1}{\sqrt{2}}\left(Y^{3/2}_{-1/2}+iY^{3/2}_{3/2}\right)$

Multiplication table

	A	B_1	B_2	E
E_1'	E_1'	E_2'	E_3'	$E_1'+E_2'+E_3'$
E_2'	E_2'	E_3'	E_1'	$E_1'+E_2'+E_3'$
E_3'	E_3'	E_1'	E_2'	$E_1'+E_2'+E_3'$

Groups T_d, O

T_d	e	$4c_3$	$4c_3^2$	$3c_2$	$3s_4$	$3s_4^3$	$6\sigma_d$	Basis functions	
O	e	$4c_3$	$4c_3^2$	$3c_2$	$3c_4$	$3c_4^3$	$6u_2$	T_d	O
E_1'	2	1	-1	0	$\sqrt{2}$	$-\sqrt{2}$	0	$\frac{1}{\sqrt{3}}[(x+iy)\beta+z\alpha]$ $\frac{i}{\sqrt{3}}[(x-iy)\alpha-z\beta]$	$\alpha,\ \beta$
E_2'	2	1	-1	0	$-\sqrt{2}$	$\sqrt{2}$	0	$\alpha,\ \beta$	$\frac{1}{\sqrt{3}}[(y+ix)z\beta+xy\alpha]$ $\frac{i}{\sqrt{3}}[(y-ix)z\alpha-xy\beta]$
G'	4	-1	1	0	0	0	0	$Y^{3/2}_{\pm 3/2},\ Y^{3/2}_{\pm 1/2}$	$Y^{3/2}_{\pm 3/2},\ Y^{3/2}_{\pm 1/2}$

Multiplication table

	A_1	A_2	E	F_1	F_2
E_1'	E_1'	E_2'	G'	$E_1'+G'$	$E_2'+G'$
E_2'	E_2'	E_1'	G'	$E_2'+G'$	$E_1'+G'$
G'	G'	G'	$E_1'+E_2'+G'$	$E_1'+E_2'+2G'$	$E_1'+E_2'+2G'$

TABLE 16.2. Decomposition of $\mathfrak{D} \times \mathfrak{D}_{1/2}$ into irreducible constituents*

Group	Representations according to which α and β transform		Representations occurring in the product of $\mathfrak{D}_{1/2}$ and the indicated single-valued representation	$u(g)$
C_1	A	A	$A \to A' + A'$	$u(e) = 1$
C_2	A_1'	A_2'	$A_1 \to A_1' + A_2'$, $A_2 \to A_1' + A_2'$	$u(c_2) = i$
C_s	A_1'	A_2'	$A_1 \to A_1' + A_2'$, $A_2 \to A_1' + A_2'$	$u(\sigma_h) = i$
C_3	B_2'	B_1'	$A_1 \to B_1' + B_2'$, $B_1 \to A_1' + B_2'$, $B_2 \to A_1' + B_1'$	$u(c_3) = -1$, $u(c_3^2) = 1$
C_4	B_2'	A_1'	$A_1 \to A_1' + B_2'$, $A_2 \to A_2' + B_1'$	$u(c_4) = (1/\sqrt{2})(1+i)$
				$u(c_2) = i$
			$B_1 \to A_1' + B_1'$, $B_2' \to A_2' + B_2'$	$u(c_4^2) = -(1/\sqrt{2})(1-i)$
S_4	B_1'	A_2'	$A_1 \to A_2' + B_1'$, $A_2 \to A_1' + B_2'$	$u(s_4) = (1/\sqrt{2})(1+i)$
				$u(c_2) = -i$
			$B_1 \to A_2' + B_2'$, $B_2 \to A_1' + B_1'$	$u(s_4^3) = -(1/\sqrt{2})(1-i)$
C_6	B_4	B_1	$A_1 \to B_1' + B_4'$, $A_2 \to B_2' + B_3'$	$u(c_6) = u(c_6^5) = i$
			$B_2 \to A_1' + B_4'$, $B_2 \to A_2' + B_3'$	$u(c_3) = -1$, $u(c_3^2) = 1$
			$B_3 \to A_2' + B_1'$, $B_4 \to A_1' + B_2'$	$u(c_2) = -i$
C_{3h}	B_2^-	B_1^+	$A_1^+ \to B_1^{+\prime} + B_2^{-\prime}$, $A_1^- \to B_1^{-\prime} + B_2^{+\prime}$	$u(s_3) = u(s_3^5) = i$
			$B_1^+ \to A_1^{+\prime} + B_2^{-\prime}$, $B_1^- \to A_1^{-\prime} + B_2^{+\prime}$	$u(c_3) = -1$, $u(c_3^2) = 1$
			$B_2^+ \to A_1^{-\prime} + B_1^{+\prime}$, $B_2^- \to A_1^{+\prime} + B_1^{-\prime}$	$u(\sigma_h) = -i$
D_3	E'		$A_1 \to E'$, $A_2 \to E'$, $E \to A_1' + A_2' + E'$	$u(c_3) = -1$; $u(c_3^2) = 1$, $u(u_2) = i$
C_{3v}	E'		$A_1 \to E'$, $A_2 \to E'$, $E \to A_1' + A_2' + E'$	$u(c_3) = -1$; $u(c_3^2) = 1$, $u(\sigma_h) = i$

* For spinor representations there may be two values of $\chi(\varphi)$, differing in sign, for each rotation φ, depending on the choice of $u(g)$. Here, for all the groups except S_4, $\chi_\alpha(\varphi) = e^{-i\varphi/2}$, $\chi_\beta(\varphi) = e^{i\varphi/2}$; for S_4 the sign is reversed. Since multiplication by $u(g)$ may reverse the parity of the representation, the indices of A and B may not correspond to the true parity.

§17. ELECTRON IN A PERIODIC FIELD

As indicated in §15, the states and spectra of any elementary excitations of an ideal crystal, such as excitations of electrons, phonons, excitons, spin waves, may be classified according to representations of the space groups. In this section we shall use group-theoretic results to characterize the wave functions and energy spectra of electrons in an ideal crystal.

The wave function of an electron moving in an ideal crystal is a solution of the Schrödinger equation (15.1)

$$\mathscr{H}\psi = E\psi, \tag{17.1}$$

where the energy operator $\mathscr{H}$ is

$$\mathscr{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{x}). \tag{17.2}$$

For the time being, we shall not include spin-orbit coupling in the operator $\mathscr{H}$ (17.2).

The potential energy $V(\boldsymbol{x})$, i.e., the self-consistent potential due to the ions and electrons forming the ideal lattice, and hence also the energy operator $\mathscr{H}$, are invariant under all transformations which take each point of the crystal to an equivalent position, i.e., under all transformations in the space group G. Consequently, by (15.2)

$$gV(\boldsymbol{x}) = V(g^{-1}\boldsymbol{x})\,g = V(\boldsymbol{x})\,g, \quad g\mathscr{H} = \mathscr{H}g. \tag{17.3}$$

The symmetry group of the operator $\mathscr{H}$ is thus the space group G, and therefore all its eigenfunctions ψ may be classified in accordance with the irreducible representations of G. As pointed out in §6, any space group contains as an abelian subgroup the group T of translations by the principal periods of the Bravais lattice. In view of the translational invariance of the potential $V(\boldsymbol{x})$, it is often called a periodic potential.

The representations of the translation group are characterized by a continuous vector $\boldsymbol{k}$ in the Brillouin zone.

A convenient choice of eigenfunctions for the energy operator $\mathscr{H}$ is the set of functions $\psi_{\boldsymbol{k}}$ that transform according to the irreducible representations of the translation group T; by (12.8) we have

$$t_{\boldsymbol{a}}\psi_{\boldsymbol{k}}(\boldsymbol{x}) = \psi_{\boldsymbol{k}}(\boldsymbol{x}-\boldsymbol{a}) = e^{-i\boldsymbol{k}\boldsymbol{a}}\psi_{\boldsymbol{k}}(\boldsymbol{x}). \tag{17.4}$$

It follows from (17.4) that the wave function $\psi_{\boldsymbol{k}}$ can be written

$$\psi_{\boldsymbol{k}} = e^{i\boldsymbol{k}\boldsymbol{x}}u_{\boldsymbol{k}}(\boldsymbol{x}). \tag{17.5}$$

The functions (17.5) are known as the Bloch functions, and the functions $u_{\boldsymbol{k}}(\boldsymbol{x})$ are the Bloch factors (or modulating factors).

The energy corresponding to state $\psi_{\boldsymbol{k}}$ is a function $E(\boldsymbol{k}) = E(k_x, k_y, k_z)$ of the vector $\boldsymbol{k}$.

In the general case equations (17.1) and (17.4) have infinitely many linearly independent solutions. We designate each linearly independent solution of (17.1) and (17.4) by an index n: $\psi_{\boldsymbol{k}n} = e^{i\boldsymbol{k}\boldsymbol{x}}u_{\boldsymbol{k}n}(\boldsymbol{x})$, and the corresponding energy is denoted by $E_n(\boldsymbol{k})$. Thus, an operator $\mathscr{H}$ with periodic potential generally has a multiband spectrum $E_n(\boldsymbol{k})$, and each branch of the spectrum is characterized by a discrete band number n. The state within a given band n is characterized by a continuous quantum number $\boldsymbol{k}$.

Different branches $E_n(k)$ may coincide at isolated points or along a curve in k-space. This touching of bands may be either accidental, i.e., due to the properties of the potential $V(x)$, or a consequence of the symmetry of the potential. In the latter case it can be investigated by group-theoretic methods.

From (17.2) and (17.5) it follows that u_{nk} satisfies the equation

$$\mathscr{H}_k u_{nk} = \mathscr{E}_n(k)\, u_{nk}, \tag{17.6}$$

where

$$\mathscr{H}_k = -\frac{\hbar^2}{2m}\nabla^2 + V(x) + \frac{\hbar k p}{m}. \tag{17.7}$$

Unlike the operator $\mathscr{H}$ (17.2), $\mathscr{H}_k$ depends on the wave vector k, since it includes the additional term $\hbar kp/m$, where p is the momentum operator. The eigenvalues $E_n(k)$ for this choice of $\mathscr{H}_k$ differ from the electron energy $\mathscr{E}_n(k)$ by the energy $\hbar^2k^2/2m$ of a free electron.

The periodicity of the functions u_{nk} is essentially a boundary condition for equation (17.6); we must therefore confine our examination of the solutions of this equation to periodic solutions.

If equation (17.6) has m linearly independent solutions u_{ik} $(i = 1, 2, \ldots, m)$, implying the existence of m linearly independent solutions $\psi_{ik} = e^{ikx} u_{ik}$ of equations (17.2), (17.5) corresponding to one energy $E(k)$, we say that there is an m-fold band degeneracy at the point k. As shown in §15, the number of linearly independent solutions of the Schrödinger equation is determined by the dimension of the irreducible representations of the symmetry group of the energy operator, in the present case the operator $\mathscr{H}_k$ (17.7). Thus the band degeneracy at the point k is determined in the general case by the dimension of the irreducible representations of the symmetry group of the operator $\mathscr{H}_k$. Because of the term $\hbar kp/m$, the operator $\mathscr{H}_k$ possesses lower symmetry than that characterized by the space group G, which is the symmetry group of the Hamiltonian $\mathscr{H}$.

Indeed, it follows from (17.7) that for any element $g \in G$

$$\begin{aligned} g\mathscr{H}_k(x) = \mathscr{H}_k(g^{-1}x) &= -\frac{\hbar^2}{2m}\nabla^2 + V(g^{-1}x) + \frac{\hbar k g^{-1} p}{m} = \\ &= -\frac{\hbar^2}{2m}\nabla^2 + V(x) + \hbar\frac{gkp}{m} = \mathscr{H}_{gk}(x). \end{aligned} \tag{17.8}$$

Thus the operator $\mathscr{H}_k$ is invariant only under transformations h in G that leave the vector k fixed, $hk = k$. For points inside the Brillouin zone, these transformations form the little group G_k introduced in §13.

Consequently, the band degeneracy at k is determined by the dimension of the irreducible representation $\mathscr{D}^k$ of the little group according to which the Bloch functions ψ_{ik} transform:

$$h\psi_{ik} = \psi_{ik}(h^{-1}x) = \sum_s \mathscr{D}^k_{si}(h)\,\psi_{sk}(x), \qquad h \in G_k.$$

The Bloch factors u_{nk} transform according to the matrix $\mathscr{D}^k(r)$ introduced in §12 (see (12.26)), which depends only on the rotational elements of the group F_k:

$$hu_{ik}(x) = u_{ik}(h^{-1}x) = \sum_s \mathscr{D}^k_{si}(r)\,u_{sk}(x); \quad h = (r|a+a), \qquad r \in F_k.$$

As demonstrated in §12, the matrices $\mathscr{D}^k(r)$ for points inside the Brillouin zone form vector representations of the crystallographic point group F_k. For

such points, therefore, the band degeneracy at $\boldsymbol{k}$ coincides with the dimension of the irreducible representations of $F_{\boldsymbol{k}}$. It is clear that band degeneracy may occur only for points of sufficiently high symmetry.

A basis for the total representation $\mathscr{D}^{\{\boldsymbol{k}\}}$ of the space group with irreducible star $\{\boldsymbol{k}\}$ is formed by the Bloch functions $\psi_{s\boldsymbol{k}_i}$, where $\boldsymbol{k}_i$ ranges over the different wave vectors in the star $\{\boldsymbol{k}\}$. As pointed out in §12, the vectors $\boldsymbol{k}_i$ may be obtained from $\boldsymbol{k}$ by applying transformations g_i: $\boldsymbol{k}_i = g_i\boldsymbol{k}$, which are elements of the space group G but not of the little group $G_{\boldsymbol{k}}$. By (12.19),

$$\psi_{s\boldsymbol{k}_i} = \psi_{s\,g_i\boldsymbol{k}} = e^{i\boldsymbol{k}_i\boldsymbol{x}} u_{s\boldsymbol{k}_i}(\boldsymbol{x}) = e^{ig_i\boldsymbol{k}\boldsymbol{x}} u_{s\,g_i\boldsymbol{k}}(\boldsymbol{x}). \tag{17.9}$$

Since all the functions belonging to one irreducible representation correspond to the same energy,

$$E(\boldsymbol{k}_i) = E(g\boldsymbol{k}) = E(\boldsymbol{k}) \tag{17.10}$$

for every $g \in G$. Thus the band structure as a whole exhibits the symmetry characterized by the crystal class F of the space group G.

The total energy degeneracy N_0 due to the lattice symmetry, equal to the dimension of an irreducible representation of the space group, is by (12.16) equal to the product of the band degeneracy m at $\boldsymbol{k}$ and the number of points in the star $\{\boldsymbol{k}\}$:

$$N_0 = mf.$$

One can distinguish two types of degeneracy in the energy spectrum: band degeneracy at a point $\boldsymbol{k}$, due to the symmetry at $\boldsymbol{k}$, and energy degeneracy, due to equal energy at different points of $\boldsymbol{k}$-space, corresponding to different points in the star of the vector $\boldsymbol{k}$.

Compatibility conditions. In crystals with sufficiently high symmetry, the Brillouin zone will always contain points or curves at which band degeneracy may occur, i.e., there are representations of the little group of dimension greater than 1. Consider any point $\boldsymbol{k}_0$ inside the Brillouin zone in whose neighborhood there are no points of higher symmetry. The band degeneracy at the point $\boldsymbol{k}_0$ is characterized by the representations of the little group $G_{\boldsymbol{k}_0}$; at a neighboring point $\boldsymbol{k}_0 + \boldsymbol{\varkappa} = \boldsymbol{k}$ we must consider the group $G_{\boldsymbol{k}}$. In general, the point $\boldsymbol{k}$ possesses lower symmetry, and so $G_{\boldsymbol{k}}$ is a subgroup of $G_{\boldsymbol{k}_0}$ and the dimensions of the irreducible representations of $G_{\boldsymbol{k}}$ are less than the dimensions of the representations of $G_{\boldsymbol{k}_0}$. Hence the band degeneracy at $\boldsymbol{k}$ is partially or completely removed. Since the group $G_{\boldsymbol{k}}$ depends only on the direction of the vector $\boldsymbol{\varkappa}$ if $\boldsymbol{\varkappa}$ is sufficiently small, the nature (but not amount) of band splitting also depends only on this direction. But if the point $\boldsymbol{k}_0$ lies on a curve of symmetry, the symmetry of the points $\boldsymbol{k}_0$ and $\boldsymbol{k}$ remains unchanged when one moves along the curve, and the band degeneracy is not removed.

The pivotal problem here is to determine which representations of $G_{\boldsymbol{k}}$ occur in a given representation $\mathscr{D}^{\boldsymbol{k}_0}$ of $G_{\boldsymbol{k}_0}$, and what representation of $G_{\boldsymbol{k}}$ is obtained from the representation $\mathscr{D}^{\boldsymbol{k}_0}$ if the degeneracy is not removed. The answers to these questions are given by relations connecting the representations at neighboring points, known as compatibility conditions.

In order to derive compatibility conditions, we proceed exactly as in the case of term splitting caused by a perturbation lowering symmetry from $G_{\boldsymbol{k}_0}$

to G_k. Thus (see §16), we must determine the coefficients in the expansion of $\mathscr{D}^{k_1}$ in terms of the representations $\mathscr{D}^k$ of G_k:

$$\mathscr{D}^{k_1} = \sum_s c_s \mathscr{D}^k_s. \tag{17.11}$$

The coefficients c_s, which indicate how many times the representation $\mathscr{D}^k_s$ occurs in $\mathscr{D}^{k_1}$, may be determined from the known characters of the representations $\mathscr{D}^{k_1}$ and $\mathscr{D}^k$, using (8.18). If c_s is not zero in (17.11), the representations $\mathscr{D}^{k_1}$ and $\mathscr{D}^k_s$ are compatible. By (12.26), for points in the Brillouin zone the matrices $\mathscr{D}^k(r)$ may be used instead of $\mathscr{D}^k(h)$ in the compatibility conditions (17.11).

Allowance for spin-orbit coupling. As shown in §16, the operator $\mathscr{H}_{so}$ should be included in the Hamiltonian $\mathscr{H}$ to allow for spin-orbital coupling. If we omit the last two relativistic terms, which do not depend on σ, from (16.1), the energy operator $\mathscr{H}$ for an electron moving in a periodic field will be

$$\mathscr{H} = \frac{p^2}{2m} + V(\boldsymbol{x}) + \frac{\hbar}{4m^2c^2}([\nabla V\, p]\sigma). \tag{17.12}$$

Correspondingly, the operator $\mathscr{H}_k$ acting on the two-component function u_{nk} is

$$\mathscr{H}_k = \frac{p^2}{2m} + V(\boldsymbol{x}) + \frac{\hbar k p}{m} + \frac{\hbar}{4m^2c^2}\Big([\nabla V\, p]\sigma\Big) + \frac{\hbar^2}{4m^2c^2}(\boldsymbol{k}[\sigma\nabla V]). \tag{17.13}$$

The operator $\mathscr{H}_k$ (17.13) can be written

$$\mathscr{H}_k = \mathscr{H}_0 + \frac{\hbar}{m}\boldsymbol{k}\pi, \tag{17.14}$$

where $\mathscr{H}_0$ is the operator (17.2), and π is the vector

$$\pi = p + \frac{\hbar}{4mc^2}[\sigma\nabla V]. \tag{17.15}$$

The second term in (17.14), as in (17.12), mixes states with different spin projections.

As usual, the symmetry group of the energy operator $\mathscr{H}$ (17.12) is the space group G, and so the states of an electron with spin in a periodic field must be classified according to the spinor representations of the space groups. All the results of §12 are valid for spinor representations. Thus, every irreducible spinor representation of the space group is characterized by the irreducible star $\{\boldsymbol{k}\}$ of the vector $\boldsymbol{k}$ and by the index of an irreducible representation of the little group G_k.

As pointed out in §12, these representations may be obtained using (12.23) if the projective representations $\mathscr{D}^k(r)$ of the crystallographic point group F_k are known.

If the wave functions ψ_{sk} at the point $\boldsymbol{k}$ transform according to an m-dimensional representation $\mathscr{D}^k$ when no allowance is made for spin-orbit coupling, when the spinor functions α and β are taken into consideration the functions $\psi_{sk}\alpha$ and $\psi_{sk}\beta$ form the basis of the $2m$-dimensional representation $\mathscr{D}^k \times \mathscr{D}_{1/2}$. According to the rules developed in §16 for determining the nature of band splitting due to spin-orbit coupling, the representation $\mathscr{D}^k \times \mathscr{D}_{1/2}$ should be expanded in terms of the irreducible spinor representations $\mathscr{D}^k_\nu$ of the little group:

$$\mathscr{D}^k \times \mathscr{D}_{1/2} = \sum_\nu c_\nu \mathscr{D}^k_\nu, \tag{17.16}$$

where c_ν are integer coefficients, determined by character theory.

If the representation $\mathcal{D}^k \times \mathcal{D}_{1/2}$ is irreducible, spin-orbit coupling does not remove band degeneracy. Instead of (17.16), one can expand the product $\mathcal{D}^k(r) \times \mathcal{D}_{1/2}$ in terms of irreducible projective representations of the point group. For points on the boundary of the Brillouin zone, the direct product $\mathcal{D}^k(r) \times \mathcal{D}_{1/2}$ of projective representations which belong to classes K_1 and K_2, respectively, should be expanded in terms of irreducible representations $\mathcal{D}^k_\nu(r)$ of class $K_3 = K_2K_1$.

The compatibility conditions are also valid for spinor representations of space groups.

Analytical properties of the Bloch functions. The Bloch functions ψ_{nk}, as functions of the continuous spectrum, will be normalized with respect to the crystal volume $\mathcal{V}$:

$$\int \psi^*_{nk} \psi_{n'k'} \, d\tau = \langle \psi_{nk} \psi_{n'k'} \rangle = \mathcal{V} \delta_{nn'} \delta_{kk'}. \tag{17.17}$$

The integration in (17.17) extends over the entire crystal volume. Since $\mathcal{V} = N\Omega_0$, where N is the number of primitive cells and Ω_0 is the volume of each cell, it follows from the periodicity of $\psi^*_{nk}\psi_{n'k'}$ and from (17.17) that the functions u_{nk} are normalized with respect to the volume of a primitive cell:

$$\langle u_{nk} u_{n'k} \rangle = \frac{1}{\Omega_0} \int_{\Omega_0} u^*_{nk} u_{n'k} \, d\tau_0 = \delta_{nn'}. \tag{17.18}$$

Here the integration extends over the volume of a primitive cell.

Note that functions u_{nk} and $u_{n'k'}$ with different k and k' are not orthogonal when $k \neq k'$, since they are eigenfunctions of different operators $\mathcal{H}_k$ and $\mathcal{H}_{k'}$.

We now consider the behavior of the wave functions near a point of degeneracy k_0. Suppose that at k_0 there are m functions $\psi_{sk_0} = e^{ik_0x} u_{sk_0}(x) (s = 1, 2 \ldots, m)$ with energy $E(k_0)$. Remaining in the neighborhood of k_0, let us move to a point $k = k_0 + \varkappa$. As indicated above, the symmetry of the wave functions at k is determined by the little group G_k, which is generally a subgroup of G_{k_0}. Therefore, as we move away from k_0, the band splits into several branches, i.e., the degeneracy is completely or partially removed. For small vectors $\varkappa$, the symmetry of the wave function and the nature of the band splitting depend only on the direction of $\varkappa$. The amount of band splitting, of course, also depends on the length of $\varkappa$. Therefore, in any small neighborhood of the degeneracy point k_0 the wave functions $\psi_{i,\, k_0+\varkappa}$ corresponding to each of the split-off bands $E_i(k_0 + \varkappa)$ depend essentially on the direction of the vector $\varkappa$ and may differ for arbitrarily small vectors $\varkappa$ in different directions, since as the point k_0 is approached the wave functions $\psi_{i,\, k_0+\varkappa}$ become a combination of degenerate functions ψ_{sk_0}, which depends essentially on the direction of approach to k. Thus, the wave functions corresponding to each of the split-off bands, as functions of k, are discontinuous at k_0. In a nondegenerate band, the wave function is continuous at any point k, since when k_0 is approached in any direction the wave function $\psi_{k_0+\varkappa}$ tends to ψ_{k_0}.

To establish the analytical properties of the functions u_{nk} and the energies $\mathcal{E}_n(k)$, we shall find it convenient to use the equation

$$(\mathcal{E}_n(k) - \mathcal{E}_{n'}(k')) \langle u_{nk} u_{n'k'} \rangle = \frac{\hbar}{m} \sum_\alpha (k_\alpha - k'_\alpha) \pi^\alpha_{nk,\, n'k'}, \tag{17.19}$$

which follows from the identities

$$\langle u_{n\boldsymbol{k}},\ \mathscr{H}_{\boldsymbol{k}'}u_{n'\boldsymbol{k}'}\rangle = \mathscr{E}_{n'}(\boldsymbol{k}')\langle u_{n\boldsymbol{k}}u_{n'\boldsymbol{k}'}\rangle,\quad \langle \mathscr{H}_{\boldsymbol{k}}u_{n\boldsymbol{k}},\ u_{n'\boldsymbol{k}'}\rangle = \mathscr{E}_{n}(\boldsymbol{k})\langle u_{n\boldsymbol{k}}u_{n'\boldsymbol{k}'}\rangle$$

and from the fact that the operator $\mathscr{H}_{\boldsymbol{k}}$ is selfadjoint. In (17.19) $\pi^{\alpha}_{n\boldsymbol{k},\,n'\boldsymbol{k}'}$ is the matrix element of the operator π^{α} evaluated for the periodic functions $u_{n\boldsymbol{k}}$:

$$\pi^{\alpha}_{n\boldsymbol{k},\,n'\boldsymbol{k}'} = \frac{1}{\Omega_0}\int\limits_{\Omega_0} u^{*}_{n\boldsymbol{k}}\,\pi^{\alpha}\,u_{n'\boldsymbol{k}'}\,d\tau_0 = p^{\alpha}_{n\boldsymbol{k},\,n'\boldsymbol{k}'} + \frac{\hbar}{4mc^2}[\sigma\nabla V]^{\alpha}_{n\boldsymbol{k},\,n'\boldsymbol{k}'}. \tag{17.20}$$

As usual, when allowance is made for spin-orbit coupling $u_{n\boldsymbol{k}}$ is a two-component function.

We first consider a band n which is nondegenerate at $\boldsymbol{k}_0$. Setting $n' = n$ in equation (17.19), let $\boldsymbol{k}'$ tend to $\boldsymbol{k}$. Using (17.18) and expanding $\mathscr{E}_n(\boldsymbol{k}')$ in series about $\boldsymbol{k}_0$, we obtain

$$\sum_{\alpha}(k_\alpha - k'_\alpha)\frac{\partial \mathscr{E}_n}{\partial k_\alpha} = \frac{\hbar}{m}\sum_{\alpha}(k_\alpha - k'_\alpha)\,\pi^{\alpha}_{n\boldsymbol{k},\,n\boldsymbol{k}'}.$$

Hence it follows that

$$\frac{\partial \mathscr{E}_n(\boldsymbol{k})}{\partial k_\alpha} = \frac{\hbar}{m}\pi^{\alpha}_{n\boldsymbol{k},\,n\boldsymbol{k}}. \tag{17.21}$$

Since $\pi^{\alpha}_{n\boldsymbol{k},\,n\boldsymbol{k}}$ is a continuous function of $\boldsymbol{k}$, it follows from (17.21) that in the case of a nondegenerate band $\mathscr{E}_n(\boldsymbol{k})$ is a continuously differentiable function of $\boldsymbol{k}$.

We now turn to the case of a band which is degenerate at $\boldsymbol{k}_0$. Consider two branches of the spectrum, i and j, and set $\boldsymbol{k} = \boldsymbol{k}_0 + \boldsymbol{\varkappa}$, $\boldsymbol{k}' = \boldsymbol{k}_0 + \lambda\boldsymbol{\varkappa}$, where λ is an arbitrary number. Then, by (17.19),

$$\mathscr{E}_j(\boldsymbol{k}_0+\boldsymbol{\varkappa}) - \mathscr{E}_i(\boldsymbol{k}_0+\lambda\boldsymbol{\varkappa})\langle u_{i,\,\boldsymbol{k}_0+\boldsymbol{\varkappa}}u_{j\boldsymbol{k}_0+\lambda\boldsymbol{\varkappa}}\rangle = \frac{\hbar}{m}(1-\lambda)\sum_{\alpha}\varkappa_\alpha\pi^{\alpha}_{i,\,\boldsymbol{k}_0+\boldsymbol{\varkappa}\cdot\,j,\,\boldsymbol{k}_0+\lambda\boldsymbol{\varkappa}}. \tag{17.22}$$

Now let $\boldsymbol{\varkappa}\to 0$. Expanding $\mathscr{E}_j(\boldsymbol{k}_0+\boldsymbol{\varkappa})$ and $\mathscr{E}_i(\boldsymbol{k}_0+\lambda\boldsymbol{\varkappa})$ in series in $\boldsymbol{\varkappa}$,

$$\mathscr{E}_j(\boldsymbol{k}_0+\boldsymbol{\varkappa}) = \mathscr{E}_j(\boldsymbol{k}_0) + \sum_{\alpha}\varkappa_\alpha\frac{\partial \mathscr{E}_i}{\partial k_\alpha} + \ldots,$$

$$\mathscr{E}_i(\boldsymbol{k}_0+\lambda\boldsymbol{\varkappa}) = \mathscr{E}_i(\boldsymbol{k}_0) + \lambda\sum_{\alpha}\varkappa_\alpha\frac{\partial \mathscr{E}_i}{\partial k_\alpha} + \ldots,$$

noting that by (17.18)

$$\lim_{\lambda\to 0}\langle u_{i,\,\boldsymbol{k}_0+\lambda\boldsymbol{\varkappa}}\,u_{j,\,\boldsymbol{k}_0+\lambda\boldsymbol{\varkappa}}\rangle = \delta_{ij},$$

and using the equality $\mathscr{E}_i(\boldsymbol{k}_0) = \mathscr{E}_j(\boldsymbol{k}_0)$, we obtain

$$\delta_{ij}\sum_{\alpha}\varkappa_\alpha\frac{\partial \mathscr{E}_i}{\partial k_\alpha}(\boldsymbol{k}_0) = \frac{\hbar}{m}\sum_{\alpha}\varkappa_\alpha\pi^{\alpha}_{i\boldsymbol{k}_0,\,j\boldsymbol{k}_0}(\boldsymbol{\varkappa}), \tag{17.23}$$

i.e., the operator $\sum_{\alpha}\varkappa_\alpha\pi^{\alpha}$, evaluated for the functions $\lim\limits_{\lambda\to 0} u_{i,\,\boldsymbol{k}_0+\lambda\boldsymbol{\varkappa}}$, is diagonal with respect to i and j, and

$$\frac{\partial \mathscr{E}_i(\boldsymbol{k}_0)}{\partial k_\alpha} = \frac{\hbar}{m}\pi^{\alpha}_{i\boldsymbol{k}_0,\,i\boldsymbol{k}_0}. \tag{17.24}$$

Since the matrix elements $\pi^{\alpha}_{i\boldsymbol{k}_0,\,i\boldsymbol{k}_0}$ are evaluated for wave functions which depend on the direction of approach to $\boldsymbol{k}_0$ and therefore have a discontinuity at

this point, it follows that the matrix elements themselves and the derivatives $\frac{\partial \mathscr{E}_l}{\partial k_\alpha}$ also have a discontinuity at k_0.

We now consider the behavior of the function $u_{n,\,k_0+\varkappa}$ near k_0. Expand this function in terms of the complete system of periodic functions u_{mk_0}. Since the expansion coefficients are the scalar products $\langle u_{n,\,k_0+\varkappa} u_{mk_0}\rangle$, we obtain from (17.19)

$$u_{n,\,k_0+\varkappa} = \frac{\hbar}{m}\sum_{\alpha m}\frac{\varkappa_\alpha \pi^\alpha_{mk_0,\,nk_0+\varkappa}}{\mathscr{E}_n(k_0+\varkappa)-\mathscr{E}_m(k_0)}\,u_{mk_0}. \tag{17.25}$$

From (17.25) we obtain the first term of the expansion of $u_{n,\,k_0+\varkappa}$ in series with respect to the small parameter $\varkappa$, for a nondegenerate band:

$$u_{n,\,k_0+\varkappa} = u_{nk_0} + \frac{\hbar}{m}\sum_{m\neq n}\frac{\varkappa_\alpha \pi^\alpha_{mk_0,\,nk_0}}{E_n(k_0)-E_m(k_0)}\,u_{mk_0}, \tag{17.26}$$

since $\mathscr{E}_n(k_0)-\mathscr{E}_m(k_0)=E_n(k_0)-E_m(k_0)$. It follows from (17.26) that for a nondegenerate band the function u_{nk} is differentiable with respect to k:

$$\frac{\partial u_{nk_0}}{\partial k^0_\alpha} = \frac{\hbar}{m}\sum_{m\neq n}\frac{\pi^\alpha_{mk_0,\,nk_0}}{E_n(k_0)-E_m(k_0)}\,u_{mk_0},$$

and thus the matrix element of the operator $\frac{\partial}{\partial k_\alpha}$ is

$$\left\langle u_{mk_0}\frac{\partial}{\partial k^0_\alpha}u_{nk_0}\right\rangle = \frac{\hbar}{m}\frac{\pi^\alpha_{mk_0,\,nk_0}}{E_n(k_0)-E_m(k_0)} \qquad (m\neq n). \tag{17.27}$$

Equation (17.26) now yields the expansion of the matrix elements $\pi^\alpha_{nk_0,\,nk_0+\varkappa}$ in terms of $\varkappa$:

$$\pi^\alpha_{nk_0,\,nk_0+\varkappa} = \pi^\alpha_{nk_0,\,nk_0} + \frac{\hbar}{m}\sum_{\beta,\,m\neq n}\frac{\varkappa_\beta \pi^\alpha_{nk_0,\,mk_0}\pi^\beta_{mk_0,\,nk_0}}{E_n(k_0)-E_m(k_0)}, \tag{17.28}$$

and from (17.21) we obtain further terms of the energy expansion near k_0 for a nondegenerate band:

$$\mathscr{E}_n(k_0+\varkappa) = \mathscr{E}_n(k_0) + \frac{\hbar}{m}\sum_\alpha \varkappa_\alpha \pi^\alpha_{nk_0,\,nk_0} + \frac{\hbar^2}{m^2}\sum_{\alpha\beta}\varkappa_\alpha\varkappa_\beta\sum_{m\neq n}\frac{\pi^\alpha_{nk_0,\,mk_0}\pi^\beta_{mk_0,\,nk_0}}{E_n(k_0)-E_m(k_0)}. \tag{17.29}$$

It follows from (17.29) that

$$\frac{\partial^2 \mathscr{E}_n(k_0)}{\partial k^0_\alpha\,\partial k^0_\beta} = \frac{\hbar^2}{m^2}\sum_{m\neq n}\frac{\pi^\alpha_{nk_0,\,mk_0}\pi^\beta_{mk_0,\,nk_0}}{E_n(k_0)-E_m(k_0)}. \tag{17.30}$$

In a similar manner one obtains further expansions of the wave functions $u_{n,\,k_0+\varkappa}$ and the energy $\mathscr{E}_n(k_0+\varkappa)$ in terms of $\varkappa$ for a nondegenerate band. Hence the wave functions and the energy are analytic functions of k near points at which there are no band degeneracies.

For a degenerate band, we divide the summation over m on the right of (17.25) into two parts: summation over bands j which belong to the given degenerate band, and summation over all other bands m. Then, for small $\varkappa$,

$$u_{l,\,k_0+\varkappa} = u_{lk_0}(\varkappa) + \frac{\hbar}{m}\sum_{m\neq n}\frac{\varkappa_\alpha \pi^\alpha_{mk_0,\,lk_0}(\varkappa)}{E_l(k_0)-E_m(k_0)}\,u_{mk_0}. \tag{17.31}$$

Here

$$u_{ik_0}(\varkappa)=\lim_{\lambda\to 0}u_{i,\,k_0+\lambda\varkappa},\qquad \pi^{\alpha}_{mk_0,\,ik_0}(\varkappa)=\lim_{\lambda\to 0}\pi^{\alpha}_{mk_0,\,ik_0+\lambda\varkappa}. \tag{17.32}$$

This yields a correction to the matrix element $\pi^{\alpha}_{ik_0,\,ik_0+\varkappa}$:

$$\pi^{\alpha}_{ik_0,\,ik_0+\varkappa}=\pi^{\alpha}_{ik_0,\,ik_0}(\varkappa)+\frac{\hbar}{m}\sum_{m\neq n_0,\,\beta}\frac{\varkappa_\beta\pi^{\alpha}_{ik_0,\,mk_0}(\varkappa)\,\pi^{\beta}_{mk_0,\,ik_0}(\varkappa)}{E_i(k_0)-E_m(k_0)}. \tag{17.33}$$

The expansion of the energy near a degeneracy point of $\mathscr{E}_i$ is

$$\mathscr{E}_i(k_0+\varkappa)=\mathscr{E}_i(k_0)+\frac{\hbar}{m}\sum_{\alpha}\varkappa_\alpha\pi^{\alpha}_{ik_0,\,ik_0}(\varkappa)+\frac{\hbar^2}{m^2}\sum_{\alpha\beta}\varkappa_\alpha\varkappa_\beta\sum_{m\neq i}\frac{\pi^{\alpha}_{ik_0,\,mk_0}(\varkappa)\,\pi^{\beta}_{mk_0,\,ik_0}(\varkappa)}{E_i(k_0)-E_m(k_0)}; \tag{17.34}$$

This expansion is formally identical to the formula (17.29) for a nondegener ate band. There is, however, an essential difference between (17.34) and (17.29). In (17.34) all the matrix elements depend on the direction of the vector $\varkappa$, so that they undergo a discontinuity at $\varkappa=0$. The expansion (17.34) for a degenerate band is thus not the usual Taylor series expansion of $\mathscr{E}_i(k_0+\varkappa)$, as in the case of a nondegenerate band. For example, if $\pi^{\alpha}_{ik_0,\,ik_0}(\varkappa)\not\equiv 0$, the second derivative of $\mathscr{E}_i(k)$ does not exist in the case of a degenerate band, since $\frac{\partial\mathscr{E}_i}{\partial k_\alpha}$ has a discontinuity.

If all the matrix elements $\pi^{\alpha}_{ik_0,\,ik_0}(\varkappa)$ vanish identically at the point of degeneracy k_0, it follows from (17.34) that the second derivative $\frac{\partial^2\mathscr{E}_i}{\partial k_\alpha\,\partial k_\beta}$ is discontinuous there, and from (17.19) that the wave functions $u_{ik_0}(\varkappa)$ diagonalize the quadratic form

$$\frac{\hbar^2}{m^2}\sum_{\alpha\beta}\varkappa_\alpha\varkappa_\beta\sum_{m}\frac{\pi^{\alpha}_{ik_0,\,mk_0}(\varkappa)\,\pi^{\beta}_{mk_0,\,jk_0}(\varkappa)}{\mathscr{E}_0(k_0)-\mathscr{E}_m(k_0)}$$

with respect to i and j.

The analytical properties of the electron energy

$$E_n(k)=\frac{\hbar^2k^2}{2m}+\mathscr{E}_n(k)$$

and the Bloch wave functions

$$\psi_{nk}=e^{ikx}u_{nk}$$

evidently coincide with the properties of $\mathscr{E}_n(k)$ and u_{nk}, since $\hbar^2k^2/2m$ and e^{ikx} are analytic functions of the vector k.

Thus, for a nondegenerate band $E_n(k)$ and ψ_{nk} are analytic functions of k, and we have

$$\begin{aligned}&\frac{\partial E_n(k)}{\partial k_\alpha}=\frac{\hbar^2}{m}k_\alpha+\frac{\hbar}{m}\pi^{\alpha}_{nk,\,nk},\\&\frac{\partial^2E_n(k)}{\partial k_\alpha\,\partial k_\beta}=\frac{\hbar^2}{m}\delta_{\alpha\beta}+\frac{\hbar^2}{m^2}\sum_{m\neq n}\frac{\pi^{\alpha}_{nk,\,mk}\pi^{\beta}_{mk,\,nk}+\pi^{\beta}_{nk,\,mk}\pi^{\alpha}_{mk,\,nk}}{E_n(k)-E_m(k)}.\end{aligned} \tag{17.35}$$

The second of equations (17.35) is known as the f-sum rule. In the case of a degenerate band, the first of equations (17.35) is always valid, the second only when $\pi^{\alpha}_{ik,\,ik}$ vanishes.

We now consider the velocity operator $v = \{x\mathcal{H}\} = \pi/m$ of an electron in a periodic field. The velocity operator is diagonal with respect to k and possesses both interband and intraband matrix elements:

$$v^{\alpha}_{n\mathbf{k},\,n'\mathbf{k}'} = \frac{1}{V}\int \psi^{*}_{n\mathbf{k}}\, v^{\alpha}\, \psi_{n'\mathbf{k}'}\, d\tau = \frac{\hbar^2}{m} k_{\alpha}\delta_{nn'}\delta_{\mathbf{k}\mathbf{k}'} + \frac{\hbar}{m}\delta_{\mathbf{k}\mathbf{k}'}\pi^{\alpha}_{n\mathbf{k},\,n'\mathbf{k}'}. \tag{17.36}$$

By (17.36) and (17.35), the diagonal element of the velocity operator is

$$v^{\alpha}_{n\mathbf{k},\,n\mathbf{k}} = \frac{1}{\hbar}\frac{\partial E_n(\mathbf{k})}{\partial k_{\alpha}}. \tag{17.37}$$

§18. TIME REVERSAL

It is clear from (15.1) that when spin-orbit coupling is neglected and no magnetic field* is present, the energy operator is real and the Schrödinger equation

$$\mathcal{H}\psi = i\hbar\frac{\partial\psi}{\partial t} \tag{18.1}$$

is invariant under time reversal: replacing t by $-t$ in (18.1) and taking complex conjugates, we obtain

$$\mathcal{H}\psi^{*} = -i\hbar\frac{\partial\psi^{*}}{\partial t}. \tag{18.2}$$

Equations (18.1) and (18.2) show that the operation of time reversal, usually denoted by K, takes the function ψ into a new function

$$K\psi = \psi^{*}, \tag{18.3}$$

which satisfies the same equation as ψ when $\mathcal{H}$ is real. The time-independent Schrödinger equation is

$$(\mathcal{H} - E)\psi = 0. \tag{18.4}$$

When the Hamiltonian is real, $\mathcal{H}^{*} = K^{-1}\mathcal{H}K = \mathcal{H}$, the eigenfunctions ψ and $K\psi$ correspond to the same energy, for the same reason as do ψ and $g\psi$, where g is an element of the symmetry group $\mathcal{G}$ of the Hamiltonian. The operation of time reversal K may therefore be regarded as a new symmetry element.

It is easy to show that K commutes with any transformation in the space group G. Since ψ and ψ^{*} transform according to complex conjugate representations $\mathcal{D}$ and $\mathcal{D}^{*}$ of this group, it follows that

$$g\psi_i = \sum_j \mathcal{D}_{ji}\psi_j \quad \text{and} \quad g(K\psi_i) = \sum_j \mathcal{D}^{*}_{ji}(K\psi_j). \tag{18.5}$$

* The quantum mechanical equations are invariant under time reversal provided velocities are reversed simultaneously, and therefore provided the directions of the currents and the magnetic field are reversed. Thus the term in $\mathcal{H}$ containing odd powers of the magnetic field $\boldsymbol{H}$ is imaginary, and

$$K^{-1}\mathcal{H}(\boldsymbol{H})K = \mathcal{H}^{*}(\boldsymbol{H}) = \mathcal{H}(-\boldsymbol{H}).$$

The operator K transforms $\psi(\boldsymbol{H})$ into $K\psi(\boldsymbol{H}) = \psi^{*}(-\boldsymbol{H})$ and couples wave functions corresponding to different energies $E(\boldsymbol{H})$ and $E(-\boldsymbol{H})$.

On the other hand,

$$Kg\psi_i = K\left(\sum_l \mathcal{D}_{li}\psi_l\right) = \sum_l \mathcal{D}^*_{li}\psi^*_l,$$

i.e.,

$$Kg = gK. \tag{18.6}$$

The eigenfunctions ψ and $K\psi$, which satisfy the same equation (18.4) and correspond to the same energy, may be either linearly independent, in which case one has two independent systems of orthonormal functions ψ and $K\psi$ for the same eigenvalue E, or linearly dependent on each other via a unitary matrix T:

$$K\psi_i = \sum_l T_{li}\psi_l. \tag{18.7}$$

In the latter case the representations $\mathcal{D}$ and $\mathcal{D}^*$ are obviously equivalent.

If ψ and $K\psi$ are linearly independent, they may transform according to either equivalent or inequivalent representations.

Thus, three cases should be distinguished*:

a) the functions ψ and $K\psi$ are linearly dependent;

b) the functions ψ and $K\psi$ are linearly independent and transform according to inequivalent representations $\mathcal{D}$ and $\mathcal{D}^*$, i.e., $\chi(g) \neq \chi^*(g)$;

c) the functions ψ and $K\psi$ are linearly independent and transform according to equivalent representations $\mathcal{D}$ and $\mathcal{D}^*$, i.e., $\chi(g) = \chi^*(g)$.

Since linearly independent functions ψ and $K\psi$ correspond to the same energy, it follows that in cases (b) and (c) invariance under time reversal causes additional degeneracy, and in these cases the representations $\mathcal{D}$ and $\mathcal{D}^*$ according to which the functions transform must be combined. Specifically, in case (b) complex conjugate inequivalent representations are combined, and in case (c) equivalent representations. Therefore, it is of practical importance to be able to distinguish these three cases, i.e., to determine when invariance under time reversal imposes additional requirements on the wave functions, due to the linear dependence of the functions ψ and $K\psi$, and when it results in additional degeneracy.

In order to answer this question we study the properties of complex conjugate representations in greater detail. In cases (a) and (c) the representations $\mathcal{D}$ and $\mathcal{D}^*$ are equivalent, i.e., their characters are real and coincide, so that there is a unitary matrix T which transforms all the matrices $\mathcal{D}(g)$ into $\mathcal{D}^*(g)$:

$$\mathcal{D}^*(g) = T^{-1}\mathcal{D}(g)T. \tag{18.8}$$

We stress that the existence of a matrix T with this property does not guarantee a linear relation of type (18.7), but if there is such a relation the matrices T in (18.7) and (18.8) coincide.

Let us consider the properties of the matrix T. Take complex conjugates on the right and left of equation (18.8):

$$\mathcal{D}(g) = T^{*-1}\mathcal{D}^*(g)T^*. \tag{18.9}$$

* This classification of representations, which is the most convenient for physical applications, differs somewhat from that customary in courses on group theory, where real representations are assigned to case (a), complex inequivalent and equivalent representations to cases (b) and (c). The two classifications agree for vector (usual) representations, but cases (a) and (c) must be interchanged for spinor representations.

Substitute $\mathcal{D}^*(g)$, as given by (18.8), into (18.9):

$$\mathcal{D}(g) = (TT^*)^{-1}\mathcal{D}(g)(TT^*). \tag{18.10}$$

Equation (18.10) means that the matrix TT^* commutes with all the matrices $\mathcal{D}(g)$ of the irreducible representation under consideration. Therefore, by Schur's first lemma (8.1a) it must be a multiple of the identity matrix, $TT^* = cI$ or $T = cT^{*-1} = c\tilde{T}$. Taking transposes on both sides of this equation, we obtain $\tilde{T} = cT = c^2\tilde{T}$. Hence $c = \pm 1$, and so there are two possible cases:

$$T = \tilde{T}, \text{ i.e., } TT^* = I, \text{ or } T = -\tilde{T}, \text{ i.e., } TT^* = -I. \tag{18.11}$$

For real matrices, $\mathcal{D}^* = \mathcal{D}$, the matrix T in equation (18.8) is obviously I and we have the first case: $T = \tilde{T}$. Now a unitary transformation of the matrix $\mathcal{D}$, taking $\mathcal{D}$ into $S\mathcal{D}S^{-1}$, takes the matrix T into $T' = STS$; thus the property (18.11) of the matrix T is preserved: $T'T'^* = TT^*$. Hence, for any representation $\mathcal{D}$ that can be made real, the matrix T must satisfy the condition $\tilde{T} = T$.

Consequently, if $\tilde{T} = -T$, the representation is essentially complex and cannot be made real.

We claim that $\tilde{T} = T$ is not only a necessary condition for the representation $\mathcal{D}$ to be real, but also sufficient, i.e., if $\tilde{T} = T$ there always exists a matrix B which transforms the representation $\mathcal{D}$ into a real form:

$$\mathcal{D}'^* = (B^{-1}\mathcal{D}B)^* = B^{-1}\mathcal{D}B = \mathcal{D}'. \tag{18.12}$$

To prove this, we first diagonalize the matrix T by a unitary transformation u: $\tau = u^{-1}Tu$, where $\tau_{ll} = e^{i\alpha_{ll}}$. This is always possible, since the matrix T is unitary. Taking transposes in the equation

$$Tu = u\tau \tag{18.13}$$

we get

$$\tilde{u}\tilde{T} = \tilde{\tau}\tilde{u}.$$

Since τ, as a diagonal matrix, is symmetric ($\tilde{\tau} = \tau$), $\tilde{T} = T$ and $\tilde{u} = u^{*-1}$, it follows that

$$Tu^* = u^*\tau. \tag{18.14}$$

The n-tuple u_{lk} $(l = 1, 2, \ldots, n)$, where n is the dimension of the matrix T, is called the k-th eigenvector of the matrix T belonging to the eigenvalue τ_k, i.e., to the k-th root of the determinant $|T - \tau| = 0$; it is denoted by u_k. Since by (18.13) an eigenvector is a solution of the system of homogeneous equations $\sum_l (T_{il} - \tau_k\delta_{il})u_{lk} = 0$, it is determined up to a constant factor c_k. In order that the matrix u remain unitary, it is necessary that $c_kc_k^* = 1$, so that $c_k = e^{i\varphi_k}$. This means that the matrices u and u^* in (18.13) and in (18.14) differ at most by a diagonal matrix c, $c_{kk'} = e^{i\varphi_k}\delta_{kk'}$; in other words, $u^* = uc$, whence

$$(uc^{1/2})^* = uc^{1/2}, \tag{18.15}$$

where $c^{1/2}$ is the matrix with elements $c_{kk'}^{1/2} = e^{i\varphi_k/2}\delta_{kk'}$. Replacing u in (18.13) by $uc^{1/2}$, we see from (18.15) that the matrix u in (18.13) may be assumed real and unitary. A matrix satisfying the condition $u^{-1} = \tilde{u}$ is said to be

orthogonal. Define a matrix $\boldsymbol{B}$ by

$$\boldsymbol{B} = u\theta u^{-1}, \tag{18.16}$$

where $\theta^2 = \tau$, i.e., θ is the diagonal matrix with elements $\theta_{ll} = \tau_{ll}^{1/2} = e^{i\alpha_{ll}/2}$. By (18.13), this matrix satisfies the following relations:

$$\boldsymbol{B}^2 = u\tau u^{-1} = \boldsymbol{T}, \quad \tilde{\boldsymbol{B}} = \tilde{u}^{-1}\tilde{\theta}\tilde{u} = u\theta u^{-1} = \boldsymbol{B}. \tag{18.17}$$

We claim that the matrix $\boldsymbol{B}$ with properties (18.17) satisfies equations (18.12), i.e., transforms $\mathcal{D}$ into real form. By (18.8) and (18.17),

$$\mathcal{D}'^{*} = (\boldsymbol{B}^{-1}\mathcal{D}\boldsymbol{B})^{*} = \boldsymbol{B}\mathcal{D}^{*}\boldsymbol{B}^{-1} = \boldsymbol{B}\boldsymbol{T}^{-1}\mathcal{D}\boldsymbol{T}\boldsymbol{B}^{-1} = \boldsymbol{B}^{-1}\mathcal{D}\boldsymbol{B} = \mathcal{D}'.$$

Thus, the condition $\boldsymbol{T}\boldsymbol{T}^{*} = \boldsymbol{I}$ is a criterion for real representations. We recall here (see §9) that real representations are representations all of whose matrices can be reduced to real form, regardless of whether the reduction is actually performed.

We now consider how the conditions imposed on the matrix $\boldsymbol{T}$ in (18.8) link up with the properties of the functions ψ and $K\psi$. We first assume that there is a relation (18.7) between the functions ψ and $K\psi$, i.e., case (a) holds. Applying the operation K to (18.7), we obtain

$$K^2\psi_i = \sum_j T_{ji}^{*} K\psi_j = \sum_{jl} T_{ji}^{*} T_{li}\psi_l = \sum_l (TT^{*})_{il}\psi_l. \tag{18.18}$$

Since $K^2\psi = K\psi^{*} = \psi$, i.e.,

$$K^2 = 1, \tag{18.19}$$

it follows that necessarily $\boldsymbol{T}\boldsymbol{T}^{*} = \boldsymbol{I}$, so that the functions transform according to a real representation $\mathcal{D}$.

Condition (18.19) is valid, however, only for vector representations, i.e. without allowance for electron spin.

As noted in §16, the Schrödinger-Pauli equation, as opposed to equation (18.1), includes a complex term which describes spin-orbit coupling:

$$\mathcal{H}_{so} = -\frac{i\hbar^2}{4m^2c^2}(\sigma[\nabla V\nabla]). \tag{18.20}$$

Thus the substitution $t \to -t$ and the transition to the complex conjugate equation transform $\mathcal{H}_{so}$ into $\mathcal{H}_{so}^{*}$, corresponding to the substitution $\sigma_i \to -\sigma_i^{*}$ Thus

$$\mathcal{H}^{*}(\sigma_i) = \mathcal{H}(-\sigma_i^{*}).$$

However, instead of the functions ψ^{*}, which are solutions of the equation $(\mathcal{H}^{*} - E)\psi^{*} = 0$, we can consider functions $\boldsymbol{S}\psi$, where $\boldsymbol{S}$ is a unitary operator which acts on the spin matrices, so chosen that in the new representation

$$\boldsymbol{S}^{-1}\mathcal{H}^{*}(\sigma_i)\boldsymbol{S} = \boldsymbol{S}^{-1}\mathcal{H}(-\sigma_i^{*})\boldsymbol{S} = \mathcal{H}(\sigma_i). \tag{18.21}$$

It is evident from (18.20) that, since $\sigma_x^{*} = \sigma_x$, $\sigma_y^{*} = -\sigma_y$, $\sigma_z^{*} = \sigma_z$, condition (18.21) implies that

$$\boldsymbol{S}^{-1}\sigma_x\boldsymbol{S} = -\sigma_x, \quad \boldsymbol{S}^{-1}\sigma_y\boldsymbol{S} = \sigma_y, \quad \boldsymbol{S}^{-1}\sigma_z\boldsymbol{S} = -\sigma_z. \tag{18.22}$$

Using the relations

$$\sigma_i\sigma_k = i\sigma_l\delta_{ikl},$$

where δ_{ikl} is the unit antisymmetric tensor, one shows easily that the unitary matrix S satisfying (18.22), coincides with σ_y up to an arbitrary phase factor. This phase factor can be assumed equal to unity, taking

$$S = S^{-1} = \sigma_y.$$

Consequently, the function $\sigma_y\psi^* = \sigma_y K_0\psi$, where K_0 is the operation of complex conjugation, satisfies the same equation as the function ψ. This function

$$\sigma_y \begin{Vmatrix} \psi_1^* \\ \psi_2^* \end{Vmatrix} = \begin{Vmatrix} -i\psi_2^* \\ i\psi_1^* \end{Vmatrix}$$

will be interpreted as the image of the function $\psi = \begin{Vmatrix} \psi_1 \\ \psi_2 \end{Vmatrix}$ under the time reversal operator K. Thus the form of the time reversal operator for spin functions is

$$K\psi = \sigma_y K_0\psi = \sigma_y\psi^*. \tag{18.23}$$

We now show that the operator K defined by (18.23) commutes with all the elements of the space group, i.e., satisfies condition (18.6). By (16.3) and (18.23),

$$gK\psi(x) = g\sigma_y\psi^*(x) = \mathcal{D}_{1/2}(g)\,\sigma_y\psi^*(g^{-1}x),$$

and

$$Kg\psi(x) = \sigma_y(\mathcal{D}_{1/2}(g)\,\psi(g^{-1}x))^* = \sigma_y\mathcal{D}^*_{1/2}(g)\,\psi^*(g^{-1}x),$$

where $\mathcal{D}^{1/2}(g)$ is the matrix according to which the spinors with spin 1/2 transform under g. By (16.2), the general form of this matrix is

$$\mathcal{D}_{1/2}(g) = \begin{Vmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{Vmatrix}.$$

It is easy to show that $\sigma_y D^*_{1/2}(g) = D_{1/2}(g)\,\sigma_y$, and so the commutation relation (18.6) is indeed fulfilled. It follows from the commutation condition that the spinor functions ψ and $K\psi$ transform according to complex conjugate representations. Indeed, if

$$g\psi_l = \sum_l \mathcal{D}_{ll}\psi_l,$$

then by (18.6)

$$gK\psi_l = Kg\psi_l = \sigma_y K_0 \sum_l \mathcal{D}_{ll}\psi_l = \sum_l \mathcal{D}^*_{ll}\sigma_y\psi_l^* = \sum_l \mathcal{D}^*_{ll}(K\psi)_l.$$

The previously cited cases (a), (b), (c) may also hold for spinor functions. In cases (a) and (c), when $\mathcal{D}$ and $\mathcal{D}^*$ are equivalent, there exists a matrix T which takes $\mathcal{D}$ into $\mathcal{D}^*$ and satisfies equations (18.8) – (18.11) and (18.18).

For spinor functions, however,

$$K^2\psi = \sigma_y K_0\sigma_y K_0\psi = \sigma_y\sigma_y^*\psi = -\psi,$$

so that, as opposed to (18.19),

$$K^2 = -1. \tag{18.24}$$

Consequently, in case (a), when there is a linear relation (18.7) between the

functions ψ and $K\psi$, the matrix T satisfies the condition

$$TT^* = K^2 I = -I,$$

i.e., the representation $\mathcal{D}$ according to which the functions ψ transform is essentially complex, and equivalent to the representation $\mathcal{D}^*$ according to which the functions $K\psi$ transform.

We have thus shown that the condition

$$TT^* = K^2 I \quad \text{or} \quad \tilde{T} = K^2 T, \text{ where } K^2 = \begin{cases} +1 \text{ for vector representations,} \\ -1 \text{ for spinor representations,} \end{cases} \tag{18.25}$$

follows necessarily from the linear dependence of ψ and $K\psi$.

We will now show that this condition is also sufficient: if $TT^* = K^2 I$, the functions ψ and $K\psi$ must be linearly dependent, except in the case of accidental degeneracy, i.e., accidental coincidence of the energies of two inequivalent representations.

Define functions

$$\psi_{i+} = \psi_i + \Theta_i, \text{ where } \Theta = TK\psi,$$

and T is the matrix defined by (18.8). Under all operation of the space group, the functions ψ_+ transform into one another, for by (18.8) $T\mathcal{D}^* = \mathcal{D}T$, and

$$\mathcal{D}\psi_+ = \mathcal{D}\psi + TK\mathcal{D}\psi = \mathcal{D}\psi + T\mathcal{D}^* K\psi = \mathcal{D}\psi_+.$$

Time reversal also transforms these functions into one another, since by (18.25)

$$K\psi_+ = K\psi + KTK\psi = T^{-1}\Theta + T^{-1}K^4\psi = T^{-1}\psi_+.$$

It is easy to see that a similar relation holds for the functions $\psi_{i-} = \psi_i - \Theta_i$

Thus, if $TT^* = K^2 I$, we can form two systems of functions ψ_+ and ψ_-, which transform independently into one another under the operations of the space group and under time reversal. If these functions are independent, accidental degeneracy occurs. But if no such degeneracy occurs, then either the functions ψ_- are linearly dependent on ψ_+, or some of them vanish identically. In either case, ψ and $K\psi$ must be linearly dependent.

Thus condition (18.25) is necessary and sufficient for case (a) to occur. Consequently, in the alternative case (c), when the functions ψ and $K\psi$ transform according to equivalent representations but are linearly independent, i.e., when time reversal causes additional degeneracy, the second condition in (18.11) must hold. Thus,

$$\begin{aligned} &\text{in case (a):} && \tilde{T} = K^2 T \quad \text{i.e.,} \quad TT^* = K^2 I; \\ &\text{in case (c):} && \tilde{T} = -K^2 T \quad \text{i.e.,} \quad TT^* = -K^2 I. \end{aligned} \tag{18.26}$$

Frobenius and Schur showed that the properties of the matrix are sufficient to determine whether the representation is real or complex, provided only that its characters are known: if the sum of characters of the squares of the group elements is equal to the order h of the group, then $T = \tilde{T}$ and the representation is real; if this sum is $-h$, then $T = -\tilde{T}$ and the representation is equivalent to its conjugate; and if the sum vanishes the representations $\mathcal{D}$ and $\mathcal{D}^*$ are complex and inequivalent.

Since we are interested in the possibility of distinguishing cases (b) and (c), in which time reversal causes additional degeneracy, from case (a), when there is no such degeneracy, we write the criterion as follows:

$$\Sigma=\frac{1}{h}\sum_{g\in\mathcal{J}}\chi(g^2)=\begin{cases}K^2- & \text{case (a)}\\ 0- & \text{case (b)}\\ -K^2- & \text{case (c)}\end{cases} \tag{18.27}$$

Let us prove this theorem.

For case (b), equation (18.27) follows directly from the orthogonality relation (8.10). By (8.15),

$$\Sigma=\frac{1}{h}\sum_{g}\chi_\mu(g^2)=\frac{1}{h}\sum_{gl}\mathcal{D}^\mu_{ll}(g^2)=\frac{1}{h}\sum_{glk}\mathcal{D}^\mu_{lk}(g)\,\mathcal{D}^\mu_{kl}(g). \tag{18.28}$$

For complex inequivalent representations, $\mathcal{D}^\mu_{kl}(g)=\mathcal{D}^{\lambda*}_{kl}(g)$, and since $\mu\neq\lambda$ it follows from (8.10) that this sum vanishes.

In cases (a) and (c), when the representations $\mathcal{D}$ and $\mathcal{D}^*$ are equivalent, we will express $\mathcal{D}^\mu_{kl}$ in (18.28) in terms of $\mathcal{D}^{\mu*}_{k'l'}$ according to (18.8). Then, using the orthogonality relation (8.10), we obtain

$$\Sigma=\frac{1}{h}\sum_{g}\sum_{iklm}\mathcal{D}^\mu_{ik}(g)\,T_{kl}\mathcal{D}^\mu_{lm}T^{-1}_{mi}=\frac{1}{h}\sum_{iklm}T_{kl}T^{-1}_{mi}\sum_{g}\mathcal{D}^\mu_{ik}(g)\,\mathcal{D}^{\mu*}_{lm}(g)=$$
$$=\frac{1}{n_\mu}\sum_{iklm}T_{kl}T^{-1}_{mi}\delta_{li}\delta_{km}=\frac{1}{n_\mu}\sum_{ik}T_{kl}T^{-1}_{kl}=\frac{1}{n_\mu}\sum_{i}(\boldsymbol{T}^*\boldsymbol{T})_{ii}.$$

By (18.26), this sum is K^2 in case (a) and $-K^2$ in case (c).

Equation (18.27) is directly applicable to point groups and finite groups in general. It is easy to prove that for the usual representations of the point groups all representations with real characters are real, i.e., belong to case (a), and all representations with complex characters belong to case (b) and consequently must be combined in pairs.

For spinor representations of these groups, one must again combine representations with complex characters, and the one-dimensional representations must also be doubled. Indeed, when $\tilde{\boldsymbol{T}}=-\boldsymbol{T}$,

$$\operatorname{Det}\boldsymbol{T}=\operatorname{Det}\tilde{\boldsymbol{T}}=\operatorname{Det}(-\boldsymbol{T})=(-1)^{n_\mu}\operatorname{Det}\boldsymbol{T}.$$

Consequently, in case (a) spinor representations must have even dimension n_μ, and therefore one-dimensional representations with real characters always belong to case (c). All other spinor representations with real characters belong to case (a).

For space groups, however, if the star includes more than one point these simple laws are not applicable, since usually only representations of the little group are available and these representations may have complex characters even if the complete representation of the space group is real. Therefore, we first transform our criterion (18.27) for space groups. The elements of a space group can be expressed as products of the fundamental elements of the group $g'=(r|\tau)$, which include only nonprimitive translations, and the elements of the translation group $(e|t)$. The latter group may be made finite formally by introducing the usual cyclic Born-von Kármán boundary conditions.

Since $(r|\tau+t)^2=(r^2|\tau+r\tau+t+rt)$, it follows by (12.27) that

$$\chi[(r|\tau+t)^2]=\sum_i\chi_{k_i}(g^2)\,e^{-it_i(t+g\tau)}=\sum_i\chi_{k_i}(g^2)\,e^{-it(k_i+g^{-1}k_i)},\quad g\in G', \tag{18.29}$$

where the summation is carried out over all points k_i of the star $\{k\}$. Therefore, upon summation over t in (18.27) only the terms with $k_i + gk_i = 0$ remain, the number of identical terms being equal to the order of the translation group, i.e., the order h of the space group divided by the number h' of fundamental elements (elements not containing primitive translations t). Thus the summation in (18.27) can be performed only over the basic elements g', with h replaced by h':

$$\Sigma = \frac{1}{h}\sum_{g\in G}\chi(g^2) = \frac{1}{h'}\sum_{g\in G'}\sum_{i}\chi_{k_i}(g^2)\,\delta_{k_i,\,-gk_i}. \tag{18.30}$$

Here, as usual, vectors differing by a reciprocal lattice vector b are treated as equal, i.e., $k_i + gk_i$ may be zero or b.

Using the fact that, by (12.24),

$$\chi_{k_i}(g^2) = \chi_{g_i k}(g^2) = \chi_k(g_i^{-1}g^2 g_i),$$

where g_i is a fixed operation mapping $k = k_1$ into k_i, we can rewrite the sum (18.30) in the form

$$\Sigma = \frac{1}{h'}\sum_{g\in G'}\sum_{i}\chi_k(g_i^{-1}g^2 g_i)\,\delta_{g_i k,\,-gg_i k} = \frac{1}{h'}\sum_{i}\sum_{g\in G'}\chi_k\left[(g_i^{-1}gg_i)^2\right]\delta_{k,\,-g_i^{-1}gg_i k}. \tag{18.31}$$

When the element g in this sum extends over all values from e to $g_{h'}$, the element $g' = g_i^{-1}gg_i$ extends in a different order over values either coinciding with g or differing from it by an integer translation. The phase factors associated with these translations for elements g such that $k + gk = 0$ all become unity. Thus the sums over g in (18.31) are independent of i and summation over i is simply multiplication by the number f of points of the star Consequently, for space groups the criterion (18.27) becomes

$$\Sigma = \frac{f}{h'}\sum_{g\in G'_k}\chi_k(g^2)\,\delta_{k,\,-gk} = \begin{cases} K^2 - \text{ case (a)} \\ 0 - \text{ case (b)} \\ -K^2 - \text{ case (c)} \end{cases} \tag{18.32}$$

Here h'/f is the number of fundamental elements of the little group G_k, i.e., elements which do not contain primitive translations The criterion (18.32) was first introduced by Herring /13.2/. The summation in (18.32) is performed over the fundamental elements $g^2 \in G'_k$ of the little group such that

$$gk = -k. \tag{18.33}$$

For spinor representations the summation in (18.27) or (18.32) must obviously be performed over all the fundamental elements of the double group, i e., the group containing the elements g^2 and $(gQ)^2$. However, since $(gQ)^2 = g^2Q^2 = g^2$, it is actually sufficient to sum only over the elements of the usual group. Of course, the characters for these elements must be taken from tables of the appropriate spinor representations of the group.*

Note that for points not on the edge of the Brillouin zone the value of the sum (18.32) is independent of whether there are nonprimitive translations in the element g, and one can substitute for $\chi(g^2)$ the values of the character

* If tables of projective representations are used, one must bear in mind that the element $g^2 = (r^2|r\tau + \tau)$ may contain a primitive translation t, and also the element Q. Accordingly, its character will differ from the character of the element $(r^2|\tau_{r^2})$ in the projective representation by the phase factor $\exp(-ikt)$ and, if r^2 includes Q, by the additional factor -1.

$\chi(r^2)$ for the crystallographic point group corresponding to G_k. Indeed, since the summation in (18.32) is performed only over elements $g=(r|\tau)$ which satisfy condition (18.33), it follows that for points within the zone

$$\chi(g^2)=\chi(r^2)\exp[-ik(r\tau+\tau)]=\chi(r^2)\exp[-i\tau(r^{-1}k+k)]=\chi(r^2).$$

Let us consider the consequences of the presence or absence of a linear relation between the functions ψ and $K\psi$ for space groups.

As indicated previously, in cases (b) and (c), when the functions ψ and $K\psi$ are linearly independent, the representations $\mathcal{D}$ and $\mathcal{D}^*$ according to which these functions transform are combined. For space groups, however, the functions $\psi=u_k e^{ikx}$ and $K\psi=(Ku_k)e^{-ikx}$ generally belong to different points of the stars $\{k\}$ and $\{-k\}$, and time reversal takes the star $\{k\}$ into the star $\{-k\}$. Thus the relation between these stars plays an essential role in combination of the representations, and for each of the previously cited cases three possibilities should be distinguished:

1) the points k and $-k$ are equivalent, i.e., $k=-k$;

2) k is not equivalent to $-k$, but the space group contains an element R which maps k onto $-k$:

$$Rk=-k;$$

3) the points k and $-k$ are in different stars.

In the last case there is no group element mapping k onto $-k$, and consequently the sum (18.32) vanishes; thus the representations $\mathcal{D}$ and $\mathcal{D}^*$ are complex and inequivalent, i.e., only case (b) is possible. Combination of these representations reduces to union of the stars $\{k\}$ and $\{-k\}$; time reversal thus implies that the energies at the points k and $-k$ are equal:

$$E(k)=E(-k). \tag{18.34}$$

Of course, condition (18.34) is also valid in all other cases, but then it is due to spatial symmetry. Thus, in case (b_3) combination of representations of the full space group does not imply combination of the representations of the little groups.

In case (a_1), the linear relation between the functions ψ and $K\psi$ implies a linear relation between the functions ψ_k and $K\psi_k$ belonging to one point of the star.

In case (a_2) we again have a linear relation, but now between the functions ψ_k and $KR\psi_k$, which also belong to one point of the star.

In the other cases (b_1), (b_2), (c_1) and (c_2), combination of the representations of the space group results in combination of the representations of the little groups, i.e., additional band degeneracy at the corresponding points of k-space.* In case (b_1) conjugate representations $\mathcal{D}^k$ and $\mathcal{D}^{*k}$, i.e., representations with conjugate characters, are combined, and in cases (c_1) and (c_2) – equivalent representations, i.e., representations with equal characters.

* Thus, it follows immediately from Herring's criterion that in crystals with an inversion center all terms at an arbitrary point of the Brillouin zone are at least doubly degenerate when allowance is made for spin. Indeed, if the little group G_k contains only the identity element, then the only element taking k into $-k$ is inversion, since if there were another element g with this property the group G_k would contain the element $gi\neq e$. Therefore, $\Sigma=\chi(i|\tau)^2=\chi(e|\tau+i\tau)=\chi(e|0)=1$. Consequently, we see from (18.32) that the spinor representations in this case belong to case (c), i.e. they are complex and combine in pairs.

The situation is more complicated in case (b_2), when the basis of the representations $\mathscr{D}^{\boldsymbol{k}}_{\mu}$ and $\mathscr{D}^{\boldsymbol{k}}_{\lambda}$ being combined comprises the functions ψ^{μ}_{l} and $\psi^{\lambda}_{l} = KR\psi^{\mu}_{l}$, where R is the operation which takes $\boldsymbol{k}$ into $-\boldsymbol{k}$, and therefore the representation μ of the little group is the complex conjugate not of the representation $\mathscr{D}^{\boldsymbol{k}}_{\lambda}$ but of the representation $\mathscr{D}^{-\boldsymbol{k}}_{\lambda}$ belonging to the point $-\boldsymbol{k}$, whose basis consists of the functions $\psi^{\lambda}_{l,-\boldsymbol{k}} = R\psi^{\lambda}_{l\boldsymbol{k}}$. In this case, by (12 24),

$$\mathscr{D}^{-\boldsymbol{k}}_{\lambda ll}(g) = \mathscr{D}^{\boldsymbol{k}}_{\lambda ll}(R^{-1}gR)$$

and

$$\mathscr{D}^{\boldsymbol{k}}_{\mu ll}(g) = \mathscr{D}^{\boldsymbol{k}*}_{\lambda ll}(R^{-1}gR),$$

whence

$$\chi^{\boldsymbol{k}}_{\mu}(g) = \chi^{\boldsymbol{k}*}_{\lambda}(R^{-1}gR). \tag{18.35}$$

Equation (18.35) defines the characters of the representation $\mathscr{D}^{\boldsymbol{k}}_{\mu}$ to be combined with $\mathscr{D}^{\boldsymbol{k}}_{\lambda}$. Since R is not an element of the little group $G_{\boldsymbol{k}}$, the elements g and $R^{-1}gR$ may be in different classes, and therefore the characters of the representations $\mathscr{D}^{\boldsymbol{k}}_{\mu}$ and $\mathscr{D}^{\boldsymbol{k}}_{\lambda}$ are not necessarily conjugates. If one of the elements $R = (\rho|\tau)$ is an element $R' = (\rho'|\tau')$ such that ρ' commutes with all elements r of the point group corresponding to elements $g = (r|\tau)$ of the little group, i. e.,

$$R'^{-1}gR' = (r|\tau + \boldsymbol{t}'), \tag{18.36}$$

where $\boldsymbol{t}' = \rho'^{-1}\tau - \tau + r\rho'^{-1}\tau' - \rho'^{-1}\tau'$ is a primitive translation, then it is convenient to choose this R' as the element R in (18.35). Then, by (18.35) and (18.36),

$$\chi^{\boldsymbol{k}}_{\mu}(g) = \chi^{\boldsymbol{k}*}_{\lambda}(g)\, e^{-i\boldsymbol{k}\boldsymbol{t}'}. \tag{18.37}$$

For example, if the point group contains inversion, which commutes with every element of the point group, the choice of $R = (i|\tau_i)$ gives $\boldsymbol{t}' = \tau_i - r\tau_i - 2\tau$.

Equations (18.35) and (18.37) are obviously also valid in cases (a_2) and (c_2), when the representations $\mathscr{D}^{\boldsymbol{k}}_{\lambda}$ and $\mathscr{D}^{\boldsymbol{k}}_{\mu}$ are equivalent, i. e., their characters are equal. By virtue of equation (18.35), these characters must satisfy the condition

$$\chi^{\boldsymbol{k}}_{\lambda}(g) = \chi^{\boldsymbol{k}*}_{\lambda}(R^{-1}gR), \tag{18.38}$$

from which it is evident that in cases (a_2) and (c_2) it is not only the characters of the full representation of the space group, which are sums of the characters of the representations for all star points, that are real, but also the sums of pairs of characters of representations of the little groups at opposite points $\boldsymbol{k}$ and $-\boldsymbol{k}$, which are, by (18.37) and (12.24),

$$\chi^{\boldsymbol{k}}_{\lambda}(g) + \chi^{-\boldsymbol{k}}_{\lambda}(g) = \chi^{\boldsymbol{k}}_{\lambda}(g) + \chi^{\boldsymbol{k}}_{\lambda}(R^{-1}gR) = 2\,\mathrm{Re}\,\chi^{\boldsymbol{k}}_{\lambda}(g).$$

Of course, the characters of the little group representations themselves may at the same time be complex. In cases (a_1) and (c_1), when the points $\boldsymbol{k}$ and $-\boldsymbol{k}$ are equivalent and $R = (e|0)$, it follows from (18.37) that these characters are always real.

We note, in conclusion, that time reversal cannot be incorporated in one group together with the symmetry operations, in the usual manner. This results from the fact that the operator K is antilinear and anti-unitary.

Indeed, for linear and unitary operators, such as spatial symmetry operators, the following relations hold when $a = \text{const}$:

$$\mathcal{D}(a\psi) = a\mathcal{D}\psi \tag{18.39}$$

and

$$\langle \mathcal{D}\psi_1 \mid \mathcal{D}\psi_2 \rangle = \langle \psi_1 \mathcal{D}^+ \mathcal{D}\psi_2 \rangle = \langle \psi_1 \psi_2 \rangle, \tag{18.40}$$

where $\langle \psi_1 \psi_2 \rangle = \int \psi_1^* \psi_2 \, d\tau$ is the integral over the configuration space. For the operator K, defined by equations (18.3) or (18.23), these relations look different:

$$K(a\psi) = a^* K\psi \tag{18.41}$$

and

$$\langle K\psi_1 \mid K\psi_2 \rangle = \langle K_0\psi_1 \mid K_0\psi_2 \rangle = \langle \psi_1 \psi_2 \rangle^*. \tag{18.42}$$

For spin functions, when K is defined by (18.23), the last equation is a consequence of the unitarity of the transformation σ_y.

We now consider the additional conditions that invariance under time reversal imposes on the matrix elements of the operator V:

$$\langle \psi_1 V \psi_2 \rangle = \int \psi_1^* V \psi_2 \, d\tau.$$

By (18.42),

$$\langle \psi_1 V \psi_2 \rangle^* = \langle K\psi_1, KV\psi_2 \rangle = \langle K\psi_1, KVK^{-1}K\psi_2 \rangle.$$

On the other hand,

$$\langle \psi_1 V \psi_2 \rangle^* = \langle \psi_2 V^+ \psi_1 \rangle.$$

Therefore,

$$\langle \psi_1 V \psi_2 \rangle = \langle K\psi_1, KVK^{-1}K\psi_2 \rangle^* = \langle K\psi_2, KV^+K^{-1}K\psi_1 \rangle. \tag{18.43}$$

We have used the equality $(KVK^{-1})^+ = KV^+K^{-1}$.

Let us treat the operation $\Theta V = KV^+K^{-1}$ as the result of time reversal acting on the operator. Since $\Theta^2 V = V$, any operator V may be split into two operators:

$$V = V_+ + V_-, \text{ where } V_+ = \tfrac{1}{2}(V + \Theta V) \text{ and } V_- = \tfrac{1}{2}(V - \Theta V).$$

With this notation, we have

$$\Theta V_\pm = KV_\pm^+ K^{-1} = fV_\pm, \text{ where } f = \begin{cases} +1 \text{ for } V_+, \\ -1 \text{ for } V_-. \end{cases} \tag{18.44}$$

Accordingly, the operator V_+ will be called even and V_- odd with respect to time reversal. This nomenclature is motivated by the fact that for even operators the mean value $\bar{V}(t) = \langle \psi V \psi \rangle$ is invariant under the substitution $t \to -t$ (i.e., $\psi \to K\psi$), whereas for odd operators this substitution changes the sign of the mean value.

Indeed, by (18.43) and (18.44),

$$K\bar{V} \equiv \langle K\psi VK\psi \rangle = \langle K^2\psi KV^+K^{-1}K^2\psi \rangle = f\langle \psi V\psi \rangle = f\bar{V}. \tag{18.45}$$

Thus operators of magnitudes which do not change sign upon time reversal, such as coordinates and energy, are even, while operators of quantities which change sign when t is replaced by $-t$, such as velocity, momentum and current, are odd. Note that operators V for which $\overline{V}$ is real are hermitian, i.e., $V^+ = V$, and if these operators do not act on the spin variables then $KV^+K^{-1} = KVK^{-1} = V^*$.

Thus, it follows from (18.43) and (18.44) that for even or odd operators invariance under time reversal imposes an additional condition on the matrix elements:

$$\langle \psi_i V \psi_j \rangle = f \langle K\psi_j V K\psi_i \rangle, \text{ where } f = \pm 1. \tag{18.46}$$

Condition (18.46) yields two useful relations for the matrix elements of Kramers conjugate functions. Thus, if $\psi_i = \psi_j$, we have from (18.45)

$$\langle K\psi_i V K\psi_i \rangle = f \langle \psi_i V \psi_i \rangle. \tag{18.47}$$

If we now set $\psi_j = K\psi_i$, it follows from (18.46) that

$$\langle \psi_i V K\psi_i \rangle = fK^2 \langle \psi_i V K\psi_i \rangle,$$

which implies that

$$\langle \psi_i V K\psi_i \rangle = 0 \text{ when } fK^2 = -1, \tag{18.48}$$

i.e., the matrix elements of an even operator between Kramers conjugate spin functions vanish, and for odd operators the matrix elements vanish on the complex conjugate coordinate functions.

In conclusion, we note that although the operation K is anti-unitary, it may be incorporated together with the unitary operations g in a special group. When this is done, if the functions ψ and $K\psi$ are linearly independent, they are also combined, to form a representation of this group, known as a corepresentation, first introduced by Wigner /I.1/. Naturally, the properties of corepresentations differ from those of the usual representations. They are considered in detail in /13.4/. When considering the effect of time reversal on the spectrum, selection rules and other characteristics, one may either make direct use of corepresentations, or start with the usual representations of space or point groups, subsequently making special allowance for the effect of time reversal. Both approaches lead to the same results. In the present book we adopt the second approach, which seems to us more meaningful from the physical standpoint.

§19. SELECTION RULES

In perturbation theory, the theory of quantum transitions, and so on, one must know the matrix elements of a given operator V between known wave functions ψ:

$$V_{ij} = \langle \psi_i V \psi_j \rangle = \int \psi_i^* V \psi_j \, dx. \tag{19.1}$$

For example, the square of the absolute value of a matrix element $|V_{ij}|^2$ determines the probability of transition from state ψ_i to state ψ_j due to a perturbation V. In many problems there is no need to calculate these matrix

elements explicitly; it is sufficient to verify whether the corresponding integrals differ from zero, to find the number of linearly independent components V_{ij}, and to establish the relation between different linearly dependent matrix elements.

Since any operator V may be expressed as the sum of l-th components of operators $V^{\varkappa l}$, which transform according to an irreducible representation $\varkappa$ of the symmetry group $\mathcal{G}$ of the Hamiltonian $\mathcal{H}_0$, whose eigenfunctions are ψ_i and ψ_j, we shall assume that not only the wave functions ψ_i^μ and ψ_j^ν but also the operators $V^{\varkappa l}$ transform according to appropriate irreducible representations $\mathcal{D}_\mu$, $\mathcal{D}_\nu$ and $\mathcal{D}_\varkappa$ of the group $\mathcal{G}$, and we shall show how a knowledge of these representations yields an answer to the above questions.

The application of group theory to selection rules is based on the following lemma: if the function $\mathcal{F}_i(x)$ transforms according to an irreducible representation $\mathcal{D}_\mu$, then the integral

$$J_i = \int \mathcal{F}_i(x)\, dx$$

is nonzero only when $\mathcal{D}_\mu$ is the identity representation $\mathcal{D}_0$.

To prove this lemma, we observe that the integral J does not change upon passage to a new coordinate system $x' = gx$, since this involves a simple substitution of variables under the integral sign. On the other hand, if g is one of the group operations, we see from (7.3) that it takes the function $g\mathcal{F}_i(x) = \mathcal{F}_i(g^{-1}x)$ into

$$g\mathcal{F}_i(x) = \sum_l \mathcal{D}_{li}(g)\, \mathcal{F}_l(x).$$

From the orthogonality relations (8.3) and (8.10) it follows that

$$\frac{1}{h} \sum_{g \in \mathcal{G}} \mathcal{D}_{li}^{\mu}(g) = \delta_{\mu 0}.$$

The last relationship is derived directly from (8.3) and (8.10) by putting $\mathcal{D}_\nu(g) = \mathcal{D}_0(g)$. Therefore, summing

$$gJ_i = \int \mathcal{F}_i(g^{-1}x)\, dx$$

over g and using the fact that $gJ_i = J_i$, we obtain

$$J_i = \frac{1}{h} \sum_{g \in \mathcal{G}} gJ_i = \frac{1}{h} \sum_l \sum_{g \in \mathcal{G}} \mathcal{D}_{li}^{\mu}(g) \int \mathcal{F}_l(x)\, dx = \delta_{\mu 0} J_i,$$

proving our assertion.

If the representation $\mathcal{D}$ according to which the functions $\mathcal{F}_i(x)$ transform is reducible, it is obvious that the integral

$$J = \int \mathcal{F}_i(x)\, dx$$

may be nonzero only if this representation contains the identity representation. Indeed, applying the operation g to $\mathcal{F}_i(x)$ and summing over g, we obtain

$$J = \frac{1}{h} \sum_g \int g\mathcal{F}_i(x)\, dx = \int P^1 \mathcal{F}_i(x)\, dx.$$

The operator

$$P^1 = \frac{1}{h}\sum_g \mathcal{D}(g)$$

is a projection operator (9.5), which determines in the set of functions $\mathcal{F}_j(x)$ a combination $\mathcal{F}_0(x)$ which transforms according to the identity representation. The function $\mathcal{F}_0(x)$ clearly differs from zero only if the representation $\mathcal{D}$ contains the identity representation.

Let us return to the integral (19.1). By (7.3), the operation g takes the functions appearing in the integrand into

$$g\psi_l^\nu = \sum_{l'} \mathcal{D}^\nu_{l'l}(g)\,\psi^\nu_{l'}, \quad g\psi_i^{\mu*} = \sum_{i'} \mathcal{D}^{\mu*}_{i'i}(g)\,\psi^{\mu*}_{i'}, \quad gV_i^\varkappa = \sum_{i'} \mathcal{D}^\varkappa_{i'i}(g)\,V^\varkappa_{i'}.$$

Therefore, the representation by which the integrand transforms is the representation with matrix elements

$$\mathcal{D}_{i'i,\,l'l,\,ri}(g) = \mathcal{D}^{\mu*}_{i'i}(g)\,\mathcal{D}^\nu_{l'l}(g)\,\mathcal{D}^\varkappa_{i'i}(g), \tag{19.2}$$

i.e., $\mathcal{D}$ is the direct product of the representations

$$\mathcal{D} = \mathcal{D}^*_\mu \times \mathcal{D}_\nu \times \mathcal{D}_\varkappa \tag{19.3}$$

and is reducible in the general case.

By the above lemma, this means that the matrix element of the operator $V^{\varkappa l}$ between functions which transform according to the representations $\mathcal{D}^*_\mu$ and $\mathcal{D}_\nu$ may differ from zero only if the direct product (19.3) contains the identity representation. By (9.24) and (8.16), this requires that the product $\mathcal{D}^*_\mu \times \mathcal{D}_\nu$ contain the representation $\mathcal{D}^*_\varkappa$. The transformation defined by

$$gV^l_{il} = \sum_{i'l'l'} \mathcal{D}^{\mu*}_{i'i}(g)\,\mathcal{D}^\nu_{l'l}(g)\,\mathcal{D}^\varkappa_{l'i}(g)\,V^{l'}_{i'l'} \tag{19.4}$$

may be regarded as the result of the operator $\mathcal{D}(g)$ acting on V^l_{il}, and the totality of $n_\mu n_\nu n_\varkappa$ different matrix elements V^l_{il} for $i = 1, 2, \ldots, n_\mu$, $j = 1, 2, \ldots, n_\nu$, $l = 1, 2, \ldots, n_\varkappa$, may be regarded as the basis of the representation $\mathcal{D}$. Successively applying all the group operations $g \in \mathcal{G}$, we can find in general h linear relations (19.4) expressing one of the elements V^l_{il} in terms of the others $V^{l'}_{i'l'}$. According to (9.5), the sum

$$P^1 V^l_{il} = \frac{1}{h}\sum_g \mathcal{D}(g)\,V^l_{il} = \frac{1}{h}\sum_g \sum_{i'l'l'} \mathcal{D}_{i'i,\,l'l,\,rl}(g)\,V^{l'}_{i'l'} \tag{19.5}$$

may be viewed as the result of the projection operator P^1 acting on V^l_{il}. In order to check whether a given matrix element is nonzero, one must apply the operator P^1, i.e., check that the sum (19.5) does not vanish.

Applying the operator P^1 to the various elements V^l_{il}, we generally obtain various functions (19.4), which transform according to the identity representation. By (19.5) each nonzero matrix element may be expressed in terms of these functions, and so the total number of linearly independent nonzero matrix elements equals the number of linearly independent invariants contained in the direct product (19.3). By (9.24), this number N_0 is

$$N_0 = \frac{1}{h}\sum_g \sum_{il} \mathcal{D}_{il,\,il,\,ll}(g) = \frac{1}{h}\sum_g \chi^*_\mu(g)\,\chi_\nu(g)\,\chi_\varkappa(g). \tag{19.6}$$

Thus, to determine the number of linearly independent nonzero elements it is sufficient to know the characters of the representations according to

which the operator itself and the wave functions transform; to determine the nonzero elements, however, one must find the invariants (19.5), and for this the representations themselves are needed.

Allowance for invariance under time reversal. As noted above, invariance under time reversal imposes an additional condition (18.46) on the matrix elements:

$$V^l_{ij} = \langle \psi^\mu_i V^\varkappa_l \psi^\nu_j \rangle = f \langle K\psi^\nu_j V^\varkappa_l K\psi^\mu_i \rangle, \tag{19.7}$$

where $f = \pm 1$ depending on whether the operator is even or odd with respect to time reversal. If the wave functions $K\psi^\mu$ and ψ^ν are linearly dependent, this condition results in additional relations, which lower the total number of linearly independent matrix elements. As pointed out in §18, the functions $K\psi^\mu$ and ψ^ν will be linearly dependent in case (a) when the functions ψ^μ and ψ^ν belong to one representation, i.e., $\mu = \nu$, and this representation $\mathscr{D}_\nu$ is real in the case of usual representations, complex and equivalent to $\mathscr{D}^*_\nu$ for spinor representations. By (18.7)

$$K\psi^\nu_i = \sum_{i'} T_{i'i} \psi^\nu_{i'}.$$

Therefore, the transformation F defined by

$$FV^l_{ij} = f \langle T\psi^\nu_j V^\varkappa_l T\psi^\nu_i \rangle = f \sum_{i'j'} T^*_{i'j} T_{j'i} V^l_{i'j'}, \tag{19.8}$$

may be regarded as the result of the operator F acting on V^l_{ij}, invariance under time reversal implying that $FV^l_{ij} = V^l_{ij}$. If the functions ψ^ν_i and $K\psi^\nu_i$ are linearly independent, the representations $\mathscr{D}^*_\nu$ and $\mathscr{D}_\nu$ are combined. In this case there are "diagonal" matrix elements

$$V_{ij} = \langle \psi^\nu_i V \psi^\nu_j \rangle, \quad V_{Ki, Kj} = \langle K\psi^\nu_i V K\psi^\nu_j \rangle$$

and "off-diagonal" elements

$$V_{Ki, j} = \langle K\psi^\nu_i V \psi^\nu_j \rangle, \quad V_{i, Kj} = \langle \psi^\nu_i V K\psi^\nu_j \rangle.$$

Condition (19.7) shows that the diagonal elements of the first and second types satisfy the relation

$$V_{Ki, Kj} = \langle K\psi^\nu_i V K\psi^\nu_j \rangle = f \langle \psi^\nu_j V \psi^\nu_i \rangle = f V_{ji} \tag{19.9}$$

and imposes an additional symmetry condition on the "off-diagonal" elements:

$$V_{Ki, j} = \langle K\psi^\nu_i V \psi^\nu_j \rangle = F V^l_{Ki, j} \equiv f \langle K\psi^\nu_j V K^2 \psi^\nu_i \rangle = f K^2 V_{Kj, i}. \tag{19.10}$$

To determine the number of linearly independent matrix elements, one can introduce the extended group consisting of the elements g and gF, where F is defined by (19.8) or (19.10). Then, by (19.8), in case (a)

$$\mathscr{D}_{i'i, j'j, \nu\nu}(Fg) = f (\mathscr{D}_\nu(g) \boldsymbol{T})^*_{i'j} (\mathscr{D}_\nu(g) \boldsymbol{T})_{j'i} \mathscr{D}^\varkappa_{\nu\nu}(g). \tag{19.11}$$

By (19.10), in cases (b) and (c), for the "off-diagonal" element $\langle K\psi^\nu_i V \psi^\nu_j \rangle$ we have*

$$\mathscr{D}_{i'i, j'j, \nu\nu}(Fg) = f K^2 \mathscr{D}^\nu_{i'j}(g) \mathscr{D}^\nu_{j'i}(g) \mathscr{D}^\varkappa_{\nu\nu}(g). \tag{19.12}$$

* For the matrix element $\langle \psi^\nu_i V K\psi^\nu_j \rangle$, one replaces $\mathscr{D}_\nu(g)$ by $\mathscr{D}^*_\nu(g)$. Accordingly, in the final equation (19.13) we have $\chi_\nu(g)$ instead of $\chi^*_\nu(g)$. This is equivalent to replacing $\chi_\varkappa(g)$ by $\chi^*_\varkappa(g)$. In case (a) these expressions coincide, since then $\chi_\nu(g) = \chi^*_\nu(g)$.

The number of linearly independent components V^l_{ij} equals the number of identity representations occurring in the extended group representation $\mathcal{D}$, which is defined by (19.4) and (19.11) in case (a) or (19.4) and (19.12) in cases (b) and (c).* Thus:

$$N_0 = \frac{1}{2h} \sum_g \sum_{ij} \mathcal{D}_{ii,\,jj,\,ii}(g) + \mathcal{D}_{ii,\,jj,\,ii}(Fg).$$

The first term of this sum may be evaluated from (19.6), for in this case $\chi^*_\mu(g) = \chi_\mu(g) = \chi_\nu(g)$, since the representation $\mathcal{D}^*_\mu$ is equivalent to $\mathcal{D}_\nu$. To evaluate the second term, we use (19.11):

$$\sum_{ij} \mathcal{D}(Fg)_{ii,\,jj,\,ii} = f \sum_{ij} (\mathcal{D}_\nu(g)\boldsymbol{T})^*_{ij} (\mathcal{D}_\nu(g)\boldsymbol{T})_{ji} \mathcal{D}^\varkappa_{ii}(g) =$$

$$= f\chi_\varkappa(g) \sum_j (\mathcal{D}_\nu(g)\boldsymbol{T}\mathcal{D}^*_\nu(g)\boldsymbol{T}^*)_{jj} = f\chi_\varkappa(g) \sum_j (\mathcal{D}_\nu(g^2)\boldsymbol{T}\boldsymbol{T}^*)_{jj} = K^2 f\chi_\varkappa(g)\chi_\nu(g^2).$$

Here we are using the fact that by (18.8) $\mathcal{D}^*_\nu(g) = \boldsymbol{T}^{-1}\mathcal{D}_\nu(g)\boldsymbol{T}$ and by (18.26) $\boldsymbol{T}\boldsymbol{T}^* = K^2$, where $K^2 = 1$ for usual representations and $K^2 = -1$ for spinor representations. In case $\mathcal{D}(Fg)$ is determined by equation (19.12), we obtain similarly

$$\sum_{ij} \mathcal{D}_{ii,\,jj,\,ii}(Fg) = fK^2 \sum_{ij} \mathcal{D}^\nu_{ij}(g)\mathcal{D}^\nu_{ji}(g)\mathcal{D}^\varkappa_{ii}(g) = K^2 f\chi_\varkappa(g)\chi_\nu(g^2),$$

i.e., in both cases,

$$N_0 = \frac{1}{2h} \sum_g \chi_\varkappa(g)\left[\chi^2_\nu(g) + K^2 f\chi_\nu(g^2)\right]. \tag{19.13}$$

Equations (19.6) and (19.13) are applicable to any finite group, in particular, to a space group, which may always be made finite, say by introducing the cyclic Born-von Kármán boundary conditions. However, their direct use in this form is not convenient for space groups, since one would then need to know the characters of the space group representations $\mathcal{D}^{\{k'\}}_\mu$, $\mathcal{D}^{\{k\}}_\nu$ and $\mathcal{D}^{\{q\}}_\varkappa$ in the complete basis, which includes the basis functions of the representations μ, ν and $\varkappa$ for all points of the stars $\{k'\}$, $\{k\}$ and $\{q\}$, respectively.

By (12.27), the characters of these representations are determined by

$$\chi(r\,|\,\tau + t) = \sum_i \chi^{k_i}(r\,|\,\tau)\, e^{-ik_i t}. \tag{19.14}$$

The summation in (19.14) extends over all points k_i of the star $\{k\}$ and χ^{k_i} is the character of a representation of the little group G_{k_i}. If $g = (r|\tau)$ is not an element of the little group G_{k_i}, then it follows from (12.23) that $\chi^{k_i}(g) = 0$ $(g \notin G_{k_i})$.

As indicated in §12, representations of space groups are usually specified not by the complete character (19.14) but by the star $\{k\}$ and the character of the appropriate representation of the little group of the G_k for one of the points of the star $\{k\}$. We therefore rework the general equations (19.6) and

* In similar fashion one can determine, for example, the number of identity representations occurring in the symmetrized or antisymmetrized product. Rather than construct the symmetrized or antisymmetrized functions (9.18) or (9.19), one assumes that all the functions ψ_{ij} are independent, introduces an index permutation operation f similar to (19.10), and sums in (9.24) over all the elements g and gf. One then has $\mathcal{D}(f) = I$ for symmetrized products and $\mathcal{D}(f) = -I$ for antisymmetrized products. This gives the same expressions as when the characters of the symmetrized or antisymmetrized products, given by (9.22) or (9.23), respectively, are summed over g.

(19.13), retaining only the characters of the fundamental elements (i.e., the elements not containing primitive translations t) of the little groups for one point k', k and q of each of the stars $\{k'\}$, $\{k\}$ and $\{q\}$.

We now consider the specific cases.

The representations $\mathcal{D}_\mu^{\{k'\}}$ and $\mathcal{D}_\nu^{\{k\}}$ belong to different energies, and the stars $\{-k'\}$ and $\{k\}$ are distinct. Matrix elements of this type determine, for example, the probability of phonon emission or absorption during indirect optical transitions, i.e., transitions involving participation of a photon and a phonon.

To determine N_0 in this case we substitute (19.14) into (19.6) and sum over all primitive translations. We obtain

$$N_0 = \frac{1}{h} \sum_g \sum_{l,l} \chi_\mu^{k'_i *}(g)\, \chi_\nu^{k_j}(g)\, \chi_\varkappa^{q_l}(g)\, \delta_{k'_i - k_j,\, q_l}. \tag{19.15}$$

Here the summation extends only over the fundamental elements $g = (r|\tau)$ of the group G, which do not contain primitive translations; h denotes the number of these elements, equal to the order of the point group. As is evident from (19.15), transitions may take place only with conservation of quasi-momentum, i.e.,

$$k'_i - k_j - q_l = 0. \tag{19.16}$$

Here, as usual, vectors which differ by a reciprocal lattice vector b are identified. Let us denote any three star points satisfying condition (19.16) by $k'_1 = k'$, $k_1 = k$, $q_1 = q$, respectively, i.e.,

$$k' - k - q = 0. \tag{19.17}$$

Applying the operations $g \in G$ to (19.17), we find other values of k'_i, k_j, q_l satisfying (19.16):

$$gk' - gk - gq = 0. \tag{19.18}$$

Note that, as shown in §12, the vectors k are affected only by "rotational" elements g, i.e., if $g = (r|\tau)$, then $gk = rk$.

Let us first assume that, as g runs through all the fundamental elements of the group G, formula (19.18) yields all values k'_i, k_j, q_l satisfying (19.16), i.e., there is no operation g outside G_k such that

$$k' - g_2 k - g_3 q = 0, \tag{19.19}$$

if g_2 is not in G_k and g_3 is not in G_q. Then, instead of summing over all i, j, l in (19.15), we may sum over all elements g. In the process, each distinct triple of vectors k'_i, k_j, q_l satisfying (19.16) occurs h_0 times, where h_0 is the number of elements g which leaves each of the vectors k', k, q invariant (up to equivalence). These elements g_0 are in each of the three groups $G_{k'}$, G_k and G_q and form their intersection G_0:

$$G_0 = G_{k'} \cap G_k \cap G_q.$$

Thus, when replacing summation in (19.15) over i, j, l by summation over g, we must divide the sum by h_0:

$$N_0 = \frac{1}{hh_0} \sum_{g'} \sum_g \chi_\mu^{*gk'}(g')\, \chi_\nu^{gk}(g')\, \chi_\varkappa^{gq}(g'). \tag{19.20}$$

By (12.24), the characters of representations of little groups for different points of the same star $\{\boldsymbol{k}\}$ are related by

$$\chi^{\boldsymbol{k}_i}(g)=\chi^{g_i\boldsymbol{k}}(g)=\chi^{\boldsymbol{k}}\left(g_i^{-1}gg_i\right), \tag{19.21}$$

where g_i is a fixed operation taking the point $\boldsymbol{k}=\boldsymbol{k}_1$ into $\boldsymbol{k}_i$ (see (12.20)).

If we substitute (19.21) into (19.20) and sum over all the fundamental elements g', letting this element run through all values from g_1' to g_h', the element $g_i^{-1}g'g_i$ runs in another order through the same values of g' or values differing from g' by a primitive translation $\boldsymbol{t}$. By condition (19.17), the phase factors associated with the translation $\boldsymbol{t}$ disappear, and so the sum

$$\begin{aligned}&\sum_{g'}\chi_\mu^{g\boldsymbol{k}'*}(g')\,\chi_\nu^{g\boldsymbol{k}}(g')\,\chi_\varkappa^{g\boldsymbol{q}}(g')=\\&=\sum_{g'}\chi_\mu^{\boldsymbol{k}'*}(g^{-1}g'g)\,\chi_\nu^{\boldsymbol{k}}(g^{-1}g'g)\,\chi_\varkappa^{\boldsymbol{q}}(g^{-1}g'g)=\sum_{g'}\chi_\mu^{\boldsymbol{k}'*}(g')\,\chi_\nu^{\boldsymbol{k}}(g')\,\chi_\varkappa^{\boldsymbol{q}}(g')\end{aligned} \tag{19.22}$$

does not depend on g and summation over g in (19.20) reduces to multiplication by the number h of fundamental elements in G. The products appearing in (19.22) differ from zero only if the element g' appears in each of the little groups $G_{\boldsymbol{k}'}$, $G_{\boldsymbol{k}}$, $G_{\boldsymbol{q}}$. Thus the final summation in (19.20) need extend only over the fundamental elements of the group $G_0=G_{\boldsymbol{k}'}\cap G_{\boldsymbol{k}}\cap G_{\boldsymbol{q}}$, whose order is h_0:

$$N_0=\frac{1}{h_0}\sum_{g_0\in G_0}\chi_\mu^{\boldsymbol{k}'*}(g_0)\,\chi_\nu^{\boldsymbol{k}}(g_0)\,\chi_\varkappa^{\boldsymbol{q}}(g_0). \tag{19.23}$$

Equation (19.23) in fact tells us how many times the representation $\mathscr{D}_\varkappa^*$ with star $\{-\boldsymbol{q}\}$ occurs in the direct product $\mathscr{D}_\mu^*\times\mathscr{D}_\nu$ of representations with stars $\{-\boldsymbol{k}'\}$ and $\{\boldsymbol{k}\}$, and condition (19.16) implies that N_0 differs from zero only if the star $\{-\boldsymbol{q}\}$ occurs in the direct product of the stars $\{-\boldsymbol{k}'\}$ and $\{\boldsymbol{k}\}$.

If (19.18) does not exhaust all the values of $\boldsymbol{k}_i'$, $\boldsymbol{k}_j$, $\boldsymbol{q}_l$ that satisfy (19.16), i.e., there is another triple of vectors $\boldsymbol{k}'=\boldsymbol{k}_1'$, $\boldsymbol{k}_2=g_2\boldsymbol{k}$, $\boldsymbol{q}_2=g_3\boldsymbol{q}$ satisfying (19.19), application of the operation g to (19.19) yields another series of vectors satisfying (19.16) but not appearing in (19.18). We thus have to add to (19.23) a second sum

$$\sum_{\bar g}\chi_\mu^{\boldsymbol{k}'*}(\bar g)\,\chi_\nu^{g_1\boldsymbol{k}}(\bar g)\,\chi_\varkappa^{g_1\boldsymbol{q}}(\bar g), \tag{19.24}$$

where $\bar g$ are the fundamental elements of the intersection $\overline{G}=G_{\boldsymbol{k}'}\cap G_{g_1\boldsymbol{k}}\cap G_{g_1\boldsymbol{q}}$, whose order is again h_0. If the stars $\{\boldsymbol{k}'\}$, $\{\boldsymbol{k}\}$, $\{\boldsymbol{q}\}$ lie in arbitrary positions, appearance of two independent relations (19.17) and (19.19) is accidental. However, if the star $\{\boldsymbol{k}\}$ coincides with the star $\{-\boldsymbol{k}'\}$, there may be two groups of vectors satisfying these relations. In that case there is an operation g_s taking $\boldsymbol{k}$ into $-\boldsymbol{k}'$:

$$-\boldsymbol{k}'=g_s\boldsymbol{k}. \tag{19.25}$$

Now if (19.25) is fulfilled for one operation g_s, it is fulfilled for all operations g_sg_k, where g_k is an arbitrary operation of the group G_k. We may then write (19.17) as

$$-\boldsymbol{k}'+\boldsymbol{k}+\boldsymbol{q}=g_s\boldsymbol{k}+\boldsymbol{k}+\boldsymbol{q}=0. \tag{19.26}$$

Permuting the first two terms, we obtain

$$\boldsymbol{k}+g_s\boldsymbol{k}+\boldsymbol{q}=0. \tag{19.27}$$

Multiplying (19.27) by g_s and using (19.25), we may write the last relationship as

$$-k' + g_s^2 k + g_s q = 0. \tag{19.27a}$$

If none of the elements g_s^2 is a product $g_{k'} g_k$ of elements of the little groups $G_{k'}$ and G_k, relation (19.27a) cannot be obtained from (19.26) by application of an operation g (without rearrangement of terms), and relations (19.26) and (19.27a) must be considered independent. In that case, N_0 is the sum of (19.23) and (19.24); moreover, as can be seen by comparing (19.19) and (19.27a), $g = g_s^2$ and $g_3 = g_s$. Expressing the characters of the representations of the groups $G_{g_s^2 k}$ and $G_{g_s q}$ in terms of the characters of the representations of the little groups G_k and G_q with the aid of (19.21), we finally obtain

$$N_0 = \frac{1}{h_0} \sum_{g_0} \chi_\mu^{k'*}(g_0) \left[\chi_\nu^k(g_0) \chi_\varkappa^q(g_0) + \chi_\nu^k(g_s^{-2} g_0 g_s^2) \chi_\varkappa^q(g_s^{-1} g_0 g_s) \right]. \tag{19.28}$$

If at least one of the elements $g_s = g_{k'} g_s' g_k$ is such that $g_s^2 = g_{k'} g_k$, then $g_{k'}^{-1} g_s \in G_q$ and relation (19.27a) obviously need not be considered separately, since it is a consequence of (19.26).*

Equation (19.28), which is valid when $g_s^2 \neq g_{k'} g_k$, may be rewritten in a more symmetric form. For this purpose we use (19.22), summing in the second term over $g_s^{-1} g_0 g_s$ instead of over g_0 and noting that, by (19.25) and (19.21),

$$\chi_\mu^{k'}(g) = \chi_\mu^{-g_s k}(g) = \chi_\mu^{-k}\left(g_s^{-1} g_0 g_s\right), \quad \chi_\mu^{k'}\left(g_s g g_s^{-1}\right) = \chi_\mu^{-k}(g). \tag{19.29}$$

We obtain

$$N_0 = \frac{1}{h_0} \sum_{g_0} \chi_\varkappa^q(g_0) \left[\chi_\mu^{-k*}(g_s^{-1} g_0 g_s) \chi_\nu^k(g_0) + \chi_\mu^{-k*}(g_0) \chi_\nu^k(g_s^{-1} g_0 g_s) \right], \tag{19.30}$$

where $g_0 \in G_0 = G_{-g_s k} \cap G_k \cap G_q$.

In determining the probabilities of direct optical transitions, i.e., transitions which occur without changes in momentum, and in a number of other problems, one is concerned with vertical transitions. In these cases $q_i = 0$, the operators $V_i^\varkappa$ are translation invariant and transform according to the representations of the point group F with characters $\chi_\varkappa(g)$. If k and $-k' = -k$ are points of one star, then $g_s = e$ and so for any operation we have $g_s^2 = g_{k'} g_k$, since g_k and g_s are elements of $G_{k'}$. In this case, therefore, equation (19.23) is always valid, the summation extending over all fundamental elements of the group G_k:

$$N_0 = \frac{1}{h} \sum_{g \in G_k} \chi_\mu^{k*}(g) \chi_\nu^k(g) \chi_\varkappa(g). \tag{19.31}$$

The representations $\mathscr{D}_\mu$ and $\mathscr{D}_\nu$ belong to the same energy. In this case the representations coincide or are combined owing to invariance under time reversal. Matrix elements of this type determine, for example, the probability of minimum-to-minimum (intervalley) transitions with absorption or emission of phonons.

* Therefore, for groups in which the products $g_{k'} g_k$ exhaust the whole group, equation (19.27a) is certainly not independent.

Let us first consider the case in which ψ^ν and $K\psi^\nu$ are linearly independent. Suppose that a transition occurs between states $\psi^\nu_{\boldsymbol{k}}$ which belong to the same representation, but generally to different points of the star, e.g., $\boldsymbol{k}$ and $\boldsymbol{k}' = g_r\boldsymbol{k}$, so that these vectors satisfy equation (19.17):

$$g_r\boldsymbol{k} - \boldsymbol{k} - \boldsymbol{q} = 0. \tag{19.32}$$

In this case N_0 is given by (19.23) but, since the representations $\mathcal{D}_\mu$ and $\mathcal{D}_\nu$ are equal, it follows from (19.21) that

$$\chi^{\boldsymbol{k}'}_\mu(g_0) = \chi^{g_r\boldsymbol{k}}_\nu(g_0) = \chi^{\boldsymbol{k}}_\nu\left(g_r^{-1}g_0g_r\right) \tag{19.33}$$

and, consequently,

$$N_0 = \frac{1}{h_0}\sum_{g_s} \chi^{\boldsymbol{k}*}_\nu(g_r^{-1}g_0g_r)\,\chi^{\boldsymbol{k}}_\nu(g_0)\,\chi^{\boldsymbol{q}}_\varkappa(g_0), \tag{19.34}$$

where

$$g_0 \in G_0 = G_{g_r\boldsymbol{k}} \cap G_{\boldsymbol{k}} \cap G_{\boldsymbol{q}}.$$

Equation (19.34) is applicable, for example, in case (b_3), when combination of the representations $\mathcal{D}_\nu$ and $\mathcal{D}^*_\nu$ reduces to combination of stars, for transitions between points belonging to one star. It is also applicable to evaluation of the number of "diagonal" components in cases (b_1), (b_2), (c_1) and (c_2), when representations of the little groups at each point of the star are combined. If none of the operations g_s^2, where g_s takes $\boldsymbol{k}$ into $-\boldsymbol{k}' = -g_r\boldsymbol{k}$, is a product $g_{\boldsymbol{k}'}g_{\boldsymbol{k}}$, then (19.23) must be replaced by (19.30). In the present case, the operation g_s may be written $g_s = g_rR^{-1}$, where R is an operation which takes $\boldsymbol{k}$ into $-\boldsymbol{k}$. Since

$$\chi^{-\boldsymbol{k}}_\mu(g) = \chi^{-\boldsymbol{k}}_\nu(g) = \chi^{\boldsymbol{k}}_\nu(R^{-1}gR), \tag{19.35}$$

it follows that

$$N_0 = \frac{1}{h_0}\sum_{g_s} \chi^{\boldsymbol{q}}_\varkappa(g_0)\left[\chi^{\boldsymbol{k}*}_\nu(g_r^{-1}g_0g_r)\,\chi^{\boldsymbol{k}}_\nu(g_0) + \chi^{\boldsymbol{k}*}_\nu(R^{-1}g_0R)\,\chi^{\boldsymbol{k}}_\nu\left(Rg_r^{-1}g_0g_rR^{-1}\right)\right]. \tag{19.36a}$$

For cases (b_1) and (c_1), when the points $\boldsymbol{k}$ and $-\boldsymbol{k}$ are equivalent, we have $R = e$ and

$$N_0 = \frac{1}{h_0}\sum_{g_s} \chi^{\boldsymbol{q}}_\varkappa(g_0)\left[\chi^{\boldsymbol{k}*}_\nu(g_r^{-1}g_0g_r)\,\chi^{\boldsymbol{k}}_\nu(g_0) + \chi^{\boldsymbol{k}*}_\nu(g_0)\,\chi^{\boldsymbol{k}}_\nu(g_r^{-1}g_0g_r)\right]. \tag{19.36b}$$

The number of linearly independent off-diagonal elements in cases (b) and (c) is determined by (19.13). In case (b_3) these off-diagonal elements correspond to a transition between points belonging to different stars, e.g., $\boldsymbol{k}_j$ and $\boldsymbol{k}'_i = -\boldsymbol{k}_i$. In all these cases the off-diagonal elements $\langle K\psi^\nu_{-\boldsymbol{k}_i} V \psi^\nu_{\boldsymbol{k}_j}\rangle$ correspond to a transition between the states $\psi^\nu_{\boldsymbol{k}_j}$ and $\psi^\mu_{\boldsymbol{k}_i} = K\psi^\nu_{-\boldsymbol{k}_i}$, and the elements $\langle \psi^\mu_{\boldsymbol{k}_i} V K\psi^\mu_{-\boldsymbol{k}_j}\rangle$ to transitions from state $\psi^\nu_{\boldsymbol{k}_j} = K\psi^\mu_{-\boldsymbol{k}_j}$ to $\psi^\mu_{\boldsymbol{k}_i}$. Moreover, if $\mathcal{D}_\mu = \mathcal{D}_\nu$ for the diagonal elements, then $\mathcal{D}_\mu = \mathcal{D}^*_\nu$ for the off-diagonal elements. By (19.33) and (18.35),

$$\chi^{\boldsymbol{k}'*}_\mu(g) = \chi^{-\boldsymbol{k}'}_\nu(g) = \chi^{\boldsymbol{k}}_\nu(g_s^{-1}gg_s), \tag{19.37}$$

where g_s is an operation which takes $\boldsymbol{k}$ into $-\boldsymbol{k}'$.

The number of linearly independent elements in case (a), where the functions ψ and $K\psi$ are linearly dependent, is again determined by equation (19.13). In this case $\mathscr{D}_\mu = \mathscr{D}_\nu$, since $\mu = \nu$, but by (18.38) the conjugate characters also satisfy condition (19.37). The first part of the sum in (19.13) differs from (19.6) only by the factor 1/2, since the quantity $(\chi_\nu(g))^2$ in (19.13) may be written $\chi^*_\mu(g)\chi_\nu(g)$ and in case (a) we have $\mu = \nu$. Therefore, this term reduces to (19.23), and it remains only to evaluate the second part of the sum in (19.13), which we denote by Σ_2.

Substituting (19.14) into (19.13) and summing over all primitive translations, we obtain the following expression:

$$\Sigma_2 = \frac{1}{2h} \sum_g \sum_{jl} \chi^{q_l}_\varkappa(g)\, \chi^{k_j}_\nu(g^2)\, \delta_{k_j + g'^{-1}k_j + q_l,\, 0}. \tag{19.38}$$

Here we have used the relation

$$\chi^k_\nu[(r \mid \tau + t)^2] = \chi^k_\nu[(r \mid \tau)^2]\, e^{-ik(t + rt)}.$$

If the vectors $-k_i = g_s k_j$, k_j, q_l satisfy only one independent relation (19.17), all the others can be obtained by successive application of operations $g \in G_k$ to (19.17):

$$gg_s k + gk + gq = 0. \tag{19.39}$$

Equation (19.39) determines all the possible values of the vectors k_i, k_j, q_l which satisfy a condition like (19.16): for this condition to hold, the vectors must satisfy the relations

$$-k_i = g'^{-1}k_j = gg_s k, \quad k_j = gk, \quad q_l = gq; \tag{19.40}$$

each triple appears in (19.39) h_0 times, where h_0 is the number of fundamental elements of the intersection G_0 of the groups G_k, $G_{g_s k}$, G_q. Thus summation over j and l in (19.38) may be replaced by summation over g, provided the sum is divided by h_0. Using (19.39) and (19.40), we can rewrite the argument of the δ-function as

$$\begin{aligned} g'^{-1}k_l + k_j + q_l &= g'^{-1}gk + gk + gq = \\ &= g'^{-1}gk - gg_s k = g\left(g^{-1}g'^{-1}g - g_s\right)k. \end{aligned}$$

Thus, proceeding as in (19.22), we can transform the sum (19.38):

$$\sum_g \sum_{g'} \chi^{gq}_\varkappa(g')\, \chi^{gk}_\nu(g'^2)\, \delta_{g^{-1}g'^{-1}gk,\, g_s k} =$$

$$= \sum_g \sum_{g'} \chi^q_\varkappa(g^{-1}g'g)\, \chi^k_\nu[(g^{-1}g'g)^2]\, \delta_{g^{-1}g'^{-1}gk,\, g_s k} = h \sum_{g'} \chi^q_\varkappa(g')\, \chi^k_\nu(g'^2)\, \delta_{g'k,\, g_s^{-1}k}.$$

The delta-function $\delta_{gk,\, g_s^{-1}k}$ differs from zero only if $g' = g_s^{-1}g_k$, where $g_k \in G_k$. Thus summation over g' may be replaced by summation over the fundamental elements of G_k. Now the product of characters in the general term of this sum differs from zero only if $g' = g^{-1}g_k$ is an element of G_q, and its square $g'^2 = (g_s^{-1}g_k)^2$ an element of G_k; hence, using (19.31) and (19.37), we can write the final expression for N_0

$$N_0 = \frac{1}{2h_0}\left[\sum_{g_0} \chi^q_\varkappa(g_0)\, \chi^k_\nu(g_0)\, \chi^k_\nu(g_s^{-1}g_0 g_s) + K^2 f \sum_{g_k} \chi^q_\varkappa(g_s^{-1}g_k)\, \chi^k_\nu((g_s^{-1}g_k)^2)\right], \tag{19.41}$$

where

$$g_0 \in G_0 = G_k \cap G_{g_s k} \cap G_q, \quad g_k \in G_k, \quad (g_s^{-1} g_k)^2 \in G_k, \quad g_s^{-1} g_k \in G_q.$$

As indicated above, if at least one of the elements g_s^2 can be represented as a product $g_{k'} g_k$, then (19.27) is not an independent relation and need not be considered separately. It is easy to show that if k and $-k$ are in one star, the condition $g_s^2 = g_{k'} g_k$ is equivalent to the conditions

$$(g_s g_k)^2 \in G_k \quad \text{and} \quad (g_s^{-1} g_k)^2 \in G_k.$$

In fact, in this case $k' = g_r k$ and $g_{k'} = g_r g_k g_r^{-1}$, but $g_r = g_s R$. Therefore, the condition $g_s^2 = g_{k'} g_k = g_s R g_k R^{-1} g_s^{-1} g_k$ implies that $(g_s^{-1} g_k)^2 = R g_k^{-1} R g_k \in G_k$. Hence, if $g_s^2 = g_{k'} g_k$ for at least one element, the second sum in (19.41) differs from zero. If none of the elements g_s satisfies this relation, the second term in (19.41) vanishes, and the first term must be replaced by (19.30). As seen from (19.37), both terms in (19.30) then coincide. Hence, in view of the quantity $2h_0$ in the denominator in (19.13), we obtain

$$N_0 = \frac{1}{h_0} \sum_{g_s} \chi_\nu^k (g_0) \chi_\nu^k (g_s^{-1} g_0 g_s) \chi_\varkappa^q (g_0), \tag{19.42}$$

where $g_0 \in G_0 = G_k \cap G_{g_s k} \cap G_q$.

Transitions between states belonging to one point of the star. As will be shown below, matrix elements of this type determine for example, the shape of the spectrum $E(k)$ at the point in question. If the matrix element is evaluated between ψ_i^ν and ψ_l^ν, and the functions $K\psi^\nu$ and ψ^ν are linearly independent, N_0 is given by (19.34). Since here $k = k'$, we have $g_r = e$, $q = 0$ and

$$N_0 = \frac{1}{h'} \sum_{g' \in G_k} |\chi_\nu^k (g)|^2 \chi_\varkappa (g). \tag{19.43}$$

The summation in (19.43) extends over all the fundamental elements g of the group G_k, since these are all elements of the point group F_k.

Equation (19.43) is applicable when the points k and $-k$ are in different stars (case (b)). If k and $-k$ are in the same star, and the functions ψ^ν and $K\psi^\nu$ are linearly independent and combine into one representation (cases (b_1), (b_2), (c_1), (c_2)), the equation determines the number of linearly independent "diagonal" elements corresponding to transitions between states ψ_i^ν and ψ_l^ν, while the number of linearly independent "off-diagonal" elements corresponding to transitions between states ψ_i^ν and $K\psi_l^\nu$, is determined by equation (19.41), which in the present case is rewritten as*

$$N_0 = \frac{1}{2h} \sum_{g \in G_k} \{\chi_\varkappa (g) \chi_\nu^k (g) \chi_\nu^k (R^{-1} g R) + K^2 f \chi_\varkappa (gR) \chi_\nu^k [(gR)^2]\}. \tag{19.44}$$

* Note that for points inside the Brillouin zone the value of $\chi[(Rg)^2]$, like that of $|\chi(g)|^2$, is independent of the nonprimitive translations in the element and coincides with the value of $\chi[(Rr)^2]$ for the point group G_k. In fact, since $Rgk = -k$, it follows that for $R = (R \mid \tau_R)$ and $g = (r \mid \tau)$

$$\chi[(Rg)^2] = \chi[(Rr)^2] \exp[-ik(Rr(\tau_R + R\tau) + \tau_R + R\tau)] = \chi[(Rr)^2] \exp[-i(\tau_R + R\tau)((Rr)^{-1} k + k)] = \chi[(Rr)^2].$$

Here the summation is performed over the fundamental elements of the group G_k, and R is any element taking k into $-k$. In cases (b_1) and (c_1), when k and $-k$ are points of one star, we have $R = e$, and N_0 is given by

$$N_0 = \frac{1}{2h} \sum_{g \in G_k} \chi_\kappa(g) [\chi_\nu^{k2}(g) + K^{2f} \chi_\nu^k(g^2)], \tag{19.45}$$

which differs from (19.13) only in that the summation extends over the fundamental elements of the little group, rather than over all the elements of the group.

In case (a), when the functions ψ^ν and $K\psi^\nu$ are linearly dependent, N_0 is again given by equation (19.44); if the points k and $-k$ are equivalent (case (a_1), equation (19.45) is valid, but when they are inequivalent, equation (19.44) must be used. Since in this case the representations $\mathscr{D}_\mu$ and $\mathscr{D}_\nu$ coincide and equation (19.37) is valid, we can rewrite (19.44) in the form

$$N_0 = \frac{1}{2h} \sum_{g \in G_k} \{\chi_\kappa(g) |\chi_\nu^k(g)|^2 + K^{2f} \chi_\kappa(gR) \chi_\nu^k[(gR)^2]\}. \tag{19.46}$$

The equations derived above completely solve the problem of determining the number of linearly independent matrix elements: they tell us whether a given transition is allowed or forbidden. In those cases in which it is also necessary to actually specify the nonzero matrix elements and to establish a relation between them, one can use the appropriate projection operators, via equation (19.5). In so doing it is sufficient to extend the summation in (19.5) only over the fundamental elements $g = (r|\tau)$ of the space group and the elements Fg that figure in the corresponding sums for the number N_0.

§20. DETERMINATION OF LINEARLY INDEPENDENT COMPONENTS OF MATERIAL TENSORS

The method of the preceding section for determining the linearly independent matrix elements is directly applicable to determination of the linearly independent nonzero components of material tensors that determine the properties of crystals, such as the conductivity tensor σ, elastic constant tensor S, etc.

Every material tensor S relates two field tensors A and B. The tensors A and B can be of different rank; in particular, they may be vectors, i.e., tensors of rank one. For example, the conductivity tensor σ relates the components of the current density j to the electric field potential $\mathscr{E}$: $j_i = \sum_k \sigma_{ik} \mathscr{E}_k$. The elastic constant tensor relates the strain tensor ε to the stress tensor T: $e_{ij} = \sum_{kl} S_{ijkl} T_{kl}$. The rank of the tensor S is the sum of ranks of the tensors A and B. Thus, let

$$A_i = \sum_k S_{ik} B_k, \tag{20.1}$$

where A_i and B_k are the components of tensors A and B. Upon transition to a new coordinate system $x' = rx$, these components transform according to the corresponding tensor representations $\mathscr{D}_A$ and $\mathscr{D}_B$ of the full spherical

group. In other words, the components A_i' and B_k' of the tensors $\boldsymbol{A}$ and $\boldsymbol{B}$ in the new coordinate system are related to the components A_i and B_k in the old system by

$$A_i' = rA_i = \sum_j \mathcal{D}^A_{ji}(r)\, A_j, \quad B_k' = rB_k = \sum_l \mathcal{D}^B_{lk}(r)\, B_l. \tag{20.2}$$

It is important to note that here, as in (2.29), one is considering the action of the operation r on the coordinate system, which is equivalent to the action of the operation r^{-1} on the tensors themselves. If the operation r is applied to the tensors, the matrices $\mathcal{D}(r)$ in (20.2) are replaced by their transposes. For a tensor of rank n, the tensor representation $\mathcal{D}_n$ is in general the direct product of n vector or pseudovector representations $\mathcal{D}_1^{\pm}$, whose characters are determined by equation (10.20).

These tensor representations are reducible and contain the representations $\mathcal{D}_j$ of the full spherical group as determined by equation (10.21), according to which

$$\mathcal{D}_{l'} \times \mathcal{D}_{l''} = \sum_{l=|l'-l''|}^{l'+l''} \mathcal{D}_l. \tag{20.3}$$

A product of representations of the same parity yields even representations $\mathcal{D}_l^+$, and a product of representations of different parity yields odd representations $\mathcal{D}_l^-$.

if the matrices $\mathcal{D}_A(r)$ and $\mathcal{D}_B(r)$ are known, it is easy to find the transformation law of the tensor $\boldsymbol{S}$. For this purpose we express B_k in terms of B_k':

$$B_k = r^{-1}B_k' = \sum_l \mathcal{D}^{B^{-1}}_{lk}(r)\, B_l' = \sum_l \mathcal{D}^{B^*}_{kl}(r)\, B_l'. \tag{20.2a}$$

Substituting this into the equation

$$A_m' = \sum_i \mathcal{D}^A_{im}(r)\, A_i = \sum_{ik} \mathcal{D}^A_{im}(r)\, S_{ik} B_k, \tag{20.4}$$

which follows from (20.1) and (20.2), we obtain

$$A_m' = \sum_{ikl} \mathcal{D}^A_{im}(r)\, \mathcal{D}^{B^*}_{kl}(r)\, S_{ik} B_l'. \tag{20.4a}$$

Since, on the other hand,

$$A_m' = \sum_l S_{ml}' B_l', \tag{20.4b}$$

it follows by comparison of (20.4a) and (20.4b) that the components of the tensor $\boldsymbol{S}$ transform to the new coordinate system as

$$S_{ml}' = rS_{ml} = \sum_{m'l'} \mathcal{D}_{m'm,\, l'l}(r)\, S_{m'l'}, \tag{20.5}$$

where

$$\mathcal{D}_{m'm,\, l'l}(r) = \mathcal{D}^A_{m'm}(r)\, \mathcal{D}^{B^*}_{l'l}(r). \tag{20.6}$$

The indices i and k in (20.4a) are here replaced for convenience by m' and l', respectively.

Thus, the components of the tensor $\boldsymbol{S}$ form a basis of a representation $\mathcal{D}_S$, the direct product of the representations $\mathcal{D}_A$ and $\mathcal{D}_B^*$:

$$\mathcal{D}_S = \mathcal{D}_A \times \mathcal{D}_B^*. \tag{20.7}$$

Equations (20.5) and (20.6) define the transformation law of the tensor component S_{ml} upon passage to a new coordinate system; they are valid for any transformation r.

In the general case, the tensor representation (20.6) is reducible and can be expanded in terms of the irreducible representations of the given space group. Naturally, the components of the tensor $\boldsymbol{S}$ transform, as do both $\boldsymbol{A}$ and $\boldsymbol{B}$, according to the translation-invariant representations, i.e., the representations corresponding to the point $\boldsymbol{k} = 0$, since the macroscopic properties of the crystals depend only on the point group F, i.e. they are the same for all space groups in the same crystal class.

If r is a symmetry element of the crystallographic point group F, so that it preserves equivalence of directions in the crystal, the components S_{ml} in the new and the old coordinate systems coincide, i.e., if $r \in F$, then

$$S_{ml} = rS_{ml} = \sum_{m'l'} \mathcal{D}^{S}_{m'm,\, l'l}(r)\, S_{m'l'}. \tag{20.8}$$

Successively applying all the operations $r \in F$, we thus obtain h relationships between S_{ml} and the other components. Summing (20.8) over r, we can express each of the components S_{ml} in terms of the invariants of the group F:

$$S_{ml} = \frac{1}{h} \sum_{r} \sum_{m'l'} \mathcal{D}^{S}_{m'm,\, l'l}(r)\, S_{m'l'} = P^{1} S_{ml}. \tag{20.9}$$

Thus, all the matrix elements may be expressed in terms of their invariant combinations, which transform according to the identity representation; consequently, the total number N_0 of linearly independent nonzero components equals the number of these linearly independent invariants, i.e., the number of identity representations occurring in the direct product (20.7). Therefore, by (9.24),

$$N_0 = \frac{1}{h} \sum_{r} \sum_{ml} \mathcal{D}^{S}_{mm,\, u}(r) = \frac{1}{h} \sum_{r} \chi_A(r)\, \chi^{*}_B(r). \tag{20.10}$$

If the representations $\mathcal{D}_A$ and $\mathcal{D}_B$ are reducible in the group F, they may be decomposed into irreducible representations by determining the components $A^{\varkappa}_{m}$ and $B^{\varkappa}_{m}$ that transform according to each irreducible representation $\mathcal{D}_{\varkappa}$ of F. The tensor components $S^{\varkappa\nu}_{ml}$ relating $A^{\varkappa}_{m}$ and B^{ν}_{l} transform according to the representation $\mathcal{D}_{\varkappa\nu} = \mathcal{D}_{\varkappa} \times \mathcal{D}^{*}_{\nu}$. As shown in §9, this product contains the identity representation only if the representations $\mathcal{D}_{\varkappa}$ and $\mathcal{D}_{\nu}$ are equal, and in that case the identity representation occurs just once in $\mathcal{D}_{\varkappa} \times \mathcal{D}^{*}_{\varkappa}$. Therefore,

$$\text{if } \mathcal{D}_A = \sum_{\varkappa} N^{A}_{\varkappa} \mathcal{D}_{\varkappa}, \quad \mathcal{D}_B = \sum_{\varkappa} N^{B}_{\varkappa} \mathcal{D}_{\varkappa}, \text{ then } N_0 = \sum_{\varkappa} N^{A}_{\varkappa} N^{B}_{\varkappa}. \tag{20.11}$$

The matrices of the representation $\mathcal{D}_{\varkappa\nu}$ according to which the components $S^{\varkappa\nu}_{ml}$ transform are defined, according to (20.6), by

$$\mathcal{D}^{\varkappa\nu}_{mm',\, u'}(r) = \mathcal{D}^{\varkappa}_{m'm}(r)\, \mathcal{D}^{\nu *}_{l'l}(r). \tag{20.12}$$

Substituting (20.12) into (20.9) and using the orthogonality relation (8.10), we obtain

$$S^{\varkappa\nu}_{ml} = \frac{1}{h} \sum_{r} \sum_{m'l'} \mathcal{D}^{\varkappa}_{m'm}(r)\, \mathcal{D}^{\nu *}_{l'l}(r)\, S^{\varkappa\nu}_{m'l'} = \frac{\delta_{\varkappa\nu}}{n_{\varkappa}} \sum_{l'm'} \delta_{m'l'} \delta_{ml} S^{\varkappa\nu}_{m'l'} = \delta_{\varkappa\nu} \delta_{ml} \frac{1}{n_{\varkappa}} \sum_{m'} S^{\varkappa\varkappa}_{m'm'}. \tag{20.13}$$

Equation (20.13) shows that for this choice of components $A_m^\varkappa$ and $B_m^\varkappa$ only the diagonal components $S_{mm}^{\varkappa\varkappa}$ differ from zero, and they are moreover equal: $S_{mm}^{\varkappa\varkappa} = S_{ll}^{\varkappa\varkappa}$ $(l = 1, 2, \ldots, n_\varkappa)$.

Note that it is assumed in (20.13) that the functions $A_m^\varkappa$ and $B_m^\varkappa$ transform according to conjugate representations. The subscript m indexes the functions of the representation. In general, equality of these subscripts in (20.13) by no means implies that the usual (coordinate) indices in the tensor components coincide. For example, in the group C_2, where the functions x and y transform according to the same one-dimensional representation B, A_1^B may denote both j_x and j_y, and B_1^B both $\mathscr{E}_x$ and $\mathscr{E}_y$; the tensor σ then has four linearly independent components: σ_{xx}, σ_{yy}, $\sigma_{xy} = \sigma_{yx}$ and σ_{zz} (the latter relating the components j_z and $\mathscr{E}_z$) which transform according to the representation A.

As we know, invariance of the equations of motion under time reversal imposes additional conditions on the kinetic coefficients. These conditions are known as the Onsager relations. They imply a connection between different kinetic tensors, such as the Peltier tensor and the thermal emf tensor, and in certain cases force the tensor components S_{ik} to be symmetric with respect to permutation of the indices i and k. Similar conditions are imposed on other material tensors. These generalized Onsager relations may be formulated as follows.*

If the rate of change of total entropy $\frac{dL}{dt}$ or internal energy $\frac{dU}{dt}$ can be expressed as a sum $-\sum_k B_k A_k$, then the tensor $\boldsymbol{S}$ relating the components of the tensors $\boldsymbol{A}$ and $\boldsymbol{B}$ according to (20.1) satisfies the condition

$$S_{ik}(\boldsymbol{H}) = S_{ki}(-\boldsymbol{H}) \tag{20.14}$$

if both operators $\boldsymbol{A}$ and $\boldsymbol{B}$ are real or imaginary, and

$$S_{ik}(\boldsymbol{H}) = -S_{ki}(-\boldsymbol{H}) \tag{20.15}$$

if one operator is real and the other imaginary.

For example, the conductivity tensor σ, the elastic constant tensor $\boldsymbol{S}$ and its inverse the stiffness tensor $\boldsymbol{C}$ satisfy condition (20.14).

The additional symmetry of the tensor $\boldsymbol{S}$ with respect to permutation of indices may also be due to the symmetry of the field tensors $\boldsymbol{A}$ and $\boldsymbol{B}$. For example, the strain tensor ε and stress tensor $\boldsymbol{P}$ are symmetric: $\varepsilon_{ik} = \varepsilon_{ki}$ and $P_{ik} = P_{ki}$. Similarly, the tensors of elastic constants $\boldsymbol{S}$ and stiffnesses $\boldsymbol{C}$ must also be symmetric with respect to permutations in the first and second pairs of indices:

$$S_{iklm} = S_{kilm} = S_{iklm} = S_{lmik}. \tag{20.16}$$

Allowance may be made for all these additional conditions in (20.4) by introducing additional symmetry elements p_i which permute the appropriate indices. When this is done, the summation in (20.10) must extend over all the elements $r, rp_1, rp_2, \ldots$, taking into account that the operation p permutes the corresponding indices on the right of (20.6). However, it is simpler to incorporate these additional conditions directly in the definition of the representation $\mathscr{D}_S$ in (20.7).

* See, for example, L.D. Landau and E.M. Lifshits, Statistical Physics, Moscow, 1964, §122. L.D. Landau and E.M. Lifshits, Electrodynamics of Continuous Media, Moscow, 1957, §88.

For example, the symmetry of the tensors ε and P with respect to index permutations implies that they transform according to a representation $\mathscr{D}$, which is the symmetrized product $[\mathscr{D}_1^2]$. By (10.23) and (10.24), for integer j',

$$[\mathscr{D}_{j'}^2] = \sum_{j=0}^{j=j'} \mathscr{D}_{2j}, \quad \{\mathscr{D}_{j'}^2\} = \sum_{j=0}^{j=j'-1} \mathscr{D}_{2j+1}, \tag{20.17}$$

so that $[\mathscr{D}_1^2] = \mathscr{D}_0 + \mathscr{D}_2$.

Symmetry (antisymmetry) of the tensor S_{ik} with respect to permutation of the indices i and k, which of course may occur only if the representations $\mathscr{D}_B$ and $\mathscr{D}_A^*$ are equal, implies that the tensor S transforms according to the symmetrized (antisymmetrized) product $\mathscr{D}_S = [\mathscr{D}_B^2]$ ($\mathscr{D}_S = \{\mathscr{D}_B^2\}$), with characters given by (9.22) ((9.23)).

In that case, if $\mathscr{D}_B = \sum_l \mathscr{D}_l$ then, by (9.22) and (9.23),

$$[\chi^2(g)] = \frac{1}{2}\left\{\left(\sum_l \chi_l(g)\right)^2 + \sum_l \chi_l(g^2)\right\} = \frac{1}{2}\sum_l \{\chi_l^2(g) + \chi_l(g^2)\} + \sum_l \sum_{i \neq l} \chi_i(g)\chi_l(g),$$

i.e.,

$$[\mathscr{D}_B^2] = \left[\left(\sum_l \mathscr{D}_l\right)^2\right] = \sum_l [\mathscr{D}_l^2] + \sum_l \sum_{i \neq l} \mathscr{D}_i \mathscr{D}_l; \tag{20.18}$$

similarly, for the antisymmetrized product,

$$\{\mathscr{D}_B^2\} = \left\{\left(\sum_l \mathscr{D}_l\right)^2\right\} = \sum_l \{\mathscr{D}_l^2\} + \sum_l \sum_{i \neq l} \mathscr{D}_i \mathscr{D}_l. \tag{20.19}$$

Note that the expressions (20.18) and (20.19) are valid regardless of whether or not some of the $\mathscr{D}_j$ are identical or whether these representations are irreducible. Thus, for example, by (20.16) – (20.18) and (20.3), the tensor S or C transforms according to the representation

$$\mathscr{D}_S = [(\mathscr{D}_0^+ + \mathscr{D}_2^+)^2] = [\mathscr{D}_0^{+2}] + [\mathscr{D}_2^{+2}] + \mathscr{D}_0^+ \mathscr{D}_2^+ = \mathscr{D}_1^+ + 2\mathscr{D}_2^+ + 2\mathscr{D}_0^+. \tag{20.20}$$

In the absence of a magnetic field, we see from (20.14) that the tensor σ transforms according to the representation

$$\mathscr{D}_\sigma = [\mathscr{D}_1^{-2}] = \mathscr{D}_2^+ + \mathscr{D}_0^+. \tag{20.21}$$

By (20.14), the Hall conductivity tensor σ_H, which describes the current density in a magnetic field via the formula $j_i = \sum_{kl} \sigma_{ikl}^H \mathscr{E}_k H_l$, is antisymmetric with respect to permutation of the first two indices, and so transforms according to the representation

$$\mathscr{D}_{\sigma_H}^H = \{\mathscr{D}_1^{-2}\}\mathscr{D}_1^+ = \mathscr{D}_1^+ \mathscr{D}_1^+ = \mathscr{D}_2^+ + \mathscr{D}_1^+ + \mathscr{D}_0^+. \tag{20.22}$$

In an isotropic medium, whose symmetry is described by the full spherical group, the number of linearly independent tensor components is equal by (20.10), to the number of identity representations $\mathscr{D}_0$ occurring in the representation $\mathscr{D}_S$ according to which the components transform. For example, each of the tensors C and S has two linearly independent components in an isotropic medium, while each of the tensors σ and σ_H has one. If the tensors A and B in (20.1) are decomposed into irreducible representations A_m^l and B_m^l of the group, it follows from (20.13) that only the diagonal components

S^{jj}_{mm} differ from zero for this choice of the components of $\boldsymbol{A}$ and $\boldsymbol{B}$, all components S_{mn} for these j's being identical. If the symmetry is lowered, the representations $\mathscr{D}_j$ with $j \geqslant 1$ (in cubic groups, with $j \geqslant 2$) become reducible and may contain the identity representation of the group. To determine the total number of identity representations in $\mathscr{D}_s$ it is then sufficient to know which of the constituents $\mathscr{D}_j$ of $\mathscr{D}_s$ contains the identity representation and how many times.