Simplification in Finding Symmetry-Adapted Eigenfunctions*

M. A. MELVIN

Department of Physics, Florida State University, Tallahassee, Florida

The problem of finding symmetry-adapted functions (SAF's) belonging to irreducible representations of a group (**R**) is examined. The problem arises when one wishes to determine the states of a complex system in terms of combinations of functions given by some simplified problem (as in the determination of molecular symmetry coordinates, or approximate molecular, atomic or nuclear eigenstates). A standard method for finding SAF's is to project any given function with respect to each row of each representation; the projection operator is the sum of operations of (**R**) each weighted by an element of the corresponding representation matrix. It is shown here that each projection operator can be written simply as a product of two factors: (1) the sum of operations in the identity-mapping or kernel subgroup (**K**) and (2) a weighted sum of operations in a *quotient set* of (**K**). The kernel operator (1) and its quotient operator (2) may often be factored again and the simplification carried on to a reduction to two-term factors, whereupon the testing of a function for its potency to contribute an SAF becomes especially simple. Kernel operators are interpreted intuitively by the symmetry principle. Several examples illustrating the application of the tables of factored projection operators are given. An auxiliary simplification occurs with degenerate representations in which the principal diagonals vanish in a set of the matrices just suitable to reduce the process to one for a subgroup (*devertebrate simplification*). The structures of all the point symmetry groups are analyzed, and tables of factored and simplified projection operators for all irreducible representations are given (except for the icosahedral and spherical groups). All of the dihedral-type groups, the tetrahedral group $\mathcal{T}$, and the didodecahedral group $\mathcal{T}^h$, respectively, admit of devertebrate simplification.

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GLOSSARY OF TERMS AND NOTATIONS

"Rep": "irreducible representation." We urge acceptance of this abbreviation for the following reasons: (a) It is much less ponderous. (b) It serves a useful discriminative function: i.e., the term "representation" can then be used to mean either "reducible representation" or one for which it is not specified whether it is irreducible or not. (c) The quantum-mechanical use of "representation" differs from the group-theoretic use. In quantum theory it refers to the choice of the particular basis or "coordinate system" in which an observable (and likewise a group-theoretic representation) may be expressed. If the word "rep" is available, it becomes possible without excessive awkwardness to introduce the well-established quantum-mechanical terminology, i.e., one may speak of a "rep in a given quantum-mechanical representation."

"jith symmetry type": "The ith row of the jth rep." If the rep is degenerate, then its symmetry types depend upon the particular choice of basis (or "coordinate system").

"Projection operator of the jith symmetry type": A properly weighted sum over the operations of the group which, when operating upon any function f, projects out the component f^{ji} which belongs to the jith symmetry type.

"kernel of a rep": Subgroup consisting of all operations which are mapped by identity matrices in the rep.

"cokernel of the jith symmetry type": Subgroup (see Appendix I) consisting of all operations which are mapped by jth rep matrices having a lone non-vanishing diagonal element equal to 1 in the ith row.

(In parentheses is given the manner of indicating the symbols in manuscript or typescript.)

Scalars: A, a, $\cdots$; complex conjugate: $\bar{A}$, $\bar{a}$
Vectors: $\mathbf{X}$, $\mathbf{x}$, (inferior tilde)
Matrices: $\mathfrak{M}$, $\mathfrak{m}$
Matrix elements: M_{ij}
Groups: $(\mathbf{R})$, $(\mathcal{R})$, or $\mathcal{R}$ (stroke through symbol from upper left to lower right)
particular groups: $\mathcal{C}_3$
Operators: In general: $\mathbf{R}$, $\mathbf{K}$ (inferior tilde)
particular operators: $\mathbf{C}_3$, $\boldsymbol{\sigma}_v$: (inferior tilde)
Group elements: see operators.
Classes: same symbol as symmetry operators, but not bold face: C_3
Characters: χ^j of jth representation.
Representations: In general: Γ^j
of particular point symmetry groups: $A_{1g}\cdots$
Functions belonging to ith row of jth rep: f^{ji}
Projection operators: In general: $\mathbf{p}$, $\mathbf{d}$ (lower case boldface) (inferior tilde)
for particular groups, e.g., $\mathcal{C}_3$: ${}^{ji}\mathbf{c}_3$ jth rep, ith row
for particular groups, e.g., symmetric group $\mathcal{S}_n$: ${}^{mi}\mathbf{s}_n$ mth rep, ith tableau
Dimension of jth representation: l^j
Orders of groups, sets: G, H, K
Quantum-mechanical operators: $\mathbf{H}_0$, $\mathbf{H}$, $\mathbf{L}^2$
Eigenvalues: E, W, $L(L+1)$

I. INTRODUCTION

IT happens in the determination of energy eigenstates of a system[1] that one encounters the following problem: It is desired to find a set of symmetry-adapted functions (SAF's) which exactly or approximately represent eigenfunctions of the complete Hamiltonian. A commonly effective procedure in dealing with the problem is to make up such SAF's as linear combinations of eigenfunctions appropriate to some simplified version of the problem; the technique for doing this is of considerable practical importance and will be the principal object of our inquiry.

The problem comes up in the determination of electronic (or nucleonic) states of atomic[2] or molecular[3] (or nuclear) systems, as well as in the analysis of molecular[4] and macroscopic[5] vibrations. That SAF determination is important for the solution of these complicated eigenstate problems follows from the existence of the very general *expansion theorem*. We shall formally discuss the theorem below; but it may be well to preface this with a verbal discussion of its meaning: Suppose that we are given some group as well as its symmetry types[1] in explicitly chosen forms (i.e., the individual rows of the matrices of all reps are given explicitly, corresponding to a definite choice of the "coordinate system" for each rep; see below). The expansion theorem then asserts that any given function F may be resolved completely into an orthogonal set of component functions or "projections," f^{ji}, each belonging to a different symmetry type of the given group. In essence the expansion theorem is a magnificent generalization of many familiar theorems, and it may be instructive to list a few examples of these, indicating in brackets their setting in the generalized theorem.

[1] The relation between the form of a Hamiltonian $\mathbf{H}$ of a system and of the form of an eigenfunction ψ of that system is, of course, quite various. But there is a universally valid relation between the *symmetry* of the Hamiltonian and the *transformation character* of its eigenfunctions. These functions can serve (singly or, in case of degeneracy, in linear combination with partners) as basis functions for reps (irreducible representations) of the symmetry group of the Hamiltonian. Given any group and its reps in some explicit form: Each of the rows, e.g., the ith, of each rep, e.g., the jth, may be considered to define a distinct "symmetry type." We may call a basis function, f^{ji}, which "belongs" [as defined by Eq. (3)] to such a jith symmetry type, a *symmetry-adapted function* (SAF).

In connection with this concept, there is one general and qualitatively important aspect of the relation between Hamiltonian and eigenfunction which does not seem to have been emphasized sufficiently in the literature: The actual symmetry of a symmetry-adapted eigenfunction, i.e. the set of operations under which it goes *exactly* into itself, is a subgroup of the symmetry of the Hamiltonian. [This relation, and the fact that it is a special case of a general Symmetry Principle, is discussed in Appendix I. For a more detailed discussion of the Symmetry Principle see M. A. Melvin, Proc. Second Can. Math. Cong. (University of Toronto Press, 1951), p. 225. In that paper, however, the connection with representation theory was not stated explicitly.] The subgroups in question are the "kernel subgroups" (for nondegenerate states) and the "cokernel subgroups" (for the eigenfunctions belonging to degenerate states). These subgroups are discussed in detail below. The corresponding "projection operators" have the property of sifting out of any given function that part of it which definitely does not belong to the given symmetry type. The projection operators for the kernels and cokernels of the point symmetry groups are listed in the tables at the end of Sec. V of this paper. It will be seen that the cokernel operators formalize the application of the symmetry principle, i.e. any function whose symmetry is not a subgroup of the Hamiltonian symmetry cannot survive the cokernel operators and therefore cannot be an eigenfunction.

[2] Here it usually presents itself in the following form: Given individual-particle eigenfunctions for a simplified Hamiltonian, one seeks SAF's which represent approximately (in special cases exactly) the eigenfunctions for the actual many particle system. The general theory, and the atomic problem, are treated by E. Wigner [*Gruppentheorie und ihre Anwendung auf die Quantenmechanik der Atomspektren* (Friedrich Vieweg und Sohn, Braunschweig, Germany, 1931; Edwards Brothers, Inc., Ann Arbor, 1944) Ch. XII]. Wigner calls SAF's "right linear combinations" of functions.

[3] In the theory of solid-state and molecular binding, approximate eigenfunctions are built up as symmetry-adapted linear combinations of atomic orbitals or products of such orbitals. A history and bibliography of the early investigations, stemming from the pioneer work of Heisenberg and Dirac, is given by J. C. Slater (*Electronic Structure of Atoms and Molecules*, Technical Report No. 3, Solid-State and Molecular Theory Group, Massachusetts Institute of Technology, Cambridge, Massachusetts). Later work on directed valence is described by J. H. Van Vleck and A. Sherman, Revs. Modern Phys. **7**, 174 (1935); G. E. Kimball, J. Chem. Phys. **8**, 188 (1940).

[4] In the theory of molecular vibrations, symmetry-adapted normal coordinates are built up as linear combinations of displacements from equilibrium positions; see, for example, J. R. Nielsen and L. H. Berryman, J. Chem. Phys. **17**, 659 (1949), or Wilson, Decius, and Cross, *Molecular Vibrations* (McGraw-Hill Book Company, Inc., New York, 1955). Here, where the number of degrees of freedom is finite, eigenfunctions reduce to eigenvectors, and SAF's are known as "symmetry coordinates."

[5] W. Ritz, Ann. Physik **28**, 737 (1909); M. A. Melvin and S. Edwards, J. Acoust. Soc. (to be published); M. A. Melvin (to be published).

(I) *Resolution of a 3-dimensional vector into orthogonal vector components* (this is an expansion in terms of SAF's belonging to the three rows of the $D^{(1)}$ rep of the rotation group—or sphere group—in three dimensions.)

(II) *Resolution of a 3-dimensional symmetric tensor into* (1) *its trace* (*a scalar*), *and* (2) *a 5-legged traceless quantity;* a physical instance is the resolution of a "strain" tensor into (1) a "dilatation" (scalar) and (2) a "shear" (traceless symmetric tensor). [This is an expansion in terms of SAF's belonging (1) to the nondegenerate rep, $D^{(0)}$, of the sphere group and (2) to the 5-dimensional rep, $D^{(2)}$, of the sphere group.]

(IIIa) *Resolution of any function* $f(\theta)$, $0\leq\theta\leq 2\pi$, *in a Fourier series.* (This is an expansion in terms of SAF's belonging to the successive reps—all nondegenerate—of the cyclic group of infinite order, the group of all rotations about a fixed axis.)

(IIIb) *Resolution of any function in terms of a complete series of orthonormal basis functions.* (This is an expansion in terms of SAF's belonging to the successive reps of the invariance group of some operator, i.e., an operator which has the basis function system as a complete set of eigenfunctions.)

It can be seen from these examples that, quite generally, the expansion theorem serves to implement the classical method of mathematical physics since before the time of Fourier: Given a "complicated problem" one first resolves it into a superposition of "simple problems," obtaining in the process a set of resolution coefficients. Next one finds the "simple solutions" to the separated problems. Finally one recombines these solutions, using the original resolution coefficients, to find the "complicated solution" of the original complicated problem. In quantum theory the third step is often not necessary because the simple solutions themselves may have direct observational meaning as eigenvalues and eigenfunctions.

The application of the expansion theorem depends upon the existence of a standard method of finding SAF's. This is described in Sec. II; it gives, for a general function F, its projection belonging to a given row of a given rep. In Sec. III it is shown how the "projection operators" involved may be factored; the factored forms will often simplify practical calculations considerably.

In brief, the formal argument is as follows: Given any rep Γ^j of the group $\mathfrak{R}$. Consider the subset $(\mathbf{K})_i{}^j$ of operations in $\mathfrak{R}$ with the following property exhibited in Γ^j: The representative matrices have, in their ith rows, a lone nonvanishing diagonal element equal to 1. It can be proved (Appendix I) that this set of operations forms a subgroup of $\mathfrak{R}$, which we call the "cokernel" subgroup $(\mathbf{K})_i{}^j$ of the ith row of the jth rep. In case the rep is nondegenerate this reduces to the identity-mapping or "kernel" subgroup $(\mathbf{K})^j$. Let the identity, plus a complete set of coset generators with respect to $(\mathbf{K})^j$, be called a *quotient set* $(\mathbf{Q})_i{}^j$ of $(\mathbf{K})_i{}^j$. There will generally be several alternative quotient sets, all equally suitable. It now follows that the jith projection operator can be written simply as a product of two factors: (1) the sum of operations in the cokernel subgroup $(\mathbf{K})_i{}^j$, (2) a weighted sum of the operations in any of the associated quotient sets $(\mathbf{Q})_i{}^j$. The cokernel operator (1) and its quotient operator (2) may often be factored again and the simplification carried on to a reduction to two-term factors, whereupon the testing of a function for its potency to contribute an SAF becomes especially simple. An important theorem in this connection is that the result of operating with a factored projection operator is independent of the order of the factors.

In Secs. IV and V the structures and reps of all the point symmetry groups are analyzed and tables of factored projection operators for all symmetry types are given. And in Sec. VI four examples are worked out to illustrate the method of factored projection operators; the first and third are from classical continuum mechanics, the second is a simple one-electron problem for a symmetric molecule, and the fourth is a three d-electron problem for a cubic crystalline system. In each case, once the table of factored projection operators (e.g., Tables III.4 and IV.2) is available, one needs to know the transformation behavior of the generating functions *only under a few key symmetry operations* (Tables Va, VIa, VIIa, and VIIIa) in order to work out in a few minutes a table of SAF's (Tables Vb, VIb, VIIb, and VIIIb). In each row of the projection-operator table one needs only to glance through the factors of the projection operator. With any of the two-term factors, it is usually apparent immediately whether the generating function will survive or not. As soon as one notes that it perishes under any factor, whichever is easiest to inspect, one writes "no" in the table of SAF's, and is through with that entry. In those cases where the generating function survives all factors of the kernel operator, and at least one quotient operator, it will survive. In such a case it is often found that certain of the factors leave it unaltered. These "neutral" factors, which neither annihilate nor build up the generating function, can all be ignored in the operational calculation by which the final SAF is found; for, since the result is independent of order, one could imagine the neutral operators all applied first, whereupon they would have made no difference.

It is evident that the generating function may survive *each* factor of the kernel operator, and yet perish under the combined action of two or more factors. The whole procedure is easily carried out systematically with the help of "key" tables like Tables Va, VIa, VIIa, and VIIIa.

A sequel to the present publication will deal with the problem of diagonalizing a perturbed Hamiltonian expeditiously. It will be shown that the tables of factored projection operators can be applied to shorten appreciably the process of finding approximate eigenvalues, or of setting up configuration-interaction secular equations from which such eigenvalues may be found.

A simplification corresponding to that developed here[6] for the finite point symmetry groups may be expected in the treatment of the full rotation(sphere) group, the double symmetry groups, and the symmetric groups. In the latter case factoring of the Young operators should prove highly useful in problems of complex atoms and nuclei.

II. ALGEBRA OF GROUP REPRESENTATIONS. GENERATION OF SYMMETRY-ADAPTED FUNCTIONS

Before presenting the formal relations governing the generation of SAF's it is worthwhile to give a brief review of the fundamentals of representation algebra. The theory actually applies to any group, but, for the sake of concreteness, let us think explicitly of a group of proper linear orthogonal transformations in three dimensions, i.e., one of the proper symmetry groups which we will discuss in detail below. Consider then any such group of pure turn operations. We shall interpret the operations as "extrinsic operations" (see Melvin, reference 1) i.e., as turns of the space-frame, while the geometrical or physical objects which are being viewed from the frame are regarded as "fixed." The description of the objects from the turned frame is naturally altered. For example, under any individual operation $\mathbf{R}$ of the group, a vector described before as $\mathbf{u}$ is now described as $\mathbf{U}$. Formally we may say that "$\mathbf{U}$ results from R operating on $\mathbf{u}$," and we may write symbolically

$$\mathbf{Ru}=\mathbf{U}.$$

Explicitly, let $\mathfrak{R}$ be the matrix in Cartesian coordinates representing the operation $\mathbf{R}$, and let $\mathfrak{u}$ and $\mathfrak{U}$ be the column matrices representing $\mathbf{u}$ and $\mathbf{U}$, respectively, then

$$\mathfrak{R}\mathfrak{u}=\mathfrak{U}.$$

The set of matrices $\mathfrak{R}$, for all $\mathbf{R}$, constitutes a representation of the group; this representation may or may not be reducible depending upon the group. [For all the cyclic and dihedral groups it is reducible, whereas for the tetrahedron, octahedron-cube, and icosahedron-dodecahedron groups it is not (see below).]

In general many other representations (homomorphic groups of matrices) of the group are possible. These representations arise for instance when a suitably chosen set of basis functions are operated on by the operations of the group. In order to make clear what this means one must define explicitly what is meant by an "operation on a function." With the particular kind of group we have chosen for illustration it is natural to think of a function of position, $f(\mathbf{x})$. The function which results when $f(\mathbf{x})$ is operated on by $\mathbf{R}$ is to be interpreted as the *same* function, but of the transformed variables, i.e., of $\mathbf{X}$:

$$\mathbf{R}f(\mathbf{x})\equiv f(\mathbf{Rx})=f(\mathbf{X})\equiv F(\mathbf{x}).$$

The last equality defines F, the *new function of the old variables* which results from $\mathbf{R}$ operating on f.

As an example, suppose that the operation to be carried out is $\mathbf{C}_4$, i.e., a quarter of a whole turn about the z-axis in the positive (counterclockwise) direction. This operation changes the description of a "fixed" vector with old components x, y, z to one with new components X, Y, Z which are equal respectively to $y, -x, z$. We write this symbolically, and in accord with the notation of crystallography,

$$\mathbf{C}_4xyz=XYZ=y\bar{x}z.$$

Now suppose that we have the function $\sin\mu x\cos\nu y$. Under $\mathbf{C}_4$ it becomes

$$\mathbf{C}_4\sin\mu x\cos\nu y=\sin\mu X\cos\nu Y=\cos\nu x\sin\mu y$$

where, as will often be convenient in solving complicated problems, we have rearranged so that the order of occurrence of xyz is alphabetic.

Suppose we have a set of functions f^i such that under all the operations of the group they mix with each other according to

$$\begin{array}{l}\mathbf{R}f^1=\sum_k R_k{}^1f^k\\ \quad\vdots\\ \mathbf{R}f^i=\sum_k R_k{}^if^k\\ \quad\vdots\end{array}$$

Then the set of matrices, $(\mathfrak{R})$, corresponding to the complete set of the operations $\mathbf{R}$, also constitutes a representation of the group. This representation may be reducible under some equivalence transformation $\mathfrak{M}^{-1}(\mathfrak{R})\mathfrak{M}$ or, alternatively, it may be a rep. However, for any group of finite order G there are only a finite number, J, of inequivalent reps. (The number J is always the same as the number of classes in the group.) Suppose these reps are given in explicit forms, i.e., the matrices are explicit. In the jth one, of dimension l^j, let the element in the ith row and kth column of that matrix which represents $\mathbf{R}$ be ${}^jR_i{}^k$. Then a function is said to be a *symmetry-adapted function* and to "belong to the ith row of the jth rep" when it is one of a set of partners which transform under $\mathbf{R}$ by mixing with each other according to

$$\mathbf{R}f^{ji}=\sum_{k=1}^{l^j}{}^jR_k{}^if^{jk}\quad(i=1,2,\cdots,l^j).\qquad(1)$$

[6] After the present investigation was completed, Dr. P. O. Löwdin and the writer discovered some of the mutual relations of our independent work. In Dr. Löwdin's work [Phys. Rev. 97, 1509 (1955); Advances in Phys. 5, 1 (1956)], factored projection operators also occur. His development of these operators is from the point of view of their definition in terms of Hermitian operators with known eigenvalues (e.g. angular momentum). The eigenvalue point of view is perhaps less universally applicable than the group-theoretic point of view; on the other hand its advantage in physical familiarity is great whenever the eigenvalue spectrum is available. It is hoped to unify the two points of view in future work.

The reason for the name may be made clear as follows: Temporarily omitting the rep label j, one can write

$$(\mathbf{R}f^1\mathbf{R}f^2\cdots)=(f^1f^2\cdots)\begin{bmatrix} \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \\ R_i^1 & R_i^2 & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot \end{bmatrix},$$

or in vector-matrix form,

$$\mathbf{Rf}=\mathfrak{f}\mathfrak{R}.$$

As we see, each $\mathbf{R}f$ involves a linear combination of all f's. $\mathbf{R}f^1$ contains f^i with coefficient R_i^1, $\mathbf{R}f^2$ contains f^i with coefficient R_i^2, etc. Thus f^i is associated with the ith row of the matrix of $\mathbf{R}$ in the process of determining the "rotated vector" $\mathbf{Rf}$ from the original $\mathbf{f}$.

We shall often have occasion to describe an f^{ji} satisfying Eq. (1) in another, equivalent, way which is perhaps more intuitive physically: We shall say that f^{ji} "belongs to the jith symmetry type."

To invert (1) one makes use of the basic orthogonality theorem of irreducible representation theory which states that[7]

$$\sum_{\mathbf{R}} {}^j\bar{R}^i{}_k\ {}^{j'}R_{i'}{}^{k'}=(G/l^j)\delta_{jj'}\delta_{ii'}\delta_{kk'}. \tag{1'}$$

Here the sum is over all the operations of the group, and the δ's are the Kronecker symbols. (The well-known orthogonality theorems for characters of reps are of course all corollaries of this.) Multiplying Eq. (1) by the complex conjugate[7] matrix element ${}^j\bar{R}^h{}_i$ and summing over $\mathbf{R}$ it follows from the basic orthogonality theorem, Eq. (1′) that the partners of f^{ji} are given by

$$f^{jh}=\frac{l^j}{G}\sum_{\mathbf{R}} {}^j\bar{R}^h{}_i\ \mathbf{R}f^{ji}. \tag{2}$$

If one sets $h=i$ in Eq. (2) one gets, as a necessary condition (it is also sufficient) for the function to belong to the ith row,

$$f^{ji}=\frac{l^j}{G}\sum_{\mathbf{R}} {}^j\bar{R}^i{}_i\ \mathbf{R}f^{ji}. \tag{3}$$

It is clear from Eq. (3) that any linear combination of ith row functions is a function of the same kind.

To find the SAF's systematically from arbitrarily given eigenfunctions we need the general expansion theorem referred to above. This theorem states: *An arbitrary function F of position, or of any other variables to which the operations* $\mathbf{R}$ *may be applied, can be expanded in a linear sum of basis-functions* (SAF's) f^{ji} ($i=1,\cdots,l^j$, $j=1\cdots J$) *where the function f^{ji} belongs to the ith row of the jth rep*:

$$F=\sum_{j=1}^{J}\sum_{i=1}^{l^j} f^{ji}. \tag{4}$$

For a proof that the f^{ji} functions form a complete set for expansion one may consult Wigner.[8] Assuming this completeness, the indicated expansion may be carried out explicitly with the help of the basic orthogonality theorem. We apply $\mathbf{R}$ to Eq. (4), multiply by ${}^j\bar{R}^i{}_i$ and sum over all $\mathbf{R}$. This gives

$$\sum_{\mathbf{R}} {}^j\bar{R}^i{}_i\mathbf{R}F=\sum_{j'}\sum_{i'}\sum_{\mathbf{R}} {}^j\bar{R}^i{}_i\mathbf{R}f^{j'i'}=(G/l^j)f^{ji}. \tag{5}$$

Thus, *for any F, the function* $\sum_{\mathbf{R}} {}^j\bar{R}^i{}_i\mathbf{R}F$ *belongs to the ith row of the jth rep and may be considered to be the "component" or "projection" of F* with respect to this row.

Now we see how one may derive SAF's systematically. One starts with arbitrary particular functions (e.g., solutions to the actual or simplified eigenfunction problem as found without regard to the full symmetry of the system). By applying Eq. (5) to a sufficient number of linearly independent particular functions one generates a complete set of SAF's appropriate to the reps as given.

III. SIMPLIFICATIONS

A. Factoring the Projection Operator

Equation (5) gives, for a general function F, a process for finding its projection belonging to a given row of a given rep. This process amounts to taking a weighted average of the results of operating on F by all the operations in the group $(\mathbf{R})$. Now, often, in taking a weighted average of any kind one finds it possible to simplify the calculation by lumping together sets of like terms, and then averaging over the sets. An exactly analogous "factoring" of the projection operator occurring in Eq. (5) is possible, and may result in a considerable simplification for practical calculation, as we shall see. Formally the argument is as follows:

Given any rep Γ^j of the group $(\mathbf{R})$. On account of homomorphism, the subset $(\mathbf{K})^j$ of operations in $(\mathbf{R})$ represented in Γ^j by identity matrices is an invariant subgroup of $(\mathbf{R})$. It is the "kernel" of the homomorphism. Let its order be g. Let the identity, $\mathbf{E}$, plus a complete set of coset generators $\mathbf{Q}'$, $\mathbf{Q}''$, $\cdots$ with respect to $(\mathbf{K})^j$ be called a *quotient set* $(\mathbf{Q})^j$ of $(\mathbf{K})^j$. There will generally be several alternative quotient sets, all equally suitable. Then, formally, the group $(\mathbf{R})$ may be factored into a "direct product" of $(\mathbf{K})^j$ and any one of its $(\mathbf{Q})^j$. More explicitly, insofar as the projection process is concerned we have the following.

First simplification theorem A, Γ^j nondegenerate.—To find for an arbitrary function F its projection belonging to Γ^j it is sufficient to average F with respect to $(\mathbf{K})^j$ *alone (i.e. project with respect to the kernel of Γ^j)*

[7] It is assumed implicitly here that all the representations are unitary. The following formulas are equally valid for nonunitary representations however if one interprets $\bar{R}^h{}_i$ to be the hith element of the matrix representing $\mathbf{R}^{-1}$: $\bar{R}^h{}_i=(\mathbf{R}^{-1})^h{}_i$.

[8] See reference 2, p. 121.

and then to take the projection of the result over a quotient set $(\mathbf{Q})^j=\mathbf{E}, \mathbf{Q}', \mathbf{Q}''$. . . . *In short, letting* R^j *represent the character (which is the same as the diagonal matrix element in a nondegenerate* Γ) *of* $\mathbf{R}$, *we have*

$$f^j=\frac{1}{G}\sum_{(\mathbf{R})}\bar{R}^j\,\mathbf{R}F=\frac{1}{G}(\sum\bar{Q}^j\,\mathbf{Q})\cdot(\sum_{(\mathbf{K})^j}\mathbf{K}F)$$

$$=\frac{1}{G}(\mathbf{E}+\bar{Q}'^j\,\mathbf{Q}'+\bar{Q}''^j\,\mathbf{Q}''+\cdots)\cdot(\sum_{(\mathbf{K})^j}\mathbf{K}F). \quad (6)$$

The projection may also be made in the reverse order, first with respect to $(\mathbf{Q})^j$ *and then with respect to* $(\mathbf{K})^j$. *The result is independent of order and of choice of* $(\mathbf{Q})^j$ *among the quotient sets of* $(\mathbf{K})^j$.

The proof of the theorem is almost self-evident. It is contained in the successive steps indicated in Eq. (6) together with the remark that the character R^j corresponding to any operation $\mathbf{R}$ is the same as that Q^j for the coset generator which, when multiplied by some element in $(\mathbf{K})$, yields $\mathbf{R}$; for, by definition, all elements in $(\mathbf{K})$ have the character 1.

A similar theorem may be stated for each row of a degenerate Γ^j, in terms of factoring with respect to the kernel subgroup of Γ^j. But actually a more extensive factoring is often possible. Consider all operations in the group whose representative matrices in Γ^j have a lone nonvanishing diagonal element equal to 1 in some given row. It is proved in Appendix I that this wider set of operations also forms a subgroup (this time not necessarily invariant), and we shall call it the "cokernel" subgroup, $(\mathbf{K})_i{}^j$, of the ith row of the jth rep. Of course, all the cokernels of a given degenerate Γ include its kernel as a common invariant subgroup.

Now, it is easy to prove in the same way that we have the following.

First simplification theorem B, Γ^j *degenerate.—To find for an arbitrary function F its projection belonging to the* i*th row of* Γ^j *it is sufficient to average F with respect to* $(\mathbf{K})_i{}^j$ *alone and then to take the* i*th row projection of this average over a quotient set* $(\mathbf{Q})_i{}^j=\mathbf{E}, \mathbf{Q}', \mathbf{Q}''$, $\cdots$. *In short*

$$f^{ji}=\frac{l^j}{G}\sum_{(\mathbf{R})}{}^i\bar{R}^i{}_i\,\mathbf{R}F=\frac{l^j}{G}(\sum{}^i\bar{Q}^i{}_i\,\mathbf{Q})\cdot(\sum_{(\mathbf{K})_i{}^j}\mathbf{K}F)$$

$$=\frac{l^j}{G}(\mathbf{E}+{}^i\bar{Q}^i{}_i{}'\,\mathbf{Q}'+{}^i\bar{Q}^i{}_i{}''\,\mathbf{Q}''+\cdots)\cdot(\sum_{(\mathbf{K})_i{}^j}\mathbf{K}F). \quad (6')$$

The projection may also be made in the reverse order, first with respect to $(\mathbf{Q})_i{}^j$ *and then with respect to* $(\mathbf{K})_i{}^j$. *The result is independent of order and of the choice of* $(\mathbf{Q})_i{}^j$ *among the quotient sets of* $(\mathbf{K})_i{}^j$.

The proof is contained in the successive steps indicated in Eq. (6′), together with the remark that the diagonal element $K_i{}^i$ in the matrix corresponding to any operation $\mathbf{K}$ is the same as the diagonal element for that coset generator which yields $\mathbf{K}$ (see Appendix I).

Very often, the "kernel (cokernel) operator" $\sum\mathbf{K}(\ )$ may be factored again and again by separating out further subgroups and quotient sets from $(\mathbf{K})$. When $(\mathbf{K})$ is a direct product of two subgroups, either in the strong or in the weak sense,[9] the factoring is especially neat. Similarly one may sometimes factor the original quotient operator further. With small enough factors, the testing and rejection of any given F as a possible source of SAF's belonging to any given (row of a) rep can be done by inspection. This is formalized in the

Second simplification theorem.—By an extension of the procedure indicated in the first theorem, the projection operator can be factored further to the form

$$f^{ji}=(\sum{}^i\bar{Q}^i{}_i\mathbf{Q})_1(\sum{}^i\bar{Q}^i{}_i\mathbf{Q})_2\cdots(\sum\mathbf{K})_1(\sum\mathbf{K})_2\cdots F, \quad (6'')$$

where the order of factors does not matter.

It is only necessary to ascertain that any one of its factors operating upon a given F gives zero to decide that F has no projection belonging to the ith row of Γ^j. When F does have a nonvanishing projection, this may be determined readily by evaluating in any order the successive effects of those factors which contribute.

The independence of the left side of Eq. (6″) of the order of factors on the right follows from the discussion in reference 9. Tables indicating the factorization (6″) for all reps of all the finite point symmetry groups (except the icosahedral groups $\mathcal{I}$ and $\mathcal{I}^h$) are given in Sec. VD.

Not only the set of rep matrices consisting of $+1$'s in the main diagonal but also the enlarged set including matrices consisting of -1's along this diagonal forms an invariant subgroup of the entire rep. It will sometimes be convenient, especially in the case of degenerate reps, to single out this larger subgroup. For brevity we will designate it the "prokernel" subgroup and the corresponding projection operator will be called the "prokernel operator."

The method of application of the tables of factored projection operators is illustrated by the examples of Sec. VI.

B. Devertebrate Simplification

Inspection of the form of the matrices in reps of various groups suggests that a simplification might be made in the method of finding SAF's in certain cases by applying Eq. (5) to a subgroup only. Such a sim-

[9] Given two groups $(\mathbf{K})$ and $(\mathbf{Q})$ which have no elements in common except the identity. A group $(\mathbf{R})$ may be said to be a direct product, in the weak sense, of $(\mathbf{K})$ and $(\mathbf{Q})$ if all products formed by taking an operation of $(\mathbf{K})$ on the left and of $(\mathbf{Q})$ on the right are included among and include all products formed in the opposite way, and likewise include and are included among the operations of $(\mathbf{R})$. It is said to be a direct product in the strong sense (this is the usual sense) if, in addition, the individual operations of the two groups commute with each other: $\mathbf{K}_p\mathbf{Q}_q=\mathbf{Q}_q\mathbf{K}_p$. For our purposes, since what occurs in the projection operator is the (weighted) sum of all the operations, direct products in the weak sense are equally admissible with those in the strong sense.

plification will be possible for the ith row of the jth rep of a group $(\mathbf{R})$ provided the following condition is satisfied: The principal-diagonal element ${}^i\bar{R}^i{}_i$ must vanish for all rep matrices except those belonging to a subgroup $(\mathbf{H})$ of $(\mathbf{R})$.

$$ {}^i\bar{R}^i{}_i=0. \quad \text{except for } \mathbf{R} \text{ in } (\mathbf{H}) \qquad (7)$$

Naturally this reduction can only occur for degenerate reps since for nondegenerate reps the matrices (characters) are never zero. Upon passage from $(\mathbf{R})$ to $(\mathbf{H})$, the irreducible matrices of dimension l^j may become reduced in such a way that the ith row now belongs to a rep of dimension $l_H{}^{ji}$ of the subgroup $(\mathbf{H})$.

If the subgroup condition (7) is satisfied, it will follow from Eq. (5) that an SAF belonging to the ith row of the jth rep of $(\mathbf{R})$ also belongs to a corresponding row of a rep in the subgroup $(\mathbf{H})$ of $(\mathbf{R})$, i.e.,

$$(f^{ji})_R=\frac{l^j}{G}\sum_{\mathbf{R}}({}^i\bar{R}^i{}_i\mathbf{R}f^{ji})_R$$
$$=\frac{Hl^j}{Gl_H{}^{ji}}\frac{l_H{}^{ji}}{H}(\sum_{\mathbf{R}}{}^i\bar{R}^i{}_i\mathbf{R}f^{ji})_H=\frac{Hl^j}{Gl_H{}^{ji}}(f^{ji})_H. \qquad (8)$$

The numerical factor in the ratio of $(f^{ji})_R$ to $(f^{ji})_H$ is of course irrelevant to the transformation character. With the help of the correspondence (8) one may be able to cut down considerably the tediousness of calculating SAF's. Whenever Eq. (7) holds one may say that row SAF simplification is possible, and that $(\mathbf{H})$ is the reducing subgroup for the ith row of the jth rep of $(\mathbf{R})$.

If we limit outselves to considering the restricted case, where there is a common reducing subgroup $(\mathbf{H})$ for all rows of a given rep, the theory simplifies. All the principal-diagonal elements of the matrices in the cosets of $(\mathbf{H})$ must then vanish simultaneously. In Sec. V we shall examine the instances in which this case of simultaneous simplification for all rows of a rep occurs among the point symmetry groups.

We may call a matrix whose principal diagonal elements all vanish a devertebrate matrix. It is clear that if simultaneous SAF simplification is to be possible there must be the proper number of cosets of devertebrate matrices in the rep, e.g., at least half of the matrices in the rep must have zero characters. However, the character of a matrix may be zero without it being devertebrate. Thus we have, as a necessary *character condition*

(C): *A necessary but not sufficient condition for* SAF *simplification to be possible simultaneously for all rows of a degenerate rep is that the characters for at least half the group elements vanish. For the existence of a simultaneously reducing subgroup of index* 3, 4, 5, $\cdots$ *the characters of at least* 2/3, 3/4, 4/5, $\cdots$, *respectively, of the group elements must vanish.*

On account of the invariance of the characters, this criterion will apply to SAF's corresponding to a given rep no matter what similarity transformation is made.

IV. THE POINT SYMMETRY GROUPS

We shall try to ascertain for all the point symmetry groups what simplifications are possible. In order to do this we must examine the reps for all these groups. As a preliminary we review their abstract group structure. This structure indicates isomorphisms and invariant

FIG. 1. The possible symmetries around a point. Except for one or two innovations the usual Schoenflies notation for the symmetry operations and groups has been used. In the illustrations of finite order groups we have not used the customary stereographic projection. Rather, for the sake of easy picturization, each representative particle in the symmetrical system is considered to be a source of rays spreading out with a fixed solid angle. In other words, a more distant particle under another particle projects in the same location but with smaller size. If the system has a mirror perpendicular to the figure axis, then this mirror coincides with the plane of projection. Likewise, if there is a center of symmetry, the plane of projection contains this center. An open circle, with a right-handed "thumb," i.e., a palm-up right hand, represents the position of a right-handed particle lying above the plane of projection. Further palm-up right hands of the same size stand for other equivalent particles obtained from the first one by symmetry turns about the figure axis. An open circle, with a left "thumb," represents the position of a left-handed particle lying above the plane of projection. Such a particle is obtained from an equivalent right-handed particle by reflection through a mirror passing through the figure axis, and is shown with the same size. Solid circles with *right* or *left* "thumbs" (and of smaller size), i.e., palm-down left or right hands—represent the corresponding left-handed or right-handed particles lying below the plane of projection. These "more distant" particles are obtained from the first ones by reflecting through the plane of projection when it is a mirror, by inverting through the figure center when it is a symmetry center, by mirror turns about the figure axis, or by half-turns about twofold axes lying in the plane of projection when these symmetry elements occur. The positions of open and solid right and left hands determine the symmetry group. The figures also show the different symmetry elements of each group. They are described as follows:

Full and dashed large circles, respectively, denote that the system has one or no mirror in the plane of projection. Such a mirror if present is designated σ_h. The operation of reflecting in σ_h is written $\boldsymbol{\sigma}_h$.

Full lines show intersections of vertical mirrors $(\boldsymbol{\sigma}_v)$ with plane of projection. The operation of reflecting in σ_v is written $\boldsymbol{\sigma}_v$.

Dashed lines indicate twofold axes of symmetry C_2 in plane of projection (dihedral-type groups). Half-turns about such axes are labeled $\mathbf{D}$ or $\mathbf{D}'$ instead of the customary $\mathbf{C}_2'$ or $\mathbf{C}_2''$.

If vertical mirrors do not coincide with D-axes, but lie between, they are labeled σ_d.

Solid ellipses, triangles, squares, hexagons, or generally p-gons, are endpoints of twofold, threefold, fourfold, sixfold, or p-fold axes, respectively; such signs in center of figures represent p-fold axes C_p in z-direction, i.e., perpendicular to plane of projection (basic operation $\mathbf{C}_p$). An (n/p)th part of a turn about the principal axis in a cyclic- or dihedral-type group is labeled $\mathbf{C}_p{}^n$. Ellipses at the end of full lines in the plane of projection indicate that intersection of σ_v with σ_h is also a C_2 axis.

Open ellipses, squares, hexagons, etc., are end points of twofold, fourfold, and sixfold alternating mirrors or "axes of rotary reflection" S_p (basic operation $\mathbf{S}_p$), respectively. (In an alternating mirror one has to rotate the system about an axis and concurrently reflect across a plane perpendicular to that axis. A twofold alternating mirror is identical with a center of symmetry ι.)

The classes within each group are indicated by writing a representative operation; the small numeral on top gives the number of operations within the class.

The symbols for the symmetry groups are essentially those of Schoenflies except that the group subtype is characterized by a superscript instead of an extra subscript. For the sake of uniformity and to make the notation discriminative we have introduced as alternatives to Schoenflies' $\mathcal{S}_{2q}$ and $\mathcal{C}_q{}^i$ the symbols $\mathcal{C}_q{}^a$ (q even) and $\mathcal{C}_q{}^a$ (q odd). The upper a in contrast with h means that the group contains only an *alternating mirror* (or rotary-reflection axis) rather than a direct mirror σ_h.

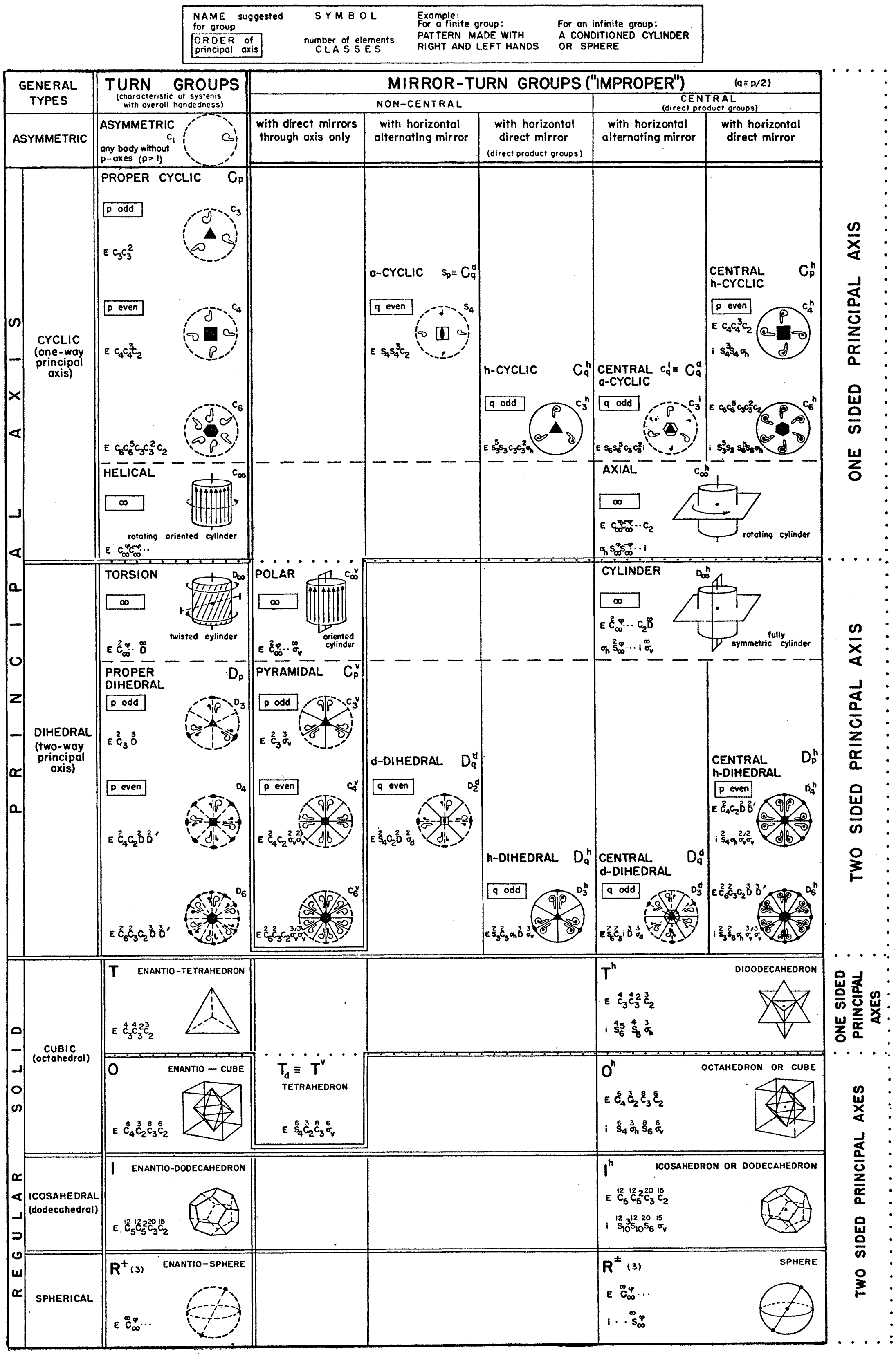

FIG. 1. (See caption on page 24.)

subgroup relations between the groups, and knowledge of these materially simplifies the problem.

The different kinds of groups and their relations may be derived concisely in two main steps.[10] First all the proper (turn) groups are derived by considering the possible regular tesselations of a sphere. This leads to the cyclic, dihedral, and regular-solid turn groups, any one of which may be designated by the generic symbol $(\mathbf{T})$.

Once the turn groups are known all the remaining point groups are derivable on the basis of the following theorem[11]:

All improper symmetry point groups are either of central type:

$$(\mathbf{A})_{\text{central}} = (\mathbf{T})(\mathcal{C}^i) \tag{9}$$

comprising the direct product of all turn groups with the origin-inversion group, or else they are of noncentral type:

$$(\mathbf{A})_{\text{noncentral}} = ((\mathbf{T}'), \mathbf{A}_r(\mathbf{T}')) \tag{9'}$$

obtained from the coset decomposition of all turn groups containing halving subgroups $(\mathbf{T}')$ (i.e., *subgroups of index* 2). $(\mathbf{A})_{\text{noncentral}}$ *is obtained from the corresponding turn group by multiplying the coset generating element* $\mathbf{T}_r$ *by the inversion operator:* $\mathbf{A}_r = \boldsymbol{\iota}\mathbf{T}_r$. *Although it is not contained in* $(\mathbf{T}')$, $\mathbf{T}_r$ *is necessarily the square root of some element in it. Any odd power of* $\mathbf{A}_r$ *will serve equally well as a coset element for* $(\mathbf{A})_{\text{noncentral}}$. *If the half-order q of* $\mathbf{T}_r$ *is odd, one of the possible coset elements is a pure reflection and then* Eq. (9′) *may be written, analogously to* Eq. (9), *in the concise form of a direct product of two subgroups.*

In Fig. 1 we present a chart[12] classifying the various types of groups, as derived on the basis of the foregoing theorem. We have illustrated all the different types by examples of systems having those symmetries; incidentally, these examples include most of the crystallographic groups, e.g., nearly all those with principal axes of order greater than two.

In the chart we have tried to exhibit clearly the isomorphisms and invariant subgroup relations between all the groups by arranging them in such a way that these relations may be read off upon inspection: All groups on the same horizontal row are isomorphic except that the central direct mirror groups, in the last column, include the others as halving (therefore invariant) subgroups. In addition, the classes of conjugate (equivalent) operations within each particular illustrative group are given, with the classes in isomorphic groups, on the same horizontal row, in corresponding order[13]; these class correspondences are easily generalized, from the examples given, to groups of any order. In Table I.1 essentially the same arrangement of groups is presented in more abstract form; invariant subgroup relations in the vertical as well as horizontal directions are easily read off. Which reps correspond to which in the various cases of isomorphic groups and invariant subgroups can be read off from standard correlation tables in the literature.

V. IRREDUCIBLE REPRESENTATIONS OF THE POINT SYMMETRY GROUPS

A. Factoring in the Cyclic-Type Groups

All the reps of every cyclic-type group are one-dimensional.[14] Explicitly, the jth rep of $\mathcal{C}_p$ consists of the jth power of $\epsilon = \exp(i2\pi/p)$ and all successive powers of ϵ^j; it is convenient to take j here with the range $0, \pm 1, \cdots \pm (p-1)/2$ (p odd), and $0, p/2, \pm 1, \cdots \pm [(p/2)-1]$ (p even). The 0-index or "identity" rep is called A, and the $p/2$-index rep (p even) is called B. All the other pairs are labeled by the conventional symbol for doubly degenerate reps, E, with the corresponding index. This calls for some explanation: Strictly, from the point of view of space-symmetry alone, there are no degenerate reps in the cyclic-type groups. However, on account of the frequent occurrence of time-inversion symmetry in physical systems, functions belonging to complex conjugate reps $(\pm j)$ are frequently degenerate with each other and the corresponding reps are conventionally taken together as forming a ("separably") degenerate rep.[5]

All the improper noncentral cyclic groups are isomorphs of $\mathcal{C}_p$ groups and therefore have the same reps. Finally, the reps of the central cyclics are obtained from those of the corresponding $\mathcal{C}_p$'s by taking the direct product with the reps of the inversion group $\mathcal{C}^i$, i.e., with $[1][1]$ and $[1][-1]$.

The general pattern of the factoring in $\mathcal{C}_p$ is as follows: The projection operator ${}^j\mathbf{c}_p$, for the jth rep of $\mathcal{C}_p$ may be summed formally to give

$${}^j\mathbf{c}_p = \sum_{k=0}^{p-1} \epsilon^{jk}\, \mathbf{C}_p{}^k = \frac{\mathbf{E} - (\epsilon^j\, \mathbf{C}_p)^p}{\mathbf{E} - \epsilon^j\, \mathbf{C}_p}, \tag{10}$$

where $\mathbf{C}_p{}^0 = \mathbf{E}$ plays the role of unity in the sum $1 + x + \cdots + x^{p-1}$. The numerator on the right may be factored according to the p roots of unity, 1, ϵ, ϵ^2,

[10] M. A. Melvin, Proc. Second Canadian Mathematical Congress (University of Toronto Press, 1951), p. 225.

[11] In essence this theorem is old. In content, if not form, it was probably known to Pierre Curie [*Oeuvres*, pp. 78, 114; Bull. de la Soc. minéralogique de France, t. **VII**, p. 418 (1884); and Compt. rend., tome C, p. 393 (1885)] who first emphasized the existence and importance of general rotary-reflection symmetries. A proof for the crystallographic point groups is given by W. H. Zachariasen [*Theory of X-Ray Diffraction in Crystals* (John Wiley and Sons, Inc., New York, 1945), p. 40]. A general proof, for all point groups, is given in Appendix II at the end of this paper.

[12] A rudimentary version of this chart, with an unfortunately original notation, will be found in the earlier paper[10] by the author. In the present version we use the standard Schoenflies notation except for slight innovations: A half-turn about a twofold axis perpendicular to the principal axis in a dihedral-type group is labeled $\mathbf{D}$ or $\mathbf{D}'$ instead of $\mathbf{C}_2$ or $\mathbf{C}_2'$.

[13] These isomorphic correspondences are not unique. Of the various possibilities one fairly natural correspondence is that exhibited in the chart.

[14] A. Speiser, *Die Theorie der Gruppen* (Verlag Julius Springer, Berlin, 1937; Dover Publications, New York, 1945), p. 179.

TABLE I. 1. Isomorphisms and invariant subgroup relations among the point symmetry groups. All groups on the same horizontal line are isomorphic with each other unless the symbol (, meaning "invariant subgroup in," appears. Within each half of the table set apart by the horizontal heavy line, each group is an invariant subgroup in a group of the type vertically below it.

	Proper			Improper						
				Noncentral				Central		
				Mirrors through axis		Horizontal alternating mirror	Horizontal direct mirror (direct product groups)	Horizontal alternating mirror	Horizontal direct mirror	
	q odd	q odd	q even	q odd	q even	q even	q odd	q odd	q odd	q even
Cyclic	$\mathcal{C}_q$						$\mathcal{C}_q{}^h$	$\mathcal{C}_q{}^a(=\mathcal{C}_q{}^i)$	($\mathcal{C}_{2q}{}^h$	
		$\mathcal{C}_{2q}$								
			$\mathcal{C}_{2q}$			$\mathcal{C}_q{}^a(=\mathcal{S}_{2q})$				($\mathcal{C}_{2q}{}^h$
	$\mathcal{C}_\infty$							($\mathcal{C}_\infty{}^h$		
Dihedral	$\mathcal{D}_\infty$			$\mathcal{C}_\infty{}^v$				($\mathcal{D}_\infty{}^h$		
	$\mathcal{D}_q$			$\mathcal{C}_q{}^v$						
		$\mathcal{D}_{2q}$		$\mathcal{C}_{2q}{}^v$			$\mathcal{D}_q{}^h$	$\mathcal{D}_q{}^d$	($\mathcal{D}_{2q}{}^h$	
			$\mathcal{D}_{2q}$		$\mathcal{C}_{2q}{}^v$	$\mathcal{D}_q{}^d$				($\mathcal{D}_{2q}{}^h$
	$\mathcal{V}(=\mathcal{D}_2)$							($\mathcal{V}^h(=\mathcal{D}_2{}^h)$		
Tetrahedral	$\mathcal{T}$							($\mathcal{T}^h$		
Cube-octahedral	$\mathcal{O}$			$\mathcal{T}^v(=\mathcal{T}_d)$				($\mathcal{O}^h$		
Dodeca-icosahedral	$\mathcal{I}$							($\mathcal{I}^h$		
Spherical	$\mathcal{R}^+(3)$							($\mathcal{R}^\pm(3)$		

$\cdots, \epsilon^{p-1}$, and we get

$$^j\mathbf{c}_p=\prod_{k=1}^{p-1}(\epsilon^k\,\mathbf{E}-\epsilon^j\,\mathbf{C}_p)=\prod_{k=1}^{p-1}(\mathbf{E}-\epsilon^{j-k}\,\mathbf{C}_p). \quad (10')$$

The factored form (10′) for the projection operators may sometimes be more useful than the familiar series form in that it indicates effectively when a function has no part in the jth row; though for actually calculating a nonvanishing part it is probably more cumbersome. We shall not discuss it any further here.

At this point we take note of the kernel subgroups and operators of the various reps of $\mathcal{C}_p$. We shall merely sketch the method of analysis since high-order cyclic groups are not common. Also we exclude the case $j=0$ (identity rep) from the discussion since in it the kernel is always $\mathcal{C}_p$ itself. From the form of the character of $\mathbf{C}_p{}^k$ in E_j, i.e., $e^{\pm ik2\pi i/p}$, it is evident that the general condition for the kth power element to belong to the kernel (prokernel) of E_j is

$$k=np/j \quad n=0,1,\cdots j-1 \quad (n=\tfrac{1}{2},\cdots j-\tfrac{1}{2}).$$

The upper limit to n is set by the fact that the largest value of k is $p-1$. It is clear that E_j for $j=1$ can never have other than the trivial kernel consisting of the identity element $\mathbf{E}$. *The same is true for any j which is relatively prime with respect to p.* Further cases may be classified according to the parity of p.

$p=2q+1$ odd.—The kernel for the rep $j=2$ (or, in general, 2^t) is also always trivial; this is a special instance of the case just described in italics. The first odd-order group for which a nontrivial kernel for $j=3$ appears is $p=9$; the kernel then consists of $\mathbf{E}$, $\mathbf{C}_3$, $\mathbf{C}_3{}^2$ and we designate the operator, which is the sum of these elements, by $\mathbf{c}_3$. The same kernel occurs with $j=3$ for all p's which are multiples of 3. A similar analysis may be given for the kernels (and prokernels) of the higher order reps.

$p=2q$ even.—The kernel of the B rep is $\mathcal{C}_q$ and we label the kernel operator $\mathbf{c}_q$. For $j=2$, the kernel is $\mathcal{C}_2$ and the operator is $\mathbf{E}+\mathbf{C}_2\equiv\mathbf{c}$. For $j=3$, the kernel is trivial unless p contains 3 as a factor, in which case the kernel is $\mathcal{C}_3$. For $j=4$, the kernel is $\mathcal{C}_2$ if p is merely simply even (q odd) but is $\mathcal{C}_4$ if p is doubly even (q even). The analysis for higher order reps is similar. Results are given in Table IIb.

TABLE I. 2. Isomorphic generating elements in the dihedral-type groups. Reducing subgroups, and projection operators for the complex reps in both cyclic- and dihedral-type groups.

Isomorphs of the proper dihedral groups	"C" element	"D" element	Invariant subgroup of "C" elements. The reducing subgroup	Projection operators for the jth rep (1st row: $+j$, 2nd row: $-j$)		
$\mathfrak{D}_p$	$\mathbf{C}_p$	$\mathbf{D}$	$\mathfrak{C}_p$	${}^j\mathbf{c}_p$		
$\mathfrak{C}_p{}^v$	$\mathbf{C}_p$	$\boldsymbol{\sigma}_v$	$\mathfrak{C}_p$	${}^j\mathbf{c}_p$		
$\mathfrak{D}_q{}^d$	$\mathbf{S}_{2q}$	$\mathbf{D}$	$\mathfrak{C}_q{}^a \equiv \mathfrak{C}_q{}^i$ q odd $\mathfrak{S}_{2q}$ q even	E_{jg}: $\mathbf{i}\cdot{}^j\mathbf{c}_q$ E_{2k}: $\mathbf{c}\cdot{}^{2k}\mathbf{s}_{2q}{}^q$	E_{ju}: ${}^{-}\mathbf{i}\cdot{}^j\mathbf{c}_q$ E_{2k+1}: ${}^{-}\mathbf{c}\cdot{}^{2k+1}\mathbf{s}_{2q}{}^q$	
q odd: $\mathfrak{D}_q{}^h$	$\mathbf{S}_q$	$\mathbf{D}$	$\mathfrak{C}_q{}^h$	E_j': $\mathbf{c}^s\cdot{}^j\mathbf{c}_q$	E_j'': ${}^{-}\mathbf{c}^s\cdot{}^j\mathbf{c}_q$	
$\mathfrak{D}_{2q}{}^h$	$\mathbf{C}_{2q}$	$\mathbf{D}$	$\mathfrak{C}_{2q}{}^h$	E_{jg}: $\mathbf{i}\cdot\mathbf{c}\cdot{}^j\mathbf{c}_q$ $\mathbf{i}\cdot{}^{-}\mathbf{c}\cdot{}^j\mathbf{c}_q$	E_{ju}: ${}^{-}\mathbf{i}\cdot\mathbf{c}\cdot{}^j\mathbf{c}_q$ ${}^{-}\mathbf{i}\cdot{}^{-}\mathbf{c}\cdot{}^j\mathbf{c}_q$	(j even) (j odd)
$q=2r$: $\mathfrak{D}_{4r}{}^h$	$\mathbf{C}_{4r}$	$\mathbf{D}$	$\mathfrak{C}_{4r}{}^h$	$\mathbf{i}\cdot\mathbf{c}\cdot(\mathbf{E}+\mathbf{C}_4)\cdot{}^j\mathbf{c}_{4r}{}^{r-1}$	${}^{-}\mathbf{i}\cdot\mathbf{c}\cdot(\mathbf{E}+\mathbf{C}_4)\cdot{}^j\mathbf{c}_{4r}{}^{r-1}$	(j double even)
				$\mathbf{i}\cdot\mathbf{c}\cdot(\mathbf{E}-\mathbf{C}_4)\cdot{}^j\mathbf{c}_{4r}{}^{r-1}$	${}^{-}\mathbf{i}\cdot\mathbf{c}\cdot(\mathbf{E}-\mathbf{C}_4)\cdot{}^j\mathbf{c}_{4r}{}^{r-1}$	(j double odd)
				$\mathbf{i}\cdot{}^{-}\mathbf{c}\cdot{}^j\mathbf{c}_{4r}{}^{2r-1}$	${}^{-}\mathbf{i}\cdot{}^{-}\mathbf{c}\cdot{}^j\mathbf{c}_{4r}{}^{2r-1}$	(j odd)

$$\mathbf{i}\equiv\mathbf{E}+\boldsymbol{\imath} \qquad \mathbf{c}\equiv\mathbf{E}+\mathbf{C}_2 \qquad \mathbf{c}^s\equiv\mathbf{E}+\boldsymbol{\sigma}_h \qquad {}^j\mathbf{s}_{2q}{}^q\equiv\mathbf{E}+\epsilon^j\,\mathbf{S}_{2q}+\dots\epsilon^{(q-1)j}\,\mathbf{S}_{2q}{}^{q-1}$$

$$({}^{-}\mathbf{i})\equiv\mathbf{E}-\boldsymbol{\imath} \qquad ({}^{-}\mathbf{c})\equiv\mathbf{E}-\mathbf{C}_2 \qquad ({}^{-}\mathbf{c}^s)\equiv\mathbf{E}-\boldsymbol{\sigma}_h \qquad {}^j\mathbf{c}_q\equiv\mathbf{E}+\epsilon^j\,\mathbf{C}_q+\dots\epsilon^{(q-1)j}\,\mathbf{C}_q{}^{q-1}$$

$${}^j\mathbf{c}_{4r}{}^s\equiv\mathbf{E}+\epsilon^{\pm j}\,\mathbf{C}_{4r}+\dots\epsilon^{\pm js}\mathbf{C}_{4r}{}^s$$

We have already implied above that the factoring of the projection operators for $\mathfrak{C}_p$ is not too important practically because the original form in Eq. (10) is fairly simple to use. What is of frequent practical value is the factoring of the projection operators of the more complex groups down to the cyclic projection operators, and to such 2-term factors as $\mathbf{c}^s\equiv\mathbf{E}+\boldsymbol{\sigma}_h$, $\mathbf{i}\equiv\mathbf{E}+\boldsymbol{\imath}$, $\cdots$; and it is this factoring on which we have mainly concentrated in the tables at the end of this paper.

Before leaving the topic, it is interesting however to consider still a third form, which is readily obtained, for the cyclic projection operators. From Eq. (10) we see that since $\epsilon^{jp}=e^{j2\pi i}=1$, and $\mathbf{C}_p{}^p=\mathbf{E}$, the operator ${}^j\mathbf{c}_p$ operating on any function F clearly gives zero unless, simultaneously, $(\mathbf{E}-\epsilon^j\,\mathbf{C}_p)F=0$. In other words, *for any function F, only that "part" which is exactly recovered under the operation $\epsilon^j\,\mathbf{C}_p$ survives the projection into the jth row.* The exact "part" which is recoverable under the operation $\epsilon^j\,\mathbf{C}_p$ is given by certain terms in the Fourier expansion of F with respect to φ, the angle about the principal axis. Only the terms in $e^{-Ki\varphi}$ where $K-j=np$ ($n=0, \pm 1, \cdots$) will recover exactly, and therefore survive, under the operation $\epsilon^j\,\mathbf{C}_p$. This is clear from the fact that this operation simply multiplies each such term by the phase factor $e^{(j-K)2\pi i/p}$. Thus, applying the general formula for the Fourier coefficients, we arrive at the expression

$${}^j\mathbf{c}_p\,F=\frac{1}{2\pi}\int_{K=np+j,\ \text{all}\ n}^{2\pi} d\varphi'\,e^{Ki(\varphi'-\varphi)}\,F(\varphi',\cdots). \qquad (10'')$$

In words we may state this as the cyclic projection theorem: *The projection of any function F upon the jth rep of the cyclic group $\mathfrak{C}_p$ is given by a regularly picked subseries of the Fourier series of F; this subseries consists of all terms of index $np+j$ where n takes on all integral values.*

For the limiting case of the full two-dimensional rotation group, $\mathfrak{C}_\infty$, this reduces to the familiar result that the projection of any function F upon the jth rep is simply the jth term in the Fourier series of F. In general, for systems with a high order of symmetry the first term or two obtained by (10″) should provide a good approximation in contrast to the series expression in Eq. (10) which becomes increasingly cumbersome for large values of p. The limiting case where only one term is retained corresponds to the "free-electron approximation" which is now being used in studies of long chain molecules. Thus (10″) appears to provide a formulation by which one may pass continuously from the linear combination atomic orbitals (LCAO) approach to the free-electron model in the study of molecular structure.

Various simplifications by factoring, according to their structure, occur for the other cyclic type groups. These are exhibited in Tables I.2, I.3, III.1a, and III.1b.

B. Simplification and Factoring in the Dihedral Type Groups

1. *The Dihedral Representations in Complex Form*

We now consider the proper dihedral groups and their isomorphs. These include the $\mathfrak{C}_p{}^v$ groups and all the improper dihedral groups with the exception of the central h-dihedral type, $\mathfrak{D}_{2q}{}^h$. Any such proper dihedral-type group (order $2p$) is generated by two elements, $\mathbf{C}$ and $\mathbf{D}$, and its abstract structure is indicated by the equations

$$\mathbf{C}^p=\mathbf{E} \quad \mathbf{D}^2=\mathbf{E} \quad \mathbf{D}^{-1}\mathbf{C}\mathbf{D}=\mathbf{C}^{-1}, \qquad (11)$$

where the collection of pth-order elements $\mathbf{C}$ form an invariant subgroup of index 2. These subgroups are of cyclic type and can be read off from Fig. 1 or Table I.1 by proceeding vertically up. The "$\mathbf{C}$" elements in the various groups are either elementary rotations or rotary reflections, whereas the "$\mathbf{D}$" elements, in every case but one, are half-turns about an axis perpendicular to the principal axis. In the case of $\mathfrak{C}_p{}^v$, $\boldsymbol{\sigma}_\mathbf{v}$ is the "$\mathbf{D}$" element (see Table I.2).

A complete set of reps for the proper dihedral groups are given by Speiser.[14] These are naturally also reps for the isomorphic groups. There are always two nondegenerate reps labeled A_1 and A_2, respectively. A_1 is the identity rep $\mathbf{C}\sim 1$, $\mathbf{D}\sim 1$ and A_2 parallels it except that $\mathbf{C}\sim 1$ and $\mathbf{D}\sim -1$. In the cases where the order p of the principal axis of the group is even, there are two more nondegenerate reps labeled B_1 and B_2, respectively. In B_1, $\mathbf{C}\sim -1$ and $\mathbf{D}\sim 1$ whereas in B_2 $\mathbf{C}\sim -1$ and $\mathbf{D}\sim -1$. The kernels and quotient sets are readily inferred and are indicated in Tables III.2–III.4.

Besides the nondegenerate reps there are $(p-1)/2$ (p odd) or $(p/2)-1$ (p even) degenerate reps. All the degenerate reps are of dimension 2. The jth one is indicated by

$$\mathbf{C}\sim\begin{pmatrix} \epsilon^j & 0 \\ 0 & \epsilon^{-j} \end{pmatrix} \quad \mathbf{D}\sim\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \epsilon\equiv\exp(2\pi i/p). \tag{12}$$

As we see, in this case devertebrate simplification is possible. By doing the calculation with its cyclic-type subgroup of "$\mathbf{C}$" elements, instead of with the dihedral-type group, one needs to find the effect $(\mathbf{R}F)$ of only half as many symmetry operations on the generating functions F; furthermore, the sum in Eq. (5), corresponding to each row, involves only half as many terms. The analysis into kernel subgroups and further simplification by factoring is then quite similar to that for the cyclic groups.

In the case of the $\mathfrak{D}_{2q}{}^h$ groups the elements $\mathbf{C}$ and $\mathbf{D}$ must be supplemented by the inversion $\boldsymbol{\imath}$ which commutes with all elements and which is represented by

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ in } E_g \quad \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \text{ in } E_u. \tag{12$'$}$$

Here again the simplifying subgroup in which reduction is possible is the invariant subgroup represented in Table I.1 vertically above the $\mathfrak{D}_{2q}{}^h$ group, i.e. $\mathfrak{C}_{2q}{}^h$.

2. *The Dihedral Representations in Real Form*

By means of a single unitary equivalence transformation it is possible to put all the reps (12) and (12′) into real forms. This is especially desirable if we wish to deal only with real basis functions. The unitary matrix which accomplishes this reality transformation is

$$\mathfrak{U}=\begin{pmatrix} 1/\sqrt{2} & i/\sqrt{2} \\ i/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}.$$

Upon operating with $\mathfrak{U}^{-1}(\ )\mathfrak{U}$ on the matrices of the jth degenerate rep of a dihedral-type group with axis of order p we find (setting $2\pi/p\equiv a$)

$$\begin{aligned} \mathbf{C}^k&\sim\begin{pmatrix} \cos kja & -\sin kja \\ \sin kja & \cos kja \end{pmatrix}, \\ \mathbf{C}^k\mathbf{D}&\sim\begin{pmatrix} -\sin kja & \cos kja \\ \cos kja & \sin kja \end{pmatrix}. \end{aligned} \tag{13}$$

In the $\mathfrak{D}_{2q}{}^h$ groups the added elements coming from $\boldsymbol{\imath}$ retain their form (12′) under this unitary transformation.

Only in certain groups and certain reps does the form (13) permit of devertebrate simplification. In any group whose principal axis is double-even in order, $p=4r$, we will get devertebrate simplification in the rep (13) corresponding to $j=r$. For then all elements of the form $\mathbf{C}^{2n+1}$ or $\mathbf{C}^{2n}\mathbf{D}$ are devertebrate and the remaining elements make up the reducing subgroups listed in Table I.3.

For example, let us consider the group $\mathfrak{D}_4{}^h$ and the E_g (or E_u) rep. Here $p=4$ and $j=1$, and the matrices corresponding to

$$\begin{array}{llll} \mathbf{C}\equiv\mathbf{C}_4 & \mathbf{C}_4{}^3 & \mathbf{D}=\mathbf{D}'_{,\pi/4} & \mathbf{C}^2\mathbf{D}=\mathbf{D}'_{,3\pi/4} \\ \boldsymbol{\imath}\mathbf{C}=\mathbf{S}_4{}^3 & \boldsymbol{\imath}\mathbf{C}^3=\mathbf{S}_4 & \boldsymbol{\imath}\mathbf{D}=\boldsymbol{\sigma}'_{\mathbf{v},\,3\pi/4} & \boldsymbol{\imath}\mathbf{C}^2\mathbf{D}=\boldsymbol{\sigma}'_{\mathbf{v},\,\pi/4} \end{array}$$

are all devertebrate according to Eq. (13). This shows that the invariant subgroup in which E_g becomes completely reduced is $\mathfrak{D}_2{}^h$, which consists of the following classes:

$$\begin{array}{llll} \mathbf{E} & \mathbf{C}_2 & (\mathbf{D}_{,0}, & \mathbf{D}_{,\pi/2}) \\ \boldsymbol{\imath} & \boldsymbol{\sigma}_\mathbf{h} & (\boldsymbol{\sigma}_{\mathbf{v},\,\pi/2}, & \boldsymbol{\sigma}_{\mathbf{v},\,0}). \end{array}$$

(The invariance of the subgroup goes, of course, with the fact that it contains a whole number of classes of $\mathfrak{D}_4{}^h$.) Thus, in determining symmetry-adapted functions of the $\mathfrak{D}_4{}^h$ group in the rep E_g we need only apply the operations of the group $\mathfrak{D}_2{}^h$. Exactly the same is true for E_u. In the same way the E reps of $\mathfrak{D}_4$, $\mathfrak{C}_4{}^v$, and $\mathfrak{D}_2{}^d$ permit of devertebrate simplification to $\mathfrak{D}_2$, $\mathfrak{C}_2{}^v$, and $\mathfrak{C}_2{}^v$, respectively.

TABLE I. 3. Reducing subgroups and kernels for the rth real rep of the group $\mathfrak{D}_{4r}$, its isomorphs, and $\mathfrak{D}_{4r}{}^h$.

$\mathfrak{D}_{4r}$ and its isomorphs	"C" element	"D" element	Reducing subgroup for the rth representation in its real form	Kernel operator	Quotient operators
$\mathfrak{D}_{4r}$	$\mathbf{C}_{4\mathbf{r}}$	$\mathbf{D}$	$\mathfrak{D}_{2r}$	$\mathbf{d}\cdot\mathbf{c}_\mathbf{r}$ $\mathbf{d}'\cdot\mathbf{c}_\mathbf{r}$	$^-\mathbf{d}'$, $\mathbf{E}-\mathbf{C}_{2\mathbf{r}}$ $^-\mathbf{d}$, $\mathbf{E}-\mathbf{C}_{2\mathbf{r}}$
$\mathfrak{C}_{4r}{}^v$	$\mathbf{C}_{4\mathbf{r}}$	$\boldsymbol{\sigma}_\mathbf{v}$	$\mathfrak{C}_{2r}{}^v$	$\mathbf{c}_\mathbf{r}\cdot\mathbf{c}^\mathbf{v}$ $\mathbf{c}_\mathbf{r}\cdot\mathbf{c}^{\mathbf{v}'}$	$^-\mathbf{c}^{\mathbf{v}'}$, $\mathbf{E}-\mathbf{C}_{2\mathbf{r}}$ $^-\mathbf{c}^\mathbf{v}$, $\mathbf{E}-\mathbf{C}_{2\mathbf{r}}$
$\mathfrak{D}_{2r}{}^d$	$\mathbf{S}_{4\mathbf{r}}$	$\mathbf{D}$	$\mathfrak{C}_{2r}{}^v$	$\mathbf{c}_\mathbf{r}\cdot\mathbf{c}^\mathbf{v}$ $\mathbf{c}_\mathbf{r}\cdot\mathbf{c}^{\mathbf{v}'}$	$^-\mathbf{c}^{\mathbf{v}'}$, $\mathbf{E}-\mathbf{C}_{2\mathbf{r}}$ $\mathbf{c}^\mathbf{v}$, $\mathbf{E}-\mathbf{C}_{2\mathbf{r}}$
$\mathfrak{D}_{4r}{}^h$	$\mathbf{C}_{4\mathbf{r}}$	$\mathbf{D}$	$\mathfrak{D}_{2r}{}^h$	$^\pm\mathbf{i}\cdot\mathbf{d}\cdot\mathbf{c}_\mathbf{r}$ $^\pm\mathbf{i}\cdot\mathbf{d}'\cdot\mathbf{c}_\mathbf{r}$	$^-\mathbf{d}'$, $\mathbf{E}-\mathbf{C}_{2\mathbf{r}}$ $^-\mathbf{d}$, $\mathbf{E}-\mathbf{C}_{2\mathbf{r}}$

TABLE I.4. Characters and matrices of the degenerate reps of the enantiocube group $\mathcal{O}$ and the tetrahedron group $\mathcal{T}_d$. The T's represent rotations about the threefold axes along cube diagonals. D_x and $D_{x'}$ represent half-turns about axes passing through and perpendicular to those midedges which are parallel to the x-axis, etc; the σ's represent mirrors perpendicular to the D's, e.g., σ_x and $\sigma_{x'}$ are those diagonal planes of the cube which are parallel to the x-axis.

	$\mathcal{O}, \mathcal{T}_d$ $\mathcal{O}$ $\mathcal{T}_d$	E $D_{z'}$ $\sigma_{z'}$	C_z D_z σ_z	C_x C_{4z}^3 S_{4z}	C_y C_{4z} S_{4z}^3	T_2 C_{4y}^3 S_{4y}	T_4 C_{4y} S_{4y}^3	T_2^2 C_{4x}^3 S_{4x}	T_4^2 C_{4x} S_{4x}^3	T_1 $D_{x'}$ $\sigma_{x'}$	T_3 D_x σ_x	T_1^2 $D_{y'}$ $\sigma_{y'}$	T_3^2 D_y σ_y
E	Characters	[2]	0 [	2][	][	0			−1][		0		]
	Matrices	$\begin{pmatrix}1&\\&1\end{pmatrix}$	$\begin{pmatrix}1&\\&1\end{pmatrix}$	$\begin{pmatrix}1&\\&1\end{pmatrix}$	$\begin{pmatrix}1&\\&1\end{pmatrix}$	$\begin{pmatrix}-1&-1\\1&\end{pmatrix}$	$\begin{pmatrix}-1&-1\\1&\end{pmatrix}$	$\begin{pmatrix}&1\\-1&-1\end{pmatrix}$	$\begin{pmatrix}&1\\-1&-1\end{pmatrix}$	$\begin{pmatrix}&1\\-1&-1\end{pmatrix}$	$\begin{pmatrix}&1\\-1&-1\end{pmatrix}$	$\begin{pmatrix}-1&-1\\1&\end{pmatrix}$	$\begin{pmatrix}-1&-1\\1&\end{pmatrix}$
		$\begin{pmatrix}&1\\1&\end{pmatrix}$	$\begin{pmatrix}&1\\1&\end{pmatrix}$	$\begin{pmatrix}&1\\1&\end{pmatrix}$	$\begin{pmatrix}&1\\1&\end{pmatrix}$	$\begin{pmatrix}1&\\-1&-1\end{pmatrix}$	$\begin{pmatrix}1&\\-1&-1\end{pmatrix}$	$\begin{pmatrix}-1&-1\\&1\end{pmatrix}$	$\begin{pmatrix}-1&-1\\&1\end{pmatrix}$	$\begin{pmatrix}-1&-1\\&1\end{pmatrix}$	$\begin{pmatrix}-1&-1\\&1\end{pmatrix}$	$\begin{pmatrix}1&\\-1&-1\end{pmatrix}$	$\begin{pmatrix}1&\\-1&-1\end{pmatrix}$
F_1	Characters	[3]	−1 [	−1][	][	1			0][		−1		]
	Matrices	(xyz)	$(\bar{x}\bar{y}z)$	$(x\bar{y}\bar{z})$	$(\bar{x}y\bar{z})$	$(\bar{y}z\bar{x})$	$(\bar{y}\bar{z}x)$	$(\bar{z}\bar{x}y)$	$(z\bar{x}\bar{y})$	(zxy)	$(\bar{z}x\bar{y})$	(yzx)	$(y\bar{z}\bar{x})$
		$(\bar{y}\bar{x}\bar{z})$	$(yx\bar{z})$	$(y\bar{x}z)$	$(\bar{y}xz)$	$(\bar{z}yx)$	$(zy\bar{x})$	$(xz\bar{y})$	$(x\bar{z}y)$	$(\bar{x}\bar{z}\bar{y})$	$(\bar{x}zy)$	$(\bar{z}\bar{y}\bar{x})$	$(z\bar{y}x)$
F_2	Characters	[3]	1 [	−1][	][	−1			0][		1		]
	Matrices	(xyz)	$(\bar{x}\bar{y}z)$	$(x\bar{y}\bar{z})$	$(\bar{x}y\bar{z})$	$(\bar{y}z\bar{x})$	$(\bar{y}\bar{z}x)$	$(\bar{z}\bar{x}y)$	$(z\bar{x}\bar{y})$	(zxy)	$(\bar{z}x\bar{y})$	(yzx)	$(y\bar{z}\bar{x})$
		(yxz)	$(\bar{y}\bar{x}z)$	$(\bar{y}x\bar{z})$	$(y\bar{x}\bar{z})$	$(z\bar{y}\bar{x})$	$(\bar{z}\bar{y}x)$	$(\bar{x}\bar{z}y)$	$(\bar{x}z\bar{y})$	(xzy)	$(x\bar{z}\bar{y})$	(zyx)	$(\bar{z}y\bar{x})$

C. Simplification and Factoring in the Regular Solid Groups

A still better result holds for the enantio-tetrahedral group $\mathcal{T}$, of order 12. It has altogether three 1-dimensional reps including the separably degenerate pair grouped under "E" and one 3-dimensional rep, F, which is given by $\mathcal{T}$ itself represented as a transformation group in Cartesian coordinates. The 1-dimensional reps are all readily factored as indicated in Table IV.1. Further the necessary condition (C) for devertebrate simplification of F to be possible holds, since the eight characters connected with the C_3 and C_3' classes all vanish. To verify whether devertebrate simplification is really possible we must find F itself. Consider a cube (Fig. 2) whose edge directions define the xyz system. Let a tetrahedron be inscribed in the cube in such a way that two opposite (criss-cross) edges of the tetrahedron coincide with the opposite diagonals of opposite faces of the cube. Then the half-turn axes of the tetrahedron lie along the xyz directions, and the operations associated with them constitute $\mathfrak{D}_2 \equiv \mathcal{V}$, an invariant subgroup of index 3 in $\mathcal{T}$. The matrices for this invariant subgroup are all diagonal. All the other operations of $\mathcal{T}$, corresponding to rotations about the threefold axes, permute the xyz axes among each other. Thus these matrices have zeros in the principal diagonal and devertebrate simplification is possible. Upon examination one sees that the successive rows in F correspond to the three nonidentity 1-dimensional reps in $\mathcal{V}$: B_3, B_2, B_1, in that order. These then simplify further according to Table III.2. The case of $\mathcal{T}^h$ runs exactly parallel to that of $\mathcal{T}$. Its reducing subgroup is $\mathcal{V}^h$, the direct product of $\mathcal{V}$ by the inversion group.

We next consider $\mathcal{O}$ and its isomorph $\mathcal{T}^v$, of order 24. One can factor the projection operators belonging to the identity rep owing to the fact, which may readily

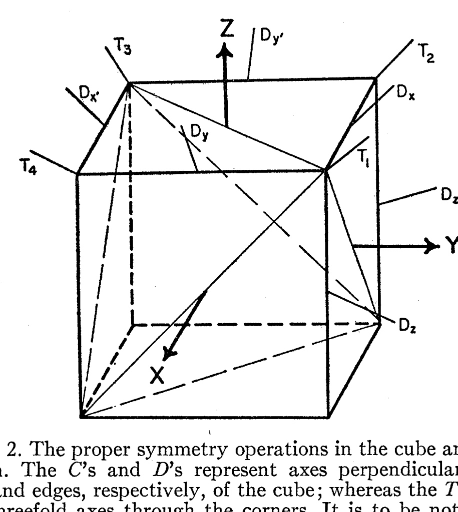

FIG. 2. The proper symmetry operations in the cube and tetrahedron. The C's and D's represent axes perpendicular to the faces and edges, respectively, of the cube; whereas the T's represent threefold axes through the corners. It is to be noted that, besides the obvious relations, the following ones also hold: $D_{x'}D_{y'}D_{z'}$ are perpendicular to T_1, $D_{x'}D_yD_z$ to T_2, $D_xD_yD_{z'}$ to T_3, and $D_xD_{y'}D_z$ to T_4.

be verified, that $\mathcal{O}$ may be written as the weak direct product of $\mathcal{V}$ and $\mathcal{D}_3$, while $\mathcal{T}^v$ may be written as the weak direct product of $\mathcal{V}$ and $\mathcal{C}_3^v$. For the second nondegenerate rep, A_2, the projection operators factor with $\mathcal{T}$ as the kernel operator. Besides the two nondegenerate reps there are three degenerate reps, of which one is of dimension 2 and two are of dimension 3. The 3-dimensional reps do not satisfy (C). The 2-dimensional rep E satisfies condition (C) since its S_4 and σ_v classes have zero characters; thus, *possibly*, it admits of devertebrate simplification with $\mathcal{T}$ as reducing subgroup. To see whether E actually admits simplification we must look at it in detail. It is derived in somewhat indefinite form by van der Waerden[15] to be

$$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix} \begin{pmatrix} & 1 \\ 1 & \end{pmatrix} \begin{pmatrix} -1 & -1 \\ & 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & \\ -1 & -1 \end{pmatrix} \begin{pmatrix} & 1 \\ -1 & -1 \end{pmatrix} \begin{pmatrix} -1 & -1 \\ 1 & \end{pmatrix} \tag{14}$$

where the six matrices are to be taken four times each. It is clear that, though it satisfies the necessary condition (C), E does not satisfy the sufficient condition

$$^{E}R_i{}^{i}=0 \quad \text{all } i, \text{ except for } \mathbf{R} \text{ in } \mathcal{T}. \tag{6'}$$

[15] B. L. van der Waerden, *Modern Algebra* (Verlag Julius Springer, Berlin, 1940; F. Ungar Company, 1950), pp. 181–2. This rep is nonunitary. We can unitarize it by the standard method, whereupon it becomes

$$\begin{pmatrix} 1 & \\ & 1 \end{pmatrix}\begin{pmatrix} -1 & \\ & 1 \end{pmatrix}\begin{pmatrix} 1/2 & -\sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}\begin{pmatrix} 1/2 & \sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}$$

$$\begin{pmatrix} -1/2 & \sqrt{3}/2 \\ -\sqrt{3}/2 & -1/2 \end{pmatrix}\begin{pmatrix} -1/2 & -\sqrt{3}/2 \\ \sqrt{3}/2 & -1/2 \end{pmatrix}.$$

Thus, in this form, E does not permit devertebrate simplification. Likewise for E_g and E_u in $\mathcal{O}^h$.

We have described the rep given in (14) as "somewhat indefinite." This is because from the way (14) is obtained[15] one does not know offhand to which operations of the group each matrix corresponds. Because the rep is not faithful there is a certain amount of arbitrariness in associating elements with matrices. But this arbitrariness is limited. Examination of the characters of the degenerate reps of $\mathcal{O}$ (Table I.4) indicates that the first of the six matrices is to be associated with $\mathbf{E}$ and the $3\mathbf{C}_2$ operations, whereas the last two matrices are associated with the $8\mathbf{C}_3$ operations. How the three other matrices of trace 0 are to be associated with the $6\mathbf{C}_4$ and $6\mathbf{C}_2$ operations is not obvious at first inspection. Upon more detailed examination, and by analogy with the more explicit F_1 rep which is faithful, we see that a consistent scheme of association is the one indicated in Table I.4 with reference to Fig. 2. The final results of factoring and row simplification of the projection operators for $\mathcal{O}$ and $\mathcal{T}^v$ are gathered together in Tables IV.2 and IV.3. The projection operators for $\mathcal{O}^h$ may be inferred immediately from those of $\mathcal{O}$.

It may be noted that the nonunitary rep (14) is more convenient for factoring than its unitary equivalent. Once the SAF's are found, they can be transformed by the unitarizing transformation to the unitary basis.

Finally we consider the icosahedral groups. The character table for $\mathcal{I}$ and a discussion of its reps is given in Speiser.[14] Upon examination one finds that (C) is not satisfied by any of the reps. Thus $\mathcal{I}$ (and likewise $\mathcal{I}^h$) does not admit of devertebrate simplification in finding SAF's for any of its degenerate reps. On account of their infrequent occurrence in Nature we shall not discuss $\mathcal{I}$ or $\mathcal{I}^h$ any further.

D. Tables of Factored Projection Operators for the Point Groups

TABLE IIa. Characters and projection operators[a] for the cyclic groups $\mathcal{C}_p$ [$(p=2,3,4,5,6)$, $(\gamma\equiv e^{2\pi i/3})$].

$\mathcal{C}_2$	E	C_2	Kernel operator	Quotient operator	Types of symmetry-adapted functions
A	1	1	$\mathbf{c}=\mathbf{E}+\mathbf{C}_2$		T_z; L_z $\alpha_{xx}, \alpha_{yy}, \alpha_{zz}, \alpha_{xy}$
B	1	-1	$\mathbf{E}$	$^{-}\mathbf{c}\equiv\mathbf{E}-\mathbf{C}_2$	T_x, T_y; L_x, L_y α_{yz}, α_{zx}

$\mathcal{C}_3$	E	C_3	C_3^2	Projection operator	Types of SAF's
A	1	1	1	$\mathbf{c}_3\equiv\mathbf{E}+\mathbf{C}_3+\mathbf{C}_3^2$	T_z; L_z $\alpha_{xx}+\alpha_{yy}, \alpha_{zz}$
E	1 1	γ $\bar{\gamma}$	$\bar{\gamma}$ γ	$^{1}\mathbf{c}_3\equiv\mathbf{E}+\gamma\mathbf{C}_3+\bar{\gamma}\mathbf{C}_3^2$ $\mathbf{E}+\bar{\gamma}\mathbf{C}_3+\gamma\mathbf{C}_3^2$	(T_x, T_y); (L_x, L_y) $(\alpha_{xx}-\alpha_{yy}, \alpha_{xy})$, $(\alpha_{yz}, \alpha_{zx})$

[a] In these and all subsequent tables the following abbreviations are used: $\mathbf{c}=\mathbf{E}+\mathbf{C}_2(z)$, $\mathbf{d}=\mathbf{E}+\mathbf{D}$, $\mathbf{c}^s=\mathbf{E}+\boldsymbol{\sigma}_h$, $\mathbf{c}^{v,d}=\mathbf{E}+\boldsymbol{\sigma}_{v,d}$, $^{-}\mathbf{c}=\mathbf{E}-\mathbf{C}_2(z)$, $^{-}\mathbf{d}=\mathbf{E}-\mathbf{D}$ $^{-}\mathbf{c}^s=\mathbf{E}-\boldsymbol{\sigma}_h$, $^{-}\mathbf{c}^{v,d}=\mathbf{E}-\boldsymbol{\sigma}_{v,d}$, and $^{j}\mathbf{c}_p\equiv\mathbf{E}+\omega^{\pm j}\,\mathbf{C}_p+\omega^{\pm 2j}\,\mathbf{C}_p^2+\cdots$ $(\omega\equiv e^{2\pi i/p})$. A further abbreviation which may be used is to put $^{\pm}\mathbf{C}_p\equiv\mathbf{E}\pm\mathbf{C}_p$ $(p\neq 2)$ or, in general, $^{\pm}{}_a\mathbf{R}\equiv\mathbf{E}\pm a\mathbf{R}$ $(\mathbf{R}^2\neq\mathbf{E})$ but, for the sake of greater explicitness, we have not done this in these tables.

TABLE IIa.—*Continued.*

$\mathcal{C}_4$	E	C_4	C_2	C_4^3	Kernel operator	Quotient operator	Types of SAF's
A	1	1	1	1	$\mathbf{c}\cdot(\mathbf{E}+\mathbf{C}_4)$		T_z; L_z $\alpha_{xx}+\alpha_{yy}$, α_{zz}
B	1	-1	1	-1	$\mathbf{c}$	$\mathbf{E}-\mathbf{C}_4$	$\alpha_{xx}-\alpha_{yy}$, α_{xy}
E	1	i	-1	$-i$		$(\mathbf{E}+i\mathbf{C}_4)\cdot{}^{-}\mathbf{c}$	(T_x, T_y); (L_x, L_y)
	1	$-i$	-1	i		$(\mathbf{E}-i\mathbf{C}_4)\cdot{}^{-}\mathbf{c}$	$(\alpha_{yz}, \alpha_{zx})$

$\mathcal{C}_5$	E	C_5	C_5^2	C_5^3	C_5^4	$\epsilon\equiv e^{2\pi i/5}$ Types of SAF's	
A	1	1	1	1	1	T_z; L_z	$\alpha_{xx}+\alpha_{yy}$, α_{zz}
E_1	1	ϵ	ϵ^2	$\bar{\epsilon}^2$	$\bar{\epsilon}$	(T_x, T_y); (L_x, L_y)	$(\alpha_{yz}, \alpha_{zx})$
	1	$\bar{\epsilon}$	$\bar{\epsilon}^2$	ϵ^2	ϵ		
E_2	1	ϵ^2	$\bar{\epsilon}$	ϵ	$\bar{\epsilon}^2$		$(\alpha_{xx}-\alpha_{yy}, \alpha_{xy})$
	1	$\bar{\epsilon}^2$	ϵ	$\bar{\epsilon}$	ϵ^2		

$\mathcal{C}_6$	E	C_6	C_3	C_2	C_3^2	C_6^5	Kernel operator	Quotient operator(s)	Types of SAF's
A	1	1	1	1	1	1	$\mathbf{c}\cdot\mathbf{c}_3$		T_z; L_z $\alpha_{xx}+\alpha_{yy}$, α_{zz}
B	1	-1	1	-1	1	-1	$\mathbf{c}_3$	$\mathbf{E}-\mathbf{C}_6$, ${}^{-}\mathbf{c}$	
E_1	1	$-\gamma^2$	γ	-1	γ^2	$-\gamma$		${}^{1}\mathbf{c}_3\cdot{}^{-}\mathbf{c}$	(T_x, T_y); (L_x, L_y)
	1	$-\gamma$	γ^2	-1	γ	$-\gamma^2$			$(\alpha_{yz}, \alpha_{zx})$
E_2	1	γ	γ^2	1	γ	γ^2	$\mathbf{c}$	${}^{1}\mathbf{c}_3{}^{*}$	$(\alpha_{xx}-\alpha_{yy}, \alpha_{xy})$
	1	γ^2	γ	1	γ^2	γ			

TABLE IIb. Projection Operators for the even-order cyclic group $\mathcal{C}_{2q}$. The product of any prokernel factor by the associated kernel operator is the prokernel operator, i.e., the sum of all operations in the prokernel subgroup each weighted by ±1, according to the corresponding diagonal matrix element in the representation.

$\mathcal{C}_{2q}$ (q odd)	Kernel operator	Prokernel factor(s)	Remaining quotient operators
A	$\mathbf{c}_{2q}\equiv\mathbf{c}\cdot\mathbf{c}_q$		
B	$\mathbf{c}_q$	${}^{-}\mathbf{c}$, $\mathbf{E}-\mathbf{C}_q$	
E_1		${}^{-}\mathbf{c}$	${}^{1}\mathbf{c}_q$
E_2	$\mathbf{c}$		${}^{2}\mathbf{c}_q$
E_3		${}^{-}\mathbf{c}$	${}^{3}\mathbf{c}_q$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
E_{q-1}	$\mathbf{c}$		${}^{q-1}\mathbf{c}_q$

$${}^{j}\mathbf{c}_q\equiv\mathbf{E}+\epsilon^{\pm j}\,\mathbf{C}_q+\cdots\epsilon^{\pm(q-1)j}\,\mathbf{C}_q{}^{q-1}$$

$\mathcal{C}_{2q=4r}$ (q even)	Kernel operator	Prokernel factor(s)	Remaining quotient operators
A	$\mathbf{c}\cdot(\mathbf{E}+\mathbf{C}_4)\cdot\mathbf{c}_{4r}{}^{r-1}$		
B	$\mathbf{c}_q$	${}^{-}\mathbf{c}$, $\mathbf{E}-\mathbf{C}_q$	
$\vdots$	$\vdots$	$\vdots$	$\vdots$
E_{2k+1}		${}^{-}\mathbf{c}$	${}^{2k+1}\mathbf{c}_{4r}{}^{2r-1}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
E_{2m}	$\mathbf{c}$	$\mathbf{E}-\mathbf{C}_4$	${}^{2m}\mathbf{c}_{4r}{}^{r-1}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
E_{4n}	$\mathbf{c}_4\equiv\mathbf{c}\cdot(\mathbf{E}+\mathbf{C}_4)$		${}^{4n}\mathbf{c}_{4r}{}^{r-1}$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
E_{2r-1}		${}^{-}\mathbf{c}$	${}^{2r-1}\mathbf{c}_{4r}{}^{2r-1}$

$${}^{j}\mathbf{c}_{4r}{}^{r-1}\equiv\mathbf{E}+\epsilon^{\pm j}\,\mathbf{C}_{4r}+\cdots\epsilon^{\pm j(r-1)}\,\mathbf{C}_{4r}{}^{r-1}$$

$${}^{j}\mathbf{c}_{4r}{}^{2r-1}\equiv\mathbf{E}+\epsilon^{\pm j}\,\mathbf{C}_{4r}+\cdots\epsilon^{\pm j(2r-1)}\,\mathbf{C}_{4r}{}^{2r-1}$$

TABLE III. 1a. Factored projection operators for the irreducible representations of the h-cyclic and the a-cyclic groups, $\mathcal{C}_q^h$ and $\mathcal{C}_q^a$ $\mathcal{C}_p^a$ and $\mathcal{C}_p^h$ $(q=1,3,5)$ $(p=2,4,6)$.

	Kernel (or prokernel) operator	Quotient operator(s). alternatives			
$\mathcal{C}_1^h=\mathcal{C}^s$				$\mathcal{C}_1^a\equiv\mathcal{C}^i$	
A'	$\mathbf{c}^s\equiv\mathbf{E}+\sigma_h$		A_g	$\mathbf{i}\equiv\mathbf{E}+\imath$	
A''	$^-\mathbf{c}^s\equiv\mathbf{E}-\sigma_h$		A_u	$^-\mathbf{i}\equiv\mathbf{E}-\imath$	
	$\mathcal{C}_3^h=\mathcal{C}_3\times\mathcal{C}^s$			$\mathcal{C}_3^a\equiv\mathcal{C}_3^i\equiv\mathcal{S}_6\equiv\mathcal{C}_3\times\mathcal{C}^i$	
A'	$\mathbf{c}_3\cdot\mathbf{c}^s$		A_g	$\mathbf{c}_3\cdot\mathbf{i}$	
A''	$\mathbf{c}_3$	$^-\mathbf{c}^s$, $\mathbf{E}-\mathbf{S}_3$	A_u	$\mathbf{c}_3$	$^-\mathbf{i}$, $\mathbf{E}-\mathbf{S}_6$
E'	$\mathbf{c}^s$	$^1\mathbf{c}_3$	E_g	$\mathbf{i}$	$^1\mathbf{c}_3$
E''	$^-\mathbf{c}^s$	$^1\mathbf{c}_3$	E_u	$^-\mathbf{i}$	$^1\mathbf{c}_3$
	$\mathcal{C}_5^h=\mathcal{C}_5\times\mathcal{C}^s$			$\mathcal{C}_5^a\equiv\mathcal{C}_5^i=\mathcal{S}_{10}=\mathcal{C}_5\times\mathcal{C}^i$	
A'	$\mathbf{c}_5\cdot\mathbf{c}^s$		A_g	$\mathbf{c}_5\cdot\mathbf{i}$	
A''	$\mathbf{c}_5$	$^-\mathbf{c}^s$, $\mathbf{E}-\mathbf{S}_5$	A_u	$\mathbf{c}_5$	$^-\mathbf{i}$, $\mathbf{E}-\mathbf{S}_{10}$
E_1'	$\mathbf{c}^s$	$^1\mathbf{c}_5$	E_{1g}	$\mathbf{i}$	$^1\mathbf{c}_5$
E_1''	$^-\mathbf{c}^s$	$^1\mathbf{c}_5$	E_{1u}	$^-\mathbf{i}$	$^1\mathbf{c}_5$
E_2'	$\mathbf{c}^s$	$^2\mathbf{c}_5$	E_{2g}	$\mathbf{i}$	$^2\mathbf{c}_5$
E_2''	$^-\mathbf{c}^s$	$^2\mathbf{c}_5$	E_{2u}	$^-\mathbf{i}$	$^2\mathbf{c}_5$
	$\mathcal{C}_2^a\equiv\mathcal{S}_4$			$\mathcal{C}_2^h=\mathcal{C}_2\times\mathcal{C}^i$	
A	$\mathbf{c}\cdot(\mathbf{E}+\mathbf{S}_4)$		A_g	$\mathbf{c}\cdot\mathbf{i}$	
B	$\mathbf{c}$	$\mathbf{E}-\mathbf{S}_4$	A_u	$\mathbf{c}$	$^-\mathbf{i}$, $^-\mathbf{c}^s$
E	$^-\mathbf{c}$	$\mathbf{E}\pm i\mathbf{S}_4$	B_g	$\mathbf{i}$	$^-\mathbf{c}$, $^-\mathbf{c}^s$
			B_u	$\mathbf{c}^s$	$^-\mathbf{c}$, $^-\mathbf{i}$
	$\mathcal{C}_4^a\equiv\mathcal{S}_8$	$(\epsilon\equiv e^{2\pi i/8})$		$\mathcal{C}_4^h=\mathcal{C}_4\times\mathcal{C}^i$	
A	$\mathbf{c}_4\cdot(\mathbf{E}+\mathbf{S}_8)$		A_g	$\mathbf{c}_4\cdot\mathbf{i}$	
B	$\mathbf{c}_4$	$\mathbf{E}-\mathbf{S}_8$	B_g	$\mathbf{c}\cdot\mathbf{i}$	$\mathbf{E}-\mathbf{C}_4$, $\mathbf{E}-\mathbf{S}_4$
E_1	$^-\mathbf{c}$	$(\mathbf{E}+\epsilon\mathbf{S}_8)\cdot(\mathbf{E}+i\mathbf{C}_4)$	A_u	$\mathbf{c}_4$	$^-\mathbf{i}$, $^-\mathbf{c}^s$, $\mathbf{E}-\mathbf{S}_4$
		$(\mathbf{E}+\bar{\epsilon}\mathbf{S}_8)\cdot(\mathbf{E}-i\mathbf{C}_4)$	B_u	$\mathbf{c}\cdot(\mathbf{E}+\mathbf{S}_4)$	$^-\mathbf{i}$, $^-\mathbf{c}^s$, $\mathbf{E}-\mathbf{C}_4$
E_2	$\mathbf{c}$	$(\mathbf{E}-\mathbf{C}_4)\cdot(\mathbf{E}\pm i\mathbf{S}_8)$	E_g	$^-\mathbf{c}\cdot\mathbf{i}$, $^-\mathbf{c}^s\cdot\mathbf{i}$	$\mathbf{E}\pm\mathbf{i}\mathbf{C}_4$
E_3	$^-\mathbf{c}$	$(\mathbf{E}-\bar{\epsilon}\mathbf{S}_8)\cdot(\mathbf{E}-i\mathbf{C}_4)$	E_u	$^-\mathbf{c}\cdot\mathbf{c}^s$, $^-\mathbf{i}\cdot\mathbf{c}^s$	$\mathbf{E}\pm\mathbf{i}\mathbf{C}_4$
		$(\mathbf{E}-\epsilon\mathbf{S}_8)\cdot(\mathbf{E}+\mathbf{i}\mathbf{C}_4)$			
	$\mathcal{C}_6^a\equiv\mathcal{S}_{12}$	$\gamma\equiv e^{2\pi i/3}$ $\epsilon\equiv e^{2\pi i/12}$		$\mathcal{C}_6^h=\mathcal{C}_6\times\mathcal{C}^i$	
A	$\mathbf{c}_6\cdot(\mathbf{E}+\mathbf{S}_{12})$		A_g	$\mathbf{c}_6\cdot\mathbf{i}$	
B	$\mathbf{c}_6$	$\mathbf{E}-\mathbf{S}_{12}$	A_u	$\mathbf{c}_6$	$^-\mathbf{i}$, $^-\mathbf{c}^s$, $\mathbf{E}-\mathbf{S}_6$, $\mathbf{E}-\mathbf{S}_3$
E_1	$^-\mathbf{c}$	$^1\mathbf{s}_{12}^6$	B_g	$\mathbf{c}_3\cdot\mathbf{i}$	$^-\mathbf{c}$, $^-\mathbf{c}^s$, $\mathbf{E}-\mathbf{C}_6$, $\mathbf{E}-\mathbf{S}_3$
E_2	$\mathbf{c}$	$^2\mathbf{s}_{12}^6$	B_u	$\mathbf{c}_3\cdot\mathbf{c}^s$	$^-\mathbf{c}$, $^-\mathbf{i}$, $\mathbf{E}-\mathbf{C}_6$, $\mathbf{E}-\mathbf{S}_6$
E_3	$^-\mathbf{c}$	$^3\mathbf{s}_{12}^6$	E_{1g}	$^-\mathbf{c}\cdot\mathbf{i}$, $^-\mathbf{c}^s\cdot\mathbf{i}$	$^1\mathbf{c}_3$
E_4	$\mathbf{c}$	$^4\mathbf{s}_{12}^6$	E_{2g}	$\mathbf{i}\cdot\mathbf{c}$	$^2\mathbf{c}_3$
E_5	$^-\mathbf{c}$	$^5\mathbf{s}_{12}^6$	E_{1u}	$^-\mathbf{c}\cdot\mathbf{c}^s$, $^-\mathbf{i}\cdot\mathbf{c}^s$	$^1\mathbf{c}_3$
			E_{2u}	$^-\mathbf{i}\cdot\mathbf{c}$, $^-\mathbf{c}^s\cdot\mathbf{c}$	$^2\mathbf{c}_3$

$$^j\mathbf{s}_{12}^6\equiv(\mathbf{E}+\epsilon^j\,\mathbf{S}_{12})\cdot(\mathbf{E}-\gamma^{2j}\,\mathbf{C}_6+\gamma^j\,\mathbf{C}_3)$$

TABLE III. 1b. Factored projection operators for the irreducible representations of the h-cyclic and the a-cyclic groups $\mathcal{C}_q^h$ and $\mathcal{C}_q^a$.

q odd

	$\mathcal{C}_q^h=\mathcal{C}_q\times\mathcal{C}^s$			$\mathcal{C}_q^a=\mathcal{C}_q^i=\mathcal{S}_{2q}=\mathcal{C}_q\times\mathcal{C}^i$	
A'	$\mathbf{c}_q\cdot\mathbf{c}^s$		A_g	$\mathbf{c}_q\cdot\mathbf{i}$	
A''	$\mathbf{c}_q$	$^-\mathbf{c}^s$, $\mathbf{E}-\mathbf{S}_q$	A_u	$\mathbf{c}_q$	$^-\mathbf{i}$, $\mathbf{E}-\mathbf{S}_{2q}$
E_1'	$\mathbf{c}^s$	$^1\mathbf{c}_q$	E_{1g}	$\mathbf{i}$	$^1\mathbf{c}_q$
E_1''	$^-\mathbf{c}^s$	$^1\mathbf{c}_q$	E_{1u}	$^-\mathbf{i}$	$^1\mathbf{c}_q$
.	.	.	.	.	.
.	.	.	.	.	.
.	.		.	.	.
$E_{(q-1)/2}''$	$^-\mathbf{c}^s$	$^{(q-1)/2}\mathbf{c}_q$	$E_{(q-1)/2,\,u}$	$^-\mathbf{i}$	$^{(q-1)/2}\mathbf{c}_q$

q even

$\mathcal{C}_q^a=\mathcal{S}_{2q}$		$(\epsilon\equiv e^{2\pi i/2q})$
A	$\mathbf{c}_q\cdot(\mathbf{E}+\mathbf{S}_{2q})$	
B	$\mathbf{c}_q$	$\mathbf{E}-\mathbf{S}_{2q}$
E_1	$^-\mathbf{c}$	$\mathbf{E}+\sum_{k=1}^{q-1}\epsilon^{\pm k}\,\mathbf{S}_{2q}^k$
E_2	$\mathbf{c}$	$\mathbf{E}+\sum_{k=1}^{q-1}\epsilon^{\pm k}\,\mathbf{S}_{2q}^k$
.	.	.
.	.	.
.	.	.
E_{q-1}	$^-\mathbf{c}$	$\mathbf{E}+\sum_{k=1}^{q-1}\epsilon^{\pm(q-1)k}\,\mathbf{S}_{2q}^k$

TABLE III. 1b.—*Continued.*

		$\mathcal{C}_{2q}^{h}=\mathcal{C}_{2q}\times\mathcal{C}^{i}$			
q odd			*q* even		
A_g	$\mathbf{c}_{2q}\cdot\mathbf{i}$		A_g	$\mathbf{c}_{2q}\cdot\mathbf{i}$	
A_u	$\mathbf{c}_{2q}$	$^{-}\mathbf{i},\ ^{-}\mathbf{c}^{s},\ \mathbf{E}-\mathbf{S}_{2q},\ \mathbf{E}-\mathbf{S}_{q}$	A_u	$\mathbf{c}_{2q}$	$^{-}\mathbf{i},\ ^{-}\mathbf{c}^{s},\ \mathbf{E}-\mathbf{S}_{2q}$
B_g	$\mathbf{c}_q^{a}=\ \mathbf{c}_q\cdot\mathbf{i}$	$^{-}\mathbf{c},\ ^{-}\mathbf{c}^{s},\ \mathbf{E}-\mathbf{C}_{2q}\ \ \mathbf{E}-\mathbf{S}_{q}$	B_g	$\mathbf{c}_q^{h}=\mathbf{c}_q\cdot\mathbf{i}$	$\mathbf{E}-\mathbf{C}_{2q},\ \mathbf{E}-\mathbf{S}_{2q}$
B_u	$\mathbf{c}_q^{h}=\ \mathbf{c}_q\cdot\mathbf{c}^{s}$	$^{-}\mathbf{c},\ ^{-}\mathbf{i},\ \ \mathbf{E}-\mathbf{C}_{2q},\ \mathbf{E}-\mathbf{S}_{2q}$	B_u	$\mathbf{c}_q^{a}=\mathbf{c}_q\cdot(\mathbf{E}+\mathbf{S}_{2q})$	$^{-}\mathbf{i},\ ^{-}\mathbf{c}^{s},\ \mathbf{E}-\mathbf{C}_{2q}$
E_{1g}	$^{-}\mathbf{c}\cdot\mathbf{i}$	$^{1}\mathbf{c}_q$	.	.	.
E_{1u}	$^{-}\mathbf{c}\cdot\mathbf{c}^{s}$		.	.	.
E_{2g}	$\mathbf{c}_2^{h}=\ \mathbf{c}\cdot\mathbf{i}$	$^{2}\mathbf{c}_q$	$E_{2k+1,\,g}$	$^{-}\mathbf{c}\cdot\mathbf{i}$	$^{2k+1}\mathbf{c}_{2q}^{\ 2r-1}$
E_{2u}	$\mathbf{c}\cdot{}^{-}\mathbf{i}$		$E_{2k+1,\,u}$	$^{-}\mathbf{c}\cdot\mathbf{c}^{s}$	
			.	.	.
E_{3g}	$^{-}\mathbf{c}\cdot\mathbf{i}$	$^{3}\mathbf{c}_q$	$E_{2m,\,g}$	$\mathbf{c}\cdot(\mathbf{E}-\mathbf{C}_4)\cdot\mathbf{i}$	$^{2m}\mathbf{c}_{2q}^{\ r-1}$
E_{3u}	$^{-}\mathbf{c}\cdot\mathbf{c}^{s}$		$E_{2m,\,u}$	$\mathbf{c}\cdot(\mathbf{E}-\mathbf{C}_4)\cdot{}^{-}\mathbf{i}$	
.	.	.	.	.	.
$E_{q-1,\,g}$	$\mathbf{c}\cdot\mathbf{i}$	$^{q-1}\mathbf{c}_q$	$E_{4n,\,g}$	$\mathbf{c}\cdot(\mathbf{E}+\mathbf{C}_4)\cdot\mathbf{i}$	$^{4n}\mathbf{c}_{2q}^{\ r-1}$
$E_{q-1,\,u}$	$\mathbf{c}\cdot{}^{-}\mathbf{i}$		$E_{4n,\,u}$	$\mathbf{c}\cdot(\mathbf{E}+\mathbf{C}_4)\cdot{}^{-}\mathbf{i}$	
			.	.	.
			$E_{2r-1,\,g}$	$^{-}\mathbf{c}\cdot\mathbf{i}$	$^{2r}\mathbf{c}_{2q}^{\ 2r-1}$
			$E_{2r-1,\,u}$	$^{-}\mathbf{c}\cdot\mathbf{c}^{s}$	

$$^{j}\mathbf{c}_{2q}^{\ s}\equiv\mathbf{E}+\epsilon^{\pm j}\,\mathbf{C}_{4r}+\cdots\epsilon^{\pm js}\,\mathbf{C}_{4r}^{\ s}$$

TABLE III. 2. Projection operators for the dihedral and pyramidal groups $\mathfrak{D}_p$ and $\mathcal{C}_p^{v}$ ($p=2,3,4,5,6$),

$$\mathbf{c}\equiv\mathbf{E}+\mathbf{C}_2(z),\quad \mathbf{d}\equiv\mathbf{E}+\mathbf{D},\quad \mathbf{c}^{s}\equiv\mathbf{E}+\boldsymbol{\sigma}_{h},\quad \mathbf{c}^{v,d}\equiv\mathbf{E}+\boldsymbol{\sigma}_{v,d},$$
$$^{-}\mathbf{c}\equiv\mathbf{E}-\mathbf{C}_2(z),\quad ^{-}\mathbf{d}\equiv\mathbf{E}-\mathbf{D},\quad ^{-}\mathbf{c}^{s}\equiv\mathbf{E}-\boldsymbol{\sigma}_{h},\quad ^{-}\mathbf{c}^{v,d}\equiv\mathbf{E}-\boldsymbol{\sigma}_{v,d}.$$

	$\mathfrak{D}_2\equiv\mathfrak{V}=(\mathcal{C}_2,\ \mathbf{D}\mathcal{C}_2)$			$\mathcal{C}_2^{v}=(\mathcal{C}_2,\ \boldsymbol{\sigma}_v\mathcal{C}_2)$	
A_1	$\mathbf{d}_2=\mathbf{d}\cdot\mathbf{c}$		A_1	$\mathbf{c}\cdot\mathbf{c}^{v}$	
B_1	$\mathbf{c}$	$^{-}\mathbf{d}$	A_2	$\mathbf{c}$	$^{-}\mathbf{c}^{v}$
B_2	$\mathbf{d}_{(y)}$	$^{-}\mathbf{c},\ ^{-}\mathbf{d}_{(x)}$	B_1	$\mathbf{c}^{v}{}_{(y)}$	$^{-}\mathbf{c},\ ^{-}\mathbf{c}^{v}{}_{(x)}$
B_3	$\mathbf{d}_{(x)}$	$^{-}\mathbf{c},\ ^{-}\mathbf{d}_{(y)}$	B_2	$\mathbf{c}^{v}{}_{(x)}$	$^{-}\mathbf{c},\ ^{-}\mathbf{c}^{v}{}_{(y)}$
	$\mathfrak{D}_3=(\mathcal{C}_3,\ \mathbf{D}\mathcal{C}_3)$			$\mathcal{C}_3^{v}=(\mathcal{C}_3,\ \boldsymbol{\sigma}_v\mathcal{C}_3)$	
A_1	$\mathbf{d}\cdot\mathbf{c}_3$		A_1	$\mathbf{c}_3\cdot\mathbf{c}^{v}$	
A_2	$\mathbf{c}_3$	$^{-}\mathbf{d}$	A_2	$\mathbf{c}_3$	$^{-}\mathbf{c}^{v}$
E		$^{1}\mathbf{c}_3$	E		$^{1}\mathbf{c}_3$
	$\mathfrak{D}_4=(\mathcal{C}_4,\ \mathbf{D}\mathcal{C}_4)$			$\mathcal{C}_4^{v}=(\mathcal{C}_4,\ \boldsymbol{\sigma}_v\mathcal{C}_4)$	
A_1	$(\mathbf{E}+\mathbf{C}_4)\cdot\mathbf{c}\cdot\mathbf{d}$		A_1	$\mathbf{c}_4\cdot\mathbf{c}^{v}$	
	$(\mathbf{E}+\mathbf{C}_4)\cdot\mathbf{c}\cdot\mathbf{d}'$				
A_2	$(\mathbf{E}+\mathbf{C}_4)\cdot\mathbf{c}$	$^{-}\mathbf{d},\ ^{-}\mathbf{d}'$	A_2	$\mathbf{c}_4$	$^{-}\mathbf{c}^{v}$
B_1	$\mathbf{d}\cdot\mathbf{c}$	$^{-}\mathbf{d},\ \mathbf{E}-\mathbf{C}_4$	B_1	$\mathbf{c}\cdot\mathbf{c}^{v}$	$^{-}\mathbf{c}^{v\prime}$
B_2	$\mathbf{c}\cdot\mathbf{d}'$	$^{-}\mathbf{d},\ \mathbf{E}-\mathbf{C}_4$	B_2	$\mathbf{c}\cdot\mathbf{c}^{v}$	$^{-}\mathbf{c}^{v}$
E	$\mathbf{d}_{(y)}$	$^{-}\mathbf{c},\ ^{-}\mathbf{d}_{(x)}$	E	$\mathbf{c}^{v}{}_{(y)}$	$^{-}\mathbf{c},\ ^{-}\mathbf{c}^{v}{}_{(x)}$
	$\mathbf{d}_{(x)}$	$^{-}\mathbf{c},\ ^{-}\mathbf{d}_{(y)}$		$\mathbf{c}^{v}{}_{(x)}$	$^{-}\mathbf{c},\ ^{-}\mathbf{c}^{v}{}_{(y)}$
	$\mathfrak{D}_5=(\mathcal{C}_5,\ \mathbf{D}\mathcal{C}_5)$			$\mathcal{C}_5^{v}=(\mathcal{C}_5,\ \boldsymbol{\sigma}_v\mathcal{C}_5)$	
A_1	$\mathbf{d}\cdot\mathbf{c}_5$		A_1	$\mathbf{c}_5\cdot\mathbf{c}^{v}$	
A_2	$\mathbf{c}_5$	$^{-}\mathbf{d}$	A_2	$\mathbf{c}_5$	$^{-}\mathbf{c}^{v}$
E_1		$^{1}\mathbf{c}_5$	E_1		$^{1}\mathbf{c}_5$
E_2		$^{2}\mathbf{c}_5$	E_2		$^{2}\mathbf{c}_5$
	$\mathfrak{D}_6=(\mathcal{C}_6,\ \mathbf{D}\mathcal{C}_6)$			$\mathcal{C}_6^{v}=(\mathcal{C}_6,\ \boldsymbol{\sigma}_v\mathcal{C}_6)$	
A_1	$\mathbf{d}\cdot(\mathbf{E}+\mathbf{C}_6)\cdot\mathbf{c}_3$		A_1	$(\mathbf{E}+\mathbf{C}_6)\cdot\mathbf{c}_3\cdot\mathbf{c}^{v}$	
A_2	$(\mathbf{E}+\mathbf{C}_6)\cdot\mathbf{c}_3$	$^{-}\mathbf{d},\ ^{-}\mathbf{d}'$	A_2	$(\mathbf{E}+\mathbf{C}_6)\cdot\mathbf{c}_3$	$^{-}\mathbf{c}^{v},\ \mathbf{c}^{v\prime}$
B_1	$\mathbf{d}\cdot\mathbf{c}_3$	$^{-}\mathbf{c},\ ^{-}\mathbf{d}'$	B_1	$\mathbf{c}_3\cdot\mathbf{c}^{v}$	$^{-}\mathbf{c},\ ^{-}\mathbf{c}^{v\prime},\ \mathbf{E}-\mathbf{C}_6$
B_2	$\mathbf{d}\cdot\mathbf{c}_3$	$^{-}\mathbf{c},\ ^{-}\mathbf{d}$	B_2	$\mathbf{c}_3\cdot\mathbf{c}^{v\prime}$	$^{-}\mathbf{c},\ ^{-}\mathbf{c}^{v},\ \mathbf{E}-\mathbf{C}_6$
E_1	$^{-}\mathbf{c}$	$^{1}\mathbf{c}_3$	E_1	$^{-}\mathbf{c}$	$^{1}\mathbf{c}_3$
E_2	$\mathbf{c}$	$^{2}\mathbf{c}_3$	E_2	$\mathbf{c}$	$^{2}\mathbf{c}_3$

TABLE III. 3. Projection operators for the *h*-dihedral and *d*-dihedral groups with odd-order axis, $\mathfrak{D}_p{}^h$ and $\mathfrak{D}_p{}^d$ ($p=3,5$).

$\mathfrak{D}_3{}^h=\mathfrak{D}_3\times\mathfrak{C}^s$			$\mathfrak{D}_3{}^d=\mathfrak{D}_3\times\mathfrak{C}^i$		
$A_1{}'$	$\mathbf{d}\cdot\mathbf{c}_3\cdot\mathbf{c}^s$		A_{1g}	$\mathbf{d}\cdot\mathbf{c}_3\cdot\mathbf{c}^d$	
$A_2{}'$	$\mathbf{c}_3\cdot\mathbf{c}^s$	${}^-\mathbf{d},\ {}^-\mathbf{c}^v$	A_{1u}	$\mathbf{d}\cdot\mathbf{c}_3$	${}^-\mathbf{i},\ \mathbf{E}-\mathbf{S}_6,\ {}^-\mathbf{c}^d$
$A_1{}''$	$\mathbf{d}\cdot\mathbf{c}_3$	${}^-\mathbf{c}^s,\ {}^-\mathbf{c}^v,\ \mathbf{E}-\mathbf{S}_3$	A_{2g}	$\mathbf{i}\cdot\mathbf{c}_3$	${}^-\mathbf{d},\ {}^-\mathbf{c}^d$
$A_2{}''$	$\mathbf{c}_3\cdot\mathbf{c}^v$	${}^-\mathbf{d},\ {}^-\mathbf{c}^s,\ \mathbf{E}-\mathbf{S}_3$	A_{2u}	$\mathbf{c}_3\cdot\mathbf{c}^d$	${}^-\mathbf{d},\ {}^-\mathbf{i},\ \mathbf{E}-\mathbf{S}_6$
E'	$\mathbf{c}^s$	${}^1\mathbf{c}_3$	E_g	$\mathbf{i}$	${}^1\mathbf{c}_3$
E''	${}^-\mathbf{c}^s$	${}^1\mathbf{c}_3$	E_u	${}^-\mathbf{i}$	${}^1\mathbf{c}_3$
	$\mathfrak{D}_5{}^h=\mathfrak{D}_5\times\mathfrak{C}^s$			$\mathfrak{D}_5{}^d=\mathfrak{D}_5\times\mathfrak{C}^i$	
$A_1{}'$	$\mathbf{d}\cdot\mathbf{c}_5\cdot\mathbf{c}^s$		A_{1g}	$\mathbf{d}\cdot\mathbf{c}_5\cdot\mathbf{c}^d$	
$A_2{}'$	$\mathbf{c}_5\cdot\mathbf{c}^s$	${}^-\mathbf{d},\ {}^-\mathbf{c}^v$	A_{1u}	$\mathbf{d}\cdot\mathbf{c}_5$	${}^-\mathbf{i},\ \mathbf{E}-\mathbf{S}_{10},\ {}^-\mathbf{c}^d$
$A_1{}''$	$\mathbf{d}\cdot\mathbf{c}_5$	${}^-\mathbf{c}^s,\ {}^-\mathbf{c}^v,\ \mathbf{E}-\mathbf{S}_5$	A_{2g}	$\mathbf{c}_5\cdot\mathbf{c}^d$	${}^-\mathbf{d},\ {}^-\mathbf{c}^d$
$A_2{}''$	$\mathbf{c}_5\cdot\mathbf{c}^v$	${}^-\mathbf{d},\ {}^-\mathbf{c}^s,\ \mathbf{E}-\mathbf{S}_5$	A_{2u}	$\mathbf{c}_5$	${}^-\mathbf{d},\ {}^-\mathbf{i},\ \mathbf{E}-\mathbf{S}_{10}$
$E_1{}'$	$\mathbf{c}^s$	${}^1\mathbf{c}_5$	E_{1g}	$\mathbf{i}$	${}^1\mathbf{c}_5$
$E_2{}'$	$\mathbf{c}^s$	${}^2\mathbf{c}_5$	E_{2g}	$\mathbf{i}$	${}^2\mathbf{c}_5$
$E_1{}''$	${}^-\mathbf{c}^s$	${}^1\mathbf{c}_5$	E_{1u}	${}^-\mathbf{i}$	${}^1\mathbf{c}_5$
$E_2{}''$	${}^-\mathbf{c}^s$	${}^2\mathbf{c}_5$	E_{2u}	${}^-\mathbf{i}$	${}^2\mathbf{c}_5$

TABLE III. 4. Projection operators for the *d*-dihedral and *h*-dihedral groups with even-order axis $\mathfrak{D}_p{}^d$ and $\mathfrak{D}_p{}^h$ ($p=2,4,6$).

$\mathfrak{D}_2{}^d=(\mathfrak{D}_2,\ \boldsymbol{\sigma}_d\mathfrak{D}_2)$			$\mathfrak{D}_2{}^h=\mathfrak{D}_2\times\mathfrak{C}^i$		
A_1	$\mathbf{d}\cdot\mathbf{c}\cdot\mathbf{c}^d$		A_{1g}	$\mathbf{i}\cdot\mathbf{c}\cdot\mathbf{d}$	
A_2	$\mathbf{c}\cdot(\mathbf{E}+\mathbf{S}_4)$	${}^-\mathbf{d},\ {}^-\mathbf{c}^d$	A_{2g}	$\mathbf{i}\cdot\mathbf{c}$	${}^-\mathbf{d},\ {}^-\mathbf{c}^v$
B_1	$\mathbf{d}\cdot\mathbf{c}$	$\mathbf{E}-\mathbf{S}_4,\ {}^-\mathbf{c}^d$	B_{1g}	$\mathbf{i}\cdot\mathbf{d}_{(y)}$	${}^-\mathbf{c},\ {}^-\mathbf{d}_{(x)},\ {}^-\mathbf{c}^v{}_{(x)},\ {}^-\mathbf{c}^s$
B_2	$\mathbf{c}\cdot\mathbf{c}^d$	$\mathbf{E}-\mathbf{S}_4,\ {}^-\mathbf{d}$	B_{2g}	$\mathbf{i}\cdot\mathbf{d}_{(x)}$	${}^-\mathbf{c},\ {}^-\mathbf{d}_{(y)},\ {}^-\mathbf{c}^v{}_{(y)},\ {}^-\mathbf{c}^s$
E	$\mathbf{d}_{(y)}$	${}^-\mathbf{c},\ {}^-\mathbf{d}_{(x)}$	A_{1u}	$\mathbf{c}\cdot\mathbf{d}$	${}^-\mathbf{i},\ {}^-\mathbf{c}^s,\ {}^-\mathbf{c}^v{}_{(x,y)}$
	$\mathbf{d}_{(x)}$	${}^-\mathbf{c},\ {}^-\mathbf{d}_{(y)}$	A_{2u}	$\mathbf{c}\cdot\mathbf{c}^v$	${}^-\mathbf{d},\ {}^-\mathbf{i},\ {}^-\mathbf{c}^s$
			B_{1u}	$\mathbf{d}_{(y)}\cdot\mathbf{c}^s,\ \mathbf{d}_{(y)}\cdot\mathbf{c}^v{}_{(x)}$	${}^-\mathbf{c},\ {}^-\mathbf{d}_{(x)},\ {}^-\mathbf{i},\ {}^-\mathbf{c}^v{}_{(y)}$
			B_{2u}	$\mathbf{d}_{(x)}\cdot\mathbf{c}^s,\ \mathbf{d}_{(x)}\cdot\mathbf{c}^v{}_{(y)}$	${}^-\mathbf{c},\ {}^-\mathbf{d}_{(y)},\ {}^-\mathbf{i},\ {}^-\mathbf{c}^v{}_{(x)}$
	$\mathfrak{D}_{4d}=(\mathfrak{D}_4,\ \boldsymbol{\sigma}_d\mathfrak{D}_4)$			$\mathfrak{D}_4{}^h=\mathfrak{D}_4\times\mathfrak{C}^i$	
A_1	$\mathbf{d}\cdot\mathbf{c}_4\cdot\mathbf{c}^d$		A_{1g}	$\mathbf{d}\cdot\mathbf{c}_4\cdot\mathbf{i}$	
A_2	$\mathbf{c}_4\cdot(\mathbf{E}+\mathbf{S}_8)$	${}^-\mathbf{d},\ {}^-\mathbf{c}^d$	A_{2g}	$\mathbf{c}_4\cdot\mathbf{i}$	${}^-\mathbf{d},\ {}^-\mathbf{d}',\ {}^-\mathbf{c}^{v,v'}$
B_1	$\mathbf{d}\cdot\mathbf{c}_4$	$\mathbf{E}-\mathbf{S}_8,\ {}^-\mathbf{c}^d$	B_{1g}	$\mathbf{d}\cdot\mathbf{c}\cdot\mathbf{i}$	$\mathbf{E}-\mathbf{C}_4,\ {}^-\mathbf{d}',\ \mathbf{E}-\mathbf{S}_4,\ {}^-\mathbf{c}^{v'}$
B_2	$\mathbf{c}_4\cdot\mathbf{c}^d$	$\mathbf{E}-\mathbf{S}_8,\ {}^-\mathbf{d}$	B_{2g}	$\mathbf{d}\cdot\mathbf{c}\cdot\mathbf{i}$	$\mathbf{E}-\mathbf{C}_4,\ {}^-\mathbf{d},\ \mathbf{E}-\mathbf{S}_4,\ {}^-\mathbf{c}^v$
E_1	${}^-\mathbf{c}$	${}^1\mathbf{s}_8{}^3$	A_{1u}	$\mathbf{d}\cdot\mathbf{c}_4$	${}^-\mathbf{i},\ \mathbf{E}-\mathbf{S}_4,\ {}^-\mathbf{c}^{s,v,v'}$
E_2	$\mathbf{c}$	$\mathbf{c}^v\cdot(\mathbf{E}-\mathbf{C}_4)$	A_{2u}	$\mathbf{c}_4\cdot\mathbf{c}^{v,v'}$	${}^-\mathbf{d},\ {}^-\mathbf{d}',\ {}^-\mathbf{i},\ \mathbf{E}-\mathbf{S}_4,\ {}^-\mathbf{c}^s$
	$\mathbf{c}$	${}^-\mathbf{c}^v\cdot(\mathbf{E}-\mathbf{C}_4)$	B_{1u}	$\mathbf{d}\cdot\mathbf{c}\cdot\mathbf{c}^{v'}$	$\mathbf{E}-\mathbf{C}_4,\ {}^-\mathbf{d}',\ {}^-\mathbf{i},\ {}^-\mathbf{c}^{s,v}$
E_3	${}^-\mathbf{c}$	${}^3\mathbf{s}_8{}^3$	B_{2u}	$\mathbf{d}'\cdot\mathbf{c}\cdot\mathbf{c}^v$	$\mathbf{E}-\mathbf{C}_4,\ {}^-\mathbf{d},\ {}^-\mathbf{i},\ {}^-\mathbf{c}^{s,v'}$
			E_g	$\mathbf{d}_{(y)}\cdot\mathbf{i}$	${}^-\mathbf{c},\ {}^-\mathbf{c}^s,\ {}^-\mathbf{d}_{(x)},\ {}^-\mathbf{c}^v{}_{(x)}$
				$\mathbf{d}_{(x)}\cdot\mathbf{i}$	${}^-\mathbf{c},\ {}^-\mathbf{c}^s,\ {}^-\mathbf{d}_{(y)},\ {}^-\mathbf{c}^v{}_{(y)}$
			E_u	$\mathbf{d}_{(y)}\cdot\mathbf{c}^s$	${}^-\mathbf{c},\ {}^-\mathbf{i},\ {}^-\mathbf{d}_{(x)},\ {}^-\mathbf{c}^v{}_{(y)}$
				$\mathbf{d}_{(x)}\cdot\mathbf{c}^s$	${}^-\mathbf{c},\ {}^-\mathbf{i},\ {}^-\mathbf{d}_{(y)},\ {}^-\mathbf{c}^v{}_{(x)}$

$$ {}^j\mathbf{s}_8{}^3\equiv\mathbf{E}+\epsilon^j\,\mathbf{S}_8+\epsilon^{2j}\,\mathbf{S}_8{}^2+\epsilon^{3j}\,\mathbf{S}_8{}^3 \qquad \epsilon\equiv e^{2\pi i/8}$$

$\mathfrak{D}_6{}^d=(\mathfrak{D}_6,\ \boldsymbol{\sigma}_d\mathfrak{D}_6)$			$\mathfrak{D}_6{}^h=\mathfrak{D}_6\times\mathfrak{C}^i$		
A_1	$\mathbf{d}\cdot\mathbf{c}_6\cdot\mathbf{c}^d$		A_{1g}	$\mathbf{d}\cdot\mathbf{c}_6\cdot\mathbf{i}$	
A_2	$\mathbf{c}_6\cdot(\mathbf{E}+\mathbf{S}_{12})$	${}^-\mathbf{d},\ {}^-\mathbf{c}^d$	A_{2g}	$\mathbf{c}_6\cdot\mathbf{i}$	${}^-\mathbf{d},\ {}^-\mathbf{d}',\ {}^-\mathbf{c}^{v,v'}$
B_1	$\mathbf{d}\cdot\mathbf{c}_6$	$\mathbf{E}-\mathbf{S}_{12},\ {}^-\mathbf{c}^d$	B_{1g}	$\mathbf{d}\cdot\mathbf{c}_3\cdot\mathbf{c}^{v'}$	$\mathbf{E}-\mathbf{C}_6,\ {}^-\mathbf{c},\ {}^-\mathbf{d}',\ \mathbf{E}-\mathbf{S}_3,\ {}^-\mathbf{c}^{s,v}$
B_2	$\mathbf{c}_6\cdot\mathbf{c}^v$	$\mathbf{E}-\mathbf{S}_{12},\ {}^-\mathbf{d}$	B_{2g}	$\mathbf{d}'\cdot\mathbf{c}_3\cdot\mathbf{c}^v$	$\mathbf{E}-\mathbf{C}_6,\ {}^-\mathbf{c},\ {}^-\mathbf{d},\ \mathbf{E}-\mathbf{S}_3,\ {}^-\mathbf{c}^{s,v'}$
E_1		${}^1\mathbf{s}_{12}$	A_{1u}	$\mathbf{d}\cdot\mathbf{c}_6$	${}^-\mathbf{i},\ \mathbf{E}-\mathbf{S}_3,\ \mathbf{E}-\mathbf{S}_6,\ {}^-\mathbf{c}^{s,v,v'}$
E_2		${}^2\mathbf{s}_{12}$	A_{2u}	$\mathbf{c}_6\cdot\mathbf{c}^{v,v'}$	${}^-\mathbf{d},\ {}^-\mathbf{d}',\ {}^-\mathbf{i},\ \mathbf{E}-\mathbf{S}_3,\ \mathbf{E}-\mathbf{S}_6,\ {}^-\mathbf{c}^s$
E_3		${}^3\mathbf{s}_{12}$	B_{1u}	$\mathbf{d}\cdot\mathbf{c}_3\cdot\mathbf{c}^s$	$\mathbf{E}-\mathbf{C}_6,\ {}^-\mathbf{c},\ {}^-\mathbf{d}',\ {}^-\mathbf{i},\ \mathbf{E}-\mathbf{S}_6,\ {}^-\mathbf{c}^v$
E_4		${}^4\mathbf{s}_{12}$	B_{2u}	$\mathbf{d}'\cdot\mathbf{c}_3\cdot\mathbf{c}^s$	$\mathbf{E}-\mathbf{C}_6,\ {}^-\mathbf{c},\ {}^-\mathbf{d},\ {}^-\mathbf{i},\ \mathbf{E}-\mathbf{S}_6,\ {}^-\mathbf{c}^v$
E_5		${}^5\mathbf{s}_{12}$	E_{1g}	$\mathbf{i}\cdot{}^-\mathbf{c}$	${}^1\mathbf{c}_3$
			E_{2g}	$\mathbf{i}\cdot\mathbf{c}$	${}^1\mathbf{c}_3{}^*$
			E_{1u}	${}^-\mathbf{i}\cdot\mathbf{c}$	${}^1\mathbf{c}_3{}^*$
			E_{2u}	${}^-\mathbf{i}\cdot\mathbf{c}$	${}^1\mathbf{c}_3$

TABLE IV. 1. Projection operators for the cubic groups $\mathcal{T}$, $\mathcal{T}^h$.

$\mathcal{T}$			$\mathcal{T}^h=\mathcal{T}\times\mathcal{C}^i$		
A	$\mathbf{t}\equiv(\mathbf{E}+\mathbf{T}_m+\mathbf{T}_n)\cdot\mathbf{c}_{(\alpha)}\cdot\mathbf{c}_{(\beta)}$ $(\alpha\neq\beta;\quad \alpha,\beta=x,y,z)$ $(m\neq n;\quad m,n=1,2,3)$		A_g	$\mathbf{i}\cdot\mathbf{t}$	
			A_u	$\mathbf{t}$	${}^{-}\mathbf{i}$
E	$\mathbf{c}_{(\alpha)}\cdot\mathbf{c}_{(\beta)}$	${}^{1}\mathbf{c}_3$	E_g	$\mathbf{i}\cdot\mathbf{c}_{(\alpha)}\cdot\mathbf{c}_{(\beta)}$	${}^{1}\mathbf{c}_3$
			E_u	${}^{-}\mathbf{i}\cdot\mathbf{c}_{(\alpha)}\cdot\mathbf{c}_{(\beta)}$	${}^{1}\mathbf{c}_3$
			F_g	$\mathbf{i}\cdot\mathbf{c}_{(x)}$ $\mathbf{i}\cdot\mathbf{c}_{(y)}$ $\mathbf{i}\cdot\mathbf{c}_{(z)}$	${}^{-}\mathbf{c}_{(y)},\ {}^{-}\mathbf{c}_{(z)}$ ${}^{-}\mathbf{c}_{(z)},\ {}^{-}\mathbf{c}_{(x)}$ ${}^{-}\mathbf{c}_{(x)},\ {}^{-}\mathbf{c}_{(y)}$
F	$\mathbf{c}_{(x)}$ $\mathbf{c}_{(y)}$ $\mathbf{c}_{(z)}$	${}^{-}\mathbf{c}_{(y)},\ {}^{-}\mathbf{c}_{(z)}$ ${}^{-}\mathbf{c}_{(z)},\ {}^{-}\mathbf{c}_{(x)}$ ${}^{-}\mathbf{c}_{(x)},\ {}^{-}\mathbf{c}_{(y)}$			
			F_u	${}^{-}\mathbf{i}\cdot\mathbf{c}_{(x)}$ ${}^{-}\mathbf{i}\cdot\mathbf{c}_{(y)}$ ${}^{-}\mathbf{i}\cdot\mathbf{c}_{(z)}$	${}^{-}\mathbf{c}_{(y)},\ {}^{-}\mathbf{c}_{(z)}$ ${}^{-}\mathbf{c}_{(z)},\ {}^{-}\mathbf{c}_{(x)}$ ${}^{-}\mathbf{c}_{(x)},\ {}^{-}\mathbf{c}_{(y)}$

TABLE IV. 2. Factored projection operators for the enantiocube (proper octahedral) group $\mathcal{O}$.
$(\mathbf{c}_{(x)}=\mathbf{E}+\mathbf{C}_x,\cdots,\quad \mathbf{c}_3=\mathbf{E}+\mathbf{T}+\mathbf{T}^2,\quad \mathbf{d}_{(x)}=\mathbf{E}+\mathbf{D}_x,\cdots)$.

$\mathcal{O}$	Kernel operator	Quotient operator(s)
A_1	$\mathbf{o}=\mathbf{v}\cdot(\mathbf{d}_3)_{\text{corner}}=\mathbf{c}_{(\alpha)}\cdot\mathbf{c}_{(\beta)}\cdot(\mathbf{c}_3\cdot\mathbf{d})_{\text{corner}}$ $(\alpha\neq\beta;\quad \alpha,\beta=x,y,z$	
A_2	$\mathbf{t}=\mathbf{c}_{(\alpha)}\cdot\mathbf{c}_{(\beta)}\cdot(\mathbf{E}+\mathbf{T}_m+\mathbf{T}_n)$ $(m\neq n;\quad m,n=1,2,3)$	$\mathbf{E}-\mathbf{C}_4,\ \mathbf{E}-\mathbf{D}$
E [a]	$\mathbf{d}_4(y)=(\mathbf{E}+\mathbf{C}_{4(y)})\cdot\mathbf{c}_{(y)}\cdot\mathbf{d}_{(y,y')}$ $\mathbf{d}_4(x)=(\mathbf{E}+\mathbf{C}_{4(x)})\cdot\mathbf{c}_{(x)}\cdot\mathbf{d}_{(x,x')}$	$\mathbf{E}-\mathbf{T}_{2,4}{}^2,\ \mathbf{E}-\mathbf{T}_{1,3},\ \mathbf{E}-\mathbf{C}_{4(x)},\ \mathbf{E}-\mathbf{C}_{4(x)}{}^3,\ \mathbf{E}-\mathbf{D}_{(x,x')}$ $\mathbf{E}-\mathbf{T}_{2,4},\ \mathbf{E}-\mathbf{T}_{1,3}{}^2,\ \mathbf{E}-\mathbf{C}_{4(y)},\ \mathbf{E}-\mathbf{C}_{4(y)}{}^3,\ \mathbf{E}-\mathbf{D}_{(y,y')}$
F_1	$\mathbf{c}_4(x)=\mathbf{c}_{(x)}\cdot(\mathbf{E}+\mathbf{C}_{4(x)})$ $\mathbf{c}_4(y)=\mathbf{c}_{(y)}\cdot(\mathbf{E}+\mathbf{C}_{4(y)})$ $\mathbf{c}_4(z)=\mathbf{c}_{(z)}\cdot(\mathbf{E}+\mathbf{C}_{4(z)})$	$\mathbf{E}-\mathbf{C}_{(y,z)},\ \mathbf{E}-\mathbf{D}_{(x,x')}$ $\mathbf{E}-\mathbf{C}_{(z,x)},\ \mathbf{E}-\mathbf{D}_{(y,y')}$ $\mathbf{E}-\mathbf{C}_{(x,y)},\ \mathbf{E}-\mathbf{D}_{(z,z')}$
F_2	$\mathbf{d}_2(x)=\mathbf{c}_{(x)}\cdot\mathbf{d}_{(x,x')}$ $\mathbf{d}_2(y)=\mathbf{c}_{(y)}\cdot\mathbf{d}_{(y,y')}$ $\mathbf{d}_2(z)=\mathbf{c}_{(z)}\cdot\mathbf{d}_{(z,z')}$	$\mathbf{E}-\mathbf{C}_{(y,z)},\ \mathbf{E}-\mathbf{C}_{4(x)},\ \mathbf{E}-\mathbf{C}_{4(x)}{}^3$ $\mathbf{E}-\mathbf{C}_{(z,x)},\ \mathbf{E}-\mathbf{C}_{4(y)},\ \mathbf{E}-\mathbf{C}_{4(y)}{}^3$ $\mathbf{E}-\mathbf{C}_{(x,y)},\ \mathbf{E}-\mathbf{C}_{4(z)},\ \mathbf{E}-\mathbf{C}_{4(z)}{}^3$

[a] Equally admissible forms of E may be given with xyz in any cyclical permutation. The representation used is the nonunitary one discussed in the text. For it: $\bar{R}^i{}_i=(\mathbf{R}^{-1})^i{}_i$.

TABLE IV. 3. Factored projection operators for the tetrahedron group $\mathcal{T}_d=\mathcal{T}^v$.
$(\mathbf{c}_{(x)}=\mathbf{E}+\mathbf{C}_{(x)},\cdots,\quad \mathbf{c}_3=\mathbf{E}+\mathbf{T}+\mathbf{T}^2,\quad \mathbf{c}^{\mathrm{v}}{}_{(x)}=\mathbf{E}+\boldsymbol{\sigma}_{(x)},\cdots)$.

$\mathcal{T}_d$	Kernel operator	Quotient operator(s)
A_1	$\mathbf{t}_{\mathrm{d}}=\mathbf{v}\cdot(\mathbf{c}_3{}^{\mathrm{v}})_{\text{corner}}=\mathbf{c}_{(\alpha)}\cdot\mathbf{c}_{(\beta)}\cdot(\mathbf{c}_3\cdot\mathbf{c}^{\mathrm{v}})_{\text{corner}}$ $(\alpha\neq\beta;\quad \alpha,\beta=x,y,z)$	
A_2	$\mathbf{t}=\mathbf{c}_{(\alpha)}\cdot\mathbf{c}_{(\beta)}\cdot(\mathbf{E}+\mathbf{T}_m+\mathbf{T}_n)$ $(m\neq n;\quad m,n=1,2,3)$	$\mathbf{E}-\mathbf{S}_4,\ \mathbf{E}-\boldsymbol{\sigma}_{\mathrm{v}}$
E [a]	$\mathbf{d}_2{}^{\mathrm{d}}(y)=(\mathbf{E}+\mathbf{S}_{4(y)})\cdot\mathbf{c}_{(y)}\cdot\mathbf{c}^{\mathrm{v}}{}_{(y,y')}$ $\mathbf{d}_2{}^{\mathrm{d}}(x)=(\mathbf{E}+\mathbf{S}_{4(x)})\cdot\mathbf{c}_{(x)}\cdot\mathbf{c}^{\mathrm{v}}{}_{(x,x')}$	$\mathbf{E}-\mathbf{T}_{2,4}{}^2,\ \mathbf{E}-\mathbf{T}_{1,3},\ \mathbf{E}-\mathbf{S}_{4(x)}{}^3,\ \mathbf{E}-\mathbf{S}_{4(x)},\ \mathbf{E}-\boldsymbol{\sigma}_{(x,x')}$ $\mathbf{E}-\mathbf{T}_{2,4},\ \mathbf{E}-\mathbf{T}_{1,3}{}^2,\ \mathbf{E}-\mathbf{S}_{4(y)}{}^3,\ \mathbf{E}-\mathbf{S}_{4(y)},\ \mathbf{E}-\boldsymbol{\sigma}_{(y,y')}$
F_1	$\mathbf{s}_4(x)=\mathbf{c}_{(x)}\cdot(\mathbf{E}+\mathbf{S}_{4(x)})$ $\mathbf{s}_4(y)=\mathbf{c}_{(y)}\cdot(\mathbf{E}+\mathbf{S}_{4(y)})$ $\mathbf{s}_4(z)=\mathbf{c}_{(z)}\cdot(\mathbf{E}+\mathbf{S}_{4(z)})$	$\mathbf{E}-\mathbf{C}_{(y,z)},\ \mathbf{E}-\boldsymbol{\sigma}_{(x,x')}$ $\mathbf{E}-\mathbf{C}_{(z,x)},\ \mathbf{E}-\boldsymbol{\sigma}_{(y,y')}$ $\mathbf{E}-\mathbf{C}_{(x,y)},\ \mathbf{E}-\boldsymbol{\sigma}_{(z,z')}$
F_2	$\mathbf{c}_2{}^{\mathrm{v}}(x)=\mathbf{c}_{(x)}\cdot\mathbf{c}^{\mathrm{v}}{}_{(x,x')}$ $\mathbf{c}_2{}^{\mathrm{v}}(y)=\mathbf{c}_{(y)}\cdot\mathbf{c}^{\mathrm{v}}{}_{(y,y')}$ $\mathbf{c}_2{}^{\mathrm{v}}(z)=\mathbf{c}_{(z)}\cdot\mathbf{c}^{\mathrm{v}}{}_{(z,z')}$	$\mathbf{E}-\mathbf{C}_{(y,z)},\ \mathbf{E}-\mathbf{S}_{4(x)}{}^3,\ \mathbf{E}-\mathbf{S}_{4(x)}$ $\mathbf{E}-\mathbf{C}_{(z,x)},\ \mathbf{E}-\mathbf{S}_{4(y)}{}^3,\ \mathbf{E}-\mathbf{S}_{4(y)}$ $\mathbf{E}-\mathbf{C}_{(x,y)},\ \mathbf{E}-\mathbf{S}_{4(z)}{}^3,\ \mathbf{E}-\mathbf{S}_{4(z)}$

[a] Equally admissible forms of E may be given with xyz in any cyclical permutation. The representation used is the nonunitary one discussed in the text, For it: $\bar{R}^i{}_i=(\mathbf{R}^{-1})^i{}_i$.

VI. EXAMPLES

A. Transverse Eigenvibrations of a Square Membrane or Plate

As an elementary macrophysical example consider the classification of eigenvibrations of a homogeneous square membrane clamped at all edges. Since its analytic solution is so simple, it provides a good example to illustrate the simplified symmetry method. Also, in it occurs an interesting "accidental" degeneracy.

Let the unit of length be chosen so that the side is of length π, let the areal density and the tension of the membrane be σ and T, respectively. Choosing the origin of coordinates in the middle, the differential equation and boundary conditions for the displacement u in the transverse direction are

$$\begin{aligned} &\nabla^2 u = \partial^2 u / c^2 \partial t^2 \quad (c^2 \equiv T/\sigma), \\ &\quad u = \partial u/\partial t = 0 \text{ at } x = \pm\pi/2 \text{ and at } y = \pm\pi/2. \end{aligned} \tag{15}$$

Particular solutions of this system are of the form

$$\begin{aligned} &\cos\mu x \cos\nu y\, e^{i\omega t}, \quad (\mu,\nu \text{ odd}) \\ &\cos\mu x \sin\nu y\, e^{i\omega t}, \quad (\mu \text{ odd}, \nu \text{ even}) \\ &\sin\mu x \cos\nu y\, e^{i\omega t}, \quad (\mu \text{ even}, \nu \text{ odd}) \\ &\sin\mu x \sin\nu y\, e^{i\omega t}, \quad (\mu \text{ even}, \nu \text{ even}), \end{aligned} \tag{15'}$$

where the angular frequency in each case is

$$\omega = c(\mu^2 + \nu^2)^{\frac{1}{2}}. \tag{16}$$

In contrast to the usual analytical procedure, it is important for the following to prefix in front of each of the particular solutions (15) the unit vector $\hat{u}$ indicating its direction. The linear combinations of the solutions, which belong to each of the symmetry types of $\mathfrak{D}_4{}^h$, may then be found. For this simple problem they

TABLE Va. Behavior of certain generating functions *versus* key operations in the $\mathfrak{D}_4{}^h$ group. The first column gives a list of symmetry operations sufficient to build all factored projection operators (see Table III.4) for $\mathfrak{D}_4{}^h$. The second column gives the ordinary cartesian transformation matrices in the abbreviated notation of crystallography; i.e., we indicate merely to which old variables the new (xyz) are equal in that order. In the remaining columns are given the transforms of the four basic types of generating functions (again new in terms of old) with the following abbreviated notation paralleling that for the coordinates themselves:

$$\begin{array}{lll} \cos\kappa x \equiv K & \sin\kappa x \equiv K' & (\kappa \equiv \mu,\nu) \\ \cos\kappa y \equiv K & \sin\kappa y \equiv K' & (K = M,N) \end{array}$$

The symbol occurring first in order after the unit vector always represents the function of x and the second represents the function of y. Thus, for example, $N'M$ represents $\sin\nu x \cos\mu y$ (ν even, μ odd).

	New xyz	$\hat{u}\,MN$	$\hat{u}\,MN'$	$\hat{u}\,M'N$	$\hat{u}\,M'N'$
$\mathbf{C}_4$	$y\bar{x}z$	$\hat{u}\,NM$	$\hat{u}\,N'M$	$-\hat{u}\,NM'$	$-\hat{u}\,N'M'$
$\mathbf{C}$	$\bar{x}\bar{y}z$	$\hat{u}\,MN$	$-\hat{u}\,MN'$	$-\hat{u}\,M'N$	$\hat{u}\,M'N'$
$\mathbf{D}_{(x)}$	$x\bar{y}\bar{z}$	$-\hat{u}\,MN$	$\hat{u}\,MN'$	$-\hat{u}\,M'N$	$-\hat{u}\,M'N'$
$\mathbf{D}_{(x)}'$	$yx\bar{z}$	$-\hat{u}\,NM$	$-\hat{u}\,N'M$	$-\hat{u}\,NM'$	$-\hat{u}\,N'M'$
$\mathbf{D}_{(y)}$	$\bar{x}y\bar{z}$	$-\hat{u}\,MN$	$-\hat{u}\,MN'$	$\hat{u}\,M'N$	$\hat{u}\,M'N'$
$\boldsymbol{\sigma}_{\mathrm{v}}$	$x\bar{y}z$	$\hat{u}\,MN$	$-\hat{u}\,MN'$	$\hat{u}\,M'N$	$-\hat{u}\,M'N'$
$\boldsymbol{\sigma}_{\mathrm{v}'}$	yxz	$\hat{u}\,NM$	$\hat{u}\,N'M$	$\hat{u}\,NM'$	$\hat{u}\,N'M'$
$\boldsymbol{\sigma}_{\mathrm{h}}$	$xy\bar{z}$	$-\hat{u}\,MN$	$-\hat{u}\,MN'$	$-\hat{u}\,M'N$	$-\hat{u}\,M'N'$

TABLE Vb. Symmetry-adapted transverse eigenvibrations of square membrane.

A_{1u}	$\hat{u}(\sin\mu x\ \sin\nu y - \sin\nu x\ \sin\mu y) \equiv \mathbf{S}_{\mu\nu}{}^-$	(μ,ν even)
A_{2u}	$\hat{u}(\cos\mu x \cos\nu y + \cos\nu x \cos\mu y) \equiv \mathbf{C}_{\mu\nu}{}^+$	(μ,ν odd)
B_{1u}	$\hat{u}(\sin\mu x\ \sin\nu y + \sin\nu x\ \sin\mu y) \equiv \mathbf{S}_{\mu\nu}{}^+$	(μ,ν even)
B_{2u}	$\hat{u}(\cos\mu x \cos\nu y - \cos\nu x \cos\mu y) \equiv \mathbf{C}_{\mu\nu}{}^-$	(μ,ν odd)
E_g	$\begin{pmatrix} \hat{u} \cos\mu y \sin\nu x \\ \hat{u} \cos\mu x \sin\nu y \end{pmatrix}$	(μ odd, ν even)

can be found by trial and error making use of the nodal properties of the particular solutions (15); but to illustrate the systematic procedure it is instructive to apply the projection operators given in Table III.4. The results for our problem utilizing the "key" Table Va are summarized in Table Vb. We see that our particular choice of basis for E_g, corresponding to the operators in Table III.4, means that the basis functions have nodal lines parallel to the x- and y-axes, respectively.

It has sometimes been considered that one has additional degeneracy besides that indicated here because one may interchange μ and ν and get the same frequency. But we see from our correctly classified SAF's, Table Vb, that this is not the case. The nondegenerate functions go into plus or minus themselves under the interchange of μ and ν, whereas the degenerate functions go into different ones *which do not however satisfy the boundary conditions;* thus there is no additional "accidental" degeneracy under exchange of μ and ν in the functions as classified in Table Vb. One notes however that there is accidental degeneracy present, in that functions belonging to different symmetries, e.g., $\mathbf{S}_{\mu\nu}{}^-$ and $\mathbf{S}_{\mu\nu}{}^+$, will have the same energy for the same μ, ν pair. Likewise for functions $\mathbf{C}_{\mu\nu}{}^+$ and $\mathbf{C}_{\mu\nu}{}^-$ belonging to A_{2u} and B_{2u}. In each case, one function goes into plus itself and one into minus itself under the operation of interchanging μ and ν. If we denote this operation by $\mathbf{Q}$ we have for example

$$\mathbf{Q}\mathbf{C}_{\mu\nu}{}^+ = +\mathbf{C}_{\mu\nu}{}^+, \quad \mathbf{Q}\mathbf{C}_{\mu\nu}{}^- = -\mathbf{C}_{\mu\nu}{}^-.$$

Because of the accidental degeneracy, one may take linear combinations of $\mathbf{C}^+$ and $\mathbf{C}^-$ and obtain such functions as

$$\cos\mu x \cos\nu y, \quad \cos\nu x \cos\mu y$$

which go into each other under $\mathbf{Q}$. Thus the accidental double degeneracy, which was "separable" in the forms of Table Vb, takes on a familiar form.[16]

For sufficiently large $\mu^2 + \nu^2$ (beginning with 65, where both $\mu_1 = 8$, $\nu_1 = 1$ and $\mu_2 = 7$, $\nu_2 = 4$ make sides of Pythagorean triangles) there are several possible μ, ν pairs and therefore functions giving the same eigen-

[16] The degeneracy in this form, together with an apparently analogous one which they have discovered in the vibrations of an elastic cube, has also been discussed by H. Ekstein and T. Schiffman (to be published). They consider its origin to be an as yet unsolved problem. Although this is true in the sense of an intrinsic explanation, it is clear that the systematic "accidental" degeneracy is described formally by the arithmetic substitution group indicated in the paper.

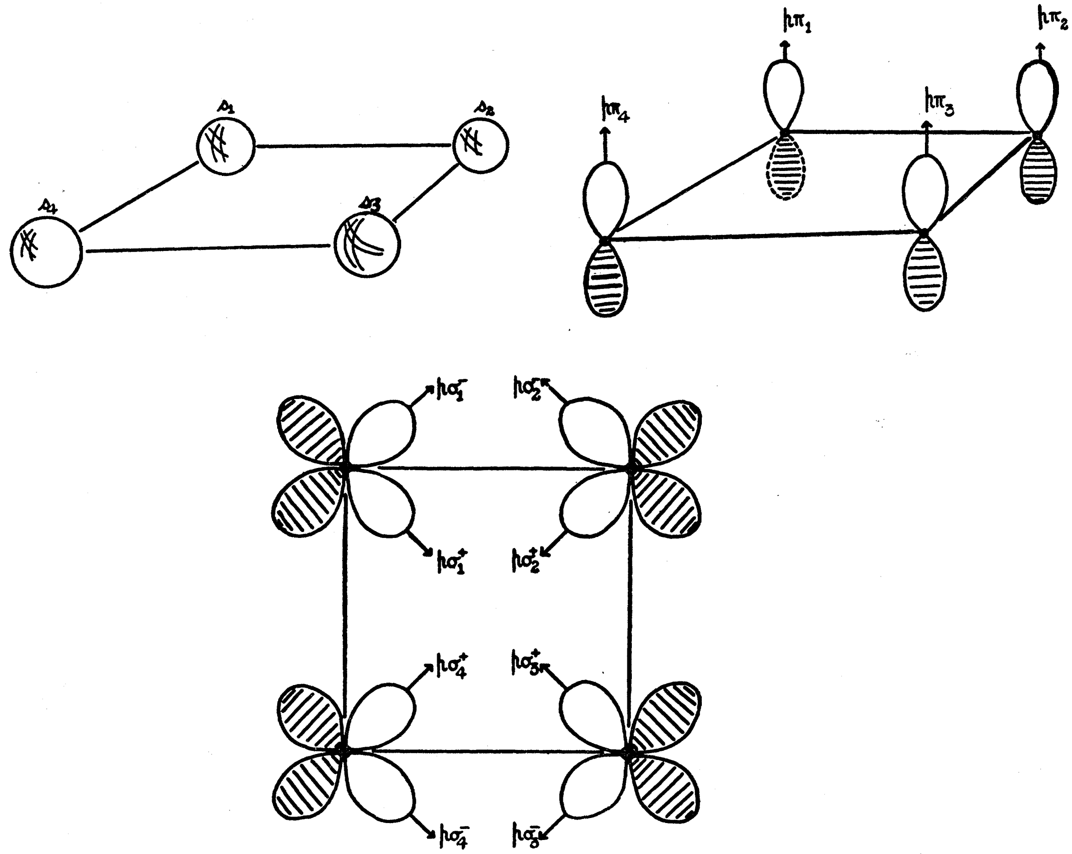

FIG. 3. s, $p\sigma$, and $p\pi$ orbitals in the "cyclobutadiene molecule."

frequency, and so we have a still higher degeneracy which, again from a purely spatial point of view, may be regarded as "accidental."

In general one may say that associated with the problem (and analogous problems in classical and quantum physics) there is an arithmetic substitution group in the "quantum numbers" μ and ν which leaves the *quantum-number formula* (eigenvalue formula) invariant; in our case this formula is given by Eq. (16) and its *quantum-number group* necessarily includes the interchange operation **Q**. When viewed with reference to the extended group, consisting of the direct product of the "quantum-number group" and the ordinary symmetry group of the system, the foregoing "accidental" degeneracy is not accidental but intrinsic. If, however, the system is subjected to some perturbation which changes the quantum-number formula, i.e., Eq. (16), and lowers its invariance group then, of course, all or part of the accidental quantum-number degeneracy may be lifted. The further development of these ideas involves the theory of arithmetic substitution groups and we shall not pursue the matter further here.

We now look briefly at the plate vibration problem. The most interesting case, corresponding to Chladni's famous experiments, is that of transverse vibrations in a square plate with free boundary. This was studied by Ritz[17] using the variational approximation method devised by him and by Rayleigh. Here approximate symmetry-adapted eigenfunctions to within a few percent are

$$
\begin{array}{lll}
A_{1u}: & \hat{u}[u_\mu(x)u_\nu(y)-u_\nu(x)u_\mu(y)] & (\mu,\ \nu \text{ odd}) \\
A_{2u}: & \hat{u}[u_\mu(x)u_\nu(y)+u_\nu(x)u_\mu(y)] & (\mu,\ \nu \text{ even}) \\
B_{1u}: & \hat{u}[u_\mu(x)u_\nu(y)+u_\nu(x)u_\mu(y)] & (\mu,\ \nu \text{ odd}) \\
B_{2u}: & \hat{u}[u_\mu(x)u_\nu(y)-u_\nu(x)u_\mu(y)] & (\mu,\ \nu \text{ even}) \\
E_g: & \begin{pmatrix} \hat{u}u_\nu(x)u_\mu(y) \\ \hat{u}u_\mu(x)u_\nu(y) \end{pmatrix} & (\mu \text{ even},\ \nu \text{ odd})
\end{array}
\tag{17}
$$

where the functions u_μ and u_ν are the eigenvibrations of of a bar with both ends free; the length of the bar is the same as the side of the plate. Taking half this length as the unit of length, and locating the origin of coordinates at the center, these bar functions for all integral values of ν are[18]

[17] W. Ritz, Ann. Physik **28**, 737 (1909).
[18] See reference 17, p. 752.

TABLE VIa. Behavior of certain generating functions *versus* key operations in the $\mathfrak{D}_4{}^h$ group. The first column gives a list of symmetry operations sufficient to build all factored projection operators for $\mathfrak{D}_4{}^h$. In the remaining columns are given the transforms of some of the 16 basic functions $s_{1,2,3,4}$, $\sigma_{1,2,3,4}{}^{\pm}$, $\pi_{13}{}^{\pm}$, $\pi_{24}{}^{\pm}$, chosen for convenience. From these basic functions 16 symmetry-adapted functions are generated in Table VIb.

					$\sigma_{1,2,3,4}{}^{\pm}=(p_x\pm p_y)_{1,2,3,4}$			$\pi_{13}{}^{\pm}\equiv p_{z1}\pm p_{z3}$		$\pi_{24}{}^{\pm}\equiv p_{z2}\pm p_{z4}$	
	s_1	s_2	s_3	s_4	$\sigma_1{}^+$	$\sigma_1{}^-$	…	$\pi_{13}{}^+$	$\pi_{13}{}^-$	$\pi_{24}{}^+$	$\pi_{24}{}^-$
$\mathbf{C}_4$	s_4	s_1	s_2	s_3	$\sigma_2{}^+$	$\sigma_2{}^-$		$\pi_{24}{}^+$	$-\pi_{24}{}^-$	$\pi_{13}{}^+$	$\pi_{13}{}^-$
$\mathbf{C}$	s_3	s_4	s_1	s_2	$\sigma_3{}^+$	$\sigma_3{}^-$		$\pi_{13}{}^+$	$-\pi_{13}{}^-$	$\pi_{24}{}^+$	$-\pi_{24}{}^-$
$\mathbf{D}_{(x)}$	s_2	s_1	s_4	s_3	$\sigma_2{}^+$	$\sigma_2{}^-$		$-\pi_{24}{}^+$	$-\pi_{24}{}^-$	$-\pi_{13}{}^+$	$-\pi_{13}{}^-$
$\mathbf{D}_{(x)}{}'$	s_1	s_4	s_3	s_2	$\sigma_1{}^+$	$-\sigma_1{}^-$		$-\pi_{13}{}^+$	$-\pi_{13}{}^-$	$-\pi_{24}{}^+$	$\pi_{24}{}^-$
$\mathbf{D}_{(y)}$	s_4	s_3	s_2	s_1	$\sigma_4{}^+$	$\sigma_4{}^-$		$-\pi_{24}{}^+$	$\pi_{24}{}^-$	$-\pi_{13}{}^+$	$\pi_{13}{}^-$
$\mathbf{i}$	s_3	s_4	s_1	s_2	$\sigma_3{}^+$	$\sigma_3{}^-$		$-\pi_{13}{}^+$	$\pi_{13}{}^-$	$-\pi_{24}{}^+$	$\pi_{24}{}^-$
$\boldsymbol{\sigma}_{\mathrm{v}}$	s_2	s_1	s_4	s_3	$\sigma_2{}^+$	$\sigma_2{}^-$		$\pi_{24}{}^+$	$\pi_{24}{}^-$	$\pi_{13}{}^+$	$\pi_{13}{}^-$
$\boldsymbol{\sigma}_{\mathrm{v}'}$	s_1	s_4	s_3	s_2	$\sigma_1{}^+$	$-\sigma_1{}^-$		$\pi_{13}{}^+$	$\pi_{13}{}^-$	$\pi_{24}{}^+$	$-\pi_{24}{}^-$
$\boldsymbol{\sigma}_{\mathrm{h}}$	s_1	s_2	s_3	s_4	$\sigma_1{}^+$	$\sigma_1{}^-$		$-\pi_{13}{}^+$	$-\pi_{13}{}^-$	$-\pi_{24}{}^+$	$-\pi_{24}{}^-$

$$\begin{aligned}
&\nu\text{ odd:}\quad u_\nu=\frac{\sinh k_\nu\ \sin k_\nu x+\sin k_\nu\ \sinh k_\nu x}{(\sinh^2 k_\nu-\sin^2 k_\nu)^{\frac{1}{2}}}\\
&\qquad\qquad\text{where }\tan k_\nu=\tanh k_\nu\\
&\nu\text{ even:}\quad u_\nu=\frac{\cosh k_\nu\ \cos k_\nu x+\cos k_\nu\ \cosh k_\nu x}{(\cosh^2 k_\nu+\cos^2 k_\nu)^{\frac{1}{2}}}\\
&\qquad\qquad\text{where }\tan k_\nu=-\tanh k_\nu.
\end{aligned}\tag{18}$$

The more nearly exact solutions obtained by Ritz differ from those given in (17) only by small added terms consisting of linear combinations of solutions all of the same symmetry type.

B. SAF's from Atomic Orbitals for a Molecule with $\mathfrak{D}_4{}^h$ Symmetry

As an elementary microphysical example we consider a "one-electron problem"; i.e., the determination of SAF's as linear combinations of atomic orbitals. These linear combinations are often taken to be a first approximation to molecular orbitals. In Fig. 3 we have diagrammed the s, $p\sigma$, and $p\pi$ atomic orbitals in a hypothetical molecule ("cyclobutadiene") of $\mathfrak{D}_4{}^h$ symmetry, and in Tables VIa and VIb we have carried out the generation of SAF's from these, taking as generating functions the orbitals of atom number 1.

C. Standing Sound Waves in a Cubic Room

We turn now to a 3-dimensional example. The eigenvibrations of the velocity potential ψ in a fluid bounded by a cubic box with side of length π, are governed by the 3-dimensional wave equation analogous to (15).

$$\nabla^2\psi=\frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2}\tag{19}$$

The boundary conditions are defined by the requirement that the velocity

$$u=-\nabla\psi\tag{20}$$

shall be zero at $x, y, z=\pm\pi/2$.

Particular solutions of these equations are of the form

$$\begin{aligned}
&\cos\lambda x\ \cos\mu y\ \cos\nu z\ e^{i\omega t}\quad(\lambda,\ \mu,\ \nu\text{ even})\\
&\cos\lambda x\ \cos\mu y\ \sin\nu z\ e^{i\omega t}\quad(\lambda,\ \mu\text{ even};\ \nu\text{ odd})\\
&\cdot\quad\cdot\quad\cdot\\
&\omega=c(\lambda^2+\mu^2+\nu^2)^{\frac{1}{2}}.
\end{aligned}$$

Omitting the common factor, $e^{i\omega t}$, the possible independent particular solutions may be written out as follows

$$\begin{array}{ll}
LMN & (\lambda,\ \mu,\ \nu\text{ even}\qquad\qquad)\\
LMN' & (\lambda,\ \mu\quad\text{even};\ \nu\quad\text{odd})\\
LM'N & (\lambda,\ \nu\quad\text{even};\ \mu\quad\text{odd})\\
LM'N' & (\lambda\qquad\text{even};\ \mu,\ \nu\text{ odd})\\
L'MN & (\mu,\ \nu\quad\text{even};\ \lambda\quad\text{odd})\\
L'MN' & (\mu\qquad\text{even};\ \lambda,\ \nu\text{ odd})\\
L'M'N & (\nu\qquad\text{even};\ \lambda,\ \mu\text{ odd})\\
L'M'N' & (\qquad\qquad\lambda,\ \mu,\ \nu\text{ odd})
\end{array}\tag{21}$$

where, as in the membrane case, we have adopted the convenient abbreviations

$$\begin{array}{lll}
\cos\kappa x\equiv K & \sin\kappa x\equiv K' & (\kappa=\lambda,\mu,\nu)\\
\cos\kappa y\equiv K & \sin\kappa y\equiv K' & (K=L,M,N)\\
\cos\kappa z\equiv K & \sin\kappa z\equiv K', &
\end{array}\tag{22}$$

and the order of the capital symbols always represents the order of the functions of x, y, and z, respectively, in that sequence.

Since we are dealing with a scalar quantity (velocity potential) in this case, there is no unit-vector prefix in front of the product wave function.

The symmetry group here is the octahedron group. It will be sufficient to find the symmetry-adapted eigenvibrations with respect to the proper-octahedron (or "enantio-cube") group, $\mathfrak{O}$, alone because the doubling of the group by including the inversion will merely lead, in a fairly obvious manner, to doubling each symmetry-adapted function: The two resulting functions under the larger group will be defined so that one is even under inversion and the other is odd.

Figure 2 shows the proper symmetry operations in

TABLE VIb. Determination of symmetry-adapted functions made up of s, $p\sigma$, and $p\pi$ atomic orbitals, respectively, for a system with $\mathfrak{D}_4{}^h$ symmetry, e.g., the well-known (and unobserved) cyclobutadiene molecule (Fig. 3).

$\mathfrak{D}_4{}^h=\mathfrak{D}_4\times\mathfrak{C}^i$			SAF's from s-orbitals. Generating function: s_1	SAF's from $p\sigma$ orbitals. Generating function: $\sigma_1{}^{\pm}\equiv(p_x\pm p_y)_1$	SAF's from p-orbitals. Generating function: $\pi_{13}{}^{\pm}=p_{z1}\pm p_{z3}$
A_{1g}	$\mathbf{d}\cdot\mathbf{c}_4\cdot\mathbf{i}$		$s_1+s_3+s_2+s_4$	$\sigma_1{}^++\sigma_3{}^++\sigma_2{}^++\sigma_4{}^+$	no
A_{2g}	$\mathbf{c}_4\cdot\mathbf{i}$	$^-\mathbf{d}$, $^-\mathbf{d}'$, $^-\mathbf{c}^{\mathrm{v},\mathrm{v}'}$	no	$\sigma_1{}^--\sigma_2{}^-+\sigma_3{}^--\sigma_4{}^-$	no
B_{1g}	$\mathbf{d}\cdot\mathbf{c}\cdot\mathbf{i}$	$\mathbf{E}-\mathbf{C}_4$, $^-\mathbf{d}'$, $\mathbf{E}-\mathbf{S}_4$, $^-\mathbf{c}^{\mathrm{v}'}$	no	$\sigma_1{}^-+\sigma_3{}^-+\sigma_2{}^-+\sigma_4{}^-$	no
B_{2g}	$\mathbf{d}\cdot\mathbf{c}\cdot\mathbf{i}$	$\mathbf{E}-\mathbf{C}_4$, $^-\mathbf{d}$, $\mathbf{E}-\mathbf{S}_4$, $^-\mathbf{c}^{\mathrm{v}}$	$s_1-s_2+s_3-s_4$	$\sigma_1\ -\sigma_2\ +\sigma_3\ -\sigma_4$	no
A_{1u}	$\mathbf{d}\cdot\mathbf{c}_4$	$^-\mathbf{i}$, $\mathbf{E}-\mathbf{S}_4$, $^-\mathbf{c}^{\mathrm{s},\mathrm{v},\mathrm{v}'}$	no	no	no
A_{2u}	$\mathbf{c}_4\cdot\mathbf{c}^{\mathrm{v},\mathrm{v}'}$	$^-\mathbf{d}$, $^-\mathbf{d}'$, $^-\mathbf{i}$, $\mathbf{E}-\mathbf{S}_4$, $^-\mathbf{c}^{\mathrm{s}}$	no	no	$\pi_{13}{}^++\pi_{24}{}^+$
B_{1u}	$\mathbf{d}\cdot\mathbf{c}\cdot\mathbf{c}^{\mathrm{v}'}$	$\mathbf{E}-\mathbf{C}_4$, $^-\mathbf{d}'$, $^-\mathbf{i}$, $^-\mathbf{c}^{\mathrm{s},\mathrm{v}}$	no	no	$\pi_{13}{}^+-\pi_{24}{}^+$
B_{2u}	$\mathbf{d}'\cdot\mathbf{c}\cdot\mathbf{c}^{\mathrm{v}}$	$\mathbf{E}-\mathbf{C}_4$, $^-\mathbf{d}$, $^-\mathbf{i}$, $^-\mathbf{c}^{\mathrm{s},\mathrm{v}'}$	no	no	no
E_g	$\mathbf{d}_y\cdot\mathbf{i}$	$^-\mathbf{c}$, $^-\mathbf{c}^{\mathrm{s}}$, $^-\mathbf{d}_x$, $^-\mathbf{c}^{\mathrm{v}}{}_x$	no	no	$\pi_{13}{}^-+\pi_{24}{}^-$
	$\mathbf{d}_x\cdot\mathbf{i}$	$^-\mathbf{c}$, $^-\mathbf{c}^{\mathrm{s}}$, $^-\mathbf{d}_y$, $^-\mathbf{c}^{\mathrm{v}}{}_y$	no	no	$\pi_{13}{}^--\pi_{24}{}^-$
E_u	$\mathbf{d}_y\cdot\mathbf{c}^{\mathrm{s}}$	$^-\mathbf{c}$, $^-\mathbf{i}$, $^-\mathbf{d}_x$, $^-\mathbf{c}^{\mathrm{v}}{}_y$	$s_1-s_3+s_4-s_2$	$\sigma_1{}^{\pm}-\sigma_3{}^{\pm}+\sigma_4{}^{\pm}-\sigma_2{}^{\pm}$	no
	$\mathbf{d}_x\cdot\mathbf{c}^{\mathrm{s}}$	$^-\mathbf{c}$, $^-\mathbf{i}$, $^-\mathbf{d}_y$, $^-\mathbf{c}^{\mathrm{v}}{}_x$	$s_1-s_3+s_2-s_4$	$\sigma_1{}^{\pm}-\sigma_3{}^{\pm}+\sigma_2{}^{\pm}-\sigma_4{}^{\pm}$	no

TABLE VIIa. Behavior of the particular solutions given by Eqs. (11) under key operations of the enantiocube group $\mathfrak{O}$. The first column gives a list of symmetry operations sufficient to build all factored projection operators for $\mathfrak{O}$. The second column gives, in crystallographic notation, the ordinary Cartesian transformation matrices corresponding to these operators: What are indicated are the old variables to which the new ones, $(x'y'z')$, are equal in that order. In the remaining columns are given the transforms of the eight basic generating functions written in the abbreviated notation defined by Eqs. (13).

		LMN	LMN'	$LM'N$	$LM'N'$	$L'MN$	$L'MN'$	$L'M'N$	$L'M'N'$
$\mathbf{C}_x$	$x\bar{y}\bar{z}$	LMN	$-LMN'$	$-LM'N$	$LM'N'$	$L'MN$	$-L'MN'$	$-L'M'N$	$L'M'N'$
$\mathbf{C}_y$	$\bar{x}y\bar{z}$	LMN	$-LMN'$	$LM'N$	$-LM'N'$	$-L'MN$	$L'MN'$	$-L'M'N$	$L'M'N'$
$\mathbf{C}_z$	$\bar{x}\bar{y}z$	LMN	LMN'	$-LM'N$	$-LM'N'$	$-L'MN$	$-L'MN'$	$L'M'N$	$L'M'N'$
$\mathbf{T}_1$	zxy	NLM	$N'LM$	NLM'	$N'LM'$	$NL'M$	$N'L'M$	$NL'M'$	$N'L'M'$
$\mathbf{T}_2$	$\bar{y}z\bar{x}$	MNL	$MN'L$	$-M'NL$	$-M'N'L$	$-MNL'$	$-MN'L'$	$M'NL'$	$M'N'L'$
$\mathbf{T}_1{}^2$	yzx	MNL	$MN'L$	$M'NL$	$M'N'L$	MNL'	$MN'L'$	$M'NL'$	$M'N'L'$
$\mathbf{D}_x$	$\bar{x}zy$	LNM	$LN'M$	LNM'	$LN'M'$	$-L'NM$	$-L'N'M$	$-L'NM'$	$-L'N'M'$
$\mathbf{D}_y$	$z\bar{y}x$	NML	$N'ML$	$-NM'L$	$-N'M'L$	NML'	$N'ML'$	$-NM'L'$	$-N'M'L'$
$\mathbf{D}_z$	$yx\bar{z}$	MLN	$-MLN'$	$M'LN$	$-M'LN'$	$ML'N$	$-ML'N'$	$M'L'N$	$-M'L'N'$
$\mathbf{D}_{z'}$	$\bar{y}\bar{x}\bar{z}$	MLN	$-MLN'$	$-M'LN$	$M'LN'$	$-ML'N$	$ML'N'$	$M'L'N$	$-M'L'N,$
$\mathbf{C}_{4x}$	$x\bar{z}y$	LNM	$-LN'M$	LNM'	$-LN'M'$	$L'NM$	$-L'N'M$	$L'NM'$	$-L'N'M'$
$\mathbf{C}_{4y}$	$zy\bar{x}$	NML	$N'ML$	$NM'L$	$N'M'L$	$-NML'$	$-N'ML'$	$-NM'L'$	$-N'M'L'$
$\mathbf{C}_{4z}$	$\bar{y}xz$	MLN	MLN'	$-M'LN$	$-M'LN'$	$ML'N$	$ML'N'$	$-M'L'N$	$-M'L'N'$

the cube. The notation is a natural generalization of that we have used for the cyclic and dihedral groups, with their unique principal axes.

Table IV.2 gives the factored projection operators for $\mathfrak{O}$, and Table VIIa gives the behavior of the various generating functions (21) under a set of key operations involved in the factored projection operators of Table IV.2. Finally Table VIIb gives the required "right linear combinations," or symmetry-adapted vibrations.

D. A Three *d*-Electron Problem for a Solid-State System with Cubic Symmetry

We consider an ion with three d-electrons in a crystal field of cubic symmetry. Examples are chrome alum[19] and chromium fluoride.[20]

The number and type of levels which can occur are obtained by the standard method.[21] In this case the method consists of reducing the product representations corresponding to a system of three isolated electrons in a field of cubic symmetry:

$$\begin{aligned}&(F_2{}^3)\rightarrow{}^4A_2+{}^2E+{}^2F_1+{}^2F_2,\\&(F_2{}^2E)\rightarrow{}^4F_1+{}^4F_2+{}^2A_1+{}^2A_2+2{}^2E+2{}^2F_1+2{}^2F_2,\\&(F_2E^2)\rightarrow{}^4F_1+2{}^2F_1+2{}^2F_2,\\&(E^3)\rightarrow{}^2E.\end{aligned}\tag{23}$$

The products on the left correspond to the only admissible types in a field of cubic symmetry, since the d-electron rep of the sphere group, $D^{(2)}$, breaks up into the E and F_2 reps of the cubic group when the symmetry is reduced to the latter. When the Coulomb interaction between the electrons is allowed for, the crystal configurations on the left break up into the level types indicated on the right. The spectral multiplicity of the levels is indicated by the upper prescript in front of the symbol for the symmetry type; the number of levels of each type is indicated by the coefficient.

We have listed only those types which are permitted

[19] This system was studied in detail by R. Finkelstein and J. H. Van Vleck, J. Chem. Phys. **8**, 790 (1940).

[20] C. M. Herzfeld has studied the strong field case of this system in detail (private communication; see Bull. Am. Phys. Soc. **29**, No. 7, 11, 1954). He has also found some of the proper basis functions for the reps (or, in our terminology, the SAF's) in terms of products of one-electron functions. He used for the projection operators (unfactored) the Young generators for the symmetric permutation group on four letters, which group is isomorphic to the octahedral group $\mathfrak{O}$.

[21] E. Wigner, Z. Physik **43**, 624 (1927); H. Bethe, Ann. phys. **3**, 133 (1929); L. Tisza, Z. Physik **82**, 48 (1933).

TABLE VIIb. Symmetry-adapted eigenvibrations for the velocity potential ψ (or the pressure $p=\rho\partial\psi/\partial t$ where $\rho=$density) in a cubic room. The factor $e^{i\omega t}$ has been omitted.[a]

A_1:	$LMN+NLM+MNL+MLN+LNM+NML\equiv[LMN]_+$ $L'M'N'+N'L'M'+M'N'L'-M'L'N'-L'N'M'-N'M'L'\equiv[L'M'N']_-$	
A_2:	$LMN+NLM+MNL-LNM-NML-MLN\equiv[LMN]_-$ $L'M'N'+N'L'M'+M'N'L'+L'N'M'+N'M'L'+M'L'N'\equiv[L'M'N']_+$	
E:	$\begin{pmatrix} LMN+NML-LNM-NLM \\ LMN+LNM-NML-MNL \end{pmatrix}\equiv E_{,1}$	$\begin{pmatrix} L'M'N'-N'M'L' \\ L'M'N'-L'N'M' \end{pmatrix}\equiv E_{,2}$
F_1:	$\begin{pmatrix} LM'N'-LN'M' \\ L'MN'-N'ML' \\ L'M'N-M'L'N \end{pmatrix}\equiv F_{1,1}$	$\begin{pmatrix} L'MN+L'NM \\ LM'N+NM'L \\ LMN'+MLN' \end{pmatrix}\equiv F_{1,2}$
F_2:	$\begin{pmatrix} LM'N'+LN'M' \\ L'MN'+N'ML' \\ L'M'N+M'L'N \end{pmatrix}\equiv F_{2,1}$	$\begin{pmatrix} L'MN-L'NM \\ LM'N-NM'L \\ LMN'-MLN' \end{pmatrix}\equiv F_{2,2}$

[a] The symbol $[LMN]_+$ is introduced for the sum of all permutations of LMN. The corresponding symbol $[LMN]_-$ represents the sum of the even permutations minus the sum of the odd permutations.

by the requirement of antisymmetry of the total space-spin wave function. Thus we have omitted those types which would appear if the products on the left were interpreted as totally symmetrized Kronecker products.[19]

The explicit forms of the SAF's corresponding to the right side of Eq. (23) are rather tedious to obtain by the usual methods. On the other hand, they are found quite quickly with the help of the factored projection operators in Table IV.2, and on the basis of Table VIIIa we have exhibited in Table VIIIb four sample sets of functions resulting from the $(F_2{}^3)$, $(F_2{}^2E)$, and (F_2E^2) crystal configurations. We have chosen as a basic set of one-electron functions

$$\begin{array}{ll} E & F_2 \\ w\equiv x^2-y^2\sim(2\gamma)_2 & X\equiv yz\sim(2\epsilon)_3 \\ v\equiv z^2-x^2\sim(2\gamma)_1-(2\gamma)_2 & Y\equiv zx\sim(2\epsilon)_2 \\ & Z\equiv xy\sim(2\epsilon)_1, \end{array} \tag{24}$$

where on the right is indicated the correspondence with the "γ" and "ϵ" functions chosen by Bethe.[22]

For symmetry we have also used the nonindependent function $u\equiv y^2-z^2=-(v+w)$.

By way of assistance in quickly obtaining the SAF's it is convenient to have the transformation properties of the X, Y, Z and u, v, w functions available, and we list these for some key operations, in an abbreviated notation similar to the crystallographic notation used in Table I.4; i.e., since the transformation matrices are all monomial, we indicate merely to which old variables the new $(XYZ)(uvw)$ are equal, in that order.

VII. SUMMARY

Given a system, however complicated. One may find its invariance group, i.e., the group of operations under which the relevant features (e.g., the equations of motion or wave equations) of the system are invariant. The complete set of "symmetry types" associated with the system are defined by the complete set of rows of the various irreducible representations (reps) of the invariance group. An efficient method has here been developed for generating, from an arbitrary basis, symmetry-adapted functions (or SAF's) belonging to any given symmetry type. The method involves the use of factored and simplified forms of the projection operators for each symmetry type. It has been worked out in detail for all the finite point symmetry groups except $\mathcal{I}$ and $\mathcal{I}^h$. It is useful in problems where one wishes to determine the states of a complicated system in terms of combinations of functions given by some simplified problem. Such problems occur in the determination of symmetry coordinates for the analysis of vibrations in macroscopic continua, crystals, or molecules; or in the determination of approximate electron (nucleon) states in crystals, molecules, and atoms (nuclei).

[22] See reference 21, p. 165.

VIII. ACKNOWLEDGMENTS

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TABLE VIIIa. Behavior of the d-electron functions listed in Eq. (24) under key operations of the enantio-cube group $\mathcal{O}$.

$\mathbf{C}_x$	$(X\bar{Y}\bar{Z})(uvw)$	$\mathbf{D}_x$	$(X\bar{Z}\bar{Y})(\bar{u}\bar{w}\bar{v})$
$\mathbf{C}_y$	$(\bar{X}Y\bar{Z})(uvw)$	$\mathbf{D}_y$	$(\bar{Z}Y\bar{X})(\bar{w}\bar{v}\bar{u})$
$\mathbf{C}_z$	$(\bar{X}\bar{Y}Z)(uvw)$	$\mathbf{D}_z$	$(\bar{Y}\bar{X}Z)(\bar{v}\bar{u}\bar{w})$
$\mathbf{T}_1$	$(ZXY)(wuv)$	$\mathbf{C}_{4x}$	$(\bar{X}Z\bar{Y})(\bar{u}\bar{w}\bar{v})$
$\mathbf{T}_2$	$(\bar{Y}Z\bar{X})(vwu)$	$\mathbf{C}_{4y}$	$(\bar{Z}\bar{Y}X)(\bar{w}\bar{v}\bar{u})$
$\mathbf{T}_1{}^2$	$(YZX)(vwu)$	$\mathbf{C}_{4z}$	$(Y\bar{X}\bar{Z})(\bar{v}\bar{u}\bar{w})$

TABLE VIIIb. Sample SAF's made up of d^3 electron functions for a system with $\mathcal{O}$ symmetry, e.g., in the chrome-alum or chromium-fluoride crystal. The SAF's are those for levels resulting from the (F_2^3), (F_2^2E), (F_2E^2) crystal configurations.

	$X\equiv yz$ $u\equiv y^2-z^2$ $(F_2^3)A_2$ quartet level, type of generating function: $Z_1X_2Y_3$	$Y\equiv zx$ $v\equiv z^2-x^2$ $(F_2^2E)E$ doublet level, type of generating function: $X_1X_2w_3$	$Z\equiv xy$ $w\equiv x^2-y^2$ $(F_2E^2)F_1$ $(F_2E^2)F_2$ doublet levels, type of generating function: $X_1w_2w_3$
A_1			
A_2	$Z_1(X_2Y_3-X_3Y_2)+Z_2(X_3Y_1-X_1Y_3)$ $+Z_3(X_1Y_2-X_2Y_1)=\mathbf{Z}\cdot\mathbf{X}\times\mathbf{Y}$		
E		$Y_1Y_2(w_3-u_3)+Z_1Z_2(v_3-u_3)$ $Z_1Z_2(u_3-v_3)\ +X_1X_2(w_3-v_3)$	
F_1			$X_1(v_2v_3-w_2w_3)$ $Y_1(w_2w_3-u_2u_3)$ $Z_1(u_2u_3-v_2v_3)$
F_2			$X_1(v_2v_3+w_2w_3)$ $Y_1(w_2w_3+u_2u_3)$ $Z_1(u_2u_3+v_2v_3)$

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APPENDIX I. VERIFICATION OF THE SYMMETRY PRINCIPLE FOR THE SYMMETRY-ADAPTED EIGENFUNCTIONS OF A HAMILTONIAN

We shall demonstrate, first, that the symmetry of a symmetry-adapted eigenfunction is a subgroup of the symmetry $\mathcal{H}$ of its Hamiltonian and, second, that this relation may be viewed as an instance of a general "Many-One Symmetry Principle" which can be formulated for both geometrical and physical systems.[1]

If an eigenfunction belongs to a nondegenerate rep Γ, its symmetry group is exactly the kernel of the homomorphism of $\mathcal{H}$ upon Γ and is therefore an invariant subgroup of $\mathcal{H}$. There remains only to consider the somewhat less obvious case of a function which belongs to the ith row of a degenerate rep Γ^j: By a simple relabeling of rows, amounting to a trivial "change" of basis, it is always possible to arrange matters so that the ith row becomes the first. The symmetry group of the eigenfunction, f^{ji}, is then that subset of the operations of $\mathcal{H}$ for which the respresenting matrices in Γ^j take the form

$$\begin{pmatrix} 1 & \mathbf{0} \\ \mathfrak{v} & \mathfrak{K} \end{pmatrix}. \tag{I.1}$$

Here $\mathbf{0}$ is a 1-row null matrix and $\mathfrak{v}$ is some 1-column matrix. The product of any two matrices of this type is another matrix of the same type, and thus the corresponding operations of $\mathcal{H}$ form a subgroup. This subgroup is the "cokernel" of the first row of the jth rep.

We note also in connection with the demonstration of the first simplification theorem B (Sec. III; A), that the product of a matrix of the form (I.1) by a general matrix of the form

$$\begin{pmatrix} r' & \mathfrak{h}' \\ \mathfrak{v}' & \mathfrak{K}' \end{pmatrix}$$

is

$$\begin{pmatrix} r' & \mathfrak{h}' \\ \mathfrak{v}r'+\mathfrak{K}\mathfrak{v}' & \mathfrak{v}\mathfrak{h}'+\mathfrak{K}\mathfrak{K}' \end{pmatrix}, \tag{I.2}$$

i.e., the first-row, first-column element of the multiplying matrix reappears.

It is clear that the cokernels of the various rows of Γ^j depend upon the explicit choice of basis. It is also clear that they all contain as a common invariant subgroup the kernel of Γ^j; the latter, which is constituted of all the identity matrices in the rep, is independent of the choice of basis.

We turn now to the demonstration that the relation between the symmetries of Hamiltonian and eigenfunction is a special case of the many-one symmetry principle. In order to state the principle concisely we need to define two terms:

Many- and One-State

In a system of any given kind let there exist two types of state description having the following relation when viewed in the complete assembly of all systems of the given kind. Suppose that *for every one of the states of the first type there is one of the second* but that *for every one of the second there are more than one of the first.* We say that the two types of states are in *many-to-one correspondence.*[23] We will call the states of the first type

[23] There is no implication in this definition that the many-one correspondence is unique. If this is assumed, then the many-one principle follows *deductively*.

the *many-states*,[24] and those of the second type the *one-states* of the system under consideration.

Now a general principle may be formulated concerning the relation between the symmetry groups of the two different types of state found in a given system.

Many-One Symmetry Principle

The symmetry of a one state may be greater, but cannot be less, than the symmetry of any of the corresponding manystates. Concisely: Many-state symmetry is a subgroup in one-state symmetry.

This principle may be proved exactly[1] for any kind of geometrical system in which there is a determinate $m:1$ correspondence between the two types of states and in which representatives of the two types occur with equal likelihood of any orientation in space, i.e., in the complete assembly of the system there is a uniform density distribution of states of each type. Then the symmetry of an m-state is a subgroup of index m in the symmetry of the 1-state. More generally, it is clear deductively that the principle holds whenever the one state is a one-valued function of many states.[23]

The principle may also be shown to hold in various cases where the densities of states and $m:1$ ratio are quantitatively indeterminate and only the many-one correspondence may be established. Just as in the analogous case of the Entropy principle, to which it may be related, the Symmetry principle is verified in various fields of reversible and irreversible physical phenomena on the basis of the specific laws which are known to hold for those phenomena. Thus it suggests itself that, if only heuristically, the principle be taken to have universal validity.

Its validity within the domain of Hamiltonian quantum mechanics is readily verified: Any quantum-mechanical system may be described by giving its Hamiltonian.[25] It may also be described by giving the complete set of possible eigenvalues and their symmetry-adapted eigenfunctions or, as we may say for brevity, eigenvalue SAF's. For *one* given Hamiltonian there are *many* eigenvalue SAF's; in fact it is generally surmised, though it does not seem to have been proved,[26] that there are always an infinite number of them. On the other hand, *one* given eigenvalue SAF corresponds to *one* Hamiltonian of which it is a characteristic solution.[27]

[24] In the paper referred to in reference 1 the names of the two type states were interchanged through an error.

[25] For a *complete* description one must of course designate a complete set of commuting observables, of which the Hamiltonian need only be one.

[26] B. L. van der Waerden, *Die Gruppentheoretische Methode in der Quantenmechanik* (Verlag Julius Springer, Berlin, 1932; Edwards Brothers, Ann Arbor, 1944), p. 5.

[27] It is readily seen that this is the case in all normal instances where the general form of the Hamiltonian is known: For a nonrelativistic many-particle system in an electrostatic field, we have the potential energy (and therefore the Hamiltonian) uniquely determined in terms of the eigenvalue W and the eigenfunction ψ as follows:

$$V=W+\sum_k \frac{\hbar^2}{2m_k}\frac{\nabla_k^2\psi}{\psi}.$$

For a relativistic one-electron system in a general electromagnetic field ($\mathbf{A}$, V) the latter (and therefore the Hamiltonian) is determined in terms of W and the 4-component wave function by inverting the Dirac system.

It is evident, from the demonstration at the beginning of this appendix, that the many-one symmetry principle is verified here.

APPENDIX II. DERIVATION OF THE IMPROPER SYMMETRY GROUPS FROM PROPER GROUPS

The determinants of the matrices representing the symmetry operations in a group are all $+1$ or -1 since the unit of volume is unaltered by a symmetry operation. In general the group may be *proper*, i.e., such that all operations are represented by matrices with determinants $+1$ (pure turns); or *improper*, i.e., such that operations with $\det=-1$ also occur.

First we establish the proposition that *the collection of proper operations in any improper group forms an invariant subgroup of index 2*, or what may be termed a halving subgroup. That the collection forms an invariant subgroup is evident from the fact that the product of two proper operations or of two improper operations is proper, while the product of a proper operation with an improper operation is improper. Next, we may draw the conclusion that the number p of proper operations in an improper group is exactly equal to the number i of improper operations. The reasoning is as follows: Take any improper operation. Multiply successively by the i different improper operations. We get i distinct proper operations (The distinctness follows from the group property of the existence of a unique right inverse.) Therefore p is at *least equal to i.* Conversely, multiply the given improper operation by the p different proper ones to obtain p distinct operations. Therefore *i is at least equal to p.* Comparing the two italicized statements, we see that $i=p$. The proper operations obviously form a halving subgroup.

It will now be demonstrated that all improper groups fall into two types and are directly derivable from the set of all proper groups once these are known. It is at once evident that for every proper group $(\mathbf{T})$ there is an improper group $(\mathbf{A})_{\text{central}}$ obtainable by taking the direct product of $(\mathbf{T})$ with the origin-inversion group $\mathcal{C}^i$. Thus

$$(\mathbf{A})_{\text{central}}=(\mathbf{T})\mathcal{C}^i \qquad \text{(II.1)}$$

and conversely, by the result of the preceding paragraph, every group containing the inversion operator $\boldsymbol{\iota}$ can be written in this form.

On the other hand, there are improper groups possible which do not contain the origin-inversion group as subgroup, i.e., do not contain the inversion $\boldsymbol{\iota}$. Such a noncentral group will be represented by the symbol $(\mathbf{A})^-$. Let $\mathbf{A}_r$ represent any one of the improper members of

$(\mathbf{A})^-$. By a familiar elementary theorem this may always be represented as compounded of inversion followed by a turn, i.e. $\mathbf{A}_r = \boldsymbol{\iota}\mathbf{T}_r$ where $\mathbf{T}_r$ is the turn corresponding to $\mathbf{A}_r$. This corresponding turn cannot be a member of the given noncentral group for, if it were, we should have

$$\mathbf{T}_r^{-1}\mathbf{A}_r = \boldsymbol{\iota}\mathbf{T}_r^{-1}\mathbf{T}_r = \boldsymbol{\iota}$$

as a member of the group contrary to hypothesis. Let us expand the group $(\mathbf{A})^-$ in cosets under its proper halving subgroup $(\mathbf{T}')$

$$(\mathbf{A})^- = (\mathbf{T}'),\ \mathbf{A}_r(\mathbf{T}') = (\mathbf{T}'),\ (\mathbf{T}')\mathbf{A}_r \qquad \text{(II.2)}$$

where $\mathbf{A}_r$ is any improper member.

From $\mathbf{A}_r(\mathbf{T}') = (\mathbf{T}')\mathbf{A}_r$, which must hold, we have also

$$\mathbf{T}_r(\mathbf{T}') = (\mathbf{T}')\mathbf{T}_r.$$

Remembering that $\mathbf{T}_r$ is not a member of $(\mathbf{T}')$, we see that the two sets $(\mathbf{T}')$ and $\mathbf{T}_r(\mathbf{T}')$ together form a new group which must be one of the proper symmetry groups, i.e.

$$(\mathbf{A}) = (\mathbf{T}'),\ \mathbf{T}_r(\mathbf{T}').$$

This proper group and the improper group (II.2) are clearly in 1-to-1 correspondence (isomorphic). In case the group $(\mathbf{A})^-$ includes among its elements a *pure reflection*, e.g., the product of an origin-inversion by the half-turn $\mathbf{C}_2$, we may choose

$$\mathbf{A}_r = \boldsymbol{\iota}\mathbf{C}_2 = \boldsymbol{\sigma}$$

which has the property that its square is the identity, and (II.2) may also be written as a direct product of two subgroups.

In summary then, we have the classification-simplifying theorem stated in Sec. IV of this paper.