Semidirect Products and Point Groups

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INTRODUCTION

ALTHOUGH the properties of the point groups are very well known, there has been recently considerable interest in them. One reason for this is that one wants to simplify the construction of symmetry-adapted functions, which requires the transform $R\phi$ of an arbitrary function ϕ under all the operations $R\phi$ of a group (see Sec. 6). This was the technique used by the author[1] to obtain spherical harmonics adapted to the irreducible representations of the point groups. In a later note,[2] I remarked that one could exploit the method for the reduction of space groups given by Bouckaert, Smoluchowski, and Wigner.[3] This is so, because all crystallographic point groups admit of an invariant subgroup that is a direct product of cyclic groups and which occupies the same position with respect to the corresponding point group as the translation group does with respect to the space group. Commenting on this remark, McIntosh[4] observed that a more powerful method was available, because the point groups could be expressed as semidirect products, a concept which had been developed some years before by Mackey.[5] Accordingly, McIntosh was able to give a very complete theory of the point groups and their representations. Whereas McIntosh based his work on the treatment of the matrix representations, the present author[6] was able to show that in most practical cases a simpler treatment was possible, if the bases of the representations, rather than the representations themselves, are taken as the starting point. In this way, moreover, the graphical character of the Bouckaert, Smoluchowski, and Wigner method can be preserved, which allows one to obtain many results without the need of laborious algebra. The purpose of this note is to provide a nonmathematical introduction to this work. Accordingly, no proofs will be given, but the reader can find them in the reference given.[6]

[1] S. L. Altmann, Proc. Camb. Phil. Soc. **53**, 343 (1957).
[2] S. L. Altmann, Progress Report No. 3, Quantum Chemistry Group, Mathematical Institute, Oxford, 1957, p. 33 (unpublished).
[3] C. P. Bouckaert, R. Smoluchowski and E. Wigner, Phys. Rev. **50**, 58 (1936).
[4] H. V. McIntosh, Symmetry adapted functions belonging to the crystallographic lattice groups, Tech. Rept. No. 58-3, RIAS, Baltimore, 1958 (unpublished); *ibid.* J. Mol. Spectr. **5**, 269 (1960).
[5] G. W. Mackey, Proc. Nat. Acad. Sci., Wash., **35**, 537 (1949); Ann. Math. **55**, 101 (1952).
[6] S. L. Altmann, Phil. Trans. Roy. Soc. (London) **A255**, 216 (1963).

1. DEFINITIONS

If two groups **N** and **C** are such that any element N_i of one commutes with any element C_j of the other

$$N_iC_j = C_jN_i \tag{1}$$

their group product (i.e., the set of all elements of the form N_iC_j) forms, as is well known, a group **G** which is the direct product of **N** and **C**: $\mathbf{N} \times \mathbf{C} = \mathbf{G}$. On the other hand, if **N** and **C** do not commute in detail but rather

$$\mathbf{N}C_j = C_j\mathbf{N} \tag{2}$$

for all $C_j \in \mathbf{N}$, then the group product forms a group which is called the semidirect product of **N** and **C**, for which we propose the notation

$$\mathbf{N} \wedge \mathbf{C} = \mathbf{G}\,. \tag{3}$$

Equation (2) means that **N** is *invariant* with respect to **C** and, as the converse will not be true in general, this means that the order of the factors in (3) is significant. We agree that the invariant subgroup will always be given first.[7]

2. THE POLES OF ROTATIONS AND THE INVARIANT SUBGROUPS

Since the invariant subgroups are much used in the theory it is useful to have a graphical method to obtain them. This requires the concept of the *poles* of a rotation, which was introduced long ago. They are the two points of the unit sphere that are left invariant by a rotation. An invariant subgroup **N** of **G** is such that its poles are only permuted among themselves by all the operations of **G**. As an example, we show by means of this rule in Fig. 1 that $\mathbf{C}_3$ and $\mathbf{D}_2$ are invariant subgroups of $\mathbf{D}_3$ and **T**, respectively.

3. THE CRYSTALLOGRAPHIC POINT GROUPS

The invariant subgroups of the eleven proper point

[7] The definition given for the semidirect product agrees with that of the "group product" given by M. J. Buerger, *Elementary Crystallography* (John Wiley & Sons, Inc., New York, 1956), p. 486.

groups can be easily obtained by the rule of Sec. 2. In the second column of Table I we list a special type of invariant subgroup which we call a *halving subgroup.* This is such that its order, that is the number of its elements, is exactly one-half that of the corresponding group. If we want to write a proper point group in the form $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$ where $\mathbf{N}$ is halving, it is clear that $\mathbf{C}$ must be a group of two elements, i.e., a group $\mathbf{C}_2$. Hence, we quickly obtain the semidirect product forms listed in the third column of Table I. $\mathbf{T}$ does not possess a halving subgroup but a semidirect product form can be easily obtained from Fig. 1.

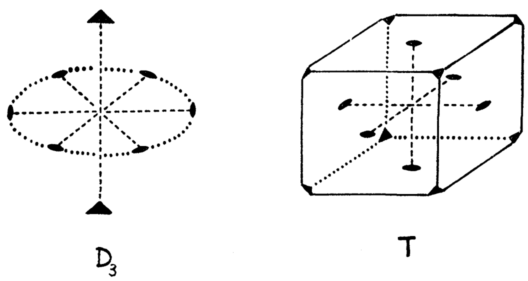

FIG. 1. The poles of invariant subgroups. In $\mathbf{D}_3$ the poles of $\mathbf{C}_3$ are denoted by the two triangles. They are invariant under the operations of $\mathbf{C}_3$ and they are permuted by the three binary rotations, the poles of which are denoted with ellipses. In $\mathbf{T}$ the poles of $\mathbf{D}_2$ are the ellipses at the ends of the axial cross. Each binary rotation leaves two of these poles invariant and permutes the rest, whereas the threefold rotations permute the binary poles cyclically.

The improper groups $\mathbf{G}'$ are of two types, with or without the inversion i, and there are two well-known prescriptions to obtain them starting from a proper group $\mathbf{G}$. The first, to obtain groups with the inversion, leads to a well-known direct product form. The second, to obtain groups without the inversion, can be reworded to express it in terms of semidirect products.

To give these prescriptions briefly, we shall use a plus sign to denote the juxtaposition of elements of two groups and a dot sign to denote a group product (later to be identified as a direct or semidirect product as the case may be). The prescriptions are:

(*i*) *Groups with inversion.* From the proper group $\mathbf{G}$ we form

$$\mathbf{G}' = \mathbf{G} + \mathbf{G}i = \mathbf{G}\cdot(E + i) \equiv \mathbf{G} \times \mathbf{C}_i\,. \quad (4)$$

Here, E is the identity operation and $\mathbf{C}_i$ the group whose elements are E and i.

(*ii*) *Groups without the inversion.* Express a proper group $\mathbf{G}$ in terms of a halving subgroup $\mathbf{N}$ as

$$\mathbf{G} = \mathbf{N} \wedge \mathbf{C}_2 \equiv \mathbf{N} + \mathbf{N}C_2\,. \quad (5)$$

Form

$$\mathbf{G}' = \mathbf{N} + \mathbf{N}C_2 i\,.$$

Since $C_2 i$ is a reflection σ, we can write

$$\mathbf{G}' = \mathbf{N} + \mathbf{N}\sigma = \mathbf{N}\cdot(E + \sigma) \equiv \mathbf{N} \wedge \mathbf{C}_s\,. \quad (6)$$

In comparing (4) and (6) notice that i commutes with any other operation, but not so σ. Hence, the different type of product that appears in each case. It should also be noticed that the second rule can be very briefly expressed as follows:

Write a proper group $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}_2$ ($\mathbf{N}$ halving).

TABLE I. Proper and improper point groups.

$\mathbf{C}_2$ and $\mathbf{C}_3$ are groups with the rotation axis and mirror plane parallel and perpendicular, respectively, to the principal axis of the invariant subgroup. The rotation axis and mirror plane in $\mathbf{C}_2'$ and $\mathbf{C}_s'$ are perpendicular and parallel, respectively, to the principal axis. The symmetry elements in $\mathbf{C}_2''$ and $\mathbf{C}_s''$ are as in $\mathbf{C}_2'$ and $\mathbf{C}_s'$ but they also bisect two secondary axes of the invariant subgroup. The threefold axis of $\mathbf{C}_3'$, $\mathbf{D}_3'$, and $\mathbf{C}_{3v}'$ is diagonal to the three binary axes of $\mathbf{D}_2$.

Proper groups	Halving subgroups	Semidirect product form	Groups with i	Groups without i
$\mathbf{C}_1$	. . .	. . .	$\mathbf{C}_i$	
$\mathbf{C}_2$	$\mathbf{C}_1$	$\mathbf{C}_1 \wedge \mathbf{C}_2$	$\mathbf{C}_{2h} = \mathbf{C}_2 \times \mathbf{C}_i$	$\mathbf{C}_s = \mathbf{C}_1 \wedge \mathbf{C}_s$
$\mathbf{C}_3$	. . .	. . .	$\mathbf{C}_{3i} = \mathbf{C}_3 \times \mathbf{C}_i$	. . .
$\mathbf{C}_4$	$\mathbf{C}_2$	. . .	$\mathbf{C}_{4h} = \mathbf{C}_4 \times \mathbf{C}_i$	$\mathbf{S}_4$
$\mathbf{C}_6$	$\mathbf{C}_3$	$\mathbf{C}_3 \wedge \mathbf{C}_2$	$\mathbf{C}_{6h} = \mathbf{C}_6 \times \mathbf{C}_i$	$\mathbf{C}_{3h} = \mathbf{C}_3 \wedge \mathbf{C}_3' \equiv \mathbf{C}_3 \times \mathbf{C}_s'$
$\mathbf{D}_2$	$\mathbf{C}_2$	$\mathbf{C}_2 \wedge \mathbf{C}_2' \equiv \mathbf{C}_2 \times \mathbf{C}_2'$	$\mathbf{D}_{2h} = \mathbf{D}_2 \times \mathbf{C}_i$	$\mathbf{C}_{2v} = \mathbf{C}_2 \wedge \mathbf{C}_s \equiv \mathbf{C}_2 \times \mathbf{C}_s'$
$\mathbf{D}_3$	$\mathbf{C}_3$	$\mathbf{C}_3 \wedge \mathbf{C}_2'$	$\mathbf{D}_{3d} = \mathbf{D}_3 \times \mathbf{C}_1$	$\mathbf{C}_{3v} = \mathbf{C}_3 \wedge \mathbf{C}_s'$
$\mathbf{D}_4$	$\mathbf{C}_4$	$\mathbf{C}_4 \wedge \mathbf{C}_2'$	$\mathbf{D}_{4h} = \mathbf{D}_4 \times \mathbf{C}_i$	$\mathbf{C}_{4v} = \mathbf{C}_4 \wedge \mathbf{C}_s'$
	$\mathbf{D}_2$	$\mathbf{D}_2 \wedge \mathbf{C}_2''$		$\mathbf{D}_{2d} = \mathbf{D}_2 \wedge \mathbf{C}_s'' = \mathbf{S}_4 \wedge \mathbf{C}_2'$
$\mathbf{D}_6$	$\mathbf{C}_6$	$\mathbf{C}_6 \wedge \mathbf{C}_2'$	$\mathbf{D}_{6h} = \mathbf{D}_6 \times \mathbf{C}_i$	$\mathbf{C}_{6v} = \mathbf{C}_6 \wedge \mathbf{C}_s'$
	$\mathbf{D}_3$	$\mathbf{D}_3 \wedge \mathbf{C}_2''$		$\mathbf{D}_{3h} = \mathbf{D}_3 \wedge \mathbf{C}_3'' = \mathbf{S}_3 \wedge \mathbf{C}_2'$
$\mathbf{T}$	. . .	$\mathbf{D}_2 \wedge \mathbf{C}_3'$	$\mathbf{T}_h = \mathbf{T} \times \mathbf{C}_i$	
$\mathbf{O}$	$\mathbf{T}$	$\mathbf{T} \wedge \mathbf{C}_2'' = \mathbf{D}_2 \wedge \mathbf{D}_3'$	$\mathbf{O}_h = \mathbf{O} \times \mathbf{C}_i$	$\mathbf{T}_d = \mathbf{T} \wedge \mathbf{C}_s'' = \mathbf{D}_2 \wedge \mathbf{C}_{3v}$

The corresponding improper group without inversion is $\mathbf{G}' = \mathbf{N} \wedge \mathbf{C}_s$.

The results of these rules for the 32-point groups are summarized in Table I.

4. TRIPLE PRODUCTS

There are two very useful relations for triple products:

$$(\mathbf{N}' \wedge \mathbf{C}') \wedge \mathbf{C} = \mathbf{N}' \wedge (\mathbf{C}' \wedge \mathbf{C}) \,, \qquad (7)$$

$$(\mathbf{N}' \wedge \mathbf{C}') \times \mathbf{C} = \mathbf{N}' \wedge (\mathbf{C}' \times \mathbf{C}) \,. \qquad (8)$$

Equation (7) is valid, when $\mathbf{N}'$ and $\mathbf{C}'$ have all poles in common or when no pole of one group is taken into a pole of another by an operation of $\mathbf{C}$. However, this condition can always be satisfied, except for cases of no interest.

As an example of (7):

$$\mathbf{O} = \mathbf{T} \wedge \mathbf{C}_2'' = (\mathbf{D}_2 \wedge \mathbf{C}_3') \wedge \mathbf{C}_2''$$
$$= \mathbf{D}_2 \wedge (\mathbf{C}_3' \wedge \mathbf{C}_2'') = \mathbf{D}_2 \wedge \mathbf{D}_3' \,,$$

(see the note at the head of Table I for an explanation of the meaning of the primes). As an example of (8):

$$\mathbf{D}_{4h} = \mathbf{D}_4 \times \mathbf{C}_i = (\mathbf{C}_4 \wedge \mathbf{C}_2') \times \mathbf{C}_i$$
$$= \mathbf{C}_4 \wedge (\mathbf{C}_2' \times \mathbf{C}_i) = \mathbf{C}_4 \wedge \mathbf{C}_{2h}' \,.$$

Many useful relations between the point groups can be obtained in this manner. Among other things, they, as well as the relations given in Sec. 3, allow us to classify very systematically the various isomorphisms between the point groups.

5. THE REPRESENTATIONS

It is well known that, if $\mathbf{G} = \mathbf{N} \times \mathbf{C}$, the representations of $\mathbf{G}$ can be obtained from those of $\mathbf{N}$ and $\mathbf{C}$ in a very simple way. We shall show in this section that, analogously, the representations of $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$ can be built up from those of $\mathbf{N}$ and $\mathbf{C}$.

5.1 The Representations of the Invariant Subgroup

We shall first consider the case when $\mathbf{N}$ is a cyclic group $\mathbf{C}_n$ of order n. The n one-dimensional representations are given by $D^k(C_r) = \exp\,(2\pi i k r/n)$ where $k,r = 1,2,\cdots n$. Here, $D^k(C_r)$ is the representative of C_r in the kth irreducible representation of the group. k is an index that labels and specifies the representation and it is very convenient for our purposes to represent it by an axial vector $\mathbf{k}$ in the direction of the axis of rotation. The modulus of $\mathbf{k}$ will take the values $1,2,\cdots n$, but it is more convenient to take the equivalent symmetrized ranges $[-\frac{1}{2}\,(n-1), \frac{1}{2}\,(n-1)]$ and $[-\frac{1}{2}\,n, \frac{1}{2}\,n - 1]$ for n odd and even, respectively. As an example of these representations and their $\mathbf{k}$ vectors, the representations of $\mathbf{C}_3$ can be seen to the left of Table II.

When $\mathbf{N} = \mathbf{D}_2 = \mathbf{C}_2 \times \mathbf{C}_2$ the representations are designated by a $\mathbf{k}$ vector of two components, which is possible because the two binary rotations involved commute. The concept of a $\mathbf{k}$ vector can still be used, with some care, when $\mathbf{N} = \mathbf{T}$.

5.2 The Representations of the Semidirect Product

Consider the group $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$, and assume that bases are available that span the irreducible representations of $\mathbf{N}$. We denote them, in row vector form, with the symbol $\langle\phi|$. We shall first treat the case when $\mathbf{N}$ is abelian (either cyclic or direct product of cyclic groups). In this case $\langle\phi|$ is one dimensional.

The first step in the prescription to form a basis of a representation of $\mathbf{G}$ is to form the *star* of the representation. This is obtained as follows. Take a basis $\langle\phi_{\mathbf{k}}|$ that corresponds to a vector $\mathbf{k}$ (i.e., to one of the irreducible representations of $\mathbf{N}$). Form all the vectors $C\mathbf{k}$ (all $C \in \mathbf{C}$). The set of all vectors thus obtained is the star of the representation. For each vector $C\mathbf{k}$ in the star there will be a basis $\langle\phi_{C\mathbf{k}}|$. A basis for the representation of $\mathbf{G}$ is obtained by forming the direct sum of the bases $\langle\phi_{C\mathbf{k}}|$ (all $C \in \mathbf{C}$). That is, we form the row vector $\langle\phi_{C_1\mathbf{k}}, \phi_{C_2\mathbf{k}}, \cdots|$.

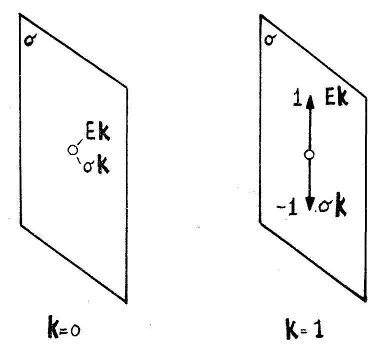

FIG. 2. The stars of $\mathbf{C}_{3v}$. In forming the star of $\mathbf{k} = 1$ it should be remembered that axial vectors change sign when reflected on their own plane.

We illustrate in Fig. 2 the stars of $\mathbf{C}_{3v} = \mathbf{C}_3 \wedge \mathbf{C}_s$. They are two, and we can see that they show an essential difference. Whereas for $\mathbf{k} = 0$ we have $\mathbf{k} = 0$ repeated twice in the star, for $\mathbf{k} = 1$ we have $\mathbf{k} = 1$ and $\mathbf{k} = -1$ in the star, and no $\mathbf{k}$ vector appears more than once in it. We shall call a *simple star* one that contains no repeated $\mathbf{k}$ vector and a *composite star* one that does.

It can be shown that a simple star corresponds to an irreducible representation. So, for $\mathbf{C}_{3v} = \mathbf{C}_3 \wedge \mathbf{C}_s$, if $\langle\phi_1|$ and $\langle\phi_{-1}|$ are the bases corresponding to $\mathbf{k} = 1$ and $\mathbf{k} = -1$, respectively, the basis of the corresponding irreducible representation of $\mathbf{C}_{3v}$ is $\langle\phi_1, \phi_{-1}|$.

The representation itself is easily obtained. The representations of the operations of $\mathbf{C}_3$ are diagonal matrices. In fact, for C_3 for instance, from the representations of $\mathbf{C}_3$ listed in Table II, we have

$$C_3\langle\phi_1| = \langle\phi_1|\,\epsilon\,,$$
$$C_3\langle\phi_{-1}| = \langle\phi_{-1}|\,\epsilon^*.$$

Hence,

$$C_3\langle\phi_1\,,\phi_{-1}| = \langle\phi_1\,,\phi_{-1}|\left[{}^{\epsilon}{}_{\epsilon^*}\right],$$

as shown in Table II. The matrix for σ_v results simply from the conditions

$$\sigma\langle\phi_1| = \langle\phi_{-1}|\,,$$
$$\sigma\langle\phi_{-1}| = \langle\phi_1|\,,$$

which follow from the way in which the star was generated. The matrices for the remaining reflections ($C_3\sigma_v$ and $C_3^2\sigma_v$) are obtained by multiplication.

To deal with composite stars we require a new concept, that of the *co-group of the* **k** *vector*, $\overline{\mathbf{K}}$. This is the group of all operations of $\mathbf{C}$ (in $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$) that leave $\mathbf{k}$ invariant. For instance in $\mathbf{C}_{3v}$, for $\mathbf{k} = 0$, this group is $\mathbf{C}_s$. The prescription to obtain an irreducible basis for a composite star is now as follows: (i) choose a basis $\langle\phi_\mathbf{k}|$ of the representation of $\mathbf{N}$ which corresponds to the $\mathbf{k}$ vector of the star and such that it belongs to an irreducible representation of $\overline{\mathbf{K}}$. (ii) Generate the star with the operations of $\mathbf{C}$ that do not belong to $\overline{\mathbf{K}}$ (i.e. avoid repeated $\mathbf{k}$ vectors in the star) and form the new basis of $\mathbf{G}$ by writing the direct sum of all the $\langle\phi_\mathbf{k}|$ for all the $\mathbf{k}$'s in the new star.

The reader can verify that the representation for $\mathbf{k} = 0$ of $\mathbf{C}_3$ generates two representations of $\mathbf{C}_{3v}$, in accordance to whether the corresponding basis is chosen to belong to either of the two irreducible representations of $\mathbf{C}_s$, in which σ_v is represented by $+1$ and -1, respectively.

When $\mathbf{N}$ is nonabelain, a basis $\langle\phi|$ of an irreducible representation of it will be multidimensional. It can be seen that, for the cases of interest in the point groups, it is enough to choose $\langle\phi|$ such that one of its columns be irreducible under $\overline{\mathbf{K}}$.

6. SYMMETRY-ADAPTED FUNCTIONS

Consider a group $\mathbf{G}$ of elements G_r, represented in the jth irreducible representation by matrices $D^j(G_r)$. The operators

$$W^j_{tu} = \textstyle\sum_r D^j(G_r)^*_{tu}G_r \tag{9}$$

are such that when applied on an arbitrary function ϕ they transform it into a function ϕ^j_t, adapted to the tth column of the jth representation. That is

$$W^j_{tu}\phi = \phi^j_t\,. \tag{10}$$

These operators satisfy the condition[8]

$$W^j_{tu}\phi^i_v = \phi^j_t\delta_{ij}\delta_{uv}\,. \tag{11}$$

Consider now $\mathbf{G} = \mathbf{N} \wedge \mathbf{C}$. We shall show that the work with the operators (9) can be much simplified by obtaining first functions that are symmetry-adapted with respect to $\mathbf{N}$. Write $\mathbf{G} = \sum_i \mathbf{N}C_i$, where, as the plus sign before, the summation sign denotes a juxtaposition of elements. Then

$$W^j_{tt} = \textstyle\sum_i \sum_s D^j(N_sC_i)^*_{tt}N_sC_i \tag{12}$$
$$= \textstyle\sum_i \sum_s D^j(C_iN_s)^*_{tt}C_iN_s \tag{13}$$
$$= \textstyle\sum_i \sum_{su} D^j(C_i)^*_{tu}D^j(N_s)^*_{ut}C_iN_s \tag{14}$$
$$= \textstyle\sum_i \sum_u D^j(C_i)^*_{tu}C_i \sum_s D^j(N_s)^*_{ut}N_s\,. \tag{15}$$

In Eq. (13) we use the relation $\mathbf{N}C = C\mathbf{N}$. Equation (14) results from the matrix multiplication rule, whereas Eq. (15) involves a mere rearrangement of

[8] For this and other properties of these operators see, for instance, S. L. Altmann, "Group Theory," in *Quantum Theory*, edited by D. R. Bates (Academic Press Inc., New York, 1962), Vol. II, p. 144.

TABLE II. The representations of $\mathbf{C}_{3v}$ in relation to those of $\mathbf{C}_3$.

C_3 is a counterclockwise rotation by $2\pi/3$. $C_3\sigma_v$ and $C_3^2\sigma_v$ are mirror planes that form angles of $2\pi/3$ and $-2\pi/3$, respectively, with σ_v.

$$\epsilon = \exp(2\pi i/3)$$

$\mathbf{C}_3$	$\mathbf{k}/\mathbf{r}$		co-group of $\mathbf{k}$	E 0	C_3 1	C_3^2 2	$\mathbf{C}_{3v}$	E	C_3	C_3^2	σ_v	$C_3\sigma_v$	$C_3^2\sigma_v$
A_1	0	star	$\mathbf{C}_s$	1	1	1	A_1	1	1	1	1	1	1
							A_2	1	1	1	-1	-1	-1
^1E	1	star	$\mathbf{C}_1$	1	ϵ	ϵ^*	E	$\begin{pmatrix}1 & \\ & 1\end{pmatrix}$	$\begin{pmatrix}\epsilon & \\ & \epsilon^*\end{pmatrix}$	$\begin{pmatrix}\epsilon^* & \\ & \epsilon\end{pmatrix}$	$\begin{pmatrix} & 1\\ 1 & \end{pmatrix}$	$\begin{pmatrix} & \epsilon\\ \epsilon^* & \end{pmatrix}$	$\begin{pmatrix} & \epsilon^*\\ \epsilon & \end{pmatrix}$
^2E	-1			1	ϵ^*	ϵ							

terms. From the description of the irreducible representations of **G** given in Sec. 5, it follows that the $D^i(N_s)$ are irreducible representations of **N**, so that the summation over s in Eq. (15) is an operator such as (9), but for the group **N**. Hence, if we apply the operator (15) on a function ϕ_t^j symmetry-adapted to **N**, and if we use Eq. (11), we obtain

$$W_{tt}^j\phi_t^j = \sum_u \sum_i D^j(C_i)^*_{tu} C_i \phi_u^j \,. \qquad (16)$$

This means that the symmetry-adapted functions with respect to **N** have to be transformed only under **C** in order to obtain symmetry-adapted functions with respect to **G**. Hence, the step-wise procedure involved in (16) requires the use of $n + m$ symmetry operations, if n and m are the orders of **N** and **C**, respectively, whereas the direct application of (9) would involve $n \cdot m$ operations.

We can see in Table II that often the matrix representatives have zero diagonal elements. This, of course, simplifies even further the work with the operators (16) and a set of rules to obtain the results in as simple a way as possible can be given.

Discussion on Treatment of Symmetry Properties

F. A. Matsen, *Chairman*

Donath: A program for applying the Boys vector-coupling reduction method for atoms has been developed. This method rests on the use of orthonormal orbitals. If we define eingangs A and B of symmetries $l_A s_A$ and $l_B s_B$, respectively, and if these eingangs have no common nl orbitals, they can be coupled to give an eingang C of symmetry LS by the use of Clesbsch–Gordan or Boys X-coefficients. Two eingangs made up of exactly the same orbitals can be used to write a new, larger eingang as follows:

$$(nl^{p+q})^{LSR} = \sum_{\substack{L_1S_1R_1\\ L_2S_2R_2}} \eta^{pq}_{LSR,L_1S_1R_1,L_2S_2R_2} \times [(nl^p)^{L_1S_1R_1}(nl^q)^{L_2S_2R_2}]^{LSR} \,.$$

These relationships are basic to a vector-coupling scheme for atoms. This scheme is convenient for introducing correlation in atoms, e.g., if we wish to introduce $2p^2$ correlation terms in Ne we obtain 3 pairs of the type:

$$[(2p^4)^1D(n_1l_1n_2l_2)^1D]^1S \,, \qquad [(2p^4)^3P(n_1l_1n_2l_2)^3P]^1S \,, \qquad [(2p^4)^1S(n_1l_1n_2l_2)^1S]^1S \,,$$

where there are 15 pairs.

The computer program developed takes any configuration and generates from this all permitted terms with whatever restrictions are introduced in the specification. More important, from any two configurations a table of the integrals over the radial coordinates is generated. This program works for all nl types of orbitals, but $l \geq 2$ eingangs which include more than 2 electrons are not permitted at present.

Coleman: About one year ago, Fukashi Sasaki, a student of Kotani, now working at Uppsala, discovered a formula which was of great usefulness in the theory of density matrices and should have wide application to systems of Fermions. If $N = p + q$, $p \leq q$, and A_N, A_p and A_q are indempotent antisymmetrizers on the N, p, and q particles, respectively, the *Sasaki's Formula* is

$$\binom{N}{p} A_N = A_p A_q \left[\sum_{i=0}^{p} (-1)^i \binom{p}{i} \binom{q}{i} (1,p+1)(2,p+2)\cdots(i,p+i) \right] A_p A_q \,,$$

where $\binom{N}{p}$ is the binomial coefficient, and $(1,\, p+1)$, etc. denotes a transposition of the first and $(p+1)$th particles. The formula appeared, for the first time to my knowledge, in Quantum Chemistry Group, Technical Report No. 78, May 1962, Uppsala University, Uppsala, Sweden (unpublished). If the factor $(-1)^i$ in Sasaki's formula is replaced by 1 the formula becomes valid for the symmetrizing operator.