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## Group Algebra, Convolution Algebra, and Applications to Quantum Mechanics\*

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The symmetry group of the Hamiltonian plays a fundamental role in quantum theory in the classification of stationary states and in studying transition probabilities and selection rules. It is here shown that the properties of the group may be given a condensed and transparent description in terms of the convolution algebra, and that Schur's lemma immediately leads to the construction of the fundamental set of projection and shift operators. The projection operators form a resolution of the identity which may be used to split the Hilbert space into orthogonal and noninteracting subspaces of infinite order. The question of the splitting of the conventional secular equations is discussed, and the explicit form of the decomposed equation is derived in terms of the convolution algebra and the characters. The theory is here discussed only for finite groups, but the results may be generalized to the compact infinite groups having a well-defined "invariant mean."

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is one of the simplest and most forceful tools for handling the quantum-mechanical applications.

The purpose of this paper is to give a short outline of the elements of group and convolution algebra and to show the direct applications to quantum mechanics. It is assumed that the reader is familiar with the elements of set theory and linear algebra: the concepts of linear independence, bases, linear operators, matrix representations, similarity transformations, eigenvalue problems, etc.<sup>1</sup> It is further assumed that the reader has some elementary knowledge of group theory: the group axioms, the concepts of subsets, subgroups, cosets, conjugate classes, etc., whereas the fundamental properties of representation theory are treated here.

**B. Functions over a Group; Invariant Mean**

*Definition of Groups*

A set  $G = \{g\}$  of objects or elements  $g$  is said to form a *group*, if the elements fulfill the following four axioms:

- (1) There exists a binary operation (for the sake of simplicity here denoted by  $\cdot$ ) such that, if  $g$  and  $h$  belong to the set, the result of the binary operation,  $g \cdot h$ , belongs also to the set,  $G$ .
- (2) The binary operation is associative so that  $(g \cdot h) \cdot k = g \cdot (h \cdot k)$ .
- (3) There exists a neutral element  $e$ , so that  $g \cdot e = e \cdot g = g$ .
- (4) Every element  $g$  has an inverse  $g^{-1}$ , such that  $g \cdot g^{-1} = g^{-1} \cdot g = e$ .

In this form, the axioms are slightly redundant, but the proper minimum definitions are given in most elementary textbooks.

The binary operation is often called “multiplication.” In general it is noncommutative, so that  $g \cdot h \neq h \cdot g$ . A group characterized by the special property  $g \cdot h = h \cdot g$  is said to be *Abelian*. The quadratic arrangement giving the results of the binary operation  $g \cdot h$  is said to be the “multiplication table” associated with the group. This table is characterized by the fact that, in each row and in each column, each element occurs once and only once.

$h$			
$g$		$\dots$	$h \dots$
$\cdot$			$\cdot$
$\cdot$			$\cdot$
$\cdot$			$\cdot$
$\cdot$			$\cdot$
$g$	$\dots$	$g \cdot h$	
$\cdot$			

“Multiplication Table”

This property is fundamental for the construction of

<sup>1</sup> See, for instance, “Linear Algebra and the Fundamentals of Quantum Theory,” Technical Note 125, Uppsala Quantum Chemistry Group, 1964 (unpublished).

the concept of the “invariant mean” basic for the convolution algebra, and, for this reason, we will repeat the simple proof: Every element  $k$  occurs at least once in the row  $g$ , depending on the multiplication relation  $g \cdot (g^{-1} \cdot k) = k$ ; it occurs further only once, since it follows from  $g \cdot h_1 = g \cdot h_2 = k$  by multiplication to the left by  $g^{-1}$  that  $h_1 = h_2 = g^{-1} \cdot k$ . A similar argument holds for the columns.

The number  $n$  of elements  $g$  in the set  $G = \{g\}$  is called the order  $|G|$  of the group; for the group we will sometimes use the notation  $G = \{g_1, g_2, g_3, \dots, g_n\}$ . In this paper, we essentially consider only *finite* groups, but certain continuous groups are mentioned in the discussion.

*Functions Over the Group*

A set of  $n$  complex numbers  $\alpha_1, \alpha_2, \alpha_3, \dots, \alpha_n$  associated with the elements  $g_1, g_2, g_3, \dots, g_n$  is called a function over the group, and the set is denoted by the symbol  $\alpha = \alpha(g)$ . If similarly  $\beta = \beta(g)$  is another function consisting of the numbers  $\beta_1, \beta_2, \beta_3, \dots, \beta_n$ , one may define the *sum*  $\alpha + \beta$  as a new function characterized by the numbers  $\alpha_1 + \beta_1, \alpha_2 + \beta_2, \alpha_3 + \beta_3, \dots, \alpha_n + \beta_n$ . If further  $c$  is an arbitrary complex constant, the symbol  $c\alpha$  will denote another function consisting of the numbers  $c\alpha_1, c\alpha_2, c\alpha_3, \dots, c\alpha_n$ .

Having defined the concepts  $\alpha + \beta$  and  $c\alpha$  in this way, we realize that all the functions  $\alpha$  form together a *linear space* closed under the operations addition and multiplication by a complex constant. In order to construct a *basis* for this space, we will consider the  $n$  functions.

$$f_k(g) = 1, \text{ for } g = g_k, \\ = 0, \text{ for } g \neq g_k, \tag{1}$$

i.e., the functions  $f_1, f_2, \dots, f_n$  consisting of the following sets of complex numbers:

$$f_1 = \{1, 0, 0, \dots, 0\}, \\ f_2 = \{0, 1, 0, \dots, 0\}, \\ \dots \dots \dots \\ f_n = \{0, 0, 0, \dots, 1\}, \tag{2}$$

respectively. It is easily shown that these functions are linearly independent and that, according to the definitions, one has the expansion theorem

$$\alpha(g) = \sum_{k=1}^n \alpha_k f_k(g), \tag{3}$$

which means that the linear space associated with the functions over the group is of order  $n = |G|$ .

*Invariant Mean*

The average value of all the complex numbers  $\alpha_1, \alpha_2, \alpha_3, \dots, \alpha_n$  for the function  $\alpha = \alpha(g)$  is called the

mean  $\bar{\alpha}$  of the function over the group:

$$\begin{aligned} \bar{\alpha} &= n^{-1}(\alpha_1 + \alpha_2 + \alpha_3 + \dots + \alpha_n) \\ &= |G|^{-1} \sum_{k=1}^n \alpha_k \equiv M\alpha(g), \end{aligned} \quad (4)$$

and we will in the following particularly use the last symbol. From the properties of the multiplication table of the group, one obtains the relations

$$\begin{aligned} M\alpha(g) &= M\alpha(g'h) = M\alpha(hg) = M\alpha(g^{-1}) \\ &= M\alpha(g^{-1}h) = M\alpha(hg^{-1}), \end{aligned} \quad (5)$$

where  $h$  is a fixed element. For this reason, the quantity  $M$  is often referred to as the *invariant mean* over the group. It is here defined only for finite groups but, by means of Haar's measure, it may also be generalized to compact infinite groups. For finite groups, we further develop this concept below.

### Group Algebra

The group axioms contain a usually noncommutative binary operation which is called "multiplication" and is denoted by a dot. In order to proceed, it is now convenient to introduce a second *binary operation* which is commutative and associative and is called "addition" and is denoted by  $+$ , and the operation "multiplication by a complex constant." Any linear combination

$$a_1g_1 + a_2g_2 + a_3g_3 + \dots + a_ng_n = \sum_k a_kg_k, \quad (6)$$

where  $a_1, a_2, a_3, \dots, a_n$  is a set of complex numbers, is called an element of the *group algebra*. The sum of two such elements is defined by the relation

$$\sum_k a_kg_k + \sum_k b_kg_k = \sum_k (a_k + b_k)g_k, \quad (7)$$

and the multiplication by a complex constant  $c$  is defined by

$$c(\sum_k a_kg_k) = \sum_k (ca_k)g_k. \quad (8)$$

The group algebra is a set closed under these two operations, and it forms hence a *linear space*. Since this space is further spanned by the elements  $g_1, g_2, g_3, \dots, g_n$ , it is of the finite order  $n = |G|$ .

It is now convenient to introduce the operation "multiplication" of two elements of the group algebra denoted by the symbol  $\times$  by combining the distributive law and the use of group multiplication  $\cdot$  in the definition:

$$(\sum_k a_kg_k) \times (\sum_l b_lg_l) = \sum_{k,l} a_kb_lg_k \cdot g_l, \quad (9)$$

which means that the result is again an element of the group algebra. The linear space is hence closed even under this operation.

### Convolution Algebra

An element of the group algebra is uniquely characterized by a set of  $n$  complex numbers, i.e., by a function over the group, and there is a one-to-one correspondence (isomorphism) between the linear space of the group algebra and the linear space formed by the functions over the group, which are both of finite order  $n = |G|$ . In order to develop the theory, it is convenient to introduce the following connection between an element  $A$  of the group algebra and a function  $\alpha$  over the group:

$$\begin{aligned} A &= n^{-1}(\alpha_1g_1^{-1} + \alpha_2g_2^{-1} + \alpha_3g_3^{-1} + \dots + \alpha_ng_n^{-1}) \\ &= |G|^{-1} \sum_{k=1}^n \alpha(g_k)g_k^{-1} = M\alpha(g)g^{-1}, \end{aligned} \quad (10)$$

where we have used the symbol  $M$  analogously to (4); we note that it has still the same invariance properties as in (5), and the "invariant mean" is going to be a fundamental concept also in group algebra.

Let us now consider two elements of the group algebra,  $A$  and  $B$ , defined by the functions  $\alpha$  and  $\beta$  over the group, respectively, so that

$$\begin{aligned} A &\leftrightarrow \alpha, & B &\leftrightarrow \beta, \\ A &= M\alpha(g)g^{-1}, & B &= M\beta(g)g^{-1}, \end{aligned} \quad (11)$$

and let us ask for the function  $\gamma$  associated with the product  $A \times B$ . Using the definition (9), introducing the substitution  $s^{-1}t^{-1} = u^{-1}$  (i.e.,  $t = us^{-1}$ ), and using the properties of the invariant mean, one finds

$$\begin{aligned} A \times B &= [M\alpha(s)s^{-1}] \times [M\beta(t)t^{-1}] \\ &= MM\alpha(s)\beta(t)s^{-1} \cdot t^{-1} \\ &= MM\alpha(s)\beta(us^{-1})u^{-1} \\ &= M[M\alpha(s)\beta(us^{-1})]u^{-1} \\ &= M\gamma(u)u^{-1}, \end{aligned} \quad (12)$$

where

$$\gamma(u) = M\alpha(s)\beta(us^{-1}). \quad (13)$$

The function  $\gamma$  defined by (13) is called the "convolution product" of the functions  $\alpha$  and  $\beta$  and will be denoted by the symbol

$$\gamma = \alpha * \beta. \quad (14)$$

This leads to the result:

$$\begin{aligned} A &\leftrightarrow \alpha, & B &\leftrightarrow \beta, \\ A \times B &\leftrightarrow \gamma = \alpha * \beta, \end{aligned} \quad (15)$$

which means that the multiplication  $\times$  in the group algebra defined by (9) corresponds uniquely to the

convolution multiplication  $\ast$  in the function space defined by (13). The linear space formed by the functions over the group extended by this operation is referred to as the "convolution algebra." It is easily shown that the convolution operation  $\ast$  is associative and distributive; this operation is of fundamental importance for the entire further development of this paper. In the following, we use the convolution operation also for matrices.

### C. Stable Subspaces and Representations

#### Stable Subspaces

The linear space formed by all elements  $A$  of the group algebra is denoted by  $V_G$  and is of finite order  $n$ . A linear space  $W$  spanned by the linearly independent elements  $A_1, A_2, \dots, A_f$  of the group algebra is a subspace of  $V_G$ , and  $W$  will be called a *proper subspace* if it is not empty and not identical to  $V_G$ ; it is evidently of order  $f$ .

Such a subspace  $W$  is said to be *stable* under the group  $G = \{g\}$ , if all elements  $g \ast W$  still belong to  $W$ . The existence of such stable subspaces is of great importance in group theory, since they automatically lead to *representations* of the group. Let

$$\mathbf{X} = \{X_1, X_2, \dots, X_f\}$$

be a basis for the subspace  $W$ ; for every element  $g$  of the group  $G$ , one has

$$g \ast X_l = \sum_k X_k \Gamma_{kl}(g), \quad (16)$$

where the quantities  $\Gamma_{kl}(g)$  are the unique expansion coefficients for the new element  $gX_l$  within the subspace  $W$ ; cf. Ref. 1, pp. 12–13. In matrix notation, this gives

$$g \ast \mathbf{X} = \mathbf{X} \Gamma(g), \quad (17)$$

where  $\Gamma(g)$  is the matrix formed by the elements  $\Gamma_{kl}(g)$ . One has further

$$\begin{aligned} (g.h) \ast \mathbf{X} &= g \ast (h \ast \mathbf{X}) = g \ast \mathbf{X} \Gamma(h) \\ &= \mathbf{X} \Gamma(g) \Gamma(h) = \mathbf{X} \Gamma(g.h), \end{aligned} \quad (18)$$

which leads to the relation

$$\Gamma(g.h) = \Gamma(g) \Gamma(h). \quad (19)$$

The matrices  $\Gamma(g)$  have hence the same multiplication table as the group  $G$ —with the binary operation  $\cdot$  replaced by matrix multiplication—and they are then said to form a *matrix representation* of the group.

For the neutral element  $e$ , one has particularly  $e \ast \mathbf{X} = \mathbf{X}$ , which implies that  $\Gamma(e)$  is a unit matrix  $\mathbf{1}$ —a property characteristic for the so-called *proper* representations. In the following, we often omit the multiplication symbol  $\ast$ .

#### Similarity Transformations

Let us now consider a nonsingular transformation  $\alpha$  of the basis  $\mathbf{X} = (X_1, X_2, \dots, X_f)$  to another basis  $\mathbf{Y} = (Y_1, Y_2, \dots, Y_f)$ :

$$\mathbf{Y} = \mathbf{X} \alpha, \quad \mathbf{X} = \mathbf{Y} \alpha^{-1}. \quad (20)$$

Denoting the matrix representations of  $g$  with respect to the two bases by  $\Gamma_X(g)$  and  $\Gamma_Y(g)$ , respectively, one obtains

$$g \mathbf{Y} = g \mathbf{X} \alpha = \mathbf{X} \Gamma_X(g) \alpha = \mathbf{Y} \alpha^{-1} \Gamma_X(g) \alpha, \quad (21)$$

which gives the relation

$$\Gamma_Y(g) = \alpha^{-1} \Gamma_X(g) \alpha. \quad (22)$$

The transformation (20) leads to a *similarity transformation* of type (22) for the matrix representations, and these are hence by no means unique.

#### Characters

The simplest invariant associated with a representation  $\Gamma(g)$  is the *trace* of the matrix, i.e., the sum of the diagonal elements:

$$\chi(g) = \text{Tr} \{ \Gamma(g) \} = \sum_k \Gamma_{kk}(g), \quad (23)$$

and this quantity is called the *character* of the representation. For the trace of a product of two matrices,  $\mathbf{R}$  and  $\mathbf{S}$ , one has the general rule:

$$\begin{aligned} \text{Tr} \{ \mathbf{R} \cdot \mathbf{S} \} &= \sum_k \{ \mathbf{R} \cdot \mathbf{S} \}_{kk} = \sum_k \sum_l R_{kl} S_{lk} \\ &= \sum_l \sum_k S_{lk} R_{kl} = \sum_l \{ \mathbf{S} \cdot \mathbf{R} \}_{ll} = \text{Tr} \{ \mathbf{S} \cdot \mathbf{R} \}. \end{aligned} \quad (24)$$

According to (22), this gives

$$\begin{aligned} \text{Tr} \{ \Gamma_Y(g) \} &= \text{Tr} \{ \alpha^{-1} \cdot \Gamma_X(g) \alpha \} \\ &= \text{Tr} \{ \Gamma_X(g) \alpha \cdot \alpha^{-1} \} = \text{Tr} \{ \Gamma_X(g) \}, \end{aligned} \quad (25)$$

i.e., the trace is invariant under the similarity transformation.

The character  $\chi(g)$  is a function over the group, which has the special property that it is constant for all elements belonging to the same conjugate class:

$$\chi(t^{-1}gt) = \chi(g), \quad (26)$$

i.e., the character  $\chi(g)$  is a *class function*. The proof follows from (19), (24), and the fact that

$$\Gamma(t^{-1}gt) = \Gamma(t^{-1}) \Gamma(g) \Gamma(t), \quad (27)$$

which gives

$$\begin{aligned} \chi(t^{-1}gt) &= \text{Tr} \{ \Gamma(t^{-1}) \cdot \Gamma(g) \Gamma(t) \} \\ &= \text{Tr} \{ \Gamma(g) \Gamma(t) \Gamma(t^{-1}) \} \\ &= \text{Tr} \{ \Gamma(gt t^{-1}) \} \\ &= \text{Tr} \{ \Gamma(g) \} = \chi(g). \end{aligned}$$

For the neutral element  $e$ , one has particularly  $\Gamma(e) = \mathbf{1}$ , and

$$\chi(e) = \text{Tr} \{ \mathbf{1} \} = f, \tag{28}$$

where  $f$  is the order of the subspace and the representation. In the following, the value of a function over the group for the neutral element  $e$  will often be denoted by the index 0, and (28) is then written in the form  $\chi_0 = f$ .

*Regular Representation*

The simplest example of a space *stable* under the group  $G = \{g\}$  is the entire space  $V_G$  associated with the group algebra. If  $A$  is an arbitrary element of  $V_G$ , the result of the operation  $g \times A$  belongs again to  $V_G$  according to (9). The space  $V_G$  is spanned by the elements  $g_1, g_2, g_3, \dots, g_n$ , which may be considered as the basis  $\mathbf{X}$ . According to a previous section, the stable space  $V_G$  leads automatically to a matrix representation of the group which is called the *regular representation* and is denoted by the symbol  $R$ . According to the multiplication table of the group, the result of the operation  $g$  is contained in the row associated with the element  $g$ :

$$g \times \{g_1, g_2, g_3, \dots, g_n\} = \{g'_1, g'_2, g'_3, \dots, g'_n\}, \tag{29}$$

and, since this row contains each element of the group once and only once, the effect of  $g$  is equivalent with a *permutation*  $P_g$  of the basis. The associated matrix representation  $\Gamma(g)$  is defined by (16):

$$g \times X_l = \sum_k X_k \Gamma_{kl}(g), \tag{30}$$

and relation (29) implies that

$$\begin{aligned} \Gamma_{kl}(g) &= 1, & \text{if } g = g_k g_l^{-1}, \\ &= 0, & \text{otherwise,} \end{aligned} \tag{31}$$

which gives the explicit form of the regular representation. We note that, in a given  $\Gamma(g)$ , each row and column contains the matrix element 1 only once whereas all other elements are zero. For a given pair  $(k, l)$  of indices, the matrix elements  $\Gamma_{kl}(g)$  are further all zero, except for a single element  $g = g_k g_l^{-1}$ . A simple way of forming all the matrices in the regular representation is hence to construct the "modified" multiplication table  $g_k \cdot g_l^{-1}$ , which immediately gives the distribution of the nonvanishing matrix elements 1 over the matrices  $\Gamma(g)$  according to (31).

Putting  $l=k$  in (31), one obtains particularly

$$\begin{aligned} \Gamma_{kk}(g) &= 1, & \text{if } g = e, \\ &= 0, & \text{otherwise,} \end{aligned} \tag{32}$$

which relation shows that only the matrix  $\Gamma(e)$  has diagonal elements which are nonvanishing. This gives for the trace of the regular representation

$$\begin{aligned} \chi(g) &= |G|, & \text{if } g = e, \\ &= 0, & \text{otherwise.} \end{aligned} \tag{33}$$

The character of the regular representation is hence vanishing over the entire group, except for the neutral element. In the following, we see that this simple result provides an important key for understanding the deeper properties of representations in general.

Formula (29) provides also a one-to-one mapping of each element  $g$  on a specific permutation  $P_g$  of  $n$  objects:

$$g \leftrightarrow P_g, \tag{34}$$

where the permutations  $P_g$  form a group having the same multiplication table as the original group. All permutations of  $n$  objects form a group, which is called the *symmetric group*  $S_n$  having the order  $n!$ . The relation (34) implies now that

$$\begin{aligned} \text{any finite group } G \text{ of order } n \text{ is isomorphic} \\ \text{with a subgroup of the total symmetric} \\ \text{group } S_n \text{ of order } n! \end{aligned} \tag{35}$$

This important theorem found by Cayley implies that the number of possible nonisomorphic groups of a certain order  $n$  is certainly *finite* depending on the fact that, since the total symmetric group  $S_n$  of all permutations is finite, it has only a finite number of subgroups.

*Reducible and Irreducible Subspaces*

A stable space is said to be *reducible* under the group, if it contains a proper subspace which is also stable under the group. If this is not the case, the space is said to be *irreducible*.

In order to show that these definitions are meaningful, it is sufficient to consider a single example, namely the one-dimensional subspace  $W_1$  spanned by the single element

$$A_1 = (1/n) (g_1 + g_2 + g_3 + \dots + g_n). \tag{36}$$

According to (29), one obtains directly  $gA_1 = A_1$ , which shows that the subspace  $W_1$  is stable under the group. The existence of this stable subspace contained in  $V_G$  shows that the entire space  $V_G$  is *reducible*. Since further the one-dimensional subspace  $W_1$  does not contain any proper subspaces whatsoever, it is certainly *irreducible*, and one has hence examples of both types of stable spaces and subspaces in the group algebra.

A representation  $\Gamma$  associated with an irreducible stable subspace is said to be an *irreducible representation*, whereas a representation  $\Gamma$  associated with a reducible stable subspace is said to be *reducible*. As an example of an irreducible representation, we will consider the representation associated with the one-dimensional subspace  $W_1$  defined by (36). From (17) and the relation  $gA_1 = A_1$ , it follows that

$$\Gamma(g) = [1], \tag{37}$$

i.e., the representation consists of one-dimensional matrices containing only the number 1. This irreducible representation is called the *identity representation* and is denoted by the symbol  $J$ .

Let us now consider a reducible stable subspace  $W$  in greater detail; it is of order  $f$ , it is spanned by the elements  $A_1, A_2, A_3, \dots, A_f$ , and the introduction of this set as a basis  $\mathbf{X}$  leads to a certain representation  $\Gamma(g)$  according to (17). According to the definition, the space  $W$  contains a proper stable subspace  $W'$  of order  $f' < f$ , which is spanned by the elements  $A'_1, A'_2, A'_3, \dots, A'_{f'}$ , and which leads to the new representation  $\Gamma'(g)$ . Let us now introduce a new basis  $\mathbf{Y}$  for the original space  $W$ , which consists of  $f$  linearly independent elements chosen so that

$$\mathbf{Y} = \{A'_1, A'_2, A'_3, \dots, A'_{f'}; A'_{f'+1}, \dots, A'_f\};$$

the new basis is related to the old one by the transformation (20), which leads to the similarity transformation (22) for the associated representations. In studying the result of the operation  $g\mathbf{Y} = \mathbf{Y}\Gamma_Y(g)$ , we note that, depending on the stability of the subspace  $W'$ , one has particularly

$$gA'_i = \sum_{k=1}^{f'} A'_k \Gamma'_{ki}(g), \tag{38}$$

which means that  $\Gamma_Y$  has the form

$$\Gamma_Y = \begin{pmatrix} -\Gamma' & \text{---} \\ \mathbf{0} & \text{---} \end{pmatrix}. \tag{39}$$

This implies that, by means of a change of basis and the associated similarity transformation, it is always possible to bring a reducible representation to the specific form (39) containing a zero matrix in the lower left-hand corner. One says that this form of the representation is *partly reduced*.

*Reducible and Decomposable Representations*

Let us start by considering some properties of the partly reduced representations. For the sake of simplicity, we use a notation in terms of submatrices:

$$\Gamma(g) = \begin{bmatrix} \Gamma_{11}(g) & \Gamma_{12}(g) \\ \mathbf{0} & \Gamma_{22}(g) \end{bmatrix}. \tag{40}$$

One has directly

$$\begin{aligned} &\Gamma(g)\Gamma(h) \\ &= \begin{bmatrix} \Gamma_{11}(g)\Gamma_{11}(h); & \Gamma_{11}(g)\Gamma_{12}(h) + \Gamma_{12}(g)\Gamma_{22}(h) \\ \mathbf{0}; & \Gamma_{22}(g)\Gamma_{22}(h) \end{bmatrix} \\ &= \Gamma(gh), \end{aligned} \tag{41}$$

which leads to the relations

$$\begin{aligned} \Gamma_{11}(gh) &= \Gamma_{11}(g)\Gamma_{11}(h), \\ \Gamma_{22}(gh) &= \Gamma_{22}(g)\Gamma_{22}(h), \\ \Gamma_{12}(gh) &= \Gamma_{11}(g)\Gamma_{12}(h) + \Gamma_{12}(g)\Gamma_{22}(h). \end{aligned} \tag{42}$$

In addition to  $\Gamma_{11}$ , the matrices  $\Gamma_{22}$  form hence a representation of the group. The meaning of the third relation is clarified below.

In connection with the study of reducibility of a space, it is natural to ask the question whether it would be possible to choose the elements  $A'_{f'+1}, A'_{f'+2}, \dots, A'_f$  in such way that they also span a *stable* subspace of order  $(f-f')$ . The existence of *one* stable subspace would then also imply the existence of a *second* stable subspace, and one says that the space  $W$  is *decomposable* into two stable subspaces. In such a case, the form (39) would contain a zero matrix also in the upper right-hand corner.

One could also ask the question whether there exists a nonlinear transformation

$$\alpha = \begin{pmatrix} \mathbf{1}_{11} & \alpha_{12} \\ \mathbf{0} & \mathbf{1}_{22} \end{pmatrix}; \quad \alpha^{-1} = \begin{pmatrix} \mathbf{1}_{11} & -\alpha_{12} \\ \mathbf{0} & \mathbf{1}_{22} \end{pmatrix}, \tag{43}$$

which brings the matrix (40) to block-diagonal form. One has

$$\begin{aligned} &\alpha^{-1}\Gamma(g)\alpha \\ &= \begin{pmatrix} \Gamma_{11}(g); & \Gamma_{11}(g)\alpha_{12} + \Gamma_{12}(g) - \alpha_{12}\Gamma_{22}(g) \\ \mathbf{0}; & \Gamma_{22}(g) \end{pmatrix}, \end{aligned} \tag{44}$$

which leads to the condition

$$\Gamma_{11}(g)\alpha_{12} + \Gamma_{12}(g) - \alpha_{12}\Gamma_{22}(g) = \mathbf{0}, \tag{45}$$

for all  $g$ . It follows from the third relation (42) that there exists a constant matrix  $\alpha_{12}$  which satisfies this condition, and that the solution has the form

$$\alpha_{12} = (\Gamma_{12} * \Gamma_{22})_0 = M \Gamma_{12}(h) \Gamma_{22}(h^{-1}). \tag{46}$$

Multiplying the third relation (42) to the right by  $\Gamma_{22}(h^{-1})$ , one obtains

$$\Gamma_{12}(gh)\Gamma_{22}(h^{-1}) = \Gamma_{11}(g)\Gamma_{12}(h)\Gamma_{22}(h^{-1}) + \Gamma_{12}(g). \tag{47}$$

Forming the invariant mean over  $h$ , one gets further

$$\begin{aligned} &\Gamma_{11}(g) M \Gamma_{12}(h) \Gamma_{22}(h^{-1}) + \Gamma_{12}(g) \\ &= M \Gamma_{12}(gh) \Gamma_{22}(h^{-1}) \\ &= M \Gamma_{12}(u) \Gamma_{22}(u^{-1}g) \\ &= \{ M \Gamma_{12}(u) \Gamma_{22}(u^{-1}) \} \Gamma_{22}(g), \end{aligned} \tag{48}$$

which proves that the quantity  $\alpha_{12}$  defined by (46) satisfies the condition (45) for all  $g$ . From (44), it follows that

$$\alpha^{-1}\Gamma(g)\alpha = \begin{bmatrix} \Gamma_{11}(g) & \mathbf{0} \\ \mathbf{0} & \Gamma_{22}(g) \end{bmatrix}, \tag{49}$$

and the representation has been partly *decomposed*.

For every finite group, a reducible representation is also decomposable; this important result is known as Maschke's theorem. It implies that every reducible stable space is also decomposable into stable subspaces. We note that the equivalence between reducibility and decomposability is not directly extendable to infinite groups.

*Transformations of Proper Representations to Unitary Form*

Let us start this section by repeating some elementary concepts in matrix theory. Let  $\mathbf{R} = \{R_{kl}\}$  be an arbitrary quadratic matrix of finite order; the Hermitian adjoint matrix  $\mathbf{R}^\dagger$  is defined through the relation

$$\{\mathbf{R}^\dagger\}_{kl} = R_{lk}^* \tag{50}$$

A matrix  $\mathbf{R}$  is said to be *normal*, if it commutes with its adjoint matrix  $\mathbf{R}^\dagger$ , so that  $\mathbf{R}\mathbf{R}^\dagger = \mathbf{R}^\dagger\mathbf{R}$ . A matrix  $\mathbf{R}$  is further said to be *self-adjoint*, if  $\mathbf{R}^\dagger = \mathbf{R}$ . All matrices may by a similarity transformation be brought to "classical canonical form"; see Ref. 1, p. 32. The normal matrices belong to an important class of matrices which may be brought to diagonal form; they are characterized by the fact that they have in general complex eigenvalues and orthogonal eigenvectors, whereas the self-adjoint matrices have real eigenvalues and orthogonal eigenvectors.

A matrix  $\mathbf{U}$  is said to be *unitary*, if it satisfies the relation:

$$\mathbf{U}^\dagger\mathbf{U} = \mathbf{U}\mathbf{U}^\dagger = \mathbf{1} \tag{51}$$

Such a matrix is a normal matrix having orthogonal eigenvectors and its eigenvalues are situated on the unit circle in the complex plane.

We now prove the fundamental theorem that, without loss of generality, any proper representation  $\Gamma(g)$  may by a similarity transformation be brought to unitary form. For this purpose, we consider the matrix  $\mathbf{S}$  defined by the relation:

$$\mathbf{S} = M \Gamma(g) \{ \Gamma(g) \}^\dagger \tag{52}$$

If the representation is unitary, one has simply  $\mathbf{S} = \mathbf{1}$ . The matrix  $\mathbf{S}$  satisfies the relations

$$\begin{aligned} \mathbf{S}^\dagger &= \mathbf{S}, & \mathbf{S} > 0, \\ \Gamma(h)\mathbf{S}\{\Gamma(h)\}^\dagger &= \mathbf{S}, \end{aligned} \tag{53}$$

for all elements  $h$  of the group. The first relation says that  $\mathbf{S}$  is self-adjoint, the second that it is positive definite, and the last one follows immediately from the properties of the invariant mean in (5):

$$\Gamma(h)\mathbf{S}\{\Gamma(h)\}^\dagger = M \Gamma(hg) \{ \Gamma(hg) \}^\dagger = \mathbf{S} \tag{54}$$

Since the matrix  $\mathbf{S}$  is self-adjoint, there exists a unitary

matrix  $\mathbf{U}$  which brings  $\mathbf{S}$  to diagonal form  $\mathbf{s}$ :

$$\mathbf{U}^\dagger\mathbf{S}\mathbf{U} = \mathbf{s} = \begin{pmatrix} s_1 & & & \\ & s_2 & & \\ & & \ddots & \\ & & & s_f \end{pmatrix}, \tag{55}$$

where  $s_i > 0$ . A proper representation is characterized by the fact that  $\Gamma(e) = \mathbf{1}_f$ , and one has hence the matrix inequalities  $\mathbf{S} \geq |G|^{-1} \Gamma(e) \{ \Gamma(e) \}^\dagger = |G|^{-1} \mathbf{1}_f$  and

$$\mathbf{s} = \mathbf{U}^\dagger\mathbf{S}\mathbf{U} \geq |G|^{-1} \mathbf{1}_f, \tag{56}$$

which imply that all the eigenvalues of  $\mathbf{s}$  are positive and larger than  $1/n$ .

The matrices  $\mathbf{s}^{1/2}$  and  $\mathbf{s}^{-1/2}$  are defined as the diagonal matrices having the positive elements  $s_k^{+1/2}$  and  $s_k^{-1/2}$ , respectively. Let us now consider the similarity transformation  $\alpha = \mathbf{U}\mathbf{s}^{1/2}$ , so that

$$\begin{aligned} \bar{\Gamma}(g) &= \alpha^{-1} \Gamma(g) \alpha \\ &= \mathbf{s}^{-1/2} \mathbf{U}^\dagger \Gamma(g) \mathbf{U} \mathbf{s}^{+1/2}. \end{aligned} \tag{57}$$

Using the fact that  $\mathbf{U}\mathbf{s}\mathbf{U}^\dagger = \mathbf{S}$ , one gets immediately

$$\begin{aligned} \bar{\Gamma}(g) \{ \bar{\Gamma}(g) \}^\dagger &= \mathbf{s}^{-1/2} \mathbf{U}^\dagger \Gamma(g) \mathbf{U} \mathbf{s}^{+1/2} \cdot \mathbf{s}^{+1/2} \mathbf{U}^\dagger \{ \Gamma(g) \}^\dagger \mathbf{U} \mathbf{s}^{-1/2} \\ &= \mathbf{s}^{-1/2} \mathbf{U}^\dagger \Gamma(g) \mathbf{S} \{ \Gamma(g) \}^\dagger \mathbf{U} \mathbf{s}^{-1/2} \\ &= \mathbf{s}^{-1/2} \mathbf{U}^\dagger \mathbf{S} \mathbf{U} \mathbf{s}^{-1/2} = \mathbf{s}^{-1/2} \mathbf{s} \mathbf{s}^{-1/2} = \mathbf{1}. \end{aligned} \tag{58}$$

Since we are dealing with finite matrices, this relation implies that the representation  $\bar{\Gamma}(g)$  is unitary, and one has

$$\{ \bar{\Gamma}(g) \}^\dagger = \{ \bar{\Gamma}(g) \}^{-1} = \bar{\Gamma}(g^{-1}). \tag{59}$$

The existence of the unitary representations leads to an important property for the characters. According to (59), one has

$$\bar{\Gamma}_{lk}(g^{-1}) = \{ \bar{\Gamma}_{kl}(g) \}^*, \tag{60}$$

and, putting  $l=k$  and summing over  $k$ , one obtains the relation

$$\chi(g^{-1}) = \{ \chi(g) \}^*, \tag{61}$$

which holds quite generally irrespective of any choice of special form of the representation.

In this connection, it is of interest to consider a special property of certain of the conjugate classes. A class  $C_g$  associated with a specific element  $g$  is said to be *ambivalent*, if it contains also the inverse element  $g^{-1}$ . This implies that, if it contains the element  $r = s^{-1}gs$ , it contains also the element  $r^{-1} = (s^{-1}gs)^{-1} = s^{-1}g^{-1}s$ . Since the characters are class functions, one has  $\chi(g) = \chi(g^{-1}) = \{ \chi(g) \}^*$ , and one obtains the theorem that *the*

character for any ambivalent class is necessarily a real quantity.

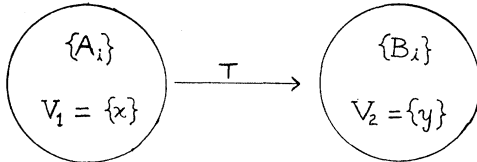
**D. Schur's Lemma and the Convolution Relations**

*Schur's Lemma*

In this section, we start by considering the general theory of linear spaces of finite order and their operators. Let  $V$  be a linear space, let  $A$  be a linear operator defined on this space, and let  $W$  be a subspace of  $V$ . The subspace  $W$  is said to be *stable* under the operation  $A$ , if  $AW$  belongs to  $W$ ; in such a case,  $W$  is also said to be an invariant subspace under  $A$ . We note that the eigenvalue problem  $AC = aC$  is equivalent with the problem of finding all the possible one-dimensional invariant subspaces.

Let us now consider a set of linear operators  $\{A_1, A_2, \dots, A_p\}$  which do not necessarily commute. The space  $V$  is said to be *reducible* under the set  $\{A_i\}$ , if there exists a proper subspace  $W$  of  $V$  which is also stable under the set  $\{A_i\}$ . If no such invariant proper subspace  $W$  exists, the space  $V$  is said to be *irreducible* under the set  $\{A_i\}$ . We note that these definitions are completely analogous with those previously introduced in the group algebra.

Schur's lemma deals with two linear spaces,  $V_1$  and  $V_2$ , and two sets of operators  $\{A_1, A_2, \dots, A_p\}$  and  $\{B_1, B_2, \dots, B_p\}$  which act on  $V_1$  and  $V_2$ , respectively. The operator  $T$  represents further a linear mapping of  $V_1$  on  $V_2$ , which is illustrated in the diagram below:



Schur's lemma is then the following theorem:

If  $TA_i = B_iT$  for all  $i = 1, 2, \dots, p$ , and the spaces  $V_1$  and  $V_2$  are both irreducible under the set of operators  $\{A_i\}$  and  $\{B_i\}$ , respectively, then either  $T = 0$ , or  $T^{-1}$  exists. (62)

The lemma is one of the most fundamental theorems in the theory of linear spaces, and particularly the applications to group algebra are of a deep-going nature.

For the proof, we denote the elements of  $V_1$  and  $V_2$  by  $x$  and  $y$ , respectively; the linear mapping has the form  $Tx = y$ . Let  $K$  be the subspace of  $V_1$  which is mapped on the zero-element  $\bar{0}$  of  $V_2$ :

$$K = \{x \mid Tx = \bar{0}\}. \tag{63}$$

We note that  $K$  is a linear space for, if  $x_1$  and  $x_2$  belong to  $K$ , then the elements  $cx_1$  and  $(x_1 + x_2)$  belong also to  $K$ . The subspace  $K$  is further invariant under  $\{A_i\}$ ,

since one has

$$T(A_i x) = TA_i x = B_i T x = B_i(\bar{0}) = \bar{0}, \tag{64}$$

which proves our statement. However, since  $V_1$  is irreducible under the set  $\{A_i\}$ , this implies that  $K$  must be an improper subspace, and one has either  $K = V_1$  or  $K = 0$ .

If  $K = V_1$ , one has  $TV_1 = 0$ , which means that  $T$  has the effect of a zero operator:  $T = 0$ .

If  $K = 0$ , one can prove that the operator  $T$  corresponds to a one-to-one mapping of the space  $V_1$  onto the space  $V_2$ , and that the inverse mapping  $T^{-1}$  hence exists. Let us first prove that  $T$  maps  $V_1$  uniquely onto  $V_2$  or onto a subspace  $W$  of  $V_2$ : let us assume that the elements  $x_1$  and  $x_2$  are both mapped on the same element  $y$ . Since  $K = 0$ , one has

$$\begin{aligned} Tx_1 &= y, & Tx_2 &= y, \\ T(x_1 - x_2) &= \bar{0}, \\ x_1 - x_2 &= 0, \\ x_1 &= x_2, \end{aligned} \tag{65}$$

which shows that the mapping is unique. Let us now consider the subspace  $W$ , defined by the relation  $W = TV_1$  or:

$$W = \{y \mid y = Tx, x \in V_1\}. \tag{66}$$

We note that  $W$  is a linear space for, if  $y_1$  and  $y_2$  are elements of  $W$ , then  $cy_1$  and  $(y_1 + y_2)$  are also elements of  $W$ . The subspace  $W$  is further invariant under the set  $B_i$ , since one has

$$y \in W, \quad B_i y = B_i T x = TA_i x = T(A_i x) = T x', \tag{67}$$

which proves the statement. However, if the space  $V_2$  is assumed to be irreducible under the set  $\{B_i\}$ , the space  $W$  must be an improper subspace of  $V_2$ , and one has either  $W = 0$  or  $W = V_2$ . In the former case, one has  $TV_1 = 0$  or  $T = 0$ , and, in the latter case, one has  $TV_1 = V_2$ , which means that  $T$  is a unique one-to-one mapping of the space  $V_1$  onto  $V_2$ , and the inverse mapping  $T^{-1}$  exists. This proves Schur's lemma.

The operators  $A_i$  and  $B_i$  are connected through the relation  $TA_i = B_iT$ . We note that, if the mapping  $T$  has an inverse  $T^{-1}$ , one obtains

$$A_i = T^{-1} B_i T, \tag{68}$$

and the operators  $A_i$  and  $B_i$  are said to be *similar* or equivalent operators on the two spaces  $V_1$  and  $V_2$ , respectively.

In the case when the two spaces are identical, i.e.,  $V_1 = V_2$  and  $A_i = B_i$ , one obtains the following special form of Schur's lemma:

If  $T$  is a linear mapping of  $V_1$  on  $V_1$ , if  $TA_i = A_i T$  for  $i = 1, 2, \dots, p$ , and if the space  $V_1$  is irreducible under the set  $\{A_i\}$ , then  $T$  must be a multiple of the identity operator  $I$ . (69)



The proof follows from the fact that one has also

$$(T - cI)A_i = A_i(T - cI), \tag{70}$$

for arbitrary values of the complex constant  $c$ . According to the general form (62) of Schur's lemma, this implies that either  $T - cI = 0$  or  $(T - cI)^{-1}$  exists. However, since the field of complex numbers is algebraically closed, there exists at least one complex number  $\lambda$  such that  $|T - \lambda I| = 0$ . For the value  $c = \lambda$ , the operator  $(T - \lambda \cdot I)$  has certainly no inverse, which leaves only the other alternative open, i.e.,  $T - \lambda \cdot I = 0$ , or

$$T = \lambda \cdot I. \tag{71}$$

This concludes the treatment of Schur's lemma.

### Convolution Relations

A representation of a group  $G = \{g\}$  is a definite set of objects  $\{A(g)\}$  associated with the elements of the group which has a binary operation  $\perp$  leading to a "multiplication table" analogous to the original one:

$$g \rightarrow A(g), \quad A(g) \perp A(h) = A(g.h). \tag{72}$$

It is easily shown that the set  $\{A(g)\}$  satisfies all four group axioms and is again a group. The most common representations of finite groups are either *linear operators* acting on a certain "carrier space" or the associated *matrices*, in which case the second binary operation  $\perp$  is simply operator or matrix multiplication, respectively.

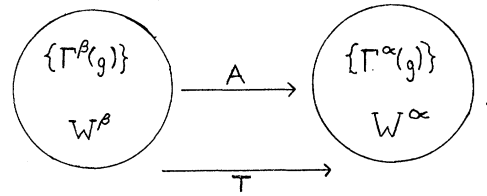
Let us start by considering the representation of the group  $G = \{g\}$  by means of the set of linear operators  $\{g\}$  acting on the group algebra  $V_G$  through the binary operation  $\times$  defined in (9). If the carrier space is instead restricted to a stable subspace  $W$  of  $V$ , we will sometimes characterize the operator  $g$  by the special symbol  $\Gamma(g)$  and, according to (16), the introduction of a specific basis leads then automatically to a matrix representation  $\Gamma(g)$  of the same order  $f$  as the subspace  $W$ :

$$\begin{array}{ccc} g \rightarrow \Gamma(g) \rightarrow \Gamma(g) \\ V_G & W & \text{order } f. \end{array} \tag{73}$$

Let us now consider two subspaces  $W^\alpha$  and  $W^\beta$  of the group algebra which are assumed to be *stable and irreducible* under the group  $G = \{g\}$ , and let their dimensions be  $f^\alpha$  and  $f^\beta$ , respectively. Let us denote the operator  $g$  when it acts on the carrier spaces  $W^\alpha$  and  $W^\beta$  by the symbols  $\Gamma^\alpha(g)$  and  $\Gamma^\beta(g)$ , respectively. After introducing a proper basis  $\mathbf{X}^\alpha$  and  $\mathbf{X}^\beta$  for each subspace, one obtains automatically the *irreducible representations*  $\Gamma^\alpha$  and  $\Gamma^\beta$  according to (17).

Let further  $A$  be an arbitrary linear operator which

maps  $W^\beta$  on  $W^\alpha$ ; in terms of the bases  $\mathbf{X}^\alpha$  and  $\mathbf{X}^\beta$ ,  $A$  is represented by a rectangular matrix of order  $f^\alpha \times f^\beta$ .



We will now introduce the fundamental operator  $T$  through the following invariant mean:

$$T = M \Gamma^\alpha(s) A \Gamma^\beta(s^{-1}), \tag{74}$$

and we note that  $T$  is a linear operator which maps the subspace  $W^\beta$  on the subspace  $W^\alpha$ . Depending on the properties (5) of the invariant mean, one obtains

$$\begin{aligned} T \Gamma^\beta(g) &= M \Gamma^\alpha(s) A \Gamma^\beta(s^{-1}g) \\ &= M \Gamma^\alpha(gu) A \Gamma^\beta(u^{-1}) \\ &= \Gamma^\alpha(g) M \Gamma^\alpha(u) A \Gamma^\beta(u^{-1}) \\ &= \Gamma^\alpha(g) T, \quad \text{for all } g \in G, \end{aligned} \tag{75}$$

which means that the operator  $T$  satisfies the properties required by the mapping in Schur's lemma (62), if one chooses  $\{A_i\}$  and  $\{B_i\}$  to be  $\{\Gamma^\beta(g)\}$  and  $\{\Gamma^\alpha(g)\}$ , respectively. Hence, this leads to the conclusion that either  $T = 0$  or  $T^{-1}$  exists.

In the case when  $T^{-1}$  exists, one has  $\Gamma^\beta = T^{-1} \Gamma^\alpha T$ , which means that  $\Gamma^\beta$  and  $\Gamma^\alpha$  are equivalent representations. If the subspaces  $W^\beta$  and  $W^\alpha$  are different from each other, this case is usually considered as comparatively "uninteresting." One focuses instead the study on the case when  $W^\beta$  and  $W^\alpha$  are identical, which according to (69) leads to the conclusion  $T = \lambda \cdot I^\alpha$ , and on the case when  $W^\beta$  and  $W^\alpha$  correspond to non-equivalent representations, which according to (62) leads to the conclusion  $T = 0$ . In order to treat both these cases simultaneously, it is convenient to introduce a special Kronecker symbol:

$$\begin{aligned} \delta^{\alpha\beta} &= 1, & \Gamma^\alpha &\equiv \Gamma^\beta, \\ &= 0, & \Gamma^\alpha &\text{ and } \Gamma^\beta \text{ are nonequivalent.} \end{aligned} \tag{76}$$

We note that the equivalent case is not included and has to be treated separately, if desired. Schur's lemma in the form (62) and (69) leads now to the conclusion  $T = \delta^{\alpha\beta} \cdot \lambda \cdot I^\alpha$ , and one obtains the result

$$T = M \Gamma^\alpha(s) A \Gamma^\beta(s^{-1}) = \delta^{\alpha\beta} \cdot \lambda \cdot I^\alpha, \tag{77}$$

where  $I^\alpha$  is the identity operator acting on the subspace  $W^\alpha$ . In this relation, it remains to determine the value of the constant  $\lambda$  in the case when  $W^\beta = W^\alpha$ . Taking the trace of both members and using (24) and the

general properties of representations, one obtains:

$$\begin{aligned} \lambda \cdot f^\alpha &= M \underset{s}{\text{Tr}} \{ \Gamma^\alpha(s) A \Gamma^\alpha(s^{-1}) \} \\ &= M \underset{s}{\text{Tr}} \{ A \Gamma^\alpha(s^{-1}) \Gamma^\alpha(s) \} \\ &= M \underset{s}{\text{Tr}} \{ A \Gamma^\alpha(e) \} = \text{Tr} \{ A \}, \end{aligned} \quad (78)$$

which gives

$$\lambda = (f^\alpha)^{-1} \text{Tr} \{ A \}. \quad (79)$$

Substitution of this value into (77) leads to the relation

$$M \underset{s}{\Gamma^\alpha}(s) A \Gamma^\beta(s^{-1}) = (f^\alpha)^{-1} \delta^{\alpha\beta} \text{Tr} \{ A \} \cdot I^\alpha \quad (80)$$

which is the fundamental formula in the theory of irreducible representations; we note that it is an immediate consequence of Schur's lemma.

In the following, we rewrite formula (80) in many different ways which are all variations of one and the same basic theme. Putting  $A = A' \Gamma^\beta(g)$ , one obtains, for instance:

$$M \underset{s}{\Gamma^\alpha}(s) A' \Gamma^\beta(g s^{-1}) = (f^\alpha)^{-1} \delta^{\alpha\beta} \text{Tr} \{ A' \Gamma^\beta(g) \} \cdot I^\alpha. \quad (81)$$

We note that, according to (13), the left-hand member is an operator depending on the fixed element  $g$  which may be considered as a convolution product of the operators  $\Gamma^\alpha$  and  $\Gamma^\beta$ , and one may write this relation symbolically in the shorthand form

$$\Gamma^\alpha \star A' \Gamma^\beta = (f^\alpha)^{-1} \delta^{\alpha\beta} \text{Tr} \{ A' \Gamma^\beta \} \cdot I^\alpha, \quad (82)$$

where  $A'$  is an arbitrary mapping of  $W^\beta$  on  $W^\alpha$ . This is probably the most condensed form one can give the fundamental theorem.

In order to proceed, we will now introduce the bases  $\mathbf{X}^\alpha$  and  $\mathbf{X}^\beta$  for  $W^\alpha$  and  $W^\beta$ , respectively. One has

$$T X_l^\beta = \sum_k X_k^\alpha T_{kl}, \quad (83)$$

which uniquely defines the rectangular matrix  $\mathbf{T} = \{ T_{kl} \}$  of order  $f^\alpha \times f^\beta$ . Introducing the rectangular matrix  $\mathbf{A}' = \{ A'_{mn} \}$  of order  $f^\alpha \times f^\beta$  associated with the arbitrary mapping  $A'$ , one may write (81) in matrix form

$$M \underset{s}{\Gamma^\alpha}(s) \mathbf{A}' \Gamma^\beta(g s^{-1}) = (f^\alpha)^{-1} \delta^{\alpha\beta} \text{Tr} \{ \mathbf{A}' \Gamma^\beta(g) \} \cdot \mathbf{1}^\alpha. \quad (84)$$

Taking the  $(k, l)$  element of this rectangular matrix and writing out the matrix multiplications, one obtains

$$\begin{aligned} \sum_{m,n} M \Gamma_{km}^\alpha(s) A'_{mn} \Gamma_{nl}^\beta(g s^{-1}) \\ = \sum_{m,n} (f^\alpha)^{-1} \delta^{\alpha\beta} A'_{mn} \Gamma_{nm}^\beta(g) \delta_{kl}. \end{aligned} \quad (85)$$

Since the matrix elements  $A'_{mn}$  are completely arbitrary, the coefficients for  $A'_{mn}$  in both members must be equal, and this gives finally the relation

$$M \underset{s}{\Gamma_{km}^\alpha}(s) \Gamma_{nl}^\beta(g s^{-1}) = (f^\alpha)^{-1} \delta^{\alpha\beta} \delta_{kl} \Gamma_{nm}^\beta(g). \quad (86)$$

This is the fundamental theorem in the theory of irre-

ducible representations expressed in terms of the matrix elements themselves; we note that it is usually easier to memorize the form (84). Using the notation (13), it may also be expressed in the convolution form

$$\Gamma_{km}^\alpha \star \Gamma_{nl}^\beta = (f^\alpha)^{-1} \delta^{\alpha\beta} \delta_{kl} \Gamma_{nm}^\beta, \quad (87)$$

which shows the importance of the convolution algebra in this connection. As we shall see later, the form (87) forms a convenient basis for the applications of group algebra to quantum mechanics.

### Some Consequences of the Convolution Relations

Let us now study some of the immediate consequences of the basic theorem (86). Putting  $\alpha = \beta$  and  $m = n$  and summing over  $m$ , one obtains

$$M \underset{s}{\Gamma_{kl}^\alpha}(s g s^{-1}) = (f^\alpha)^{-1} \delta_{kl} \chi^\alpha(g), \quad (88)$$

or

$$M \underset{s}{\Gamma^\alpha}(s g s^{-1}) = (f^\alpha)^{-1} \chi^\alpha(g) \cdot \mathbf{1}^\alpha. \quad (88')$$

If the variable element  $s$  runs over the entire group  $G$ , the variable  $sgs^{-1}$  runs over the conjugate class  $C_g$  associated with the element  $g$ ; if the entire class contains  $h_g$  elements, every element will further be repeated  $|G|/h_g$  times in the summation over  $s$ , and one obtains the formula

$$M \underset{s}{f}(s g s^{-1}) = h_g^{-1} \sum_{t \in C_g} f(t), \quad (89)$$

for any quantity  $f$  which depends on the elements of the group. Formula (88') implies then that, *if an irreducible representation  $\Gamma^\alpha$  is averaged over a conjugate class, the result will be proportional to a unit matrix with the factor  $(f^\alpha)^{-1} \chi^\alpha$* . It is rather interesting to check this simple theorem with the existing tables of irreducible representations.

Let us now return to the fundamental theorem in the form (87). Putting  $m = k$  and summing over  $k$ , one obtains

$$\chi^\alpha \star \Gamma_{nl}^\beta = (f^\alpha)^{-1} \delta^{\alpha\beta} \Gamma_{nl}^\beta. \quad (90)$$

Putting  $n = l$  and summing over  $l$ , one gets further

$$\chi^\alpha \star \chi^\beta = (f^\alpha)^{-1} \delta^{\alpha\beta} \chi^\beta. \quad (91)$$

This is the basic *convolution theorem for the characters* of the irreducible representations. The relation (91) may also be written in the form

$$M \underset{s}{\chi^\alpha}(s) \chi^\beta(g s^{-1}) = (f^\alpha)^{-1} \delta^{\alpha\beta} \chi^\beta(g). \quad (92)$$

For  $g = e$ , one obtains the special formula

$$M \underset{s}{\chi^\alpha}(s) \chi^\beta(s^{-1}) = \delta^{\alpha\beta}, \quad (93)$$

which is called the *orthogonality relations* for the characters; it may be written in the condensed form  $(\chi^\alpha \star \chi^\beta)_e = \delta^{\alpha\beta}$ . In this connection, the relation (61) is also very useful. We note that the orthogonality

relations are hence a special case of the convolution relations, but that the latter may not be derived from the former. Schur's lemma and the associated general convolution relations (87) reveal some very deep-going properties of the irreducible representations, which are not easily found in some other way.

**E. Properties of Irreducible Representations**

*Spectral Analysis of Arbitrary Representations*

Let  $W$  be an arbitrary stable subspace of the group algebra having the basis  $\mathbf{X}$  leading to the representation  $\Gamma$  according to (17). An important problem is to investigate whether the subspace  $W$  is *irreducible* under the group  $G = \{g\}$  or whether it is decomposable into irreducible subspaces.

For this purpose, we first assume that the space is reducible which means that it is also decomposable, according to Maschke's theorem. This implies that there exists a similarity transformation  $\alpha$  which brings the representation  $\Gamma$  to block-diagonal form:

$$\alpha^{-1}\Gamma\alpha = \begin{bmatrix} \Gamma^{\alpha_1} & & & & \\ & \Gamma^{\alpha_2} & & & \\ & & \Gamma^{\alpha_3} & & \\ & & & \ddots & \\ & & & & \ddots \end{bmatrix}, \quad (94)$$

where the diagonal blocks are assumed to be irreducible. A specific irreducible representation  $\Gamma^\alpha$  may occur  $\nu^\alpha$  times in the right-hand side, and  $\nu^\alpha$  is said to be the frequency of  $\Gamma^\alpha$  in  $\Gamma$ . Forming the trace of both members of (94), one obtains

$$\chi(g) = \sum_{\alpha} \nu^{\alpha} \chi^{\alpha}(g), \quad (95)$$

where  $\chi = \text{Tr} \{\Gamma\}$  is the character of the given representation  $\Gamma$ . Using (91), one gets further

$$\begin{aligned} \chi * \chi^{\beta} &= \sum_{\alpha} \nu^{\alpha} \chi^{\alpha} * \chi^{\beta} = \sum_{\alpha} \nu^{\alpha} (f^{\alpha})^{-1} \delta^{\alpha\beta} \chi^{\beta} \\ &= \nu^{\beta} (f^{\beta})^{-1} \chi^{\beta}. \end{aligned} \quad (96)$$

Putting  $g=e$ , one obtains particularly  $(\chi * \chi^{\beta})_0 = \nu^{\beta}$ , or

$$\nu^{\alpha} = (\chi * \chi^{\alpha})_0 = M_s \chi(s) \chi^{\alpha}(s^{-1}), \quad (97)$$

which relation determines the frequency  $\nu^{\alpha}$ , provided that one knows the characters of the irreducible representations.

A very interesting relation is obtained by considering the "square" of the character  $\chi$  in the convolution

algebra. Using (91), one gets directly

$$\begin{aligned} \chi * \chi &= \left( \sum_{\alpha} \nu^{\alpha} \chi^{\alpha} \right) * \left( \sum_{\beta} \nu^{\beta} \chi^{\beta} \right) \\ &= \sum_{\alpha} \sum_{\beta} \nu^{\alpha} \nu^{\beta} \chi^{\alpha} * \chi^{\beta} \\ &= \sum_{\alpha} \sum_{\beta} \nu^{\alpha} \nu^{\beta} (f^{\alpha})^{-1} \delta^{\alpha\beta} \chi^{\beta} \\ &= \sum_{\alpha} (\nu^{\alpha})^2 (f^{\alpha})^{-1} \chi^{\alpha}. \end{aligned} \quad (98)$$

Putting  $g=e$ , one obtains particularly

$$(\chi * \chi)_0 = \sum_{\alpha} (\nu^{\alpha})^2. \quad (99)$$

This relation shows that, a necessary and sufficient condition that a representation  $\Gamma$  is irreducible is that its character  $\chi$  satisfies the equation

$$(\chi * \chi)_0 = 1. \quad (100)$$

The necessity follows, of course, also from relation (91), but formula (99) shows also the sufficiency. We note particularly that the quantity  $(\chi * \chi)_0$  is always an integer.

*Completeness Relation*

In order to proceed, it is now convenient to introduce a special function over the group  $E(g)$  defined through the relation

$$\begin{aligned} E(g) &= |G|, \quad \text{if } g=e \\ &= 0, \quad \text{if } g \neq e. \end{aligned} \quad (101)$$

From the definition (13) of the convolution product follows immediately

$$E * \alpha = \alpha, \quad (102)$$

for an arbitrary function  $\alpha$  over the group, and the function  $E$  may hence be characterized as the *identity function* in the convolution algebra.

Let us now apply the analysis in terms of irreducible subspaces to the entire space  $V_G$  of the group algebra. This space is associated with the *regular representation*  $\Gamma_R$  which is explicitly defined by (31), and its character  $\chi_R$  given by (33) is apparently identical with the identity function:

$$\chi_R(g) = E(g). \quad (103)$$

The frequency analysis of the regular representation is now easily performed. Substitution of (103) into (97) gives

$$\nu^{\alpha} = (E * \chi^{\alpha})_0 = \chi^{\alpha}(e) = f^{\alpha}, \quad (104)$$

i.e., the frequency of the irreducible representation  $\Gamma^{\alpha}$  in the regular representation  $\Gamma_R$  equals the order  $f^{\alpha}$  of the representation:  $\nu^{\alpha} = f^{\alpha}$ . Substituting this result into (95), one obtains

$$E(g) = \sum_{\alpha} f^{\alpha} \chi^{\alpha}(g), \quad (105)$$

which relation will be described as a "resolution of the

identity" in the convolution algebra. Putting  $g=e$ , one obtains particularly

$$|G| = \sum_{\alpha} (f^{\alpha})^2, \tag{106}$$

which is often referred to as the *completeness relation* for the irreducible representations.

The functions  $f^{\alpha}\chi^{\alpha}$  serve the purpose of "projection operators" in the convolution algebra. One may write relation (91) in the form

$$f^{\alpha}\chi^{\alpha} * f^{\beta}\chi^{\beta} = \delta^{\alpha\beta} f^{\beta}\chi^{\beta}, \tag{107}$$

which means that they are idempotent and mutually exclusive and, according to (105), they form also a resolution of the identity. In Sec. I.F, we return to this problem and utilize these important properties.

*Square Form of Character Table*

The characters  $\chi^{\alpha}(g)$  are class functions, and it may be convenient to list them in the form of a rectangular table, where the rows are labeled by the irreducible representations  $\alpha_1, \alpha_2, \dots, \alpha_M$  and the columns are labeled by the conjugate classes  $C_1, C_2, \dots, C_N$ :

$\alpha$	$C_1$	$C_2$	$C_3$	$\dots$	$C_N$
$\alpha_1$	$\chi^{\alpha_1}(C_1)$	$\chi^{\alpha_1}(C_2)$	$\chi^{\alpha_1}(C_3)$	$\dots$	$\chi^{\alpha_1}(C_N)$
$\alpha_2$	$\chi^{\alpha_2}(C_1)$	$\chi^{\alpha_2}(C_2)$	$\chi^{\alpha_2}(C_3)$	$\dots$	$\chi^{\alpha_2}(C_N)$
$\alpha_3$	$\chi^{\alpha_3}(C_1)$	$\chi^{\alpha_3}(C_2)$	$\chi^{\alpha_3}(C_3)$	$\dots$	$\chi^{\alpha_3}(C_N)$
$\dots$	$\dots$	$\dots$	$\dots$	$\dots$	$\dots$
$\alpha_M$	$\chi^{\alpha_M}(C_1)$	$\chi^{\alpha_M}(C_2)$	$\chi^{\alpha_M}(C_3)$	$\dots$	$\chi^{\alpha_M}(C_N)$

(108)

The number of irreducible representations is  $M$ , and the number of conjugate classes is  $N$ . According to (93), one has the orthonormality relation

$$M \chi^{\alpha}(s) \{ \chi^{\beta}(s) \}^* = \delta^{\alpha\beta}, \tag{109}$$

which may also be written in the form:

$$\sum_{k=1}^M \{ (h_k/|G|)^{1/2} \chi^{\alpha}(C_k) \} \{ (h_k/|G|)^{1/2} \chi^{\beta}(C_k) \}^* = \delta^{\alpha\beta}, \tag{110}$$

where  $h_k$  is the number of elements in the conjugate class  $C_k$ .

The functions over the classes form a linear space of order  $N$ , which may be spanned by a basis consisting of  $N$  linearly independent functions. The characters  $\chi^{\alpha}(C)$  form a set of  $M$  orthogonal and hence linearly independent functions, and one has directly the inequality  $M \leq N$ , since the number of linearly independent functions can never exceed the order of the space.

In order to study whether there is any orthogonality between the columns of the character table, we start

by considering the lemma:

$$\chi^{\alpha}(r)\chi^{\alpha}(g) = f^{\alpha} M \chi^{\alpha}(rsgs^{-1}). \tag{111}$$

The proof follows from (86) and the fact that

$$\begin{aligned} f^{\alpha} M \chi^{\alpha}(rsgs^{-1}) &= f^{\alpha} M \sum_s \Gamma_{kk}^{\alpha}(rsgs^{-1}) \\ &= f^{\alpha} \sum_{kl} M \Gamma_{kl}^{\alpha}(r) \Gamma_{lk}^{\alpha}(sgs^{-1}) \\ &= \sum_{kl} \Gamma_{kl}^{\alpha}(r) \delta_{lk} \chi^{\alpha}(g) \\ &= \sum_k \Gamma_{kk}^{\alpha}(r) \chi^{\alpha}(g) \\ &= \chi^{\alpha}(r) \chi^{\alpha}(g). \end{aligned} \tag{112}$$

Putting  $g=t^{-1}$ , summing over all  $\alpha$ , and using (105), one obtains

$$\begin{aligned} \sum_{\alpha} \chi^{\alpha}(r) \chi^{\alpha}(t^{-1}) &= M \left[ \sum_s f^{\alpha} \chi^{\alpha}(rst^{-1}s^{-1}) \right] \\ &= ME(rst^{-1}s^{-1}). \end{aligned} \tag{113}$$

The identity function  $E$  is nonvanishing only if  $rst^{-1}s^{-1}=e$ , i.e.,  $r=s^{-1}ts$ , which means that  $r$  and  $t$  belong to the same conjugate class. If  $r$  and  $t$  belong to *different* conjugate classes, one has hence the result:

$$\sum_{\alpha} \chi^{\alpha}(r) \{ \chi^{\alpha}(t) \}^* = 0, \tag{114}$$

which shows that different columns of the character table are orthogonal. Let us now consider the case when  $r=t$ ; since  $r=s^{-1}rs$  for  $|G|/h_r$  elements  $s$ , one obtains from (113) that

$$\sum_{\alpha} | \chi^{\alpha}(r) |^2 = |G|/h_r, \tag{115}$$

where  $h_r$  is the number of elements in the conjugate class  $C_r$ . One may combine the relations (114) and (115) into the single orthonormality relation:

$$\sum_{\alpha} \{ (h_k/|G|)^{1/2} \chi^{\alpha}(C_k) \} \{ (h_l/|G|)^{1/2} \chi^{\alpha}(C_l) \}^* = \delta_{kl}, \tag{116}$$

which is the counterpart to (110) for the columns of the character table.

One may now introduce the functions  $f(\alpha_k)$  over all irreducible representations having the symbol  $\alpha_k$  as argument; it is evident that these functions form a linear space of order  $M$ . The characters in a given column forms such a function over the irreducible representations. Because of the orthogonality relations (114), one has  $N$  linearly independent functions of this type which leads to the condition  $N \leq M$ .

Since we have previously obtained the condition  $M \leq N$ , one has apparently  $M=N$ , i.e., the character table has square form, and the *number of the irreducible representations equals the number of classes*. We note that the proof given here depends on the "resolution of the identity" as expressed in (105).

*Dual Representations*

In the previous section, it has been seen that the character table is square, and we will now show another elementary "symmetry property" in this table. For this purpose, we will consider the dual or *contragredient representation*  $\Lambda$  to an arbitrary representation  $\Gamma$  defined through the relation:

$$\Lambda(g) = \Gamma^{\text{tr}}(g^{-1}), \tag{117}$$

where  $\Gamma^{\text{tr}}$  denotes the transpose of  $\Gamma$  obtained by interchanging rows and columns, so that  $\Gamma_{kl}^{\text{tr}} = \Gamma_{lk}$ . That  $\Lambda$  is a representation follows from the fact

$$\begin{aligned} \Lambda(g)\Lambda(h) &= \Gamma^{\text{tr}}(g^{-1})\Gamma^{\text{tr}}(h^{-1}) = [\Gamma(h^{-1})\Gamma(g^{-1})]^{\text{tr}} \\ &= [\Gamma(h^{-1}g^{-1})]^{\text{tr}} = \Gamma^{\text{tr}}[(gh)^{-1}] = \Lambda(gh). \end{aligned} \tag{118}$$

For the trace, one obtains according to (61):

$$\begin{aligned} \text{Tr} \{ \Lambda(g) \} &= \text{Tr} \{ \Gamma^{\text{tr}}(g^{-1}) \} \\ &= \text{Tr} \{ \Gamma(g^{-1}) \} \\ &= \chi(g^{-1}) = \{ \chi(g) \}^*, \end{aligned} \tag{119}$$

which means that the dual representation  $\Lambda$  has a character which is the *complex conjugate* of the character of the representation  $\Gamma$ .

The spectral content (94) of an arbitrary representation  $\Gamma$  is characterized by the frequencies  $\nu^\alpha$  which are completely determined by the character  $\chi = \text{Tr} \{ \Gamma \}$  according to (97). A representation  $\Gamma$  is said to be *self-dual*, if the dual representation  $\Lambda$  is either identical with  $\Gamma$  or equivalent with  $\Gamma$ . In both case, one has

$$\chi(g) = \{ \chi(g) \}^*, \tag{120}$$

which means that the associated character  $\chi$  is necessarily real. On the other hand, if a character  $\chi$  is real, the dual representation  $\Lambda$  and  $\Gamma$  have the same character, and they are hence equivalent. This leads to the theorem that *a representation is self-dual, if and only if, the associated character is a real function over all classes.*

Let us now consider the irreducible representations  $\Gamma^\alpha$  and their dual representations  $\Lambda^\alpha$ . It follows from (100) that, if  $(\chi * \chi)_0 = 1$  for  $\chi = \chi^\alpha$ , then the same is true also for the complex conjugate character  $\chi = (\chi^\alpha)^*$ ; this means that the dual representations  $\Lambda^\alpha$  are also irreducible. Considering the frequency of  $\Gamma^\alpha$  in  $\Lambda^\alpha$ , one obtains by using (97):

$$\nu^\alpha = M_s \chi^{\Lambda^\alpha}(s) \chi^\alpha(s^{-1}) = M_s \chi^\alpha(s^{-1}) \chi^\alpha(s^{-1}), \tag{121}$$

i.e.,

$$\begin{aligned} M_s \{ \chi^\alpha(s) \}^2 &= 1, \quad \text{if } \Gamma^\alpha \text{ self-dual,} \\ &= 0, \quad \text{if } \Gamma^\alpha \text{ not self-dual.} \end{aligned} \tag{122}$$

Summing over all the irreducible representations, this gives

$$\sum_\alpha M_s \{ \chi^\alpha(s) \}^2 = n^\alpha, \tag{123}$$

where  $n^\alpha$  is the total number of self-dual representations.

It is now possible to rewrite the double sum in (123) in another way. Starting from the orthogonality relation (116), one has

$$\sum_\alpha (h_k / |G|) \chi^\alpha(C_k) \{ \chi^\alpha(C_i) \}^* = \delta_{ki}. \tag{124}$$

If  $C_k$  is a specific conjugate class, we will let us the symbol  $C'_k$  denote the class of the inverse elements. If  $C_k = C'_k$ , the class is said to be *ambivalent*. According to (61), one has

$$\chi^\alpha(C'_k) = \{ \chi^\alpha(C_k) \}^*, \tag{125}$$

which gives the previously mentioned theorem that ambivalent classes have real characters. From (124), one obtains further

$$\begin{aligned} \sum_\alpha (h_k / |G|) \chi^\alpha(C_k) \chi^\alpha(C'_k) \\ = 1, \quad \text{if } C_k \text{ is ambivalent} \\ = 0, \quad \text{if } C_k \text{ is not ambivalent.} \end{aligned} \tag{126}$$

Summing over all classes, one gets finally

$$\sum_\alpha M_s \{ \chi^\alpha(s) \}^2 = n_o, \tag{127}$$

where  $n_o$  is the total number of ambivalent classes. Comparing (123) and (127), one obtains  $n^\alpha = n_o$  and the theorem that *the total number of self-dual irreducible representations equals the number of ambivalent classes.* One can also express the theorem in the statement that the character table contains as many real rows as it has real columns.

Let us now study the dual representations in some greater detail. If  $\Gamma^\alpha$  is *self-dual*,  $\Lambda^\alpha$  and  $\Gamma^\alpha$  are related through a similarity transformation  $\mathbf{S}$ :

$$\Lambda = \mathbf{S}^{-1} \Gamma \mathbf{S}, \tag{128}$$

where, for the sake of simplicity, we have temporarily omitted the index  $\alpha$  of the irreducible representation under consideration. According to the definition (117), one has further

$$\Lambda = (\Gamma^{-1})^{\text{tr}} = (\Gamma^{\text{tr}})^{-1}. \tag{129}$$

Combining (128) and (129), one obtains

$$\begin{aligned} \Gamma = (\Lambda^{-1})^{\text{tr}} &= (\mathbf{S}^{-1} \Gamma^{-1} \mathbf{S})^{\text{tr}} = \mathbf{S}^{\text{tr}} (\Gamma^{-1})^{\text{tr}} (\mathbf{S}^{-1})^{\text{tr}} \\ &= \mathbf{S}^{\text{tr}} \Lambda (\mathbf{S}^{-1})^{\text{tr}} = \mathbf{S}^{\text{tr}} \mathbf{S}^{-1} \Gamma \mathbf{S} (\mathbf{S}^{-1})^{\text{tr}} \\ &= [\mathbf{S} (\mathbf{S}^{-1})^{\text{tr}}]^{-1} \Gamma [\mathbf{S} (\mathbf{S}^{-1})^{\text{tr}}], \end{aligned} \tag{130}$$

i.e.,

$$[\mathbf{S} (\mathbf{S}^{-1})^{\text{tr}}] \Gamma = \Gamma [\mathbf{S} (\mathbf{S}^{-1})^{\text{tr}}]. \tag{131}$$

Since  $[\mathbf{S} (\mathbf{S}^{-1})^{\text{tr}}]$  commutes with all the matrices  $\Gamma^\alpha(g)$  of the irreducible representation  $\alpha$ , Schur's lemma (69)

says that  $[\mathbf{S}(\mathbf{S}^{-1})^{\text{tr}}]$  must be a multiple of the unit matrix  $\mathbf{1}^\alpha$ :

$$\mathbf{S}(\mathbf{S}^{-1})^{\text{tr}} = c \cdot \mathbf{1}. \tag{132}$$

Taking the determinant of both sides, one obtains

$$c^f = |\mathbf{S}| \cdot |\mathbf{S}^{-1}| = 1, \tag{133}$$

which relation shows that the possible values of  $c$  are limited to be the unit roots of order  $f^\alpha$ . In the special case when  $\mathbf{\Lambda} = \mathbf{\Gamma}$ , one says that  $\mathbf{\Gamma}$  is self-dual in an identical sense, and one has then  $\mathbf{S} = \mathbf{1}$  and  $c = 1$ .

In order to proceed, we now consider *all* irreducible representations  $\mathbf{\Gamma}^\alpha$  irrespective of whether they are self-dual or not. Let  $\mathbf{\Gamma}^\alpha$  have the dual representation  $\mathbf{\Lambda}^\alpha$ , which is equivalent with the representation  $\mathbf{\Gamma}^{\alpha'}$ , so that one has

$$\mathbf{\Lambda}^\alpha = \mathbf{S}^{-1} \mathbf{\Gamma}^{\alpha'} \mathbf{S}. \tag{134}$$

We note that  $\mathbf{S}$  has the special property (132), only when  $\mathbf{\Gamma}^\alpha$  is self-dual, so that  $\alpha' = \alpha$ . According to the definition (117), one has  $\Lambda_{kl}^\alpha(s) = \Gamma_{lk}^\alpha(s^{-1})$ . Using the definitions and the convolution relation (87), one obtains the following transformation:

$$\begin{aligned} M_s \chi^\alpha(sgs) &= M_s \sum_k \Gamma_{kk}^\alpha(sgs) \\ &= M_s \sum_{kl} \Gamma_{kl}^\alpha(s) \Gamma_{lk}^\alpha(g) \\ &= \sum_{kl} M \Lambda_{lk}^\alpha(s^{-1}) \Gamma_{lk}^\alpha(g) \\ &= \sum_{kl} \Lambda_{lk}^\alpha * \Gamma_{lk}^\alpha \\ &= \sum_{kl} \{\mathbf{S}^{-1} \mathbf{\Gamma}^{\alpha'} \mathbf{S}\}_{lk} * \Gamma_{lk}^\alpha \\ &= \sum_{kl} \sum_{mn} (\mathbf{S}^{-1})_{lm} \Gamma_{mn}^{\alpha'} S_{nk} * \Gamma_{lk}^\alpha \\ &= \sum_{kl} \sum_{mn} (\mathbf{S}^{-1})_{lm} \Gamma_{mn}^{\alpha'} * \Gamma_{lk}^\alpha S_{nk} \\ &= \sum_{kl} \sum_{mn} (\mathbf{S}^{-1})_{lm} (f^\alpha)^{-1} \delta^{\alpha' \alpha} \delta_{km} \Gamma_{ln}^\alpha(g) S_{nk} \\ &= (f^\alpha)^{-1} \delta^{\alpha' \alpha} \sum_{lmn} \Gamma_{ln}^\alpha(g) S_{nm} (\mathbf{S}^{-1})^{\text{tr}}_{ml} \\ &= (f^\alpha)^{-1} \delta^{\alpha' \alpha} \text{Tr} \{ \mathbf{\Gamma}^\alpha(g) \mathbf{S} (\mathbf{S}^{-1})^{\text{tr}} \}. \end{aligned} \tag{135}$$

For  $\alpha' \neq \alpha$ , the right-hand member vanishes. For  $\alpha' = \alpha$ , one can use the relation (132), and this gives the final formula

$$M_s \chi^\alpha(sgs) = c (f^\alpha)^{-1} \delta^{\alpha' \alpha} \chi^\alpha(g), \tag{136}$$

where the coefficient  $c$  enters. Taking the complex conjugate of this relation and observing that it holds in the same form for  $g^{-1}$  instead of  $g$ , one gets further  $c^* = c$ , i.e., the constant  $c$  must necessarily be real. Since one has also  $c^f = 1$ , this implies that one can only have the value  $c = 1$  for odd orders  $f^\alpha$ , whereas one can

have  $c = \pm 1$ , if  $f^\alpha$  is even:

$$\begin{aligned} c^\alpha &= 1, & f^\alpha &= \text{odd}, \\ c^\alpha &= \pm 1, & f^\alpha &= \text{even}. \end{aligned} \tag{137}$$

The constant  $c^\alpha$  is through the relation (136) directly connected with the characters, and the question is what conclusions one may draw from its value. Putting  $\alpha' = \alpha$  and  $g = e$  into (136), one obtains particularly

$$c^\alpha = M \chi^\alpha(s^2), \tag{138}$$

i.e.,  $c^\alpha$  is the average value of the character  $\chi^\alpha$  over the "diagonal" of the multiplication table of the group.

Since the value of  $c^\alpha$  is independent of the choice of the form of the representation, it may be convenient to study the *unitary* representations in some greater detail. For such a representation, one has particularly

$$\mathbf{\Lambda} = (\mathbf{\Gamma}^{-1})^{\text{tr}} = \mathbf{\Gamma}^*, \tag{139}$$

i.e., the dual representation  $\mathbf{\Lambda}$  is identical with the *complex conjugate* representation  $\mathbf{\Gamma}^*$ . If the matrices  $\mathbf{\Gamma}$  are unitary, the same applies to the matrices  $\mathbf{\Lambda}$ , and we will now prove that the matrix  $\mathbf{S}$  in the transformation (128) is unitary except for a constant factor. From  $\mathbf{\Lambda} = \mathbf{S}^{-1} \mathbf{\Gamma} \mathbf{S}$  and  $\mathbf{\Gamma} = (\mathbf{S} \mathbf{\Lambda} \mathbf{S}^{-1})^{\text{tr}}$ , it follows that

$$\begin{aligned} \mathbf{\Gamma} &= (\mathbf{\Gamma}^{-1})^\dagger = (\mathbf{S} \mathbf{\Lambda}^{-1} \mathbf{S}^{-1})^\dagger = (\mathbf{S}^{-1})^\dagger \mathbf{\Lambda} \mathbf{S}^\dagger \\ &= (\mathbf{S}^\dagger)^{-1} \mathbf{S}^{-1} \mathbf{\Gamma} \mathbf{S} \mathbf{S}^\dagger = (\mathbf{S} \mathbf{S}^\dagger)^{-1} \mathbf{\Gamma} (\mathbf{S} \mathbf{S}^\dagger), \end{aligned} \tag{140}$$

and

$$(\mathbf{S} \mathbf{S}^\dagger) \mathbf{\Gamma} = \mathbf{\Gamma} (\mathbf{S} \mathbf{S}^\dagger), \tag{141}$$

i.e.,  $\mathbf{S} \mathbf{S}^\dagger$  commutes with all the matrices  $\mathbf{\Gamma}^\alpha(g)$  of the irreducible representation  $\alpha$ . According to Schur's lemma (69), one can then draw the conclusion that  $\mathbf{S} \mathbf{S}^\dagger$  must be a multiple of the unit matrix:

$$\mathbf{S} \mathbf{S}^\dagger = \lambda \cdot \mathbf{1}^\alpha. \tag{142}$$

Taking the  $(k, k)$  element of this relation, one obtains

$$\lambda = \sum_i |S_{ki}|^2,$$

which shows that  $\lambda$  is a positive constant. Introducing the new matrix  $\mathbf{U} = \lambda^{-1/2} \mathbf{S}$ , one has

$$\mathbf{\Lambda} = \mathbf{U}^{-1} \mathbf{\Gamma} \mathbf{U}, \quad \mathbf{U}^\dagger \mathbf{U} = \mathbf{1}, \tag{143}$$

i.e.,  $\mathbf{\Lambda}$  and  $\mathbf{\Gamma}$  are related through a unitary transformation  $\mathbf{U}$ . According to (132), one has further:

$$\mathbf{U} (\mathbf{U}^{-1})^{\text{tr}} = c \cdot \mathbf{1}, \tag{144}$$

or

$$\mathbf{U} \mathbf{U}^* = c \cdot \mathbf{1}, \tag{145}$$

where  $c = \pm 1$  is the characteristic constant to be investigated.

Let us now consider the special case when a *unitary transformation*  $\mathbf{\Gamma}$  has only real elements or is equivalent with such a real representation. One has

$$\mathbf{\Lambda} = \mathbf{\Gamma}^* = \mathbf{\Gamma}, \tag{146}$$

i.e., the representation is self-dual in the identical sense, and one has  $\mathbf{U}=\mathbf{1}$  and  $c=+1$ . One can now also prove the reverse theorem that, if  $c=+1$ , there exists at least one representation of  $\Gamma^\alpha$  which is completely real.

For this purpose, let us consider an arbitrary irreducible representation  $\Gamma^\alpha$  having  $c^\alpha=+1$ . Let us further introduce the similarity representation:

$$\bar{\Gamma}^\alpha = (\mathbf{U}^* - e^{i\phi} \cdot \mathbf{1}) \Gamma^\alpha (\mathbf{U}^* - e^{i\phi} \cdot \mathbf{1})^{-1}, \quad (147)$$

where the complex number  $e^{i\phi}$  is chosen so that it is not an eigenvalue of the matrix  $\mathbf{U}^*$ , which satisfies the relation  $\mathbf{U}\mathbf{U}^*=\mathbf{1}$ . One obtains directly

$$\begin{aligned} \bar{\Gamma}^* &= (\mathbf{U} - e^{-i\phi} \cdot \mathbf{1}) \Gamma^* (\mathbf{U} - e^{-i\phi} \cdot \mathbf{1})^{-1} \\ &= (\mathbf{U} - e^{-i\phi} \cdot \mathbf{1}) \Lambda (\mathbf{U} - e^{-i\phi} \cdot \mathbf{1})^{-1} \\ &= (\mathbf{U} - e^{-i\phi} \cdot \mathbf{1}) \mathbf{U}^{-1} \Gamma \mathbf{U} (\mathbf{U} - e^{-i\phi} \cdot \mathbf{1})^{-1} \\ &= e^{-i\phi} (e^{i\phi} \cdot \mathbf{1} - \mathbf{U}^{-1}) \Gamma (e^{i\phi} \cdot \mathbf{1} - \mathbf{U}^{-1})^{-1} e^{i\phi} \\ &= (\mathbf{U}^* - e^{i\phi} \cdot \mathbf{1}) \Gamma (\mathbf{U}^* - e^{i\phi} \cdot \mathbf{1})^{-1} = \bar{\Gamma}, \quad (148) \end{aligned}$$

which implies that the representation  $\bar{\Gamma}^\alpha$  is real. By means of the procedure outlined in Sec. I.C, it is then also possible to construct a real unitary representation of  $\Gamma^\alpha$ .

The case  $c=+1$  occurs always for self-dual irreducible representations of *odd order*  $f^\alpha$ , and such representations can hence always be written in real form. The case  $c=-1$  may occur only for *even orders*  $f^\alpha$ , and it is evident from the theorem given above that such representations can never be brought to real form by any similarity transformation. It may be shown by some simple examples that this case really occurs in the theory of finite groups.

In summary, we can say that, if a row in the character table contains any complex member, the irreducible representation is certainly *not self-dual*, and one has the theorem:

$$M\chi^\alpha(sgs) = 0. \quad (149)$$

If, on the other hand, a row in the character table contains only real numbers, the associated representation is certainly *self-dual*. For representations of *odd orders*, one has the additional theorem that they can always be brought to real form by a similarity transformation. One has further

$$M\chi^\alpha(sgs) = (f^\alpha)^{-1} \chi^\alpha(g), \quad f^\alpha = \text{odd}. \quad (150)$$

For representations of *even orders*, one should investigate the quantity

$$c^\alpha = M\chi^\alpha(s^2)$$

which has only the values  $c^\alpha = \pm 1$ . If  $c^\alpha = +1$ , the representation can always be brought to real form, whereas, for  $c^\alpha = -1$ , this is not the case. One has the additional theorem

$$M\chi^\alpha(sgs) = \pm (f^\alpha)^{-1} \chi^\alpha(g), \quad f^\alpha = \text{even}. \quad (151)$$

This exhausts the possibilities contained in the relation (136). A study of the dual representations gives hence some rather interesting additional information about the properties of the character table and the associated irreducible representations.

The derivations in this section about dual representations are essentially inspired by Sec. 5.8 in Chapter II of Laurens Jansen's monograph "Introduction to the Theory of Finite Groups with Applications to Quantum Chemistry and Solid-State Physics," but the treatments are by no means identical, and the reader may find many additional points of view by consulting Jansen's paper. (Preprint from the Battelle Memorial Institute, Geneva.)

## F. Splitting of the Group Algebra

### Basic Projection and Shift Operators

In Sec. I.C, we have shown that every reducible stable space may be decomposed into stable subspaces (Maschke's theorem), and we will now study the *decomposition of the entire space  $V_G$  associated with the group algebra into irreducible subspaces*. The spectral analysis of the regular representation in the previous section shows that there will be  $f^\alpha$  different subspaces which all lead to the same irreducible representation  $\Gamma^\alpha$ .

For this purpose, we recall that there is an isomorphism  $A \leftrightarrow \alpha$  between the group algebra  $V_G = \{A\}$  and the linear space  $\{\alpha\}$  formed by all functions  $\alpha$  over the group expressed in relation (10):

$$A = M\alpha(s) s^{-1}. \quad (152)$$

We note further, if  $A \leftrightarrow \alpha$  and  $B \leftrightarrow \beta$  are two elements of the group algebra, one has the product rule (15):

$$A \times B \leftrightarrow \gamma = \alpha * \beta. \quad (153)$$

Let us now consider the elements  $P_{km}^\alpha$  of the group algebra which correspond to the matrix elements  $\Gamma_{km}^\alpha$  of the irreducible representation  $\Gamma^\alpha$  considered as "functions over the group." It turns out to be convenient to introduce an extra factor  $f^\alpha$ , so we will use the definitions

$$\begin{aligned} P_{km}^\alpha &= f^\alpha \Gamma_{km}^\alpha, \\ P_{km}^\alpha &= f^\alpha M \Gamma_{km}^\alpha(s) s^{-1}. \quad (154) \end{aligned}$$

In Sec. I.D, we have shown that, as an immediate consequence of Schur's lemma, one obtains the convolution relation (87), which may now be written in the form

$$f^\alpha \Gamma_{km}^\alpha * f^\beta \Gamma_{nl}^\beta = \delta^{\alpha\beta} \delta_{kl} f^\beta \Gamma_{nm}^\beta. \quad (155)$$

According to (153) and (154), this implies that the elements  $P_{km}^\alpha$  have the following basic multiplication rule

$$P_{km}^\alpha \times P_{nl}^\beta = \delta^{\alpha\beta} \delta_{kl} P_{nm}^\beta. \quad (156)$$

This rule is also of main importance in the later appli-

cations to quantum mechanics. In the following, we will often omit the multiplication symbol  $\times$ .

In studying the consequences of (156), we will start with the "diagonal" elements  $P_{kk}^\alpha$ . Putting  $m=k$ ,  $n=l$  in (156) and modifying the right-hand member slightly, one obtains

$$P_{kk}^\alpha \times P_{ll}^\beta = \delta^{\alpha\beta} \delta_{kl} P_{ll}^\beta, \tag{157}$$

i.e.,  $\{P_{kk}^\alpha\}^2 = P_{kk}^\alpha$ , and  $P_{kk}^\alpha \times P_{ll}^\alpha = 0$  for  $k \neq l$ . The diagonal elements are hence idempotent and mutually exclusive, and they form a set of *projection operators* which are of fundamental importance in splitting the space  $V_G$  of the group algebra. They form further a "resolution of the identity":

$$e = \sum_\alpha \sum_k P_{kk}^\alpha, \tag{158}$$

where  $e$  is the neutral element in the group which serves as the "identity element" in the group algebra. The proof follows from the fact that the neutral element  $e$  in the group algebra corresponds to the identity function  $E$  defined by (101):

$$e \leftrightarrow E. \tag{159}$$

According to (105), one has further

$$E = \sum_\alpha f^\alpha \chi^\alpha = \sum_\alpha \sum_k f^\alpha \Gamma_{kk}^\alpha, \tag{160}$$

which corresponds to the relation (158) in the group algebra.

The space  $V_G$  of the group algebra is of order  $|G|$  and, according to (106), one has

$$|G| = \sum_\alpha (f^\alpha)^2. \tag{161}$$

It is remarkable that there is a total of

$$\sum_\alpha (f^\alpha)^2 = |G|$$

elements  $P_{km}^\alpha$  defined by (154), and the question is whether they are linearly independent and may be used to span the group algebra. For this purpose, it is convenient to study an element  $A$  which may be written as a linear superposition of the elements  $P_{km}^\alpha$ :

$$A = \sum_\alpha \sum_{km} P_{km}^\alpha a_{km}^\alpha, \tag{162}$$

where we will now determine the coefficients  $a_{km}^\alpha$ . Multiplying to the left by a specific element  $P_{km}^\alpha$ , and changing the dummy indices in the summation, one obtains

$$\begin{aligned} P_{km}^\alpha \times A &= P_{km}^\alpha \times \sum_\beta \sum_{ln} P_{ln}^\beta a_{ln}^\beta \\ &= \sum_\beta \sum_{ln} \delta^{\alpha\beta} \delta_{kn} P_{lm}^\beta a_{ln}^\beta \\ &= \sum_l P_{lm}^\alpha a_{lk}^\alpha \\ &= f^\alpha \sum_l M \Gamma_{lm}^\alpha(s) a_{lk}^\alpha s^{-1}. \end{aligned} \tag{163}$$

Putting the coefficients of the element  $e$  of both sides equal, one obtains

$$a_{mk}^\alpha = (f^\alpha)^{-1} \{P_{km}^\alpha \times A\}_e. \tag{164}$$

The result implies particularly that, if  $A=0$ , one has necessarily all  $a_{km}^\alpha=0$ , which proves that all the elements  $P_{km}^\alpha$  are linearly independent. Since their number equals the order  $|G|$  of the space, the elements  $P_{km}^\alpha$  may be used as a *basis* for the group algebra, and an *arbitrary element*  $A$  may now be expressed in the form (162). If the element  $A$  corresponds to the function  $\alpha$  through the mapping  $A \leftrightarrow \alpha$ , one obtains from (164) the following expression for the expansion coefficients

$$a_{km}^\alpha = \{\Gamma_{mk}^\alpha * \alpha\}_0. \tag{165}$$

The quantity  $A_{km}^\alpha = P_{km}^\alpha a_{km}^\alpha$  will be described as the "component" of the arbitrary element  $A$  along the base element  $P_{km}^\alpha$ , and we note that  $A_{km}^\alpha$  may also be found from the formula

$$A_{km}^\alpha = P_{mm}^\alpha A P_{kk}^\alpha, \tag{166}$$

where  $P_{kk}^\alpha$  is one of the fundamental projection operators.

In discussing the basic elements  $P_{km}^\alpha$ , it is often convenient to arrange them in terms of a series of matrices:

$$P^\alpha: \begin{pmatrix} P_{11}^\alpha & P_{12}^\alpha & P_{13}^\alpha & \cdots & P_{1f}^\alpha \\ P_{21}^\alpha & P_{22}^\alpha & P_{23}^\alpha & \cdots & P_{2f}^\alpha \\ P_{31}^\alpha & P_{32}^\alpha & P_{33}^\alpha & \cdots & P_{3f}^\alpha \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ P_{f1}^\alpha & P_{f2}^\alpha & P_{f3}^\alpha & \cdots & P_{ff}^\alpha \end{pmatrix} \tag{167}$$

of order  $f^\alpha \times f^\alpha$ , one for each irreducible representation  $\Gamma^\alpha$ . Let us now consider the subspace  $W_k^\alpha$  spanned by the elements  $\{P_{km}^\alpha\}$  in a specific row:

$$W_k^\alpha: \{P_{k1}^\alpha, P_{k2}^\alpha, P_{k3}^\alpha, \dots, P_{kf}^\alpha\}. \tag{168}$$

According to (166), this space is characterized by the projection operator  $P_{kk}^\alpha$  acting on the *right-hand side* of the elements of the group algebra. We will now see that the space  $W_k^\alpha$  is *stable* under the operations of the group  $G = \{g\}$ . By using the properties (5) of the invariant mean and the definitions, one obtains

$$\begin{aligned} g P_{km}^\alpha &= f^\alpha M \Gamma_{km}^\alpha(s) g s^{-1} \\ &= f^\alpha M \Gamma_{km}^\alpha(tg) t^{-1} \\ &= f^\alpha M \sum_t \Gamma_{kt}^\alpha(t) \Gamma_{tm}^\alpha(g) t^{-1} \\ &= \sum_t P_{kt}^\alpha \Gamma_{tm}^\alpha(g), \end{aligned} \tag{169}$$

which proves the statement. The representation associated with the stable subspace  $W_k^\alpha$  is further the irreducible representation  $\Gamma^\alpha$ . The subspaces  $W_k^\alpha$  associated with the rows of the matrices (167) give hence



the desired decomposition of the space  $V_G$  of the entire group algebra into stable irreducible subspaces:

$$V_G \doteq \sum_{\alpha} \sum_k W_k^{\alpha}. \quad (170)$$

We note that there are  $f^{\alpha}$  different irreducible subspaces  $W_k^{\alpha}$  for  $k=1, 2, 3, \dots, f^{\alpha}$  which are all associated with the same irreducible representation  $\Gamma^{\alpha}$ ; this result corresponds to the previously found frequency theorem (104).

According to (168) and (169), a *single row*  $\{\Gamma_{km}^{\alpha}\}$  of an irreducible representation  $\alpha$  determines the stable subspace  $W_k^{\alpha}$  and hence the entire representation  $\Gamma^{\alpha}$ . This means that a single row of an irreducible representation determines also all the other rows—at least implicitly. One can better understand this result, if one studies the consequences of the general convolution relation (87). For  $\alpha=\beta$  and  $k=1$ , one obtains

$$\Gamma_{nm}^{\alpha} = f^{\alpha} \Gamma_{km}^{\alpha} * \Gamma_{nk}^{\alpha}, \quad (171)$$

which relation gives an arbitrary matrix element explicitly expressed in terms of a single row  $k$  and a single column  $k$ . For a *unitary* representation, one has further  $\Gamma_{nk}^{\alpha}(s^{-1}) = \{\Gamma_{kn}^{\alpha}(s)\}^*$ , which means that the elements of the column  $k$  may also be derived from the elements in the row  $k$ , and relation (171) gives then the explicit formula desired. According to (88), the characters  $\chi^{\alpha}$  may further be found from the special relation

$$\begin{aligned} \chi^{\alpha}(g) &= f^{\alpha} M \Gamma_{kk}^{\alpha}(sgs^{-1}) \\ &= (f^{\alpha}/h_G) \sum_{t \in C_G} \Gamma_{kk}^{\alpha}(t), \end{aligned} \quad (172)$$

i.e., the characters may be found from the diagonal elements  $\Gamma_{kk}^{\alpha}$  in the row  $k$ . Relations of the type (171) and (172) may be of importance in connection with problems where it is essential to *store information* about the irreducible representations in smallest possible space, e.g., in group theoretical calculations by means of electronic computers.

According to the fundamental relation (156), one obtains directly

$$P_{mn}^{\alpha} * P_{km}^{\alpha} = P_{kn}^{\alpha}, \quad (173)$$

and the operator  $P_{mn}^{\alpha}$  may hence be characterized as a *shift operator*  $m \rightarrow n$  which takes one from the  $m$ th element in the  $k$ th row to the  $n$ th element in the same row. They are of fundamental importance in the quantum-mechanical applications.

In concluding this section, we will finally consider also the subspaces  $R_k^{\alpha}$  spanned by the elements in a column  $\{P_{mk}^{\alpha}\}$  of the matrix (167) for fixed  $k$ . Such a subspace is characterized by the projection operator  $P_{kk}^{\alpha}$  acting to the left of the group algebra, but we note that it is *not stable* under the operations of the group  $G = \{g\}$ , and that it is hence of smaller interest in connection with the decomposition of the group algebra. The subspaces  $R_k^{\alpha}$  are, however, of importance in the quantum-mechanical applications.

### Character Projection Operators

In the previous section, we have described the complete decomposition of the group algebra  $V_G$  into stable irreducible subspaces  $W_k^{\alpha}$  by means of the elements  $P_{km}^{\alpha}$  associated with the irreducible representations  $\Gamma^{\alpha}$ . We now investigate how far one can proceed with the decomposition, if one knows the characters  $\chi^{\alpha}$  alone and not the complete matrices. For this purpose, we introduce the operators:

$$Q^{\alpha} = \sum_k P_{kk}^{\alpha} = f^{\alpha} M \chi^{\alpha}(s) s^{-1}, \quad (174)$$

which means that  $Q^{\alpha}$  is the element of the group algebra associated with the function  $f^{\alpha} \chi^{\alpha}$ , so that  $Q^{\alpha} \leftrightarrow f^{\alpha} \chi^{\alpha}$ . From the relations (105) and (107) follows immediately

$$e = \sum_{\alpha} Q^{\alpha}, \quad (175)$$

$$Q^{\alpha} * Q^{\beta} = \delta^{\alpha\beta} Q^{\beta}, \quad (176)$$

it is the elements  $\{Q^{\alpha}\}$  form a set of projection operators which are idempotent, mutually exclusive, and form a resolution of the identity. Using the fact that the characters  $\chi^{\alpha}(s)$  are class functions and putting  $s = g^{-1}tg$ , one obtains

$$\begin{aligned} gQ^{\alpha} &= f^{\alpha} M \chi^{\alpha}(s) g s^{-1} \\ &= f^{\alpha} M \chi^{\alpha}(g^{-1}tg) t^{-1}g = Q^{\alpha} * g, \end{aligned} \quad (177)$$

which shows that  $Q^{\alpha}$  commutes with all elements  $g$  of the group, and that it hence belongs to the so-called *center* of the group algebra. For the space  $V^{\alpha}$  defined by  $Q^{\alpha}$ , one has particularly

$$\begin{aligned} V^{\alpha} &= Q^{\alpha} V_G Q^{\alpha} \\ &= Q^{\alpha} V_G = V_G Q^{\alpha}, \end{aligned} \quad (178)$$

and, according to (170) and (174), one obtains

$$V^{\alpha} \doteq \sum_k W_k^{\alpha}, \quad (179)$$

i.e., the space  $V^{\alpha}$  is the direct sum of all the  $f^{\alpha}$  irreducible subspaces  $W_k^{\alpha}$  associated with representation  $\Gamma^{\alpha}$ . This implies that the space  $V^{\alpha}$  is stable and reducible and of the order  $(f^{\alpha})^2$ , and this is also about as far as one can go in the decomposition of  $V_G$ , if one knows the characters only. In order to proceed further, one needs additional tools. As we shall see later, the character projection operators play anyway an important role in the quantum-mechanical applications.

### Class Operators

The conjugate class associated with the element  $g$  has previously been denoted by the symbol  $C_g$ , whereas  $C'_g$  denoted the class of the inverse elements. In this connection, it is further convenient to introduce the

class operator  $C(g)$  through the relation:

$$C(g) = M \underset{s}{s^{-1}gs} = h_g^{-1} \sum_{t \in C_g} t, \quad (180)$$

where  $h_g$  is the number of elements in  $C_g$ . Using the properties of the invariant mean, one obtains directly

$$\begin{aligned} hC(g) &= M \underset{s}{hs^{-1}gs} = M \underset{s}{(sh^{-1})^{-1}g(sh^{-1})h} \\ &= \{M \underset{t}{t^{-1}gt}\} h = C(g)h, \end{aligned} \quad (181)$$

i.e., the operators  $C(g)$  commute with all the elements of the group. This means that the operators  $C(g)$  all belong to the "center" of the group, which may be spanned by either the projection operators  $Q^\alpha$  associated with the irreducible representations or the class operators  $C(g)$ . The fact that the number of irreducible representations and the number of conjugate classes must both be the same as the order of the space associated with the "center" of the group algebra gives the deeper reason why the number of irreducible representations equals the number of classes, i.e., why the character table has the form of a square.

Let us now consider the class operators in some greater detail. According to (174), one has

$$\begin{aligned} Q^\alpha &= f^\alpha M \underset{s}{\chi^\alpha(s^{-1})s} \\ &= (f^\alpha / |G|) \sum_k h_k \chi^\alpha(C'_k) C(k), \end{aligned} \quad (182)$$

where the index  $k$  goes over the conjugate classes. This relation gives the explicit expression for the coefficients of the expansion of  $Q^\alpha$  in terms of the class operators. Using (124), one obtains further

$$\begin{aligned} \sum_\alpha (f^\alpha)^{-1} Q^\alpha \chi^\alpha(C_i) \\ &= \sum_k \sum_\alpha (h_k / |G|) \chi^\alpha(C'_k) \chi^\alpha(C_i) C(k) \\ &= \sum_k \delta_{ki} C(k) = C(i), \end{aligned} \quad (183)$$

which gives the inverse relation

$$C(k) = \sum_\alpha (f^\alpha)^{-1} \chi^\alpha(C_k) Q^\alpha. \quad (184)$$

Of particular interest is the product

$$\begin{aligned} C(k)Q^\alpha &= \sum_\beta (f^\beta)^{-1} \chi^\beta(C_k) Q^\alpha Q^\beta \\ &= \sum_\beta (f^\beta)^{-1} \chi^\beta(C_k) \delta^{\alpha\beta} Q^\beta \\ &= (f^\alpha)^{-1} \chi^\alpha(C_k) Q^\alpha, \end{aligned} \quad (185)$$

or

$$C(k)Q^\alpha = (f^\alpha)^{-1} \chi^\alpha(C_k) Q^\alpha, \quad (186)$$

which relation shows that the elements  $Q^\alpha$  are the *eigenelements* of the class operators  $C(k)$  and that the associated eigenvalues are  $(f^\alpha)^{-1} \chi^\alpha(C_k)$ . This implies

that the class operator  $C(g)$  satisfies the characteristic equation

$$\prod_\alpha \{C(g) - (f^\alpha)^{-1} \chi^\alpha(g)\} = 0, \quad (187)$$

for a fixed element  $g$ .

Formula (176) gives the multiplication table for the projection operators  $Q^\alpha$ , and we will now derive also the multiplication table for the class operators. According to (184), (176), and (182), one obtains

$$\begin{aligned} C(k)C(l) &= \sum_{\alpha\beta} (f^\alpha f^\beta)^{-1} \chi^\alpha(C_k) \chi^\beta(C_l) Q^\alpha Q^\beta \\ &= \sum_\alpha (f^\alpha)^{-2} \chi^\alpha(C_k) \chi^\alpha(C_l) Q^\alpha \\ &= \sum_\alpha \sum_m (f^\alpha)^{-1} (h_m / |G|) \chi^\alpha(C_k) \chi^\alpha(C_l) \chi^\alpha(C'_m) C(m) \\ &= \sum_m \left\{ \sum_\alpha (f^\alpha)^{-1} (h_m / |G|) \chi^\alpha(C_k) \chi^\alpha(C_l) \chi^\alpha(C'_m) \right\} C(m), \end{aligned} \quad (188)$$

which gives the result

$$\begin{aligned} C(k)C(l) &= \sum_m a(k, l, m) C(m), \\ a(k, l, m) &= (h_m / |G|) \sum_\alpha (f^\alpha)^{-1} \chi^\alpha(C_k) \chi^\alpha(C_l) \chi^\alpha(C'_m). \end{aligned} \quad (189)$$

This is the multiplication table for the class operators with the coefficients  $a(k, l, m)$  expressed in terms of the characters.

We note that both the class operators  $C(k)$  and the projection operators  $Q^\alpha$  are utilized in describing the *center* of the group algebra, i.e., the set of all elements of  $V_G$  which commute with all elements  $g$  of the group, and that the two descriptions are unified in the eigenvalue relation (186).

## II. APPLICATIONS TO QUANTUM MECHANICS

### A. Approximate Solution of the Schrödinger Equation; Groups as Constants of Motion

#### *Basic Principles of Quantum Mechanics*

The fundamental problem in quantum mechanics is the solution of the Schrödinger equation

$$H\Psi = -(\hbar/2\pi i) (\partial\Psi/\partial t), \quad (190)$$

where  $H$  is the Hamiltonian of the physical system under consideration and  $\Psi = \Psi(X)$  is its wave function in the configuration space associated with the composed coordinate  $X = (x_1, x_2, x_3, \dots, x_N)$ . The quantity  $N$  is the number of particles, and  $x_k = (r_k, \zeta_k)$  is the combined space-spin coordinate for particle  $k$ . The solution of (190) is often expressed in the form

$$\Psi = U\Psi_0, \quad (191)$$

where  $U = U(t, t_0)$  is the *evolution operator* which takes

the system from its initial state characterized by the wavefunction  $\Psi_0$  at  $t=t_0$  to its final state at time  $t$ . If the Hamiltonian does not contain the time  $t$ , the evolution operator has the simple form

$$U = \exp \{ -(2\pi i/\hbar) H_{\text{op}}(t-t_0) \}. \quad (192)$$

Most physical interpretations of quantum mechanics are built on the concept of "expectation values." A physical quantity is represented by the linear operator  $F$ , and the *expectation value* of  $F$  in the physical situation characterized by the wave function  $\Psi$  is defined by the expression:

$$\bar{F} = \langle \Psi | F\Psi \rangle / \langle \Psi | \Psi \rangle \equiv \langle F_{\text{op}} \rangle_{\Psi}, \quad (193)$$

where  $\langle \Psi_1 | \Psi_2 \rangle$  is the *scalar product* of the two wave functions  $\Psi_1$  and  $\Psi_2$ .

The fundamental *superposition principle* in quantum mechanics says that, if  $\Psi_1$  and  $\Psi_2$  are wave functions representing physical states, one can also give physical significance to the wave functions  $(\Psi_1 + \Psi_2)$  and  $c\Psi_1$ , where  $c$  is an arbitrary complex constant. The set  $\{\Psi\}$  of all wave functions forms hence a linear space, and a study of (190) and (191) shows that the evolution operator  $U$  is a *linear operator* defined on this space.

A "scalar product"  $\langle \Psi_1 | \Psi_2 \rangle$  is a complex number associated with two elements of a linear space which fulfills the following four axioms:

- (1)  $\langle \Psi_1 | \Psi_2 + \Psi_3 \rangle = \langle \Psi_1 | \Psi_2 \rangle + \langle \Psi_1 | \Psi_3 \rangle$ ,
  - (2)  $\langle \Psi_1 | c\Psi_2 \rangle = c\langle \Psi_1 | \Psi_2 \rangle$ ,
  - (3)  $\langle \Psi_1 | \Psi_2 \rangle = \langle \Psi_2 | \Psi_1 \rangle^*$ ,
  - (4)  $\langle \Psi | \Psi \rangle \geq 0$ , and  $\langle \Psi | \Psi \rangle = 0$ , only if  $\Psi = 0$ .
- (194)

In "abstract quantum theory," these four axioms take about the same place as the group axioms in the theory of "abstract groups." We note that the fourth axiom is of particular structural importance and that it immediately leads to the Schwarz inequality, the triangular inequality, and, the famous *uncertainty relations* characteristic for quantum mechanics. In treating infinite spaces, one adds two more axioms about convergence properties and denseness, and the space  $\{\Psi\}$  has then the character of an *abstract Hilbert space*.

The Hermitian adjoint  $F^\dagger$  of an arbitrary linear operator  $F$  is defined through the relation

$$\langle \Psi_1 | F^\dagger \Psi_2 \rangle = \langle \Psi_2 | F\Psi_1 \rangle^* = \langle F\Psi_1 | \Psi_2 \rangle, \quad (195)$$

which is often referred to as the "turn-over-rule," one has  $(F+G)^\dagger = F^\dagger + G^\dagger$  and  $(FG)^\dagger = G^\dagger F^\dagger$ . An operator which satisfies the relation  $F^\dagger = F$  is said to be *self-adjoint* or Hermitian, but we note that, in the theory of the infinite Hilbert space, this concept is much more complicated than is indicated here depending on the fact that the domain of the operator has to be properly included in the discussion of the operator properties.

It is generally assumed in quantum mechanics that the Hamiltonian  $H$  is self-adjoint, so that  $H^\dagger = H$ . Using (193), (190), and (195), one obtains for the time derivative of an expectation value:

$$d\bar{F}/dt = (2\pi i/\hbar) \langle HF - FH \rangle_{\Psi} + (\partial F/\partial t)_{\Psi}, \quad (196)$$

which is Heisenberg's equation of motion. Time-independent operators  $\Lambda$  which commute with the Hamiltonian, so that

$$H\Lambda = \Lambda H, \quad (196')$$

have expectation values  $\bar{\Lambda}$  which remain constant in time, and such operators are referred to as *constants of motion*.

If the Hamiltonian  $H$  does not contain the time  $t$ , one may separate the variables  $X$  and  $t$  in (190), and one is led to study the time-independent Schrödinger equation

$$H\Psi_k = E_k\Psi_k, \quad (197)$$

subject to the proper boundary conditions for discrete and continuous states. For self-adjoint Hamiltonians, the set of the eigenfunctions  $\{\Psi_k\}$  is orthonormal and under rather general assumptions complete, and this set may hence be used as a basis for the Hilbert space. Letting the evolution operator (192) work on both sides of the resolution of the identity  $\sum_k |\Psi_k\rangle\langle\Psi_k| = 1$ , one obtains

$$U = \sum_k \exp [-(2\pi i/\hbar) E_k(t-t_0)] |\Psi_k\rangle\langle\Psi_k|, \quad (198)$$

which is the "spectral resolution" of this operator. Substitution of this expression into (191) gives finally

$$\Psi(X, t) = \sum_k \exp [-(2\pi i/\hbar) E_k(t-t_0)] \Psi_k(X) \langle\Psi_k | \Psi_0\rangle, \quad (199)$$

which is the well-known "expansion in stationary states." We note that the relations (198) and (199) should be interpreted symbolically, that one should sum over the discrete eigenvalues  $E_k$  and integrate over the continuous part of the spectrum, and that the series expansions imply only "convergence in the mean"—which is the only type of convergence of importance in quantum mechanics.

#### Variation Principle and Secular Equation

From the relation (197), it follows that  $\langle\Psi_k | H\Psi_k\rangle = E_k\langle\Psi_k | \Psi_k\rangle$ , i.e.,

$$E_k = \langle\Psi_k | H\Psi_k\rangle / \langle\Psi_k | \Psi_k\rangle, \quad (200)$$

which relation implies that the eigenvalue  $E_k$  is the expectation value of  $H$  with respect to the physical state characterized by the eigenfunction  $\Psi_k$ . Let us now consider the integral

$$I = \langle\Phi | H\Phi\rangle / \langle\Phi | \Phi\rangle \equiv \langle H_{\text{op}} \rangle_{\Phi}, \quad (201)$$

for arbitrary trial wave functions  $\Phi$ . Putting  $\Phi = \Psi_k + \delta\Phi$ , using the relation  $(H - E_k)\Psi_k = 0$  and the turn-over rule

(196) for the self-adjoint operator  $(H-E)$ , one obtains

$$I - E_k = \langle \Phi | H - E_k | \Phi \rangle / \langle \Phi | \Phi \rangle$$

$$= \langle \delta\Phi | H - E_k | \delta\Phi \rangle / \langle \Phi | \Phi \rangle \quad (202)$$

where the right-hand member is quadratic in  $\delta\Phi$  and hence of the second order in the variation. Since the first-order variation is missing, one has  $\delta I = 0$  or

$$\delta \langle H_{op} \rangle_{av} = 0, \quad (203)$$

which relation is referred to as the *variation principle*. An important consequence is also that the integral  $I$  forms an upper bound for the ground state energy:

$$I \geq E_0. \quad (204)$$

The variation principle is of particular importance in determining approximate solutions to the Schrödinger equation (197). Let us assume that one has a *basic set*  $\{\Phi_k\}$  of finite order  $M$  characterized by the metric matrix  $\mathbf{\Delta} = \{\Delta_{kl}\}$  having the elements

$$\Delta_{kl} = \langle \Phi_k | \Phi_l \rangle, \quad (205)$$

and that one has the problem of determining the coefficients  $c_k$  in the expansion

$$\Phi = \sum_k \Phi_k c_k, \quad (206)$$

so that  $\Phi$  becomes an approximate eigenfunction which is as accurate as possible. Introducing the energy matrix  $\mathbf{H} = \{H_{kl}\}$  having the elements

$$H_{kl} = \langle \Phi_k | H \Phi_l \rangle \equiv \langle \Phi_k | H | \Phi_l \rangle, \quad (207)$$

one obtains for the expectation value (201):

$$I = \langle \Phi | H \Phi \rangle / \langle \Phi | \Phi \rangle$$

$$= (\sum_{kl} c_k^* \langle \Phi_k | H \Phi_l \rangle c_l) / (\sum_{kl} c_k^* \langle \Phi_k | \Phi_l \rangle c_l)$$

$$= \sum_{kl} c_k^* H_{kl} c_l / \sum_{kl} c_k^* \Delta_{kl} c_l$$

$$= \mathbf{c}^\dagger \mathbf{H} \mathbf{c} / \mathbf{c}^\dagger \mathbf{\Delta} \mathbf{c}, \quad (208)$$

where  $\mathbf{c}$  is the row vector  $\mathbf{c} = \{c_k\}$ , and  $\mathbf{c}^\dagger$  is the column vector  $\mathbf{c}^\dagger = \{c_k^*\}$ . Varying the coefficient  $\mathbf{c}$  and putting  $\delta I = 0$ , one obtains

$$(\mathbf{H} - I \cdot \mathbf{\Delta}) \mathbf{c} = \mathbf{0}, \quad (209)$$

which is a system of linear equations of order  $M$ . If all the functions  $\Phi_k$  are really linearly dependent, this system has a nontrivial solution, if and only if the determinant of the coefficients is vanishing, i.e.,

$$|\mathbf{H} - I \cdot \mathbf{\Delta}| = 0. \quad (210)$$

This so-called *secular equation* has  $M$  solutions for the parameter  $I$ , say  $I = \varepsilon_1, \varepsilon_2, \varepsilon_3, \dots, \varepsilon_M$ . These are approximate eigenvalues and, according to the separation theorem, one has

$$\varepsilon_k \geq E_k, \quad (211)$$

i.e., the solutions to the secular equation form in order upper bounds to the true eigenvalues.

If the basis  $\Phi = \{\Phi_k\}$  is *orthonormal*, i.e.,

$$\mathbf{\Delta} = \langle \Phi | \Phi \rangle = \mathbf{1},$$

one has no problem with the linear independence of the basis. However, in many quantum-mechanical applications, the basis  $\Phi$  occurs naturally in a non-orthogonal form, and one should then study the properties of the metric matrix  $\mathbf{\Delta}$  in greater detail. This matrix is *positive definite*, i.e.,

$$\mathbf{\Delta} > 0, \quad (212)$$

which follows from the fact that, for any set  $\mathbf{a} = \{a_k\}$  of complex numbers, one has

$$\mathbf{a}^\dagger \mathbf{\Delta} \mathbf{a} = \sum_{kl} a_k^* \Delta_{kl} a_l = \sum_{kl} a_k^* \langle \Phi_k | \Phi_l \rangle a_l$$

$$= \langle \sum_k \Phi_k a_k | \sum_l \Phi_l a_l \rangle > 0. \quad (213)$$

We note that the relation  $\mathbf{a}^\dagger \mathbf{\Delta} \mathbf{a} = 0$ , according to the fourth axiom in (194), necessarily implies  $\sum_k \Phi_k a_k = 0$ , i.e., that the functions  $\{\Phi_k\}$  are linearly dependent. The smallest value of the quantity  $\mathbf{a}^\dagger \mathbf{\Delta} \mathbf{a}$ , subject to the condition  $\mathbf{a}^\dagger \mathbf{a} = 1$ , is called the *measure of linear independence* of the set  $\Phi = \{\Phi_k\}$ . Observing that the metric matrix  $\mathbf{\Delta}$  is self-adjoint, i.e.,  $\mathbf{\Delta}^\dagger = \mathbf{\Delta}$ , one can now by means of the variation principle identify the measure of linear independence with the smallest eigenvalue  $\mu_1$  of  $\mathbf{\Delta}$ .

This result shows that it may be of importance to study the eigenvalues  $\mu_1, \mu_2, \dots, \mu_M$  of  $\mathbf{\Delta}$ , which we assume will be arranged in increasing order. Let  $\mathbf{U}$  be the unitary matrix which brings  $\mathbf{\Delta}$  to diagonal form  $\mathbf{y}$ :

$$\mathbf{U}^\dagger \mathbf{\Delta} \mathbf{U} = \mathbf{y} = \begin{pmatrix} \mu_1 & & & & \\ & \mu_2 & & & \\ & & \cdot & & \\ & & & \cdot & \\ & & & & \mu_M \end{pmatrix}. \quad (214)$$

In order to construct an orthonormal set from the basis  $\Phi$ , one may use the classical procedure by Schmidt in which the functions are introduced *successively* in order  $\Phi_1, \Phi_2, \Phi_3, \dots, \Phi_M$ . The author has suggested two more orthogonalization procedures: the *symmetric orthonormalization* (1948) based on the linear transformation

$$\phi = \Phi \mathbf{\Delta}^{-1/2}, \quad (215)$$

which gives

$$\langle \phi | \phi \rangle = \mathbf{\Delta}^{-1/2} \langle \Phi | \Phi \rangle \mathbf{\Delta}^{-1/2} = \mathbf{\Delta}^{-1/2} \mathbf{\Delta} \mathbf{\Delta}^{-1/2} = \mathbf{1},$$

and the *canonical orthonormalization* (1956) based on the transformation

$$\phi' = \Phi \mathbf{U} \mathbf{y}^{-1/2}, \quad (216)$$

which gives

$$\begin{aligned} \langle \phi' | \phi' \rangle &= \mathbf{u}^{-1/2} \mathbf{U}^\dagger \langle \Phi | \Phi \rangle \mathbf{U} \mathbf{u}^{-1/2} \\ &= \mathbf{u}^{-1/2} \mathbf{U}^\dagger \mathbf{\Delta} \mathbf{U} \mathbf{u}^{-1/2} = \mathbf{u}^{-1/2} \mathbf{u} \mathbf{u}^{-1/2} = 1. \end{aligned}$$

One may write this relation in the form

$$\phi'_k = (\mu_k)^{-1/2} \sum_l \Phi_l U_{lk}, \quad (217)$$

and, for the square of the coefficients of the elements  $\Phi_l$ , one obtains

$$\sum_l |U_{lk} / (\mu_k)^{1/2}|^2 = \mu_k^{-1}. \quad (218)$$

This implies that, if the eigenvalues  $\mu_1, \mu_2, \dots$ , are small, the sum of the absolute square of the coefficients become correspondingly large.

If the system  $\Phi$  has *approximate linear dependencies*, i.e., if the smallest eigenvalues  $\mu_1, \mu_2, \dots$ , are negligibly small in the accuracy used in the study, which is often the case with the systems conventionally used in the quantum-mechanical applications, one cannot simply remove the difficulty by an arbitrary orthonormalization, since the coefficients are going to “blow up,” and one is going to lose significant figures. On the other hand, if one has approximate linear dependencies in the basis, the secular equation (210) will be *almost identically vanishing* for all values of the parameter  $I$ , and it will become very difficult to determine the actual eigenvalues  $\varepsilon$  with any degree of accuracy.

In the case of approximate linear dependencies, it is hence necessary to reduce the order of the space  $\Phi = \{\Phi_k\}$ , and this can be performed in an *optimum* way by using the canonical orthonormalization (217) in which the resulting functions  $\phi'_k$  are arranged after the measures of linear independence  $\mu_k$ . If the value of  $\mu_1$  is too small for the accuracy required, we will remove the function  $\phi'_1$  and consider the next eigenvalue  $\mu_2$ , etc. In this way, one can systematically diminish the order of the space, until one obtains a meaningful secular equation (210).

There is another way of *testing the linear independence* of a set  $\Phi$ , which will now be mentioned for the sake of some later applications. Since the determinant of a matrix is invariant under similarity transformations, one has

$$|\Delta_{kl}| = \prod_{k=1}^M \mu_k \geq 0, \quad (219)$$

where the equality sign holds, if and only if the set  $\Phi$  is linearly dependent. For  $M=2$ , relation (219) reduces to Schwarz's inequality

$$\begin{vmatrix} \langle \Phi_1 | \Phi_1 \rangle & \langle \Phi_1 | \Phi_2 \rangle \\ \langle \Phi_2 | \Phi_1 \rangle & \langle \Phi_2 | \Phi_2 \rangle \end{vmatrix} \geq 0, \quad (220)$$

and for  $M=3, 4, 5, \dots$ , etc., one obtains interesting generalizations of this theorem. We note that all the

principal minors of the metric matrix  $\mathbf{\Delta}$  will necessarily be nonnegative, and that such a determinant will vanish only if there is a linear dependence between the basic elements involved. One can now use this theorem to construct a procedure for determining the order  $n$  of the space spanned by the elements

$$\Phi = \{\Phi_1, \Phi_2, \dots, \Phi_M\},$$

where  $n \leq M$ .

For this purpose, it is convenient to introduce a set of successive quantities  $D_1, D_2, D_3, \dots, D_M$ , defined through the relations:

$$\begin{aligned} D_1 &= \sum_k \langle \Phi_k | \Phi_k \rangle; \\ D_2 &= \sum_{k < l} \begin{vmatrix} \langle \Phi_k | \Phi_k \rangle & \langle \Phi_k | \Phi_l \rangle \\ \langle \Phi_l | \Phi_k \rangle & \langle \Phi_l | \Phi_l \rangle \end{vmatrix}; \\ D_3 &= \sum_{k < l < m} \begin{vmatrix} \langle \Phi_k | \Phi_k \rangle & \langle \Phi_k | \Phi_l \rangle & \langle \Phi_k | \Phi_m \rangle \\ \langle \Phi_l | \Phi_k \rangle & \langle \Phi_l | \Phi_l \rangle & \langle \Phi_l | \Phi_m \rangle \\ \langle \Phi_m | \Phi_k \rangle & \langle \Phi_m | \Phi_l \rangle & \langle \Phi_m | \Phi_m \rangle \end{vmatrix}; \\ &\dots\dots\dots \\ D_M &= \begin{vmatrix} \langle \Phi_1 | \Phi_1 \rangle & \langle \Phi_1 | \Phi_2 \rangle & \dots & \langle \Phi_1 | \Phi_M \rangle \\ \langle \Phi_2 | \Phi_1 \rangle & \langle \Phi_2 | \Phi_2 \rangle & \dots & \langle \Phi_2 | \Phi_M \rangle \\ \dots & \dots & \dots & \dots \\ \langle \Phi_M | \Phi_1 \rangle & \langle \Phi_M | \Phi_2 \rangle & \dots & \langle \Phi_M | \Phi_M \rangle \end{vmatrix}. \quad (221) \end{aligned}$$

We note that  $D_k$  is simply the sum of all different Graam's determinants of type (219) which may be obtained by selecting  $k$  elements out of the set  $\{\Phi_1, \Phi_2, \dots, \Phi_M\}$ . One has the inequality  $D_k \geq 0$ , and the equality sign holds if and only if every selection of  $k$  elements is linearly dependent, i.e.,  $k > n$ . This implies that, *in the sequence  $D_1, D_2, D_3, \dots, D_M$ , the order of the space is given by the index of the last non-vanishing quantity  $D$ , i.e.,*

$$D_n \neq 0, \quad D_{n+1} = D_{n+2} = \dots = 0. \quad (222)$$

Even in this procedure, one may notice the existence of approximate linear dependencies, since the quantities  $D_k$  may turn out to be exceedingly small from a certain value of the index  $k$ , even if they are not exactly vanishing.

In conclusion, we observe that the order  $n$  of the space spanned by a set of elements  $\{\Phi_1, \Phi_2, \dots, \Phi_M\}$  equals the number of non-vanishing eigenvalues  $\mu_k$  of the metric matrix  $\mathbf{\Delta}$  or the number of non-vanishing quantities in the set  $\{D_1, D_2, \dots, D_M\}$ .

#### Groups as Constants of Motion

For many of the applications to quantum mechanics, it is not necessary to specify any particular *realization* of the scalar product  $\langle \Psi_1 | \Psi_2 \rangle$ , as long as this quantity satisfies the four basic axioms (194). In conventional

theory, one is often using the particular definition:

$$\langle \Psi_1 | \Psi_2 \rangle = \int \Psi_1^*(X) \Psi_2(X) (dX), \quad (223)$$

where the integral goes over the entire configuration space with the coordinate  $X = (x_1, x_2, x_3, \dots, x_N)$ , but it will not be necessary for us to confine ourselves to this special realization.

Let  $g$  be a linear operator which acts on the composed coordinate  $X = (x_1, x_2, \dots, x_N)$  in a specific way, so that  $X' = (x'_1, x'_2, \dots, x'_N) = gX$ . Such an operator will be called a *symmetry operator*, if it leaves the volume element invariant

$$(dX') = (dX), \quad (224)$$

i.e., if the Jacobian of  $X'$  with respect to  $X$  equals unity. As examples of symmetry operations, we will here only mention reflections in a point or in a plane, rotations a certain angle around an axis, permutations of the particle coordinates, etc.

Let us now further define the action of  $g$  on an arbitrary wave function  $\Phi = \Phi(X)$  by means of the relation

$$g\Phi(X) = \Phi(g^{-1}X). \quad (225)$$

This definition is almost universally used, since it is in accordance with the definition of an operator product; one has

$$\begin{aligned} gh\Phi(X) &= g\{h\Phi(X)\} = g\Phi(h^{-1}X) \\ &= g\Phi\{h^{-1}(X)\} = \Phi\{h^{-1}(g^{-1}X)\} \\ &= \Phi\{h^{-1}g^{-1}X\} = \Phi\{(gh)^{-1}X\}. \end{aligned} \quad (226)$$

Putting  $X'' = g^{-1}X$ , one obtains for the scalar product of two such functions

$$\begin{aligned} \langle g\Phi_1 | g\Phi_2 \rangle &= \int \Phi_1^*(g^{-1}X) \Phi_2(g^{-1}X) (dX) \\ &= \int \Phi_1^*(X'') \Phi_2(X'') (dX'') = \langle \Phi_1 | \Phi_2 \rangle, \end{aligned} \quad (227)$$

i.e.,

$$\langle \Phi_1 | g^\dagger g - 1 | \Phi_2 \rangle = 0, \quad (228)$$

for all functions  $\Phi_1$  and  $\Phi_2$ . This is possible, only if  $g^\dagger g = 1$ , which means that the symmetry operators are *unitary* with respect to the scalar product (223):

$$g^\dagger g = gg^\dagger = 1. \quad (229)$$

In the following, we will say that an operator  $g$  is a symmetry operator if it fulfills relation (229), irrespective of the particular realization of the scalar product.

Let us now assume that there exists a set of symmetry operators which form a group  $G = \{g\}$  and that, for every function  $\Phi = \Phi(X)$ , one has  $gH\Phi = Hg\Phi$  according to the definition (225). In such a case, one has

$$gH = Hg, \quad (230)$$

and one says that the group  $G$  consists of a set of *constants of motion*.

The constants of motion are used in quantum theory

to classify the stationary states, and in Ref. 1, the author has shown how one may carry out a *component analysis* of an arbitrary trial function with respect to a single constant of motion  $\Lambda$  or with respect to a set of such constants  $(\Lambda_1, \Lambda_2, \Lambda_3, \dots)$  which commute between themselves. The component analysis is based on a resolution of the identity into a sum of projection operators  $O_k$  which are idempotent and mutually exclusive, so that

$$O_k^2 = O_k, \quad O_k O_l = 0 (k \neq l), \quad 1 = \sum_k O_k, \quad (231)$$

and it is shown that this analysis always leads to a lowering of the expectation value of the energy.

If the group  $G = \{g\}$  is Abelian, one may directly apply this technique. In a more general case, however, the procedure has to be modified to take into account the fact that the elements  $g$  of the group usually do not commute. In this connection, the importance of the *group algebra* introduced in Sec. I.B becomes suddenly clear in a new way, since we are now going to use the definition:

$$\left(\sum_k a_k g_k\right)\Phi(X) = \sum_k a_k \Phi(g_k^{-1}X), \quad (232)$$

which implies that the commutative operation of "addition" in the group algebra is going to correspond to the "addition" of wave functions according to the superposition principle.

If the group  $G = \{g\}$  is non-Abelian, one cannot use the group elements in general to classify the stationary states. However, the class operators  $C(g)$  defined by (189) commute with all the elements of the group and hence also mutually:

$$C(g)C(h) = C(h)C(g). \quad (233)$$

According to (229), one has  $g^\dagger = g^{-1}$ , and this implies that the class operators are self-adjoint only for the ambivalent classes. Using (181), one could now construct the product-projection operators as defined in Ref. 1, but we note that these eigenoperators are also defined in (186). In analogy with (231), one has

$$Q^\alpha Q^\beta = \delta^{\alpha\beta} Q^\beta, \quad e = \sum_\alpha Q^\alpha, \quad (234)$$

and we note that the operators  $Q^\alpha$  are self-adjoint:

$$(Q^\alpha)^\dagger = Q^\alpha. \quad (235)$$

Let us now derive the Hermitian adjoint to an arbitrary operator  $P_{km}^\alpha$  defined by (154). For a complex number  $c$ , one has simply  $c^\dagger = c^*$ . Using the definitions and the fact that  $s^\dagger = s^{-1}$ , one obtains

$$\begin{aligned} (P_{km}^\alpha)^\dagger &= (f^\alpha)^{-1} M \left\{ \Gamma_{km}^\alpha(s) \right\}^* (s^{-1})^\dagger \\ &= (f^\alpha)^{-1} M \Gamma_{mk}^\alpha(s^{-1}) s = P_{mk}^\alpha, \end{aligned} \quad (236)$$

i.e.,

$$(P_{km}^\alpha)^\dagger = P_{mk}^\alpha. \quad (237)$$

This implies that the diagonal operators  $P_{kk}^\alpha$  are self-

adjoint. Since they further satisfy the relations

$$P_{kk}^\alpha P_{ll}^\beta = \delta^{\alpha\beta} \delta_{kl} P_{ll}^\beta, \quad e = \sum_\alpha \sum_k P_{kk}^\alpha, \quad (238)$$

analogous to (231), one could expect that the set  $\{P_{kk}^\alpha\}$  could be used for a *component analysis* of a still more deep-going nature than the one based on the set  $\{Q^\alpha\}$ . We will now show that, for the non-Abelian groups, a new feature exists depending on the existence of the *shift operators*, and that this leads to a discussion of the important phenomenon of *degeneracy* of the energy levels.

#### *Splitting of the Secular Equation by Means of Group Algebra*

Let us now study the classification of the eigenstates of the Hamiltonian  $H$  under the assumption that  $G = \{g\} = \{g_1, g_2, g_3, \dots, g_n\}$  is a group of constants of motion satisfying (230).

Let us further assume that a *single* trial wavefunction  $\Phi = \Phi(X)$  is given and should be subject to "component analysis." For this purpose, we introduce the associated functions

$$\Phi_k = g_k \Phi, \quad (239)$$

which are formed from  $\Phi$  by means of the symmetry operations  $g_k$ . We will now consider the space  $V_\Phi$  spanned by the set  $\{\Phi_1, \Phi_2, \dots, \Phi_n\}$ , where  $n = |G|$ . The metric matrix has the elements

$$\begin{aligned} \Delta_{kl} &= \langle \Phi_k | \Phi_l \rangle = \langle g_k \Phi | g_l \Phi \rangle \\ &= \langle \Phi | g_k^{-1} g_l \Phi \rangle \\ &= \Delta(g_k^{-1} g_l), \end{aligned} \quad (240)$$

where we have introduced the notation  $\Delta(g) = \langle \Phi | g \Phi \rangle$ , which defines a function over the group which will be called the *metric function*. It consists of  $n$  complex numbers which all enter the rows of the matrix  $\Delta$  in various permutations depending on the multiplication table of the group. One obtains further

$$\begin{aligned} \Delta(g^{-1}) &= \langle \Phi | g^{-1} \Phi \rangle = \langle \Phi | g^\dagger \Phi \rangle = \langle g \Phi | \Phi \rangle \\ &= \langle \Phi | g \Phi \rangle^* = \{\Delta(g)\}^*. \end{aligned} \quad (241)$$

For the matrix elements of the Hamiltonian, one obtains similarly

$$\begin{aligned} H_{kl} &= \langle \Phi_k | H \Phi_l \rangle = \langle g_k \Phi | H g_l \Phi \rangle \\ &= \langle \Phi | g_k^{-1} H g_l \Phi \rangle = \langle \Phi | H g_k^{-1} g_l \Phi \rangle \\ &= H(g_k^{-1} g_l), \end{aligned} \quad (242)$$

where  $H(g) = \langle \Phi | H g \Phi \rangle$  is the *Hamiltonian function* over the group. Since the Hamiltonian is self-adjoint, one has also the property

$$\begin{aligned} H(g^{-1}) &= \langle \Phi | H g^{-1} \Phi \rangle = \langle g H \Phi | \Phi \rangle \\ &= \langle \Phi | H g \Phi \rangle^* = \{H(g)\}^*. \end{aligned} \quad (243)$$

In the following, it is convenient to introduce the operator  $K = H - \varepsilon \cdot 1$ . and the associated function  $\bar{K}(g) = \langle \Phi | (H - \varepsilon \cdot 1) g \Phi \rangle$  which both contain the energy parameter  $\varepsilon$ .

Let us now first assume that the space  $V_\Phi$  is of order  $|G|$ . In such a case, one says that the trial wavefunction is completely without symmetry properties. The secular equation (210) takes now the form

$$|K(g_k^{-1} g_l)| = |\langle \Phi | H - \varepsilon \cdot 1 | g_k^{-1} g_l \Phi \rangle| = 0, \quad (244)$$

and is of order  $|G| \times |G|$ . The question is to what an extent this secular equation can be simplified by using the splitting properties of the constants of motion  $G = \{g\}$  and particularly the projection operators  $P_{kk}^\alpha$  in the relations (238).

The order of the space  $V_\Phi$  is determined by the number of non-vanishing eigenvalues of the metric matrix  $\Delta$  defined by (240) or by the number of non-vanishing quantities in the series  $D_1, D_2, D_3, \dots$ , defined by (221). If the order is smaller than  $|G|$ , one says that  $\Phi$  has certain symmetry properties, and, if  $g \Phi = \Phi$  for all  $g$ , one says that  $\Phi$  is totally symmetric. Even the question of the order of the space  $V_\Phi$  may be essentially simplified by the use of the group algebra.

Starting out from the resolution of the identity in (238), we will first introduce the component analysis:

$$\Phi = e \Phi = \left( \sum_\alpha \sum_k P_{kk}^\alpha \right) \Phi = \sum_\alpha \sum_k \Phi_{kk}^\alpha, \quad (245)$$

where we have used the symbol  $\Phi_{kk}^\alpha = P_{kk}^\alpha \Phi$ . Introducing the general notation

$$\Phi_{km}^\alpha = P_{km}^\alpha \Phi = \int^\alpha M \Gamma_{km}^\alpha(s) s^{-1} \Phi, \quad (246)$$

we observe that, according to (173), the functions  $\Phi_{km}^\alpha$  in the  $k$ th row may be obtained from the "diagonal" function  $\Phi_{kk}^\alpha = P_{kk}^\alpha \Phi$  by means of the shift operator  $P_{km}^\alpha$ :

$$\Phi_{km}^\alpha = P_{km}^\alpha \Phi_{kk}^\alpha. \quad (247)$$

There is a total of

$$\sum_\alpha (f^\alpha)^2 = |G|$$

functions  $\Phi_{km}^\alpha$ , and they are conveniently arranged in terms of matrices analogous to (167):

$$\Phi^\alpha: \begin{bmatrix} \Phi_{11}^\alpha & \Phi_{12}^\alpha & \Phi_{13}^\alpha & \dots & \Phi_{1f}^\alpha \\ \Phi_{21}^\alpha & \Phi_{22}^\alpha & \Phi_{23}^\alpha & \dots & \Phi_{2f}^\alpha \\ \Phi_{31}^\alpha & \Phi_{32}^\alpha & \Phi_{33}^\alpha & \dots & \Phi_{3f}^\alpha \\ \dots & \dots & \dots & \dots & \dots \\ \Phi_{f1}^\alpha & \Phi_{f2}^\alpha & \Phi_{f3}^\alpha & \dots & \Phi_{ff}^\alpha \end{bmatrix} \quad (248)$$

where  $f = f^\alpha$  is the order of the matrix. These functions span also the space  $V_\Phi$ , which is easily shown by

considering the relation

$$\begin{aligned}
 g\Phi &= g\left(\sum_{\alpha} \sum_k P_{kk}^{\alpha}\right)\Phi \\
 &= \left[\sum_{\alpha} \sum_{kl} P_{kl}^{\alpha} \Gamma_{lk}^{\alpha}(g)\right]\Phi \\
 &= \sum_{\alpha} \sum_{kl} \Gamma_{lk}^{\alpha}(g) \Phi_{kl}^{\alpha}. \tag{248'}
 \end{aligned}$$

Let us now study the metric matrix formed by the functions  $\Phi_{km}^{\alpha}$ . Using (237) and (156), we obtain

$$\begin{aligned}
 \langle \Phi_{km}^{\alpha} | \Phi_{ln}^{\beta} \rangle &= \langle P_{km}^{\alpha} \Phi | P_{ln}^{\beta} \Phi \rangle \\
 &= \langle \Phi | P_{mk}^{\alpha} P_{ln}^{\beta} \Phi \rangle \\
 &= \langle \Phi | \delta^{\alpha\beta} \delta_{mn} P_{lk}^{\alpha} | \Phi \rangle \\
 &= \delta^{\alpha\beta} \delta_{mn} \langle \Phi | P_{lk}^{\alpha} | \Phi \rangle. \tag{249}
 \end{aligned}$$

The occurrence of the Kronecker symbols  $\delta^{\alpha\beta}$  and  $\delta_{mn}$  shows that functions associated with different irreducible representations are automatically orthogonal, and that functions associated with different columns of one and the same representations are also orthogonal.

Since the Hamiltonian commutes with all elements  $g$  of the group, it commutes also with the operators  $P_{km}^{\alpha}$  algebra. For the matrix elements of the Hamiltonian, one obtains

$$\begin{aligned}
 \langle \Phi_{km}^{\alpha} | H | \Phi_{ln}^{\beta} \rangle &= \langle P_{km}^{\alpha} \Phi | H | P_{ln}^{\beta} \Phi \rangle \\
 &= \langle \Phi | P_{km}^{\alpha} H P_{ln}^{\beta} | \Phi \rangle \\
 &= \langle \Phi | H P_{km}^{\alpha} P_{ln}^{\beta} \Phi \rangle \\
 &= \delta^{\alpha\beta} \delta_{mn} \langle \Phi | H | P_{lk}^{\alpha} \Phi \rangle. \tag{250}
 \end{aligned}$$

This implies that functions  $\Phi_{km}^{\alpha}$  associated with different irreducible representations are *noninteracting* with respect to the Hamiltonian  $H$ , and that the same applies also to functions associated with different rows of one and the same representation.

In summary, one obtains for the matrix elements entering the secular equation:

$$\begin{aligned}
 \langle \Phi_{km}^{\alpha} | K | \Phi_{ln}^{\beta} \rangle &= \delta^{\alpha\beta} \delta_{mn} \langle \Phi | H - \varepsilon \cdot 1 | P_{lk}^{\alpha} \Phi \rangle \\
 &= \delta^{\alpha\beta} \delta_{mn} f^{\alpha} M \Gamma_{lk}^{\alpha}(s) \langle \Phi | H - \varepsilon \cdot 1 | s^{-1} \Phi \rangle \\
 &= \delta^{\alpha\beta} \delta_{mn} f^{\alpha} M \Gamma_{lk}^{\alpha}(s) K(s^{-1}) \\
 &= \delta^{\alpha\beta} \delta_{mn} f^{\alpha} \{ \Gamma_{lk}^{\alpha} * K \}_0, \tag{251}
 \end{aligned}$$

i.e., each nonvanishing matrix element is essentially a convolution product between the function  $f^{\alpha} \Gamma_{lk}^{\alpha}$  and the function  $K$ .

In order to proceed, it is now necessary to discuss the order of the space  $V_{\Phi}$ , since any linear dependence between the basis functions is going to lead to secular equations which are identically vanishing. Let us first observe that, if any diagonal component  $\Phi_{kk}^{\alpha}$  is not identically vanishing, the entire row  $\Phi_{km}^{\alpha}$  is non-

vanishing and consists of  $f^{\alpha}$  mutually orthogonal functions. From (249), one obtains particularly

$$\begin{aligned}
 \langle \Phi_{km}^{\alpha} | \Phi_{km}^{\alpha} \rangle &= \langle \Phi | P_{kk}^{\alpha} | \Phi \rangle \\
 &= \langle \Phi_{kk}^{\alpha} | \Phi_{kk}^{\alpha} \rangle, \tag{249'}
 \end{aligned}$$

which relation shows that all functions in the same row have the same norm. The orthogonality property is a consequence of the general relations (249). We note further that, according to (169), the functions in such a row form a basis for the irreducible representation  $\Gamma^{\alpha}$ , i.e.,

$$g\Phi_{km}^{\alpha} = \sum_l \Phi_{kl}^{\alpha} \Gamma_{lm}^{\alpha}(g). \tag{252}$$

The functions  $\Phi_{km}^{\alpha}$  associated with different irreducible representations are both orthogonal and noninteracting with respect to  $H$ . It is perhaps even more remarkable that the same applies also to functions associated with *different columns* of one and the same irreducible representation; each column forms, so to say, a little isolated world by itself. For the matrix elements between functions associated with the  $m$ th column, one obtains according to the general formula (251):

$$\begin{aligned}
 \langle \Phi_{km}^{\alpha} | H - \varepsilon \cdot 1 | \Phi_{lm}^{\alpha} \rangle &= \langle \Phi | H - \varepsilon \cdot 1 | P_{lk}^{\alpha} \Phi \rangle \\
 &= f^{\alpha} \{ \Gamma_{lk}^{\alpha} * K \}_0, \tag{251'}
 \end{aligned}$$

which means that the result is going to be independent of the value of  $m=1, 2, 3, \dots, f^{\alpha}$ .

Our study shows that the splitting of the space  $V_{\Phi}$  by means of the basis  $\{\Phi_{km}^{\alpha}\}$  leads to orthogonal and noninteracting subspaces associated with the different irreducible representations and different columns within one and the same representation. Each such subspace corresponds further to a "block" of the secular equation, and we note each one of the columns of  $\Gamma^{\alpha}$  gives rise to an identical block, which is thus repeated  $f^{\alpha}$  times. This implies that every eigenvalue associated with such a block is going to be repeated  $f^{\alpha}$  times; *the eigenvalue is hence degenerate of order  $f^{\alpha}$* . This is an important consequence of the non-Abelian properties of the group, which is here demonstrated for the approximate eigenvalues associated with the simplest possible secular equation, and we will later show that a similar degeneracy theorem holds also for the exact energy levels.

In order to construct the secular equation for the problem explicitly, it is necessary to study the order of the space  $V_{\Phi}$  and its subspaces in greater detail. Let  $n^{\alpha}$  be the order of the space  $V_{\Phi^{\alpha}} = Q^{\alpha} V_{\Phi}$ , which is spanned by the functions

$$Q^{\alpha} \Phi_k = Q^{\alpha} g_k \Phi = g_k Q^{\alpha} \Phi = g_k \Phi^{\alpha}, \tag{253}$$

where

$$\Phi^{\alpha} = Q^{\alpha} \Phi = f^{\alpha} M \chi^{\alpha}(s) s^{-1} \Phi. \tag{254}$$

Let further  $n_m^{\alpha}$  be the order of the space  $V_{\Phi^{\alpha}}$ ,  $m = P_{mm}^{\alpha} V_{\Phi}$  associated with the  $m$ th column of the matrix  $\Phi^{\alpha}$  in (248). Since all the column spaces are orthogonal



and have the same order, depending on the existence of the shift relation (247), one obtains

$$n^\alpha = \sum_m n_m^\alpha = f^\alpha n_m^\alpha, \tag{255}$$

which shows that the order of the space  $V_{\Phi^\alpha}$  must be an integer multiple of  $f^\alpha$ , i.e.,  $n^\alpha = 0, f^\alpha, 2f^\alpha, 3f^\alpha, \dots, (f^\alpha)^2$ .

Let us now calculate the order  $n_m^\alpha$  of the column space  $V_{\Phi, m}^\alpha$  by studying the associated series of numbers  $D_1, D_2, D_3, \dots, D_M$  defined by (221). The set of elements to be investigated is  $\{\Phi_{km}^\alpha\}$  for  $k=1, 2, \dots, f^\alpha$ , so one has  $M=f^\alpha$ . Using (249), (246), and the definitions, one obtains

$$\begin{aligned} D_1 &= \sum_k \langle \Phi_{km}^\alpha | \Phi_{km}^\alpha \rangle \\ &= \sum_k \langle \Phi | \Phi_{kk}^\alpha \rangle \\ &= f^\alpha \sum_k M \Gamma_{kk}^\alpha(s) \langle \Phi | s^{-1} \Phi \rangle \\ &= f^\alpha M \chi^\alpha(s) \Delta(s^{-1}). \end{aligned} \tag{256}$$

$$\begin{aligned} D_2 &= \sum_{k < l} \begin{vmatrix} \langle \Phi_{km}^\alpha | \Phi_{km}^\alpha \rangle & \langle \Phi_{km}^\alpha | \Phi_{lm}^\alpha \rangle \\ \langle \Phi_{lm}^\alpha | \Phi_{km}^\alpha \rangle & \langle \Phi_{lm}^\alpha | \Phi_{lm}^\alpha \rangle \end{vmatrix} \\ &= \frac{1}{2} \sum_{k, l} \begin{vmatrix} \langle \Phi | \Phi_{kk}^\alpha \rangle & \langle \Phi | \Phi_{lk}^\alpha \rangle \\ \langle \Phi | \Phi_{kl}^\alpha \rangle & \langle \Phi | \Phi_{ll}^\alpha \rangle \end{vmatrix} \\ &= \frac{1}{2} (f^\alpha)^2 \sum_{k, l, s, t} M M [\Gamma_{kk}^\alpha(s) \Gamma_{ll}^\alpha(t) \Delta(s^{-1}) \Delta(t^{-1}) \\ &\quad - \Gamma_{lk}^\alpha(s) \Gamma_{kl}^\alpha(t) \Delta(s^{-1}) \Delta(t^{-1})] \\ &= \frac{1}{2} (f^\alpha)^2 M M \{ \chi^\alpha(s) \chi^\alpha(t) - \chi^\alpha(st) \} \Delta(s^{-1}) \Delta(t^{-1}), \end{aligned} \tag{257}$$

and similarly

$$\begin{aligned} D_3 &= (3!)^{-1} (f^\alpha)^3 M M M \{ \chi^\alpha(s) \chi^\alpha(t) \chi^\alpha(u) \\ &\quad - \chi^\alpha(s) \chi^\alpha(tu) - \chi^\alpha(t) \chi^\alpha(us) \\ &\quad - \chi^\alpha(u) \chi^\alpha(st) + \chi^\alpha(stu) + \chi^\alpha(sut) \} \\ &\quad \times \Delta(s^{-1}) \Delta(t^{-1}) \Delta(u^{-1}). \end{aligned} \tag{258}$$

It is now easy to generalize this result. Following W. Byers-Brown<sup>2</sup> we now introduce the following special functions of the characters:

$$\begin{aligned} B_1^\alpha(s) &= \chi^\alpha(s), \\ B_2^\alpha(s, t) &= \frac{1}{2} \{ \chi^\alpha(s) \chi^\alpha(t) - \chi^\alpha(st) \}, \\ B_3^\alpha(s, t, u) &= (3!)^{-1} \{ \chi^\alpha(s) \chi^\alpha(t) \chi^\alpha(u) \\ &\quad - \chi^\alpha(s) \chi^\alpha(tu) - \chi^\alpha(t) \chi^\alpha(us) \\ &\quad - \chi^\alpha(u) \chi^\alpha(st) + \chi^\alpha(stu) + \chi^\alpha(sut) \}, \\ &\dots \\ B_r^\alpha(s_1, s_2, \dots, s_r) &= (r!)^{-1} \sum_{P_r} (-1)^P \chi(P_r). \end{aligned} \tag{259}$$

Here  $P$  is a permutation of the elements  $s_1, s_2, \dots, s_r$  and, if  $P$  has the cycle structure  $P = (1) (3) (254) \dots$ , one has the definition

$$\chi^\alpha(P) = \chi^\alpha(s_1) \chi^\alpha(s_3) \chi^\alpha(s_2 s_5 s_4) \dots, \tag{260}$$

with one character-factor for each cycle. Using these functions, one obtains the general formula

$$\begin{aligned} D_r &= (f^\alpha)^r M M \dots M B_r^\alpha(s_1, s_2, \dots, s_r) \\ &\quad \times \Delta(s_1^{-1}) \Delta(s_2^{-1}) \dots \Delta(s_r^{-1}). \end{aligned} \tag{261}$$

It is perhaps somewhat surprising that the quantities  $D_1, D_2, D_3, \dots$ , which are associated with a column  $\{\Phi_{km}^\alpha\}$  depend only on the characters  $\chi^\alpha$  and not on the elements of the irreducible representation  $\Gamma^\alpha$ . This can perhaps be understood, if one realizes that the quantities  $\bar{D}_j$  for the basis  $\{g_k \Phi^\alpha\}$  for  $j=r f^\alpha$  are proportional to the  $f^\alpha$ th power of the quantities  $D_r$ . The explicit proof above is due to Byers-Brown.

One can now repeat the same arguments for the determinants formed by the matrix elements between the functions  $\{\Phi_{km}^\alpha\}$  in the column  $m$  with respect to the operator  $K = H - \varepsilon \cdot 1$ . Let us introduce a series of quantities

$$\begin{aligned} D_1(K) &= \sum_k \langle \Phi_{km}^\alpha | K | \Phi_{km}^\alpha \rangle, \\ D_2(K) &= \sum_{k < l} \begin{vmatrix} \langle \Phi_{km}^\alpha | K | \Phi_{km}^\alpha \rangle & \langle \Phi_{km}^\alpha | K | \Phi_{lm}^\alpha \rangle \\ \langle \Phi_{lm}^\alpha | K | \Phi_{km}^\alpha \rangle & \langle \Phi_{lm}^\alpha | K | \Phi_{lm}^\alpha \rangle \end{vmatrix}, \\ &\dots \end{aligned} \tag{262}$$

If the order of the space  $V_{\Phi, m}^\alpha$  is  $n_m^\alpha$ , it is evident that all the quantities  $D_r(K)$  are going to *vanish identically*, i.e., for all values of the parameter  $\varepsilon$ , if  $r = n_m^\alpha + 1, n_m^\alpha + 2, \dots$ . The reverse theorem is also true, depending on the fact that the operator  $K$  is positive definite,  $K > 0$ , for  $\varepsilon < E_0$ . For  $r = n_m^\alpha$ , the quantity  $D_r(K)$  is going to vanish only for certain values of the parameter  $\varepsilon$  equal to the eigenvalues  $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_r$ . Repeating the same simplification as before, one obtains

$$\begin{aligned} D_r(K) &= (f^\alpha)^r M M \dots M B_r^\alpha(s_1, s_2, \dots, s_r) \\ &\quad \times K(s_1^{-1}) K(s_2^{-1}) \dots K(s_r^{-1}), \end{aligned} \tag{263}$$

which is Byers-Brown's formula. It should be observed that the eigenvalues  $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_r$  associated with a specific column depend only on the characters  $\chi^\alpha$  but not on any individual elements of the irreducible representation  $\Gamma^\alpha$ . In this connection, it is also interesting to study the quantity  $\bar{D}_j(K)$  associated with the basis  $\{g_k \Phi^\alpha\}$  for  $j = f^\alpha n_m^\alpha$ . We note that the eigenvalues  $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_r$  in the total secular equation are going to be repeated once for every column, and that the corresponding energy levels are hence degenerate of

<sup>2</sup> W. Byers-Brown, in *Quantum Theory of Atoms, Molecules, and the Solid State*, A Tribute to John C. Slater (Academic Press Inc., New York, 1966), p. 123.

order  $f^\alpha$ , provided that the values  $\varepsilon_1, \varepsilon_2, \dots, \varepsilon_r$  are all different.

*Secular Equation in Terms of Convolution Algebra*

It is now possible to simplify the expressions (261) and (263) still further by using convolution algebra. The convolution multiplication  $*$  defined by (13) is associative and, considering a fixed element  $g$ , one has

$$\begin{aligned} \alpha * \beta &= M \alpha(s) \beta(g s^{-1}); \\ \alpha * \beta * \gamma &= M M \alpha(s) \beta(t s^{-1}) \gamma(g t^{-1}); \\ \alpha * \beta * \gamma * \delta &= M M M \alpha(s) \beta(t s^{-1}) \gamma(u t^{-1}) \delta(g u^{-1}); \\ \dots \end{aligned} \tag{264}$$

Convolution products are usually noncommutative, so that  $\beta * \alpha \neq \alpha * \beta$ . However, depending on the properties of the invariant mean, one has always  $(\beta * \alpha)_0 = (\alpha * \beta)_0$ . Since the operator  $Q^{\alpha \leftrightarrow f^\alpha \chi^\alpha}$  commutes with every element  $A \leftrightarrow \alpha$  of the group algebra, i.e.,  $Q^\alpha A = A Q^\alpha$ , one obtains for the associated functions

$$\chi^\alpha * \alpha = \alpha * \chi^\alpha, \tag{265}$$

where  $\alpha$  is an arbitrary function over the group.

In the formulas (261) and (263), one has sums of the type

$$M \chi(s) \Delta(s^{-1}), \quad M M \chi(st) \Delta(s^{-1}) \Delta(t^{-1}), \dots$$

which we can now rewrite in terms of convolution products:

$$\begin{aligned} M \chi^\alpha(s) \Delta(s^{-1}) &= (\chi^\alpha * \Delta)_0, \\ M M \chi^\alpha(st) \Delta(s^{-1}) \Delta(t^{-1}) &= M M \chi^\alpha(u) \Delta(tu^{-1}) \Delta(t^{-1}) \\ &= (\chi^\alpha * \Delta * \Delta)_0, \\ M M M \chi^\alpha(stu) \Delta(s^{-1}) \Delta(t^{-1}) \Delta(u^{-1}) \\ &= M M M \chi^\alpha(s_1) \Delta(s_2 s_1^{-1}) \Delta(s_3 s_2^{-1}) \Delta(s_3^{-1}) \\ &= (\chi^\alpha * \Delta * \Delta * \Delta)_0. \end{aligned} \tag{266}$$

From (256)–(258), one gets

$$\begin{aligned} D_1 &= f^\alpha (\chi^\alpha * \Delta)_0, \\ D_2 &= \frac{1}{2} (f^\alpha)^2 \{ (\chi^\alpha * \Delta)_0^2 - (\chi^\alpha * \Delta * \Delta)_0 \}, \\ D_3 &= (3!)^{-1} (f^\alpha)^3 \{ (\chi^\alpha * \Delta)_0^3 - 3 (\chi^\alpha * \Delta)_0 (\chi^\alpha * \Delta * \Delta)_0 \\ &\quad + 2 (\chi^\alpha * \Delta * \Delta * \Delta)_0 \}, \\ \dots \end{aligned} \tag{267}$$

By means of (261), one obtains the general formula

$$D_r = (r!)^{-1} (f^\alpha)^r \sum_P^{S_r} (-1)^P \Delta_p, \tag{268}$$

where  $\Delta_p$  is defined below; if  $P$  belongs to the conjugate class characterized by the cycle structure  $1^{\lambda_1} 2^{\lambda_2} 3^{\lambda_3} \dots$ , one has simply

$$\begin{aligned} \Delta_p &= (\chi^\alpha * \Delta)_0^{\lambda_1} (\chi^\alpha * \Delta * \Delta)_0^{\lambda_2} (\chi^\alpha * \Delta * \Delta * \Delta)_0^{\lambda_3} \dots \\ &= (\chi^\alpha * \Delta)_0^{\lambda_1} (\chi^\alpha * \Delta^{[2]})_0^{\lambda_2} (\chi^\alpha * \Delta^{[3]})_0^{\lambda_3} \dots, \end{aligned} \tag{269}$$

where we have used the special symbol  $\alpha^{[n]}$  to denote a ‘‘convolution power’’:  $\alpha^{[n]} = \alpha * \alpha * \alpha * \dots * \alpha$ . A still further simplification is possible, if one observes that, according to (107), the function  $f^\alpha \chi^\alpha$  is *idempotent* in the convolution algebra

$$(f^\alpha \chi^\alpha)^{[n]} = f^\alpha \chi^\alpha. \tag{270}$$

Using (265), one obtains

$$\begin{aligned} \chi^\alpha * \Delta * \Delta &= (f^\alpha)^{-1} (f^\alpha \chi^\alpha * \Delta) * (f^\alpha \chi^\alpha * \Delta) \\ &= (f^\alpha)^{-1} (f^\alpha \chi^\alpha * \Delta)^{[2]}; \\ \chi^\alpha * \Delta * \Delta * \Delta &= (f^\alpha)^{-1} (f^\alpha \chi^\alpha * \Delta)^{[3]}; \\ \dots \end{aligned} \tag{271}$$

Introducing the special function

$$\begin{aligned} \Delta^\alpha &= f^\alpha \chi^\alpha * \Delta = f^\alpha M \chi^\alpha(s) \Delta(g s^{-1}) \\ &= f^\alpha M \chi^\alpha(s) \langle \Phi | g s^{-1} | \Phi \rangle = \langle \Phi | g | \Phi^\alpha \rangle, \end{aligned} \tag{272}$$

one obtains finally

$$\begin{aligned} \Delta_p &= (f^\alpha)^{-\lambda_1 + \lambda_2 + \lambda_3 + \dots} \\ &\quad \times (\Delta^\alpha)_0^{\lambda_1} (\Delta^\alpha * \Delta^\alpha)_0^{\lambda_2} (\Delta^\alpha * \Delta^\alpha * \Delta^\alpha)_0^{\lambda_3} \dots \end{aligned} \tag{273}$$

It should be observed that the function  $\Delta^\alpha$  contains the same numbers as the overlap matrix associated with the basis  $\{g_k \Phi^\alpha\}$ .

In order to study the secular equation, it is convenient to introduce the special function

$$\begin{aligned} K^\alpha &= f^\alpha \chi^\alpha * K = f^\alpha M \chi^\alpha(s) K(g s^{-1}) \\ &= f^\alpha M \chi^\alpha(s) \langle \Phi | H - \varepsilon \cdot 1 | g s^{-1} \Phi \rangle \\ &= \langle \Phi | H - \varepsilon \cdot 1 | g \Phi^\alpha \rangle, \end{aligned} \tag{274}$$

which may be described as the "projection" of the function  $K$  on the space associated with the irreducible representation  $\Gamma^\alpha$  in the convolution algebra. For the matrix elements of  $(H - \varepsilon \cdot 1)$  with respect to the basis  $\{g_k \Phi^\alpha\}$ , one obtains

$$\langle g_k \Phi^\alpha | H - \varepsilon \cdot 1 | g_l \Phi^\alpha \rangle = K^\alpha(g_k^{-1} g_l), \quad (275)$$

i.e., the rows of this matrix consists of various permutations of the numbers associated with the function  $K^\alpha$ . However, instead of studying the sum  $\bar{D}_j(K)$  of all the principal minors of order  $j = f^\alpha n_m^\alpha$ , we will consider the quantity  $D_r(K)$  for  $r = n_m^\alpha$ . Simplifying the expression (263) by the methods outlined above, we obtain the final formula

$$\begin{aligned} D_r(K) &= (r!)^{-1} (f^\alpha)^r \sum_P (-1)^P K_P^\alpha, \\ P &= (1^{\lambda_1} 2^{\lambda_2} 3^{\lambda_3} \dots) \\ K_P^\alpha &= (f^\alpha)^{-(\lambda_1 + \lambda_2 + \lambda_3 + \dots)} \\ &\times (K^\alpha)_0^{\lambda_1} (K^\alpha * K^\alpha)_0^{\lambda_2} (K^\alpha * K^\alpha * K^\alpha)_0^{\lambda_3} \dots \end{aligned} \quad (276)$$

It is hence possible to evaluate  $D_r(K)$  for various values of the parameter  $\varepsilon$ , if one knows the function  $K^\alpha$  and its powers in the convolution algebra. One has particularly

$$\begin{aligned} K_0^\alpha &= \langle \Phi | H - \varepsilon \cdot 1 | \Phi^\alpha \rangle, \\ (K^\alpha * K^\alpha)_0 &= M \int \langle \Phi | H - \varepsilon \cdot 1 | g \Phi^\alpha \rangle^2, \\ &\dots \end{aligned} \quad (277)$$

It should be emphasized that the formulas obtained are essentially of principal interest, and that the proper modifications of these formulas for numerical purposes have to be studied in greater detail. One should be particularly careful to avoid such approximate linear dependencies as may destroy the accuracy of the numerical result. The best way to approach this problem is probably to evaluate the measures of linear independence of the column set  $\{\Phi_{km}^\alpha\}$ , i.e., to determine the eigenvalues of the associated metric matrix. This may be performed by studying the quantity  $D_r(L)$  for  $L = 1 - \mu \cdot 1$  and  $r = n_m^\alpha$ . If the smallest eigenvalues  $\mu_1, \mu_2, \dots$ , are almost negligible in the accuracy under consideration, it may be worthwhile to carry out a canonical orthonormalization according to (217) and a reduction of the order of the space  $V_{\Phi, m}^\alpha$  before proceeding. The practical problems involved will be the subject for further investigations.

## B. Symmetry Properties of the Exact Eigenfunctions of the Hamiltonian

### General Degeneracy Theorem

In the previous section, we have studied some special properties of the approximate solutions to the Schrödinger equation which are direct consequences of the fact that the Hamiltonian  $H$  commutes with all the elements  $g$  of a group  $G = \{g\}$ . We will now investigate the corresponding properties of the exact eigenfunctions to the Hamiltonian.

Let us assume that  $\Psi$  is a normalizable function which satisfies the time-independent Schrödinger equation

$$H\Psi = E\Psi. \quad (278)$$

Let us further introduce the functions

$$\Psi_{km}^\alpha = P_{km}^\alpha \Psi, \quad (279)$$

and arrange them in terms of matrices of the type (248). Since  $gH = Hg$ , one has further  $P_{km}^\alpha H = H P_{km}^\alpha$ , i.e., the elements  $P_{km}^\alpha$  are also constants of motion. One obtains directly

$$\begin{aligned} H\Psi_{km}^\alpha &= H P_{km}^\alpha \Psi = P_{km}^\alpha H \Psi = P_{km}^\alpha E \Psi \\ &= E P_{km}^\alpha \Psi = E \Psi_{km}^\alpha, \end{aligned} \quad (280)$$

which implies that every non-vanishing function  $\Psi_{km}^\alpha$  is also an eigenfunction to  $H$  associated with the eigenvalue  $E$ .

In order to discuss the degeneracy problem in greater detail, we will start from the component analysis

$$\Psi = e\Psi = \left( \sum_\alpha \sum_k P_{kk}^\alpha \right) \Psi = \sum_\alpha \sum_k \Psi_{kk}^\alpha. \quad (281)$$

Since the functions in the right-hand member are all orthogonal, one obtains

$$\langle \Psi | \Psi \rangle = \sum_\alpha \sum_k \langle \Psi_{kk}^\alpha | \Psi_{kk}^\alpha \rangle \neq 0, \quad (282)$$

which means that at least one of the norms  $\|\Psi_{kk}^\alpha\|$  has to be non-vanishing for a specific pair of values  $(\alpha, k)$ . In such a case, the entire  $k$ th row may be created by means of the shift operator:

$$\Psi_{km}^\alpha = P_{km}^\alpha \Psi_{kk}^\alpha, \quad (283)$$

and we note that all these functions have the same norm  $\|\Psi_{km}^\alpha\| = \|\Psi_{kk}^\alpha\| \neq 0$ . The row functions  $\{\Psi_{km}^\alpha\}$  are further orthogonal (and hence linearly independent),

and they form a basis for the irreducible representation  $\Gamma^\alpha$ :

$$g\Psi_{km}^\alpha = \sum_n \Psi_{kn}^\alpha \Gamma_{nm}^\alpha(g). \tag{284}$$

If  $\|\Psi_{kk}^\alpha\| \neq 0$ , one can hence draw the conclusion that the energy eigenvalue  $E$  has a degeneracy of at least order  $f^\alpha$ , and that the associated eigenfunctions transform according to the irreducible representation  $\Gamma^\alpha$ .

In the ideal case, only a single term  $\|\Psi_{kk}^\alpha\|^2$  in the sum (282) is nonvanishing, which means that  $\Psi = \Psi_{kk}^\alpha$ . Starting out from this function, we have constructed the entire row  $\{\Psi_{km}^\alpha\}$  according to (283), and these functions span a certain linear space of order  $f^\alpha$  associated with the eigenvalue  $E$ . If all the eigenfunctions to  $H$  having the eigenvalue  $E$  belong to this linear space, one says that the degeneracy is completely classified by the group  $G = \{g\}$ . The eigenfunctions are then interrelated through the symmetry operations  $g$ , and the order of the degeneracy is exactly  $f^\alpha$ .

There is, of course, nothing which prevents two or more norms in the sum (282) from being nonvanishing, and, in such a case, the degeneracy is of a more complicated nature being associated with two or more nonvanishing rows in the matrices (248). The degeneracy is still classified by the two symbols  $(\alpha, k)$ , but the eigenfunctions in different rows are no longer interrelated by the symmetry operations  $g$  which only connect functions within one and the same row. In such a case, one speaks of an accidental degeneracy. The systematic occurrence of accidental degeneracies is usually taken as an indication that one has not found all the possible constants of motion  $g$ , that there may exist additional symmetry operations which connect the seemingly noninterrelated wavefunctions of different rows, and that the group  $G = \{g\}$  is a subgroup of a larger group which may classify the degeneracy completely. In this connection, it may be convenient to use a slightly different approach.

### Unitary Group of the Hamiltonian

Let us consider the set  $\{g\}$  which consists of all unitary constants of motion of the Hamiltonian:

$$G_H = \{g \mid gH = Hg, g^\dagger g = gg^\dagger = 1\}. \tag{285}$$

One has immediately the theorem that the set  $G_H$  forms a group. If  $g$  and  $h$  are two operators belonging to  $G_H$ , one has

$$\begin{aligned} (gh)H &= g(hH) = g(Hh) = (gH)h = (Hg)h \\ &= H(gh), \end{aligned}$$

$$(gh)^\dagger(gh) = h^\dagger g^\dagger gh = h^\dagger h = 1, \tag{286}$$

which means that also  $gh$  belongs to  $G_H$ . Multiplying the relation  $gH = Hg$  to the left and to the right by  $g^{-1}$ ,

one obtains

$$Hg^{-1} = g^{-1}H, \tag{287}$$

which means that  $g^{-1}$  belongs to  $G_H$ . Since further the set  $G_H$  contains the identity operator  $1$  as neutral element, the set  $G_H$  forms a group called the unitary group of the Hamiltonian.

Let us now introduce the set  $W_E$  of all normalizable eigenfunctions  $\Psi$  of the Hamiltonian  $H$  associated with the eigenvalue  $E$ :

$$W_E = \{\Psi \mid H\Psi = E\Psi; \langle\Psi \mid \Psi\rangle = \text{finite}\}. \tag{288}$$

This set forms a linear space which is stable under all the operations in the group  $G_H = \{g\}$ , since one has

$$\begin{aligned} H(g\Psi) &= g(H\Psi) = g(E\Psi) = E(g\Psi), \\ \langle g\Psi \mid g\Psi\rangle &= \langle\Psi \mid \Psi\rangle. \end{aligned} \tag{289}$$

The arguments in the previous section lead us now to the following hypothesis:

The unitary group  $G_H$  of the Hamiltonian is complete, if all the subspaces  $W_E$  are irreducible under  $G_H$ . (290)

If the subspace  $W_E$  is irreducible under  $G_H$ , it must be possible to span the space by using the functions  $\{\Psi_{km}^\alpha\}$  in a single row, which means that they are all interrelated by the symmetry operations. If, on the other hand, the subspace  $W_E$  is reducible under  $G_H$ , one must apparently use functions from two or more rows  $\{\Psi_{km}^\alpha\}$  to span  $W_E$ , which means that there are functions associated with the degeneracy which are not interrelated by the operators  $\{g\}$  under consideration. In such a case, one should look for new symmetry operations commuting with  $H$ , which should connect the previously noninterrelated spaces.

It is probably very hard if not impossible to prove a theorem of type (290) in general; instead one has to work through the examples of systems having accidental degeneracies one-by-one to find the complete unitary groups of the Hamiltonian. Important examples have been treated by McIntosh and by Moshinsky, who have also shown how accidental degeneracies may be utilized for other purposes in quantum mechanics.

The conjecture expressed in (290) may also be formulated so that "there are no accidental degeneracies" and the development has shown that this is a valuable working hypothesis in the study of degeneracies by means of the unitary group of the Hamiltonian. The cases investigated so far have shown that, in solving the Schrödinger equation, all degeneracies may be completely classified by the group  $G_H = \{g\}$  consisting of all unitary constants of motion.

### C. Summary and Discussion

In this paper, the splitting of the quantum-mechanical secular equation by means of group theory has been

discussed. Starting from the isomorphism between the elements  $A$  of the group algebra and the functions  $\alpha$  over the group,  $A \leftrightarrow \alpha$ , expressed in terms of the invariant mean (10):

$$A = M \underset{s}{\alpha}(s) s^{-1}, \quad (291)$$

we derived the multiplication rule (15)

$$\begin{aligned} A \leftrightarrow \alpha, \quad B \leftrightarrow \beta, \\ A \times B \leftrightarrow \gamma = \alpha * \beta, \end{aligned} \quad (292)$$

with the convolution product defined by (13):

$$\gamma(g) = M \underset{s}{\alpha}(s) \beta(g s^{-1}). \quad (293)$$

After the definition of the concept of irreducible stable subspaces of the group algebra and the proof of Schur's lemma, we reached the relation (77):

$$T = M \underset{s}{\Gamma^\alpha}(s) A \Gamma^\beta(s^{-1}) = \delta^{\alpha\beta} \cdot \lambda \cdot I^\alpha, \quad (294)$$

where the constant has the value  $\lambda = (f^\alpha)^{-1} \text{Tr} \{A\}$ . Putting  $A = A' \Gamma^\beta(g)$ , we obtain the convolution relation (82):

$$\Gamma^\alpha * A' \Gamma^\beta = (f^\alpha)^{-1} \delta^{\alpha\beta} \text{Tr} \{A' \Gamma^\beta\} \cdot I^\alpha, \quad (295)$$

where  $A'$  is an arbitrary constant operator. In terms of the matrix elements, this gave relation (87):

$$\Gamma_{km}^\alpha * \Gamma_{nl}^\beta = (f^\alpha)^{-1} \delta^{\alpha\beta} \delta_{kl} \Gamma_{nm}^\beta. \quad (296)$$

For the basic elements of the group algebra defined through the equivalence  $P_{km}^\alpha \leftrightarrow f^\alpha \Gamma_{km}^\alpha$ , this lead to the fundamental multiplication rule:

$$P_{km}^\alpha \times P_{nl}^\beta = \delta^{\alpha\beta} \delta_{kl} P_{nm}^\beta. \quad (297)$$

For symmetry operators satisfying the relation  $ss^\dagger = s^\dagger s = 1$ , we obtained  $(P_{km}^\alpha)^\dagger = P_{mk}^\alpha$  according to (237). Combination with (297) gives then the following two relations:

$$\begin{aligned} P_{km}^{\alpha\dagger} \times P_{ln}^\beta &= \delta^{\alpha\beta} \delta_{mn} P_{lk}^\beta; \\ P_{km}^{\alpha\dagger} \times HP_{ln}^\beta &= \delta^{\alpha\beta} \delta_{mn} HP_{lk}^\beta, \end{aligned} \quad (298)$$

which are equivalent with the formulas (249) and (250) basic for the quantum-mechanical applications. These relations show that functions  $\Phi_{km}^\alpha = P_{km}^\alpha \Phi$  associated with different irreducible representations or with different columns of the same representation are not only orthogonal but also noninteracting with respect to  $H$ ; products associated with the same column ( $\alpha = \beta, m = n$ ) are further independent of the index  $m$ . Functions  $\Phi_{km}^\alpha$  in one and the same row are further mutually orthogonal and form a basis for the irreducible representation  $\Gamma^\alpha$ .

The secular equation associated with the functions  $\Phi_{km}^\alpha$  in a specific column  $m$  was finally shown to be

dependent only on the characters  $\chi^\alpha$  and not on the individual matrix elements of  $\Gamma^\alpha$ , and explicit expressions for the characteristic equation in terms of the convolution algebra were derived. The technique used seems to be simple and forceful, and the direct connection between Schur's lemma (294) and the two basic formulas (298) in the quantum-mechanical applications becomes clear and transparent.

The treatment is here confined to *finite groups*, and the fundamental tool is the invariant mean. This concept may be generalized to *compact infinite groups*, and many theorems here proven for finite groups may in this way be extended also to the infinite case.

In this connection, it is perhaps worthwhile to observe that, in the quantum-mechanical applications, there are two types of continuous groups which are of essential importance, namely those associated with translational and rotational symmetry. The main problem is again to find a resolution of the identity in terms of a set of projection operators which are idempotent and mutually exclusive. The projection operators associated with the primitive translations in crystal symmetry as well as those associated with angular momenta have been treated in Ref. 1 and in a series of published papers, and it seems as if all the essential physical results could be obtained by using these elementary tools.

In the studies of the spectral resolution of the Hamiltonian carried out by von Neumann and other specialists on the theory of Hilbert space, the "resolution of the identity" in terms of a set of projection operators plays a fundamental role. We have here used a similar approach also in studying the constants of motion, and the "component analysis" of a trial wavefunction turns out to be a valuable tool in the quantum-mechanical applications.

These ideas are also of importance in generalizing the independent-particle model, and for a more detailed study of "The Projected Hartree-Fock Method," the reader is referred to an article by Löwdin.<sup>3</sup>

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<sup>3</sup> Per-Olov Löwdin, in *Quantum Theory of Atoms, Molecules, and the Solid State*, A Tribute to John C. Slater (Academic Press Inc., New York, 1966), p. 601.