Group Theory and Its Applications

VOLUME I

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Preface

The importance of group theory and its utility in applications to various branches of physics and chemistry is now so well established and universally recognized that its explicit use needs neither apology nor justification. Matters have moved a long way since the time, just thirty years ago, when Condon and Shortley, in the introduction to their famous book, "The Theory of Atomic Spectra", justified their doing "group theory without group theory" by the statement that ". . . the theory of groups . . . is not . . . part of the ordinary mathematical equipment of physicists." The somewhat adverse, or at least sceptical, attitude toward group theory illustrated by the telling there of the well-known anecdote concerning the Weyl-Dirac exchange,* has been replaced by an uninhibited and enthusiastic espousal. This is apparent from the steadily increasing number of excellent textbooks published in this field that seek to instruct ever widening audiences in the nature and use of this tool. There is, however, a gap between the material treated there and the research literature and it is this gap that the present treatise is designed to fill. The articles, by noted workers in the various areas of group theory, each review a substantial field and bring the reader from the level of a general understanding of the subject to that of the more advanced literature.

The serious student and beginning research worker in a particular branch should find the article or articles in his specialty very helpful in acquainting him with the background and literature and bringing him up to the frontiers of current research; indeed, even the seasoned specialist in a particular branch will still learn something new. The editor hopes also to have the treatise serve another useful function: to entice the specialist in one area into becoming acquainted with another. Such ventures into novel fields might be facilitated by the recognition that similar basic techniques are applied throughout; e.g., the use of the Wigner-Eckart theorem can be recognized as a unifying thread running through much of the treatise.

The applications of group theory can be subdivided generally into two broad areas: one, where the underlying dynamical laws (of interactions) and therefore all the resulting symmetries are known exactly; the other, where

*After a seminar on spin variables and exchange energy which Dirac gave at Princeton in 1928, Weyl protested that Dirac had promised to derive the results without use of group theory. Dirac replied: "I said I would obtain the results without previous knowledge of group theory" (Condon and Shortley, "The Theory of Atomic Spectra", pp. 10–11. Cambridge Univ. Press, 1953).

these are as yet unknown and only the kinematical symmetrics (i.e. those of the underlying space-time continuum) can serve as a certain guide.

In the first area, group theoretical techniques are used essentially to exploit the known symmetries, either to simplify numerical calculations or to draw exact, qualitative conclusions. All (extra-nuclear) atomic and molecular phenomena are believed to belong to this category; the central chapters in this book deal with such applications, which, until relatively recently, formed the bulk of all uses of group theory.

In the second major area, application of group theory proceeds essentially in the opposite direction: It is used to discover as much as possible of the underlying symmetries and, through them, learn about the physical laws of interaction. This area, which includes all aspects of nuclear structure and elementary particle theory, has mushroomed in importance and volume of research to an extraordinary degree in recent times; the articles in the second half of the treatise are devoted to it.

In part as a consequence of these developments, physical scientists have been forced to concern themselves more profoundly with mathematical aspects of the theory of groups that previously could be left aside; questions of topology, representations of noncompact groups, more powerful methods for generating representations as well as a systematic study of Lie groups and their algebras in general belong in this category. They are treated in the earlier chapters of this book.

Considerations of both space and timing have forced omission from this volume of articles dealing with several important areas of applied group theory like molecular spectra, hidden symmetry and "accidental" degeneracy, group theory and computers, and others. These will be included in a second volume, currently in preparation.

Complete uniformity and consistency of notation is an ideal to be striven for but difficult to attain; it is especially hard to achieve when, as in the present case, many different and widely separated specialities are discussed, each of which usually has a well-established notational system of its own which may not be reconcilable with an equally well-established one in another area. In the present book uniformity has been carried as far as possible, subject to these restrictions, except where it would impair clarity.

The glossary of symbols included is expected to be of help; a few general remarks about notation follow: different mathematical entities are generally distinguished by different type fonts: vectors in bold face ($\mathbf{A}$, $\mathbf{H}$, $\mathbf{M}$, $\mathbf{u}$, $\boldsymbol{\alpha}$, $\boldsymbol{\Sigma}$), matrices in bold face sans serif ($\boldsymbol{\mathsf{A}}$, $\boldsymbol{\mathsf{M}}$, $\boldsymbol{\mathsf{R}}$, $\boldsymbol{\mathsf{u}}$), operators in script ($\mathscr{C}$, $\mathscr{H}$, $\mathscr{R}$) (though certain special Hamiltonians are indicated by italic sans serif H); spaces, fields, etc., by bold face German ($\mathfrak{C}$, $\mathfrak{H}$, $\mathfrak{R}$, $\mathfrak{B}$). The asterisk (*) denotes the complex conjugate, the dagger (†) the adjoint, and the tilde (~) the transpose. Different product signs are used as follows: $\times$, number product; $\boldsymbol{\times}$, vector cross product; X, the general (Cartesian) product of sets, the (outer) direct product of groups and representations; $\boxtimes$, the inner direct product of groups and representations (of the same group), and $\wedge$, the semidirect product; $\oplus$ denotes the direct sum.

It would be highly presumptuous for the editor to commend the authors for the quality of their contributions; however, I would like to thank them publicly and most sincerely for the spirit in which they cooperated in matters of selection of subject matter or emphasis, notation, style, etc., often sacrificing or modifying individual preferences for the sake of greater unity for the work as a whole. This made the task of the editor a much more enjoyable and less harassing one than it might otherwise have been.

It is also a great pleasure to thank the publisher, Academic Press, Inc., and the printers for the patience, devotion, diligence, and consummate skill with which they handled the uncommonly complex manuscripts. In spite of this diligence and skill misprints and errors undoubtedly still exist and the editor expresses his gratitude in advance to any reader who will point them out.

The dedication of this volume to the late G. Racah is a mark of appreciation for the monumental contribution he has made to group theory and its applications and a token of the esteem in which his person and his work is held by the editor and the contributors. It also symbolizes the sorrow and sense of loss which his tragic and untimely death caused. His contribution to this volume, which had been solicited, would have added luster and its absence leaves a void. On a more personal note, Professor Racah was the first to teach me theoretical physics and to stimulate my interest in it and in group theory. I owe him a debt of gratitude which cannot adequately be expressed, much less repaid.

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Brooklyn, New York
April 1968

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The Algebras of Lie Groups and Their Representations

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I. Introduction

A Lie group is defined as a topological group whose identity element has a neighborhood that is homeomorphic to a subset of an r-dimensional Euclidean space, where r is then called the order or dimension of the Lie group (*1*). Thus, a Lie group combines in one entity two distinct structures, a topological structure and a group-theoretic structure. The topological properties of the Lie group have far-reaching implications for the algebraic, or group-theoretic, structure. These implications are largely contained in the theorem that states that a Lie group (and in fact any topological group) is *homogeneous*, that is, for any given pair of points X, Y in the group manifold G there exists a homeomorphism f: $G \to G$ such that $f(X) = Y$. Thus, we need state and examine the local properties of a Lie group only in the neighborhood of a single point, e.g., the identity element; the homogeneity of the manifold then enables us to derive the same properties at any other point. Let us consider an analytic function $F(X)$ defined over the group manifold and examine $F(X)$ in a small neighborhood of the identity $X = 0$ where it takes the form

$$F(X) = F(0) + \sum_{i,j=1}^{r} \mu_j^i \left[\frac{\partial F(X)}{\partial X^i}\right]_{X=0} X^j \equiv F(0) + \sum_{j=1}^{r} X^j [x_j F(X)]_{X=0} \quad (1.1)$$

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where the x_i are linearly independent differential operators over the parameter space. These differential operators act as the generators of infinitesimal transformations and obey the commutation relations

$$[x_i, x_j] = (ij^k)\, x_k, \tag{1.2}$$

which serve to define the *structure constants* (ij^k). In order to assure that an infinitesimal transformation of the group can be integrated to obtain a finite transformation, it can be shown that the generators must also obey the Jacobi condition

$$[[x_i, x_j], x_k] + [[x_j, x_k], x_i] + [[x_k, x_i], x_j] = 0. \tag{1.3}$$

This set of generators, then, which is closed under the operation of commutation, and the set of all their linear combinations is called the *Lie algebra* of the group, and there exists a Lie algebra for every Lie group. The conditions (1.2) and (1.3) can be expressed as conditions on the structure constants:

$$(ij^k) = -(ji^k), \tag{1.4}$$

$$(ij^k)(kl^m) + (li^k)(kj^m) + (jl^k)(ki^m) = 0 \qquad \text{(Jacobi condition)}. \tag{1.5}$$

Lie further demonstrated that if we are given any r^3 constants (ij^k) that satisfy the relations (1.4) and (1.5), then we can integrate the generators that specify the infinitesimal transformations of a group and so determine the group itself, that is, the structure constants *alone* determine a group of continuous transformations. This group, however, is determined only up to a local isomorphism; the integration of the generators gives us a representation of the universal covering group, while other groups that are multiply connected may have the same local properties, that is, the same Lie algebra and the same structure constants.

In the study of Lie groups, then, we achieve an enormous simplification by restricting our attention to the Lie algebra and its representations. We need deal only with a finite number of elements, the Lie algebra, rather than a continuous infinity in order to establish a system of basis vectors for a representation space for the group. The algebra, because of its integrability, determines all the structures that have the desired properties of transformation under the finite elements of the group. In particular, we can determine all the irreducible unitary representations of a group by performing only the much easier construction of all the Hermitian representations and sets of basis vectors for the Lie algebra. Hence it is worth our while to study Lie algebras in some detail.

In the present chapter we shall restrict our attention to the problem of the classification of the compact real semisimple Lie algebras and review the work originally done by Killing (*2*) and Cartan (*3*). In a continuation of this chapter, which will be published in a subsequent volume, we shall apply this apparatus to a systematic treatment of the representation theory of the groups of n-dimensional unitary matrices and to a determination of all tensor operators in $U(n)$, using the techniques of the boson calculus and the Gel'fand and Weyl systems of basis vectors (*4*).

A Lie algebra is defined abstractly as a linear space of elements x_i with coefficients in any field (for our purposes the real or complex numbers) and a product defined by the foregoing relations (1.2) that satisfies (1) the condition of antisymmetry (or equivalently $[x,x]=0$); (2) the Jacobi condition (1.3); and, of course, (3) the usual conditions of linearity:

$$[ax_i, x_j] = a[x_i, x_j],$$
$$[x_i + x_j, x_k] = [x_i, x_k] + [x_j, x_k]. \tag{1.6}$$

Hence a Lie algebra is a particular instance of a nonassociative algebra; the Jacobi condition holds instead of the property of associativity. The property of antisymmetry and that provided by the Jacobi condition are expressed by conditions on the structure constants given earlier by (1.4) and (1.5).

We wish to show now that there exists a Lie algebra for every set of structure constants that satisfy these conditions, and we shall do this by the explicit construction of a model. A linear correspondence $x \to X$ of a Lie algebra L into a set of linear transformations X of a vector space S is called a *representation* of the Lie algebra if $[x,y] \to XY - YX$, where x, $y \in L$ and X and Y are transformations of S. We shall write $XY - YX = [X, Y]$. These linear transformations, or matrices, are called representations, and the vector space S is called the carrier space of the representation. The vectors in the carrier space then span the representation space, and the set of matrices X itself is loosely called a representation. Since physics is concerned with Lie groups that are themselves groups of linear transformations and therefore representations of themselves, the concept of matrix representation of Lie groups and their Lie algebras is of fundamental importance.

We remark now that the particular linear mappings of L into L that we define as $x \to x' = [y,x]$, where x, $y \in L$, and that we shall denote as $x' = [y,x] \equiv (\operatorname{ad} y)\, x$, have the property

$$(\operatorname{ad} y_1 \operatorname{ad} y_2 - \operatorname{ad} y_2 \operatorname{ad} y_1)\, x = [y_1, [y_2, x]] - [y_2, [y_1, x]]$$
$$= [[y_1, y_2], x] = (\operatorname{ad}[y_1, y_2])\, x, \tag{1.7}$$

which can be written as

$$[\operatorname{ad} y_1, \operatorname{ad} y_2] = \operatorname{ad}[y_1, y_2]. \tag{1.7a}$$

(We have made use here of the Jacobi condition.) It follows from (1.7a), then, that the linear transformations ad y are a (faithful) representation of L, which we call ad L, the *adjoint representation*. The reader should note that the idea of a representation of the Lie algebra by transformations induced in the algebra itself as a carrier space, though easy to grasp and seemingly trivial, is nonetheless very important and underlies the entire treatment to follow. In fact, the theory of the classification of semisimple Lie algebras *is* nothing more than the theory of the adjoint representation.

When we introduce a coordinate system in L, it becomes possible to specify matrix elements of ad y explicitly. Let x_i be the generators of L which we now take to define the basis (specified by the index i) and let $x = r^i x_i$ be an arbitrary element of L. Then

$$(\operatorname{ad} x_j)\, x = r^i [x_j, x_i] = r^i (ji^k)\, x_k, \tag{1.8}$$

and we note that the r^i and the x_j transform contragrediently to each other. The matrix elements of the adjoint representation are then seen to be simply the structure constants of L which are specified by our chosen basis

$$(\operatorname{ad} x_j)_{ki} = (ji^k). \tag{1.9}$$

These, then, are the desired matrices for our model, since we can write the Jacobi identity for the structure constants as

$$-(ij^a)(\operatorname{ad} x_a)_{lk} + (\operatorname{ad} x_j)_{ak}(\operatorname{ad} x_i)_{la} + (-\operatorname{ad} x_i)_{ak}(\operatorname{ad} x_j)_{la} = 0, \tag{1.10}$$

and this relation proves that structure constants that satisfy antisymmetry and the Jacobi condition "belong" to a Lie algebra.

The transformations of the adjoint representation of the Lie algebra (which, by Lie's fundamental theorem, can be integrated to yield the *adjoint group*), can be regarded as acting either on the abstract elements x or on the coordinates r^i, and we shall write indiscriminately $f(r^i) = f(x)$ for a fixed basis, i.e., the generators x_i. More complicated functions of x than linear ones, in fact polynomials, are defined indirectly (through $x \equiv r^i x_i$) as functions of r^i. [Note that only the operation of "commutation," Eq. (1.2), is defined for the elements x, and no other; in a representation, however, there exist two multiplication operations: one is the ordinary associative matrix multiplication AB, and the other, the commutation operation $[A, B] = AB - BA$, is expressed in terms of the former, but only this operation has a counterpart in the abstract Lie algebra.]

From Eq. (1.7) it follows that

$$\begin{aligned} [\operatorname{ad} y, \operatorname{ad} x] &= \operatorname{ad}((\operatorname{ad} y)\, x), \\ [\operatorname{ad} y, [\operatorname{ad} y, \operatorname{ad} x]] &= \operatorname{ad}((\operatorname{ad} y)(\operatorname{ad} y)\, x) \equiv \operatorname{ad}((\operatorname{ad} y)^2 x), \end{aligned} \tag{1.11}$$

hence we may apply the Baker-Campbell-Hausdorff formula

$$\exp(\theta A)\beta\exp(-\theta A) = \beta + \frac{\theta}{1!}[A,\beta] + \frac{\theta^2}{2!}[A,[A,\beta]] + \cdots \tag{1.12}$$

to obtain the transformations of the adjoint group:

$$[\exp(\theta\,\mathrm{ad}\,y)](\mathrm{ad}\,x)[\exp(-\theta\,\mathrm{ad}\,y)] = \mathrm{ad}(\exp(\theta\,\mathrm{ad}\,y)\,x). \tag{1.13}$$

The essential point of Lie's theory is that the conditions that are necessary for the integrability of a Lie algebra, namely, antisymmetry and the Jacobi condition, are also in general sufficient for integration in the neighborhood of the identity. The integration of representations is not a problem and proceeds directly by matrix exponentiation.

We turn now to the problem of the explicit classification of Lie algebras and their representations. First we introduce some definitions: the subset $x_{\bar{a}}$ of generators span a Lie *subalgebra* $\bar{L}$ if and only if $[x_{\bar{a}}, x_{\bar{b}}] \in \bar{L}$. In terms of the structure constants, $(\bar{a}, \bar{b}^k) = 0$ unless $k = \bar{c}$ also designates a member of the subalgebra. The condition for an *invariant subalgebra* is $[x_{\bar{a}}, x_b] \in \bar{L}$ for any $x_b \in L$. We can also write, in this case, $[\bar{L}, x] \in \bar{L}$. Note that an invariant subalgebra is therefore an *ideal* in L under the commutation operation. The condition for the invariance of a subalgebra in terms of the structure constants is then $(\bar{a}b^k) = 0$ unless $k = \bar{k}$ denotes a member of the subalgebra. Further, $\bar{L}$ is an Abelian subalgebra if $(\bar{a}\bar{b}^k) = 0$ for all $\bar{a}, \bar{b}, k$, and is an *invariant Abelian subalgebra* if both conditions hold; that is, if $(\bar{a}j^k) \neq 0$ only if $x_j \in L$, $x_k \in \bar{L}$.

A Lie algebra that possesses no invariant subalgebras at all is called *simple*, and simple Lie algebras belong to simple Lie groups. It is important here to note that a simple Lie group is one that possesses no invariant Lie subgroups; it may possess invariant *finite* subgroups, since these have no elements in a sufficiently small neighborhood of the identity except the identity itself. A Lie algebra (group) that possesses no invariant Abelian subalgebra (invariant Abelian Lie subgroup) is called *semisimple*. Of course, the property of simplicity implies that of semisimplicity. It will be seen later that a semisimple Lie algebra (group) can be represented as a direct sum (direct product) of simple Lie algebras (groups).

In order to establish a criterion for semisimplicity, which was first introduced by Cartan, let us construct the tensor (to be interpreted later as a *metric* tensor):

$$g_{ab} \equiv \mathrm{tr}(\mathrm{ad}\,x_a\,\mathrm{ad}\,x_b) = \sum_{ik}(ai^k)(bk^i). \tag{1.14}$$

Cartan's criterion states that *a Lie algebra is semisimple if and only if g_{ab} is nonsingular.*

Proof. The proof of necessity is easy. Suppose that L is not semisimple and hence has an Abelian invariant subalgebra $\bar{L}$ whose elements are $x_{\bar{a}}$. Then

$$g_{\bar{a}b} = \sum_{ik} (\bar{a}i^k)(bk^i) = \sum_{\bar{i}k} (\bar{a}i^k)(b\bar{k}^i) = \sum_{\bar{i}k} (\bar{a}\bar{i}^k)(b\bar{k}^{\bar{i}}) = 0, \tag{1.15}$$

where we have used the conditions on the structure constants that characterize an Abelian invariant subalgebra. This expression vanishes; hence g_{ab} has an entire row $g_{\bar{a}b}$ of zeros and thus is singular. The proof of the sufficiency of the Cartan criterion is more difficult and makes use of Cartan's second criterion of solvability, which we shall discuss in Section IV. We shall defer consideration of the sufficiency proof until Section IV, then, when we shall have developed the necessary tools. At present we shall merely prove the trivial theorem: If g_{ab} is singular, then L has an invariant subalgebra; that is, L is not simple.

Proof. We can construct the linear space L^* of all $x^* = w^a x_a$ such that $\operatorname{tr}(\operatorname{ad} x^* \operatorname{ad} x_b) = w^a \operatorname{tr}(\operatorname{ad} x_a \operatorname{ad} x_b) = w^a g_{ab} = 0$ for all $x_b \in L$. Since g_{ab} is singular, L^* is not empty. For any x_b, $x_c \in L$ we can write

$$\begin{aligned}\operatorname{tr}(\operatorname{ad}[x_c, x^*] \operatorname{ad} x_b) &= \operatorname{tr}([\operatorname{ad} x_c, \operatorname{ad} x^*] \operatorname{ad} x_b) = \operatorname{tr}(\operatorname{ad} x^* [\operatorname{ad} x_b, \operatorname{ad} x_c]) \\ &= (bc^d) \operatorname{tr}(\operatorname{ad} x^* \operatorname{ad} x_d) = 0,\end{aligned} \tag{1.16}$$

by the definition of x^*. Hence all $[x_c, x^*]$ belong to L^* and L^* is an invariant subalgebra. Note that for any two elements x^*, $y^* \in L^*$ we have in particular

$$\operatorname{tr}(\operatorname{ad} x^* \operatorname{ad} y^*) = 0, \tag{1.17}$$

a fact that we shall need later in our treatment of the second solvability criterion of Cartan.

In this study we shall restrict our attention to compact Lie algebras defined over the field of real numbers. We say that a Lie algebra is compact if it is isomorphic to the Lie algebra of a Lie group whose manifold is a compact set. It can be shown that for a compact Lie group all irreducible matrix representations are finite-dimensional and equivalent to unitary representations (Peter-Weyl theorem); hence all representations of their Lie algebras are similarly finite-dimensional and equivalent to Hermitian representations. These properties are not shared by noncompact groups. For noncompact groups all† the faithful irreducible unitary representations are infinite-dimensional and there exists a nondenumerable infinity of them, that is, there exist series of irreducible unitary representations that are labeled by continuous values of the invariants. For compact groups, on the other hand, all irreducible unitary representations are finite-dimensional and occur only in discrete series. For both

† Except of course the identity representation.