GROUP THEORY MADE EASY FOR SCIENTISTS AND ENGINEERS

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PREFACE

One might be tempted to ask "Yet another book on Group Theory?" This book is different, however, in that it aims to help the advanced undergraduate, the beginning graduate student, or the industrial researcher who would like to be familiar with the tools of symmetry without having to wade through elaborate mathematical proofs. Extensive theory to be found in most texts on group theory has been avoided; instead, attention is concentrated on discussion of illustrative problems. The choice of material has been dictated by the experience gained in teaching group theory courses, and the areas covered include atomic physics, nuclear physics, particle physics, solid-state physics, and molecular physics. We believe this is a useful addition to the existing literature, one that seeks to supplement rather than duplicate other treatments of the subject, and one that students of mathematics, chemistry, or engineering will also find useful.

The informal approach in this book is motivated by the desire to acquaint the uninitiated with the fundamentals of Group Theory. Chapters 1 - 4 go over the bare essentials and one who needs a quick grasp of the tools can afford to omit Chapters 5 - 8. Each of the latter chapters is meant to familiarize the student with the applications in different fields at the level of background preparation. The book as a whole is designed for a one semester course for students who had courses in Calculus, Elementary Linear Algebra and Modern Physics or Introductory Quantum Mechanics, although Chapters 1 - 4 can be gone through even without the last mentioned preparation.

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CHAPTER ONE

MATRICES, ALGEBRAS

MATRICES

We will briefly review some properties of square matrices that are helpful in understanding group representations. In the following matrix

$$U = \begin{pmatrix} -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix}$$

we know that the determinant of the matrix can be expanded using the elements in any row:

$$-\frac{1}{\sqrt{2}} \begin{vmatrix} 0 & -\frac{i}{\sqrt{2}} \\ 1 & 0 \end{vmatrix} + 0 \begin{vmatrix} -\frac{i}{\sqrt{2}} & -\frac{i}{\sqrt{2}} \\ 0 & 0 \end{vmatrix} + \frac{1}{\sqrt{2}} \begin{vmatrix} -\frac{i}{\sqrt{2}} & 0 \\ 0 & 1 \end{vmatrix}$$

$$\det U = -\frac{1}{\sqrt{2}}\left(\frac{i}{\sqrt{2}}\right) + 0(0) + \frac{1}{\sqrt{2}}\left(-\frac{i}{\sqrt{2}}\right) = -i$$

$$-\frac{i}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right) + 0(0) - \frac{i}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\right) = -i$$

$$0(0) + 1(-i) + 0(0) = -i \qquad (1)$$

Defining a *reduced cofactor* as the cofactor multiplying the element of each row in the expansion of the determinant divided by the value of the determinant, we obtain a corresponding matrix of reduced cofactors, the so-called *contragredient matrix*

$$\begin{pmatrix} -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{i}{\sqrt{2}} & 0 & \frac{i}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix} \qquad (2)$$

The transpose of this contragredient matrix is the *inverse of U*. Thus

$$U^{-1} = \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \end{pmatrix} \qquad (3)$$

$$U\,U^{-1} = U^{-1}\,U = 1$$

where 1 is the unit matrix, $\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$. If each element of a matrix is replaced by its complex conjugate and if the rows and columns are then interchanged (transposed), the result is called the *adjoint matrix*

$$U^{+} = \begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \end{pmatrix} \qquad (4)$$

We notice in the above instance, however, U^{+} is the same as U^{-1}. Such matrices are known as *unitary matrices*. In this unitary matrix U any two rows, treated as vectors, are orthogonal, and each row normalizes to unity:

$$\left(\frac{i}{\sqrt{2}}, 0, \frac{i}{\sqrt{2}}\right)\begin{pmatrix} -\frac{1}{\sqrt{2}} \\ 0 \\ \frac{1}{\sqrt{2}} \end{pmatrix} = -\frac{i}{2} + 0 + \frac{i}{2} = 0 \quad \text{(orthogonality of rows 2 and 1)}$$

$$\left(\frac{i}{\sqrt{2}}, 0, \frac{i}{\sqrt{2}}\right)\begin{pmatrix} -\frac{i}{\sqrt{2}} \\ 0 \\ -\frac{i}{\sqrt{2}} \end{pmatrix} = \frac{1}{2} + 0 + \frac{1}{2} = 1 \quad \text{(row 2 normalized).} \tag{5}$$

The columns have similar properties. If a matrix is *equal* to its adjoint it is called a *Hermitean matrix*. For instance,

$$H = \begin{pmatrix} -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & \frac{i}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{i}{\sqrt{2}} & 0 \end{pmatrix} = H^{+} \tag{6}$$

Let A and B be two 2 x 2 matrices

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \quad B = \begin{pmatrix} e & f \\ g & h \end{pmatrix} \tag{7}$$

Two 4 x 4 matrices are derived from these two matrices, the direct sum $A \oplus B$ and the direct product $A \otimes B$

$$A \oplus B = \begin{pmatrix} a & b & 0 & 0 \\ c & d & 0 & 0 \\ 0 & 0 & e & f \\ 0 & 0 & g & h \end{pmatrix}, \quad B \oplus A = \begin{pmatrix} e & f & 0 & 0 \\ g & h & 0 & 0 \\ 0 & 0 & a & b \\ 0 & 0 & c & d \end{pmatrix}$$

$$A \otimes B = \begin{pmatrix} aB & bB \\ cB & dB \end{pmatrix} = \begin{pmatrix} ae & af & be & bf \\ ag & ah & bg & bh \\ ce & cf & de & df \\ cg & ch & dg & dh \end{pmatrix}$$

$$B \otimes A = \begin{pmatrix} ea & eb & fa & fb \\ ec & ed & fc & fd \\ ga & gb & ha & hb \\ gc & gd & hc & hd \end{pmatrix} \qquad (8)$$

The trace of either direct product matrix (the sum of diagonal elements) is seen to be (a + d) (e + h), which is the product of the traces of the two factors in the direct product.

$U\,H'\,U^{-1}$ is called a similarity transformation of a matrix H', U being the transforming matrix. Matrix multiplication shows

$$\underset{U}{\begin{pmatrix} -\frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ -\frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ 0 & 1 & 0 \end{pmatrix}} \underset{H'}{\begin{pmatrix} 0 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 0 \end{pmatrix}} \underset{U^{-1}}{\begin{pmatrix} -\frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \\ 0 & 0 & 1 \\ \frac{1}{\sqrt{2}} & \frac{i}{\sqrt{2}} & 0 \end{pmatrix}} = \underset{\lambda_i \delta_{ij}}{\begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{pmatrix}}$$

or, symbolically,

$$U\,H'U^{-1} = \lambda_i \delta_{ij} \qquad (9)$$

where H' is the matrix $\begin{pmatrix} 0 & 0 & -1 \\ 0 & 2 & 0 \\ -1 & 0 & 0 \end{pmatrix}$

and $\lambda_1 = 1$, $\lambda_2 = -1$, $\lambda_3 = 2$. The Kronecker symbol δ_{ij} has the usual meaning

$$\begin{aligned} \delta_{ij} &= 1 \qquad i = j \\ &= 0 \qquad i \neq j \end{aligned} \qquad (10)$$

U is said to diagonalize H' through a similarity transformation, and the diagonal elements are the *eigenvalues* of H'. Notice the trace of the diagonal matrix, that is, the sum of eigenvalues is 1 - 1 + 2 = 2 which is also the trace of H'. This illustrates the well-known theorem, of importance in group theory, that the trace of a matrix is invariant to a similarity transformation. The

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general procedure for diagonalizing any matrix is to be found in standard texts, for instance D. E. Littlewood (1970) *A University Algebra*.

ALGEBRAS

An algebra in which the associative law of multiplication is valid is called a *linear associative algebra*. The set of all n x n square matrices (matrix elements complex numbers) forms an algebra of order n^2, called the *total matrix algebra*. The basis elements e_{ij} of such an algebra satisfy

$$e_{ij}\, e_{kl} = 0 \qquad j \neq k$$

$$e_{ij}\, e_{jl} = e_{il} \qquad (11)$$

For n = 2 these are

$$e_{11} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix},\ e_{12} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix},\ e_{21} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix},\ e_{22} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}$$

In other words, the general basis element matrix e_{ij} has 1 in the i-th row and j-th column and zeroes elsewhere.

Several interesting results follow when the basis elements of an algebra are isomorphic to the elements of a group; the multiplication table of the algebra will in this case also be the Cayley table for the group. We illustrate the important properties of such algebras with the help of two finite groups: the Abelian cyclic group C_4 and the group C_{3v} (isomorphic to S_3 or D_3).

We assume the elements of C_4 to be isomorphically represented by basis elements e_i such that E (identity element of the group) → e_1, $C_4 \to e_2$, $C_4^2 \to e_3$, $C_4^3 \to e_4$. It is obvious that the constants of multiplication in the algebra are all either 1 or 0 because of the fundamental group property. The common multiplication table is

	e_1	e_2	e_3	e_4
e_1	e_1	e_2	e_3	e_4
e_2	e_2	e_3	e_4	e_1
e_3	e_3	e_4	e_1	e_2
e_4	e_4	e_1	e_2	e_3

$e_i\, e_j = \gamma_{ijk}\, e_k \qquad \gamma_{ijk} = 1 \text{ or } 0$

A general element of the algebra is $X = \sum_{i=1}^{4} x_i e_i$ where x_i are the chosen complex numbers. We notice that there also exists an element of the algebra $e_1 = \sum_{i=1}^{4} \varepsilon_i e_i$, where $\varepsilon_1 = 1$, $\varepsilon_2 = 0 = \varepsilon_3 = \varepsilon_4$, which commutes with every element of the algebra,

$$e_1 x = x\, e_1 = x \tag{12}$$

e_1 is called the *modulus of the algebra*. Furthermore, $e_1^2 = e_1$, and for this reason e_1 is said to be an *idempotent*. The product of no other element with e_1 vanishes; hence e_1 is also called the *principal idempotent*. From Eq. (12) we see

$$\begin{aligned} X^2 = (x_1^{\,2} + x_3^{\,2} + 2x_2x_4)e_1 &+ (2x_1x_2 + 2x_2x_4)e_2 \\ &+ (x_2^{\,2} + 2x_1x_3 + x_4^{\,2})e_3 \\ &+ (2x_1x_4 + 2x_2x_3)e_4 \end{aligned} \tag{13}$$

and this cannot be 0 unless all x_i are 0. An element x of an algebra is said to be nilpotent if $x^n = 0$ for some integer n. This algebra is thus not nilpotent and contains an idempotent element. This is a particular application of a theorem that says every algebra that is not nilpotent contains an idempotent element.

We now ask the question: Given x, can we find another element of the algebra $y = \sum_i y_i e_i$ such that it satisfies the equation

$$xy = \omega y$$

or

$$(x-\omega)y = 0 \tag{14}$$

where ω is a number. If we carry out the multiplication x y and collect coefficients of e_i, this equation takes the form

$$[\quad]e_1 + [\quad]e_2 + [\quad]e_3 + [\quad]e_4 = 0 \tag{15}$$

Since e_i, by definition, are nonzero, each coefficient in Eq. (15) must vanish, and we have four linear equation in y_i, which can be written in matrix form

$$\begin{pmatrix} x_1-\omega & x_4 & x_3 & x_2 \\ x_2 & x_1-\omega & x_4 & x_3 \\ x_3 & x_2 & x_1-\omega & x_4 \\ x_4 & x_3 & x_2 & x_1-\omega \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = 0 \tag{16}$$

As is well known, for a nontrivial solution the determinant of this matrix $\Delta(x)$, a polynomial in ω of degree 4, has to vanish. $\Delta(x)$ is called the *characteristic determinant* and $\Delta(x) = 0$ the *characteristic equation*.

In the case of a semisimple algebra it can be shown that the characteristic equation can be reduced, by a similarity transformation of the matrix equation, to a product of factors that cannot further be reduced. In our example the unitary matrix

$$U = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{i}{2} & -\frac{1}{2} & -\frac{i}{2} \\ \frac{1}{2} & -\frac{1}{2} & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{i}{2} & -\frac{1}{2} & \frac{i}{2} \end{pmatrix} \tag{17}$$

reduces the matrix equation to

$$U[(x-\omega y)y]U^{-1} = 0 \tag{18}$$

$$\begin{pmatrix} (x_1+x_2+x_3+x_4-\omega) & 0 & 0 & 0 \\ 0 & (x_1+ix_2-x_3-ix_4-\omega) & 0 & 0 \\ 0 & 0 & (x_1-x_2+x_3-x_4-\omega) & 0 \\ 0 & 0 & 0 & (x_o-ix_2-x_3+ix_4-\omega) \end{pmatrix} = 0 \tag{19}$$

The characteristic equation is thus reduced to four linear factors, each of the first degree in x_i

$$(x_1+x_2+x_3+x_4-\omega)\ (x_1+ix_2-x_3-ix_4-\omega)\ (x_1-x_2+x_3-x_4-\omega)$$
$$(x_1-ix_2-x_3+ix_4-\omega) = 0 \tag{20}$$

The number of irreducible factors being 4 is a consequence of there being <u>four</u> elements of the algebra (in this case, all the elements!) that <u>commute</u> with every element of the algebra. That each factor is linear in the numbers x_i and raised to the first power is related to the fact that

$$\sum_\mu (n_\mu \times n_\mu) = 4 = \text{order of the algebra}$$

where n_μ is the degree of the x_i in each factor, and also the power of that factor in the product. This indirectly verifies the theorem that a semisimple algebra is equivalent to a direct sum of total matrix algebras, here a sum of four 1 x 1 matrix algebras. Of significance is the fact that the C_4 group has <u>four</u> classes. If, for instance, we choose $x_1 = x_2 = x_3 = 0$ and $x_1 = 1$ as the numbers defining the element κ, then the roots of the characteristic equation will be

$$\omega = 1, i, -1, -i$$

These are the one-dimensional matrix algebras into which the given algebra decomposes. These numbers are familiar from the character table of C_4!

A more illuminating example is the algebra of order 6 with basis elements e_1, e_2, e_3, e_4, e_5, e_6 isomorphic to the elements of the Group C_{3v} with the correspondences

$$e_1 \to E,\ e_2 \to A,\ e_3 \to B,\ e_4 \to C,\ e_5 \to D,\ e_6 \to F$$

The multiplication table of these elements is shown in Table I.

TABLE I. MULTIPLICATION TABLE OF THE ALGEBRA

	e_1	e_2	e_3	e_4	e_5	e_6
e_1	e_1	e_2	e_3	e_4	e_5	e_6
e_2	e_2	e_1	e_5	e_6	e_3	e_4
e_3	e_3	e_6	e_1	e_5	e_4	e_2
e_4	e_4	e_5	e_6	e_1	e_2	e_3
e_5	e_5	e_4	e_2	e_3	e_6	e_1
e_6	e_6	e_3	e_4	e_2	e_1	e_5

We now list a few properties of this algebra

1. The algebra has a modulus e_1 because $e_1 e_i = e_i\, e_1 = e_i$ for $i = 1,2,..6$.
2. The algebra has an idempotent that is also a principal idempotent $e_1^{\ 2} = e_1$, there does not exist an e_j for which $e_1 e_j = 0$ or $e_j e_1 = 0$.
3. The subset of elements e_1, e_5, e_6 forms an algebra in itself; this is then a subalgebra of the algebra (also with a modulus). However, the products $e_i e_1$, $e_1 e_i$, $e_i e_5$, $e_5 e_i$, $e_i e_6$, $e_6 e_i$ where e_i is any element of the main algebra, are

not all members of this subalgebra. For instance, $e_4 e_5 = e_2$, and e_2 is not in the subset. When this does not happen, the subalgebra is not an "invariant subalgebra". An algebra that does not have an invariant subalgebra is called a "*simple*" *algebra*. This, then, is a simple algebra.

4. This algebra does not have a nilpotent element, that is, $e_i^n \neq 0$ for any e_i and for any n. It is obvious that the subalgebra does not have a nilpotent element either. Algebras having no nilpotent invariant subalgebras are called *semisimple*. Our algebra is, therefore, a semisimple algebra. Naturally, all simple algebras are semisimple.

5. The following theorems are at once satisfied:

   A simple algebra always contains an idempotent element.

   Every algebra that does not possess a modulus has a nilpotent invariant subalgebra.

   A semisimple algebra always has a modulus.

   If an algebra has a modulus e_1, this element is a principal idempotent and the only one.

The important consequence of the algebra being semisimple is that it is equivalent to a direct sum of total matrix algebras. This can be seen a little more explicitly with the help of the characteristic equation.

The characteristic equation of x is

$$\begin{vmatrix} x_1-\omega & x_2 & x_3 & x_4 & x_6 & x_5 \\ x_2 & (x_1-\omega) & x_5 & x_6 & x_4 & x_3 \\ x_3 & x_6 & (x_1-\omega) & x_5 & x_2 & x_4 \\ x_4 & x_5 & x_6 & (x_1-\omega) & x_3 & x_2 \\ x_5 & x_4 & x_2 & x_3 & (x_1-\omega) & x_6 \\ x_6 & x_3 & x_4 & x_2 & x_5 & (x_1-\omega) \end{vmatrix} = 0 \qquad (21)$$

a polynomial in ω of the sixth degree. A simple algebraic multiplication goes to show that there are three linear sets that commute with every element of the algebra:

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