Group Theory for Physicists

Group theory helps readers in understanding energy spectrum and the degeneracy of systems possessing discrete symmetry and continuous symmetry. This text covers two essential aspects of group theory, namely discrete groups and Lie groups. Important concepts including permutation groups, point groups, and irreducible representation related to discrete groups are discussed with the aid of solved problems. Topics such as the matrix exponential, the circle group, tensor products, angular momentum algebra, and the Lorentz group are explained to help readers in understanding the quark model and the corresponding bound states of quarks. Real life applications including molecular vibration, level splitting perturbation, and the orthogonal group are also covered. Application-oriented solved problems and exercises are interspersed throughout the text to reinforce understanding of the key concepts.

Pichai Ramadevi is Professor of Physics at the Indian Institute of Technology Bombay, India. She has taught courses including general relativity, group theory methods, particle physics, quantum mechanics and quantum physics. She has published more than 50 papers in journals of national and international repute. Her research interests include string theory, knot theory, quantum field theory, and supersymmetry.

Varun Dubey is a researcher at the International Center for Theoretical Sciences, Bangalore, India. His research interests include probability theory, stochastics in quantum dynamics, and geometric quantization.

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with Applications

Pichai Ramadevi
Varun Dubey

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Preface

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In our day-to-day life as well as in the laboratories, we observe patterns with symmetry. These could be in the symmetric shape of the wings of a butterfly, the arrangement of atoms in a molecule, the shape of nuclei as inferred by advanced experimental techniques, among many others. Group theory is a mathematical formulation of such symmetries. While group theory is of interest in mathematics, the prevalence of symmetries in the physical world enable it to find applications in several other disciplines. For instance, the synthesis of molecules in chemistry, crystallographic structures in physics, elasticity properties in continuum mechanics, etc., require the basics of the symmetry principles.

Understanding complex physical systems in nature by solving complicated mathematical equations can be a daunting task. Group theory offers an elegant and powerful framework to extract certain details about such complex systems. For example, the underlying group symmetry can assert whether a given scattering or decay process is allowed or forbidden without performing any explicit computation. This book employs solved examples as well as a variety of exercises (sometimes drawn from sources listed in the Bibliography) to help the reader appreciate the role of group theory in explaining certain experimental observations. We have tried to balance between the formal mathematical aspects and the applications so that the student can effortlessly absorb the group theory arguments behind ad hoc postulates and

selection rules. The contents and presentation style enable undergraduate students to connect with the physics they have learned, or will be learning in courses like quantum mechanics, continuum mechanics, atomic and molecular physics, condensed matter physics, nuclear physics, and particle physics in their undergraduate curriculum.

A comprehensive understanding of the concepts in this book will build a strong foundation, preparing the students for further study in diverse areas such as theoretical condensed matter physics or high energy physics, theory including string theory. The first four chapters address discrete group concepts and their applications. The introductory chapter contains definitions and examples, including permutation group. Chapter 2 contains discussion on molecular symmetry, broadly known as point groups. After an initial review of vector spaces and group action on vector spaces, Chapter 3 elaborates on reducible and irreducible representation, character tables, tensor products and their decomposition. This provides the necessary background to determine the vibrational modes of molecules, splitting of degenerate energy level due to impurity or defect which breaks the symmetry of the system partially or completely, and selection rules for transition between energy levels. These applications are elaborated in Chapter 4.

Continuous groups (also known as Lie groups) are discussed in Chapter 5 and Chapter 6. Some of the concepts and notations elaborated in the context of discrete groups are useful while studying systems possessing continuous group symmetry. The key highlights of these two chapters are: (i) Young diagram presentation of irreducible representations for both permutation group as well as special unitary groups which clarifies concepts like tensor products and the decomposition of irreducible representations; (ii) a warm-up on angular momentum algebra which naturally facilitates the description of formal aspects of special unitary group where we introduce weight vectors, root vectors and the Dynkin diagrams; (iii) orthogonal groups and their applications to the energy spectrum of hydrogen atom.

The task of structuring this book in print form would not have been possible without the help of our colleagues and students. We are grateful to Deepak and Himanshu for their timely help in fixing LYX syntax errors which we faced while compiling the chapters. We would like to thank Vivek for helping us with the drawings for some of the figures. We would also like to thank Adiba for helping us in typesetting two sections in LYX package, as well as for proof reading the contents of this book. Our thanks are due also to Himanshu, Aman, Gurbir, Anish, Amihay, Ayaz, Saswati, Zodin, Lata, and Abhishek for their help and valuable comments during various stages in the progress of the book. Besides these students, we greatly appreciate Urjit, Uma, Punit, Pradeep, and Vikram for their comments. Finally, we would like to thank our family members for their encouragement.

We envision that the book will be most suited to teachers offering a one-semester group theory course to undergraduate students. It is also of relevance to researchers embarking on a study of this field. We wish all the readers enjoy their journey through the contents.

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1

Introduction

We observe objects in nature to have some pattern or symmetry. In fact, the symmetries inherent in any physical system play a very crucial role in the study of such systems. Group theory is a branch of mathematics that facilitates classification of these symmetries. Hence learning the group theory tools will prove useful to studying applications in physics. Readers will particularly appreciate the power and elegance of the group theoretical techniques in reproducing the experimental observations.

Before delving into its applications, it is important to understand the concept of an abstract group from a purely mathematical standpoint. In this chapter, we present the formal definition of a group and also the notations which will be followed in the rest of the book.

1.1 Definition of a Group

Definition 1. A group G is a set on which is defined a binary operation called the *product* having the following properties:

1. Closure: For all a and b in G, the product ab is in G. Here a and b need not be distinct.
2. Associativity: $(ab)c = a(bc)$ for all a, b and c in G.
3. Existence of Identity: There exists a unique e in G such that $ae = ea = a$ for all a in G. e is called the identity element of the group.
4. Existence of Inverse: For every a in G there exists a unique b in G such that $ab = ba = e$. b is called the inverse of a and is conventionally denoted by a^{-1}.

In addition to the above mentioned axioms, if it is also true that $ab = ba$ for all a and b in G, then G is said to be an *abelian group*. It must be noted that the property of being abelian is special in the sense that not all groups need be abelian. In any group, it is trivial to prove the following statements:

$$\begin{aligned} ax &= bx \Rightarrow a = b \\ xa &= xb \Rightarrow a = b \\ (ab)^{-1} &= b^{-1}a^{-1}. \end{aligned} \tag{1.1.1}$$

Due to the obvious simplicity of the definition, many familiar sets in mathematics are indeed seen to be examples of groups.

Example 1. The set of all integers Z is a group if the group product is taken to be the usual addition of integers. This group is clearly abelian and has an infinite number of elements.

□

Example 2. The set of all complex numbers C is a group under addition of complex numbers. This group again is abelian and infinite. □

Example 3. The set $C - \{0\}$ is an infinite abelian group under the usual multiplication of complex numbers. □

Example 4. The set of all 2×2 matrices with complex entries is an infinite abelian group under matrix addition. □

Example 5. The set of all invertible 2×2 matrices with complex entries is an infinite *non-abelian* group under matrix multiplication. □

A group G that contains a finite number of elements is called a *finite group*. The number of elements in a finite group G is called the *order* of the group and is denoted by $|G|$. For any element a in a group and a positive integer n, a^n represents $aa...a$ where there are n factors in the product. Similarly a^{-n} represents $(a^{-1})^n$. Before looking at some examples of finite groups, the following definition may be noted.

Definition 2. A subset S of elements of a group G is said to generate G if every element of G can be expressed as a finite product of finite powers of elements (or their inverses) of S in some order. If the set S is finite then the group G is said to be *finitely generated*. The elements of the minimal set S that generates a group G are called the *generators* of the group and S itself is called the *generating set*. A group whose generating set contains a single element is said to be a *cyclic group*.

A group is completely specified if its generators are known along with all the relations that exist between them. It is important to realize that a group may have more than one generating set. In case of finite groups though, the number of elements in all possible generating sets is the same.

Table 1.1 Klein-4 Group V

V	e	a	b	ab
e	e	a	b	ab
a	a	e	ab	b
b	b	ab	e	a
ab	ab	b	a	e

Example 6. The set $\{e\}$ along with the relation $e^2 = e$ generates the trivial group $\{e\}$ called the identity group of order 1. Henceforth, this group would be represented by the symbol E. □

Example 7. The set $\{a\}$ along with the relation $a^2 = e$ generates the group $\{e, a\}$ of order 2. □

Example 8. The set $\{a\}$ along with the relation $a^n = e$ (n being a positive integer) generates the cyclic group $\{e, a, a^2, \ldots, a^{n-1}\}$ of order n. Henceforth, this group would be represented by the symbol C_n. □

Example 9. The set $\{a, b\}$ along with the relations $a^2 = b^2 = e$ and $ab = ba$ generates the abelian group $V = \{e, a, b, ab\}$. The group V is called the Klein-4 group. It is useful to depict this group in the form of a multiplication table showing all possible products of various group elements as in Table 1.1. Such a table can be drawn for all finite groups. □

Example 10. A slightly less trivial example is that of a finite group generated by the set $\{a, b\}$ where a and b satisfy the relations $a^2 = b^3 = e$ and $ab = b^2a$. The generated group $\mathfrak{S}(3) = \{e, a, b, b^2, ab, ab^2\}$ is of order 6 and is non-abelian (Table 1.2). Any product involving a finite number of a's and b's can be reduced to one of the elements of $\mathfrak{S}(3)$ by use of the relations on a and b. The notation $\mathfrak{S}(3)$ will be clarified later. □

Table 1.2 Symmetric Group $\mathfrak{S}(3)$

$\mathfrak{S}(3)$	e	a	b	b^2	ab	ab^2
e	e	a	b	b^2	ab	ab^2
a	a	e	ab	ab^2	b	b^2
b	b	ab^2	b^2	e	a	ab
b^2	b^2	ab	e	b	ab^2	a
ab	ab	b^2	ab^2	a	e	b
ab^2	ab^2	b	a	ab	b^2	e

1.2 Subgroups

Definition 3. A subset H of a group G is called a subgroup if H is a group under the product operation defined on G. The identity group E and the group G are both subsets of the group G and are called the *trivial subgroups* of G. Other subgroups of G are called *non-trivial subgroups*.

For a subset H of a group G to be a subgroup, H must satisfy all the axioms stated in the Definition 1. If H is closed under the group product and every element of H has its inverse in H, then other axioms are automatically satisfied since H is merely a subset of the group G. If G is a finite group, then the condition on H to be a subgroup of G is even simpler: H would then just have to be closed under the group product.

Given a finite group G, it is easy to find cyclic subgroups of G. For example, if a is an element of G, all positive integral powers of a are also elements of G. G being a finite group implies that there are only finitely many integral powers of a which are distinct elements of G. This could happen only if there was some minimum positive integer n for which $a^n = e$, so that further powers of a would merely be repetitions of elements in the set $H = \{e, a, \ldots, a^{n-1}\}$. But then we have generated a cyclic subgroup H of G. The order of the subgroup generated by a is also called the order of the element a. Evidently, the order of every element of a finite group is finite.

Example 11. $\mathfrak{S}(3)$ has $\{e, a\}$, $\{e, ab\}$, $\{e, ab^2\}$, $\{e, b, b^2\}$ as its cyclic subgroups. □

Two subsets of a group G are said to be equal if they contain the same elements. If A and B are two subsets of G, then AB is the set of all elements of G which are equal to the product of an element of A with an element of B in that order. It is worth noting that AB and BA need not be equal sets. Suppose that H is a subgroup of G. If a is any element of G, Ha denotes a subset of G containing elements of the form ha where h runs through all the elements of H. Then Ha is called a *left coset* of the subgroup H. In the same way, a *right coset* aH can be defined. From hereon, by a coset we mean a left coset. It is evident that $H = He$, and therefore H is one of the cosets of H. Every element of G belongs to some coset of H because the coset Ha definitely contains a which could be any arbitrary element of G. Thus each and every coset of H contains every possible element of G. It is possible that two distinct elements a, b of G may belong to the same coset of H. This can happen only if there is some h in H such that $ha = b$, or in other words, ab^{-1} is in H. Also, two different cosets of H are disjoint. Suppose the two cosets had a common element a, then both the cosets must be equal to the coset Ha indicating that the intersection between two different cosets must be a null set. Hence for the finite group G, all the cosets of H contain same number of elements and are disjoint whose union is equal to G. This proves the important *Lagrange's theorem* which states that the order of every subgroup H of a finite group G divides the order of G. Lagrange's theorem does not imply that a subset of a finite group is definitely a subgroup if the number of elements in the subset divides the group order.

A group G may have several subgroups of various orders. Let H be a non-trivial subgroup of G. If a is an element of G, then aHa^{-1} is a set which contains elements of form aha^{-1} for every h in H. It can be verified that aHa^{-1} is also a subgroup of G. By choosing a different a each time, we can generate all possible subgroups of the form aHa^{-1}. Such subgroups are called *conjugate subgroups*. It is possible that one may get the same subgroup for different choices of a. If it turns out that for every choice of a, $aHa^{-1} = H$, then H is said to be a *normal subgroup* or *invariant subgroup*. Normal subgroups are special in the sense that they are invariant under conjugation by all the elements of the group, i.e., if k is an element of a normal subgroup K, then for all a in G, aka^{-1} is again an element of K. Further $aKa^{-1} = K \Rightarrow aK = Ka$, i.e., the left and right cosets of a normal subgroup are identical. The trivial subgroups of G are clearly normal. If G is abelian then every subgroup of G is normal. In case G has no non-trivial normal subgroups then G is said to be a *simple group*. Groups of prime order are examples of simple groups.

Example 12. Consider the group $\mathfrak{S}(3)$. With the notation $H_a = \{e,\ a\}$ for the cyclic subgroup generated by a and using the relations on the generators a and b, the following can be verified

$$aH_aa^{-1} = H_a;\ (ab)H_a(ab)^{-1} = H_{ab^2};\ (ab^2)H_a(ab^2)^{-1} = H_{ab}.$$

Thus H_a, H_{ab}, H_{ab^2} are conjugate subgroups. Also, H_b can be seen to be a normal subgroup of $\mathfrak{S}(3)$ and hence $\mathfrak{S}(3)$ is not a simple group. In fact H_b is the only non-trivial normal subgroup of $\mathfrak{S}(3)$. □

The non-trivial normal subgroups of a group play an important role in the study of the group's structure. If K is a normal subgroup of the group G, then the set of cosets of K is also a group, called the *factor group* of G with K. The factor group is denoted as G/K. Let Ka and Kb be two cosets of K. Defining the product of the two cosets $(Ka)(Kb)$ to be the set that contains elements of G which are equal to the product of an element of Ka with an element of Kb in that order. Then the elements of $(Ka)(Kb)$ have the form $k_1ak_2b = k_1ak_2a^{-1}ab = k_1k_3ab = k_4\ ab$. When k_1 takes all values in K, k_4 also takes all values in K. Thus $(Ka)(Kb) = Kab$ and we have closure in the set of cosets of K under the defined product. Associativity follows from $(KaKb)Kc = KabKc = K(ab)c = Ka(bc) = KaKbc = Ka(KbKc)$. The coset K serves as the identity in G/K and $(Ka)^{-1} = Ka^{-1}$. This proves G/K is a group.

1.3 Conjugacy Classes

Suppose a is an element of a group G. The set of all elements of G which are equal to gag^{-1} for some choice of g in G is called the *conjugacy class* of the element a. The elements of a conjugacy class are said to be conjugate elements of G. Conjugate elements, even though distinct, have important common properties. One

such property is that if a and b are conjugate then both must have same order. For instance, if a has order n and $b = gag^{-1}$ for some g, then

$$b^m = \underbrace{(gag^{-1})(gag^{-1})\ldots(gag^{-1})}_{m \text{ factors}} = ga^m g^{-1}. \tag{1.3.1}$$

The smallest positive integer m for which $ga^m g^{-1}$ is equal to e is clearly n. Hence b has the same order as a. The above expression also proves that if a and b are conjugate then so are their equal powers. Additionally, if a is conjugate to $b(a = gbg^{-1})$ and b is conjugate to $c(b = hch^{-1})$, then $a = ghch^{-1}g^{-1} = (gh)c(gh)^{-1}$. It follows that a is conjugate to c. The property of being conjugate is for this reason *transitive*.

The conjugate elements of G belong to the same conjugacy class. As every element of G is in its own conjugacy class $(a = eae^{-1})$, the whole group G can be divided into several conjugacy classes. It is important that two different conjugacy classes cannot have a common element. For if there was a common element, then that element would be conjugate to all the elements in both the conjugacy classes. By the transitivity property, it follows that the elements in the two classes would be conjugate and therefore must belong to the one and same class. The conjugacy classes of a group decompose the group into mutually exclusive sets. In case of an abelian group, the conjugacy classes consist of the individual group elements.

Example 13. Consider $\mathfrak{S}(3)$. Since $geg^{-1} = e$ for all g in $\mathfrak{S}(3)$, $\{e\}$ forms a conjugacy class. Also $bab^{-1} = bab^2 = ab^4 = ab$ and $(b^2)a(b^2)^{-1} = b^2ab = b^4a = ba = ab^2$, thus $\{a,\ ab,\ ab^2\}$ is a conjugacy class. $aba^{-1} = aba = b^2 \cdot a^2 = b^2$, and it follows $\{b,\ b^2\}$ is a conjugacy class. We note finally that

$$\mathfrak{S}(3) = \{e\} \cup \{a,\ ab,\ ab^2\} \cup \{b,\ b^2\}. \qquad \square$$

1.4 Further Examples of Groups

Two important groups are considered here in light of the concepts introduced in previous sections. They are namely: the *Quaternion Group* and the *Dihedral Group*. The quaternion group is a group structure on algebraic entities called *quaternions*. Quaternions were first considered in connection to classical mechanics. They have deep significance as regards mathematical constructs in various physical theories. We do not intend to explore this significance, but we would like to understand what quaternions are in principle. The dihedral group is of importance in the study of symmetries of a regular polygon. We will often encounter the dihedral group in later chapters.

The Quaternion Group Q

The quaternion group Q has 8 elements. Explicitly, the group $Q = \{e, s, i, j, k, si, sj, sk\}$. Various elements satisfy the relationships

$$s^2 = e; i^2 = j^2 = k^2 = ijk = s.$$

The symbols $i,\ j,\ k$ can be regarded as imaginary units, e as the real unit and s as negative e. The defining relations specify the group completely. The relation $i^2 = ijk$ implies $i = jk$. Likewise, $j = ki$ and $k = ij$. One may note the cyclic nature of these equalities. Furthermore, $i^2 = j^2 \Rightarrow (ji)(ij) = e$. Because $ij = k$ and $(sk)k = e$, it follows $ij = sji$. Likewise, $jk = skj$ and $ki = sik$. The identity element e obviously commutes with all the elements of Q, but so does the element s. For example, $i = jk \Rightarrow si = sjk$ and $ijk = s \Rightarrow sjk = is$. It follows that $si = is$. In a similar fashion it may be shown s commutes with j and k and hence with all the elements of Q. To sum up, we may note the relations that follow from the defining relationships.

$$\begin{aligned} i = jk, &\quad j = ki, &\quad k = ij, \\ ij = sji, &\quad jk = skj, &\quad ki = sik, \\ si = is, &\quad sj = js, &\quad sk = ks. \end{aligned}$$

The non-trivial subgroups of Q can be of order 2 or 4. The subgroup of order 2 is $\{e,\ s\}$. The three subgroups of order 4 are $\{e,\ s,\ i,\ si\}$, $\{e,\ s,\ j,\ sj\}$ and $\{e,\ s,\ k,\ sk\}$. Each of the order-4 subgroups is isomorphic to the cyclic group C_4. It can be verified that all the subgroups of Q are normal in Q. The conjugacy classes of Q can be found from the relationships given above. Since e and s commute with all the elements, they are the only elements in their respective classes. Since $jij^{-1} = sijj^{-1} = si$, it follows i and si are conjugate. Similarly, j and sj are conjugate, and also k and sk are conjugate. The decomposition of Q in conjugacy classes is.

$$Q = \{e\} \cup \{s\} \cup \{i,\ si\} \cup \{j,\ sj\} \cup \{k,\ sk\}.$$

The Dihedral Group $D_n (n \geq 3)$

The dihedral group D_n has $2n$ elements. It can be generated by the symbols r and s satisfying the relationships as under

$$r^n = s^2 = e,\ sr = r^{-1}s.$$

Explicitly, $D_n = \{e,\ s,\ r,\ r^2,\ \ldots r^{n-1},\ sr,\ sr^2,\ \ldots sr^{n-1}\}$. Any product of a finite number of r's and s's can be reduced to one of the group elements using the defining relationships. Consider

$$r^k s = \underbrace{rr\ldots r}_{k \text{ factors}} \quad s = \underbrace{rr\ldots r}_{k-1 \text{ factors}} \quad sr^{-1} = sr^{-k} = sr^{n-k},$$

and likewise in other cases. The subgroup $\{e,\ s\}$ is the smallest non-trivial subgroup. The cyclic subgroup generated by r, $\{e,\ r,\ r^2,\ \ldots r^{n-1}\}$ is a normal subgroup of D_n. If a

positive integer k is a divisor of n then r^k will generate a cyclic subgroup of D_n. In order to calculate the conjugacy classes, the following relationships are useful:

$$sr^k s = r^{-k},$$
$$r^{-k} s r^k = s r^{2k},$$
$$(sr^t) r^k (sr^t)^{-1} = s r^t r^k r^{-t} s = r^{-k}.$$

In the case when n is $2p+1$, there are $p+2$ classes. The decomposition of D_{2p+1} into classes is

$$D_{2p+1} = \{e\} \cup \underbrace{\{r, r^{2p}\} \cup \{r^2, r^{2p-1}\} \cup \ldots \{r^p, r^{p+1}\} \cup}_{p \text{ classes}} \tag{1.4.1}$$
$$\cup \{s, sr, sr^2, \ldots sr^{2p}\}.$$

In the case when n is $2p$, there are $p+3$ classes. The decomposition of D_{2p} is seen to be

$$D_{2p} = \{e\} \cup \{r^p\} \cup \underbrace{\{r, r^{2p-1}\} \cup \ldots \{r^{p-1}, r^{p+1}\}}_{p-1 \text{ classes}} \cup \tag{1.4.2}$$
$$\cup \{s, sr^2, \ldots sr^{2p-2}\} \cup \{sr, sr^3, \ldots sr^{2p-1}\}.$$

1.5 Homomorphism of Groups

A *homomorphism* between two groups is a function from one to the other that preserves products. More specifically, a function φ from a group G to a group T is a homomorphism if for all $a,\ b$ in G

$$\varphi(ab) = \varphi(a)\varphi(b). \tag{1.5.1}$$

Here the notation $\varphi(a)$ stands for the member of T which is the image of a under the function φ. If a and b are both chosen to be identity element e of G then $\varphi(e) = [\varphi(e)]^2$ and it follows that the identity of G is mapped to the identity of T. Also, if $b = a^{-1}$, then $\varphi(e) = \varphi(a)\varphi(a^{-1})$ and it follows that $\varphi(a^{-1}) = [\varphi(a)]^{-1}$. In other words, under a homomorphism, identity is mapped to identity and inverse is mapped to inverse. The subset K of G which contains all the elements which are mapped to the identity of T is called the *kernel* of the homomorphism φ. It can be shown that the kernel K is a normal subgroup of G. In fact all the normal subgroups of G would cause a homomorphism of G into some group. It can be also shown that all elements of a coset of K are mapped to the same element of T.

Example 14. Let $C_2 = \{E,\ A\}$ where C_2 is the cyclic group of order 2 in our notation and E here is the identity element of C_2. Consider a function φ from $\mathfrak{S}(3)$ to C_2 defined as

$$\varphi(e) = \varphi(b) = \varphi(b^2) = E,$$

$$\varphi(a) = \varphi(ab) = \varphi(ab^2) = A.$$

Then φ is a homomorphism. The kernel of this homomorphism is the normal subgroup H_b. □

When the kernel of a homomorphism is simply the trivial group E, then the homomorphism is one to one. In this case the two groups are said to be *isomorphic*. Isomorphic groups are essentially the same group and differ merely in the manner of labelling of their elements. In the study of *point groups*, it will be seen that some of them are isomorphic groups. In case of the group $\mathfrak{S}(3)$, the factor group $\mathfrak{S}(3)/H_b$ is isomorphic to the group C_2. In notation,

$$C_2 \cong \mathfrak{S}(3)/H_b. \tag{1.5.2}$$

Suppose now that φ_1 is a homomorphism from G_0 into G_1 and that φ_2 is a homomorphism from G_1 into G_2. It is then possible to compose φ_1 and φ_2 together to give a homomorphism ψ from G_0 into G_2. For $a \in G_0$, define ψ so that

$$\psi(a) = \varphi_2(\varphi_1(a)).$$

It is easy to show that with the above definition, ψ is a homomorphism from G_0 into G_2.

1.6 The Symmetric Group

Consider a set of n distinct letters $\{1, 2, \ldots n\}$ arranged in that order. Any rearrangement of this set of elements is called a *permutation*. For example, if $n = 3$, then all the permutations are

$$\begin{aligned}
\pi_1 &= \begin{pmatrix} 1 & 2 & 3 \\ 1 & 2 & 3 \end{pmatrix}; \quad \pi_4 = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} \\
\pi_2 &= \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}; \quad \pi_5 = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} \\
\pi_3 &= \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix}; \quad \pi_6 = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 1 & 2 \end{pmatrix}.
\end{aligned}$$

A permutation that leaves the positions of all the letters unchanged is called the identity permutation. In the example above, π_1 is the identity permutation. Remember that the exchange amongst columns in the above elements denote the same permutation operation. That is,

$$\pi_5 = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 1 & 3 \\ 3 & 2 & 1 \end{pmatrix}.$$

A product operation may be defined in the set of permutations so that the product of two permutations is another permutation. The operation of forming the product of two permutations can be most easily understood by considering the concrete case of $n = 3$. Consider the product $\pi_2\pi_5$. π_2 takes 1 to 2 and π_5 takes 2 to 3, thus $\pi_2\pi_5$ takes 1 to 3. In this manner the action of $\pi_2\pi_5$ can be ascertained on all the letters

$$\begin{aligned}
\pi_2\pi_5 &= \begin{pmatrix} 1 & 2 & 3 \\ 2 & 1 & 3 \end{pmatrix}\begin{pmatrix} 2 & 1 & 3 \\ 3 & 2 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{pmatrix} = \pi_4, \\
\pi_5\pi_2 &= \begin{pmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \end{pmatrix}\begin{pmatrix} 2 & 3 & 1 \\ 1 & 3 & 2 \end{pmatrix} = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 3 & 2 \end{pmatrix} = \pi_3.
\end{aligned}$$

Similarly, one may verify that the product so defined is associative. Also $(\pi_2)^{-1} = \pi_2$, $(\pi_3)^{-1} = \pi_3$, $(\pi_4)^{-1} = \pi_4$, $(\pi_5)^{-1} = (\pi_5)^2 = \pi_6$, $(\pi_6)^{-1} = (\pi_6)^2 = \pi_5$. Thus the set of permutations on three letters is a group. In fact, this is the same group as $\mathfrak{S}(3)$ if we identify π_1 with e, π_2 with a, π_5 with b, π_6 with b^2, π_4 with ab and π_3 with ab^2. Since $\mathfrak{S}(3)$ is the group of all permutations on 3 letters, it is called the *symmetric group* of degree 3. In the general case of permutations on n letters, $\mathfrak{S}(n)$ is called the symmetric group of degree n. The order of $\mathfrak{S}(n)$ is $n!$, the total number of permutations of n letters. Subgroups of $\mathfrak{S}(n)$ are called *permutation groups*. The very important *Cayley's Theorem* states that every group is isomorphic to a permutation group which is embedded in some symmetric group. In particular, if G is a group of order n, then it is isomorphic to a subgroup of $\mathfrak{S}(n)$. In order to see this, label the elements of G so that $G = \{g_1(= e),\ g_2,\ \ldots g_n\}$. Let g be some element of G. If every element of G is multiplied with g from right, then we have a permutation π_g induced on the letters $\{g_1,\ g_2,\ \ldots g_n\}$ which can be written as

$$\pi_g = \begin{pmatrix} g_1 & g_2 & \cdots & g_n \\ g_1g & g_2g & \cdots & g_ng \end{pmatrix}.$$

Another element h of G induces a permutation π_h so that the product $\pi_g\pi_h$ is given by

$$\begin{aligned}
\pi_g\pi_h &= \begin{pmatrix} g_1 & g_2 & \cdots & g_n \\ g_1g & g_2g & \cdots & g_ng \end{pmatrix}\begin{pmatrix} g_1 & g_2 & \cdots & g_n \\ g_1h & g_2h & \cdots & g_nh \end{pmatrix} \\
&\Rightarrow \quad \pi_g\pi_h = \begin{pmatrix} g_1 & g_2 & \cdots & g_n \\ g_1gh & g_2gh & \cdots & g_ngh \end{pmatrix} \\
&\Rightarrow \quad \pi_g\pi_h = \pi_{gh}.
\end{aligned}$$

This proves that the mapping $g \to \pi_g$ is a homomorphism (Equation 1.5.1). Because two distinct elements of G induce distinct permutations, it follows that the group G and the set of permutations $\{\pi_{g_1},\ \pi_{g_2},\ \ldots \pi_{g_n}\}$ are isomorphic. This proves the Cayley's Theorem for finite groups.

A permutation can also be represented as a product of disjoint *permutation cycles*. Consider the following permutation on 7 letters.

$$\pi = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 5 & 7 & 3 & 4 & 6 & 1 & 2 \end{pmatrix}.$$

π permutes the letters 1, 5, 6 among themselves, and also 2, 7 among themselves while leaving 3 and 4 in their places. This can also be represented as

$$1 \overset{\pi}{\to} 5 \overset{\pi}{\to} 6 \overset{\pi}{\to} 1,\ 2 \overset{\pi}{\to} 7 \overset{\pi}{\to} 2,\ 3 \overset{\pi}{\to} 3,\ 4 \overset{\pi}{\to} 4.$$

Here $(1,5,6)$ is a three-cycle, $(2,7)$ is a two-cycle, (3) and (4) are one-cycles. It is now simpler to write $\pi = (1,5,6)(2,7)(3)(4)$. Since elements in one-cycles are unmoved by the permutation, it is redundant to mention them [for this reason it is conventional to represent the identity permutation simply by the empty cycle $()$]. The decomposition of π in disjoint cycles is therefore

$$\pi = (1,5,6)(2,7).$$

The cycle decomposition is particularly useful in carrying out calculations with permutations. Consider another permutation

$$\sigma = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 1 & 4 & 6 & 5 & 7 & 3 & 2 \end{pmatrix} = (3,6)(2,4,5,7).$$

The products $\pi\sigma$ and $\sigma\pi$ can be easily read from the cycle decompositions of the two to be

$$\pi\sigma = (1,7,4,5,3,6);\ \sigma\pi = (1,5,2,4,6,3).$$

It may be noted that π (product of a two-cycle and a three-cycle) and σ (product of a two-cycle and a four-cycle) have different cycle structure while $\sigma\pi$ and $\pi\sigma$ both has the same six-cycle structure. Further, $(1,5,2,4,6,3)$, $(5,2,4,6,3,1)$ and $(3,1,5,2,4,6)$ represent the same permutations, i.e., positions in a cycle can be changed cyclically without affecting the permutation.

The inverse of a permutation can be obtained by inspection. For example, π is a product of a three-cycle and a two-cycle. Since both the cycles are disjoint, π^{-1} would be a product of the inverses of the two cycles. A two-cycle like (2, 7) is called a *transposition*. It is obvious that the inverse of a transposition is the transposition itself. As for the three-cycle $(1,5,6)$, its inverse should take 5 to 1, 1 to 6 and 6 to 5, i.e., $(1,5,6)^{-1} = (1,6,5)$. Thus $\pi^{-1} = (1,6,5)(2,7)$, and calculating similarly, $\sigma^{-1} = (3,6)(2,7,5,4)$.

Since a transposition interchanges positions of only two letters, it is the most elementary type of permutation. It is natural to expect that all permutations can be

built up from transpositions. It can be checked readily that the k-cycle (1, 2, .., k) is equivalent to a product of $k-1$ transpositions

$$(1,2,\ldots,\ k) = (1,2)(1,3)\ldots(1,\ k).$$

As any permutation is a product of disjoint cycles, it can be expressed as a product of transpositions. Depending on whether an odd or an even number of transpositions are involved in the product, the permutation is called *odd* or *even* correspondingly. No permutation is both even and odd.

In the symmetric group $\mathfrak{S}(n)$, it is evident that not all elements would have similar cycle structure. Any permutation in $\mathfrak{S}(n)$ can be written as a product of disjoint i_k k-cycles, where k ranges from 1 to n as in

$$\underbrace{\left(a_1^{(1)}\right)\ldots\left(a_{i_1}^{(1)}\right)}_{i_1 1-\text{cycles}}\underbrace{\left(b_1^{(1)},b_1^{(2)}\right)\ldots\left(b_{i_2}^{(1)},b_{i_2}^{(2)}\right)}_{i_2 2-\text{cycles}}\ldots$$

$$\ldots\underbrace{\left(t_1^{(1)},t_1^{(2)},\ldots t_1^{(n)}\right)\ldots\left(t_{i_n}^{(1)},t_{i_n}^{(2)},\ldots t_{i_n}^{(n)}\right)}_{i_n n-\text{cycles}}$$

It is clear that $\Sigma_{k=1}^{n} k i_k = n$, where some of the i_k's can be 0. Using elementary combinatorics, it can be proved that the total number of such permutations is given by the following expression:

$$n!\prod_{k=1}^{n}\frac{1}{i_k!(k)^{i_k}}. \tag{1.6.1}$$

The significance of having identical cycle structure is that all such elements are conjugate in $\mathfrak{S}(n)$ and hence belong to the same conjugacy class. Suppose that σ and π are permutations on same set of letters. Let them be represented by:

$$\sigma = (a_{11}\ldots a_{1s_1})(a_{21}\ldots a_{2s_2})\ldots\ (a_{t1}\ldots a_{ts_t}),$$

$$\pi = \begin{pmatrix} a_{11} & \cdots & a_{1s_1} & a_{21} & \cdots & a_{2s_2} & \cdots & a_{t1} & \cdots & a_{ts_t} \\ b_{11} & \cdots & b_{1s_1} & b_{21} & \cdots & b_{2s_2} & \cdots & b_{t1} & \cdots & b_{ts_t} \end{pmatrix}.$$

Consider the action of $\pi^{-1}\sigma\pi$ on b_{11} : $b_{11} \overset{\pi^{-1}}{\to} a_{11} \overset{\sigma}{\to} a_{12} \overset{\pi}{\to} b_{12}$, which means that $\pi^{-1}\sigma\pi$ sends b_{11} to b_{12} and so on. In effect,

$$\pi^{-1}\sigma\pi = (b_{11}\ldots b_{1s_1})(b_{21}\ldots b_{2s_2})\ldots\ (b_{t1}\ldots b_{ts_t})$$

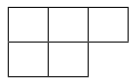
and the conclusion is that conjugate elements have the same cycle structure. From the above it is also clear that given two permutations in $\mathfrak{S}(n)$ having identical cycle structures (the RHS of σ and $\pi^{-1}\sigma\pi$), one can always find a permutation in $\mathfrak{S}(n)$(the RHS of π) so that the first two permutations are related via conjugation by the third.

The conjugacy classes of $\mathfrak{S}(n)$ are distinguished by the cycle structure of elements in the class. Expression 1.6.1 gives the number of permutations in a conjugacy class of a specified cycle structure.

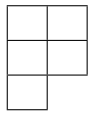
The number of conjugacy classes in $\mathfrak{S}(n)$ is the number of ways in which n can be expressed as a sum of positive integers. For example, if $n = 5$ then there are 7 partitions of n, namely $1+1+1+1+1, 1+2+2, 3+2, 1+4$, 1+1+1+2, 1+1+3 and 5. $\mathfrak{S}(5)$ therefore has 7 conjugacy classes. These conjugacy classes may be conveniently represented by *Young diagrams*. A Young diagram is an arrangement of a certain number of boxes in left justified rows such that the number of boxes in a row is at least as large as the number of boxes in the row below it. Below are listed the Young diagrams for conjugacy classes of $\mathfrak{S}(5)$.

1. The Identity class contains the identity permutation as its only member. The identity is simply the product of 5 one-cycles.

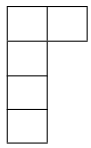
2. Product of 2 two-cycles and 1 one-cycle



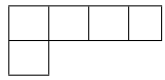
3. Product of 1 three-cycle and 1 two-cycle



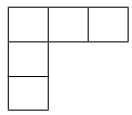
4. Product of 1 four-cycle and 1 one-cycle



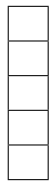
5. Product of 1 two-cycle and 3 one-cycles



6. Product of 1 three-cycle and 2 one-cycles



7. A five-cycle



In the symmetric group $\mathfrak{S}(n)$, the set of all even permutations forms a group called the *alternating group* $\mathfrak{U}(n)$. That $\mathfrak{U}(n)$ is a group follows from the fact that product of two even permutations is an even permutation. The conjugates of an even permutation would have identical cycle structure, and therefore would all be even. It follows that $\mathfrak{U}(n)$ is a normal subgroup of $\mathfrak{S}(n)$. This further implies that the factor group $\dfrac{\mathfrak{S}(n)}{\mathfrak{U}(n)}$ is the set of cosets of $\mathfrak{U}(n)$. Suppose now

$$\frac{\mathfrak{S}(n)}{\mathfrak{U}(n)} = \{\mathfrak{U}(n),\ \mathfrak{U}(n)(1,2),\ O_1,\ \ldots\}.$$

Here $\mathfrak{U}(n)(1,2)$ is a coset of $\mathfrak{U}(n)$ obtained by multiplying all elements of $\mathfrak{U}(n)$ with the transposition (1, 2) and O_1 is another coset of $\mathfrak{U}(n)$ containing only odd permutations. Then $O_1\mathfrak{U}(n)(1,2)$ is also a coset of $\mathfrak{U}(n)$. $O_1\mathfrak{U}(n)(1,2)$ can contain only even permutations. Because the only coset of $\mathfrak{U}(n)$ containing even permutations is $\mathfrak{U}(n)$ itself, we have $O_1\mathfrak{U}(n)(1,2) = \mathfrak{U}(n)$. $\mathfrak{U}(n)$ is the identity of the factor group and it follows that $O_1 = [\mathfrak{U}(n)(1,2)]^{-1}$ But $[\mathfrak{U}(n)(1,2)]^{-1} = \mathfrak{U}(n)(1,2)$ and we have the result that there are only two cosets of $\mathfrak{U}(n)$, one being $\mathfrak{U}(n)$ and the other being the set of all odd permutations. Thus the order of the group $\mathfrak{U}(n)$ is $\dfrac{n!}{2}$.

1.7 Direct and Semi-direct Products

Two groups G_1 and G_2 can be used to form a larger group G by a construction called the *direct product* of groups. The direct product of G_1 and G_2 is denoted as $G = G_1 \times G_2$. Every element of G should be uniquely expressible as a product of an element of G_1 and an element of G_2. In forming the direct product, $G_1 \times G_2$ is not distinguished from $G_2 \times G_1$. Consequently, every element of G_1 should commute with every element of G_2. With these properties, it can be seen that G_1 and G_2 are normal subgroups of G. The only element common to G_1 and G_2 is the identity, for if g_1 is in G_1 and g_2 is in G_2, then $g_1 g_2 g_1^{-1} g_2^{-1} = e$ because of commutation. Because G_1 is normal $g_1(g_2 g_1^{-1} g_2^{-1})$ is an element of G_1, and because G_2 is normal $(g_1 g_2 g_1^{-1}) g_2^{-1}$ is an element of G_2, and both are equal to the identity element. It is clear that $|G| = |G_1| \times |G_2|$.

Example 15. Consider the groups $C_2 = \{e,\ a\}$ and $C_3 = \{e,\ b,\ b^2\}$. From the prescription above, the direct product

$$C_2 \times C_3 = \{e,\ a,\ b,\ b^2,\ ab,\ ab^2\}.$$

It may now be noted that the element ab generates the group $C_2 \times C_3$, and order of ab is 6. In fact $C_2 \times C_3$ is isomorphic to C_6. In other words

$$C_6 = C_2 \times C_3.$$ □

In the general case, a direct product may be constructed for any number of groups, the groups themselves being finite or infinite. We do not present this construction here. Finally it may be noted that a finite group G may be expressed as a direct product of its normal subgroups $K_1,\ K_2, .,\ K_s$ under the following conditions:

1. $G = K_1 K_2 \ldots K_s$.
2. Every element of G is uniquely expressible as a product of elements from each of the normal subgroups K_i.

In a group G, let K be a non-trivial normal subgroup. Let T be another non-trivial subgroup of G such that the identity is the only common element in K and T. Due to normality of K, we have $KT = TK$. Suppose all the group elements $g_i \in G$ can be written as product $k_i t_j$ where $k_i \in K$ and $t_i \in T$. That is, $G = KT$. In this circumstance, G is said to be a *semi-direct product* of K by T. The notation for the same is

$$G = K \rtimes T.$$

Notice the positioning of the groups K and T about $\rtimes$. For t_1 and t_2 in T, Kt_1 and Kt_2 are cosets of K. These two cosets will be same only if $t_1 t_2^{-1}$ is in K. Because $t_1 t_2^{-1}$ is a member of both K and T, from aforementioned conditions on K and T it follows that $t_1 = t_2$. The conclusion is that distinct elements of T are in distinct cosets of K and therefore can be chosen as the coset representatives. Additionally Kt_i, with t_i in T exhaust all the cosets of K in G since $G = KT$. If the subgroup T is also normal in G then G is the direct product $K \times T$.

Example 16. It was noted in Section 1.6 that the alternating group $\mathfrak{U}(n)$ is a normal subgroup of $\mathfrak{S}(n)$. For $n \geq 3$, let T be the group of order 2 generated by a transposition such as (1, 2). Then

$$\mathfrak{S}(n) = \mathfrak{U}(n) \times T.$$ □

Exercises

1. For the following sets S and binary operation $*$ on S, determine which of the group axioms stated in Definition 1 are satisfied
   1) $S = N,\ m * n = \max\{m,\ n\}$ for $m,\ n$ in N.
   2) $S = Z,\ m * n = m + n + 1$ for $m,\ n$ in Z.
   3) S is the set of $n \times n$ invertible real matrices $(\mathrm{n} \geq 2),\ A * B = [AB + BA]$.
2. Prove the statements in Equations 1.1.1.
3. Show that a subset H of a finite group G is a subgroup of G if H is closed under the group product.
4. If H is a subgroup of G and a is any arbitrary element of G, then show that aHa^{-1} is a subgroup of G.
5. Write the multiplication table of D_3 and determine the conjugacy classes.
6. If K is a normal subgroup of the group G and A is any subset of elements of G, show that $KA = AK$.
7. For subsets A and B of a group G, let AB represent the subset of G containing elements ab such that a is in A and b is in B. If A and B are subgroups of G, and at least one of them is normal in G, show that every finite product of elements of A and B is an element of AB.
8. With reference to Equation 1.5.1, show that the kernel K of the homomorphism ϕ is a subgroup of G. Further show that K is a normal subgroup of G.
9. In a homomorphism ϕ, is it always true that the orders of the element a and its image $\phi(a)$ are equal? What if ϕ is an isomorphism?
10. Find an isomorphism between a set of positive reals (a group under ordinary multiplication) and all the reals (a group under ordinary addition).
11. Of the groups C_4, D_2 and the Kelin-4 group V, which are the isomorphic groups? Are the groups D_4 and Q isomorphic?
12. Consider the group D_4. List all its conjugacy classes and its subgroups. Are all the non-trivial subgroups of D_n cyclic?
13. Show that all possible products generated by the Pauli matrices $i\sigma_1$ and $i\sigma_2$ form a group. Write the multiplication table of this group and determine the conjugacy classes. This group is isomorphic to which one of the groups considered in the chapter?

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}.$$

14. Show that the composition of homomorphisms defined in Section 1.5 is again a homomorphism.

15. Consider the direct product $C_2 \times C_6$ and state whether it is isomorphic to the cyclic group C_{12}.
16. For the symmetric group $\mathfrak{S}(6)$, determine the number of conjugacy classes and the number of permutations belonging to each class. Prepare a Young diagram representation of the classes as illustrated for $\mathfrak{S}(5)$ in the text.
17. Prove that the number of elements belonging to a conjugacy class in $\mathfrak{S}(n)$ is given by Expression 1.6.1.
18. Show that the alternating group $\mathfrak{A}(n)$ is generated by the set of all the three-cycles on n letters.
19. Consider the group $\mathfrak{S}(4)$. Determine its conjugacy classes and the number of elements in each class. Repeat the same exercise for $\mathfrak{A}(4)$. Do the elements appearing in a conjugacy class in $\mathfrak{S}(4)$ appear in the same class in $\mathfrak{A}(4)$?
20. In the group $\mathfrak{S}(4)$, consider the subgroups

$$V = \{(),\ (1,2),\ (3,4),\ (1,2)(3,4)\}$$

and $V_N = \{(),\ (1,2)(3,4),\ (1,3)(2,4),\ (1,4)(2,3)\}$. Show that V_N is normal in $\mathfrak{S}(4)$ while V is not. Realize $\mathfrak{S}(4)$ as a semi-direct product of V_N with another subgroup of $\mathfrak{S}(4)$.

21. Verify $(1,\ 2,\ 3,\ \ldots a,\ a+1,\ \ldots n) = (a,\ a+1,\ \ldots n)(1,2,3,\ \ldots a)$.
22. The generators of the symmetric group $\mathfrak{S}(n)$ are $(1,2), (1,2,\ldots n)$. Verify this statement for $\mathfrak{S}(4)$.
23. Let $P_i = (i, i+1)$ denote transposition element of $\mathfrak{S}(n)$ involving neighbouring objects. Show that

$$P_i P_{i+1} P_i = P_{i+1} P_i P_i;\ P_i P_j = P_j P_i \text{ for } |i-j| \geq 2.$$

Incidentally, these relations are similar to the defining relations of generators $b_i's$ of *braid group* $\mathfrak{B}(\mathfrak{n})$ which emerge as natural symmetry of exchange of neighbouring objects in a two-dimensional plane with $b_i^2 \neq P_i^2 = \mathrm{I}$.

2

Molecular Symmetry

In this chapter, we will focus on the symmetries possessed by molecules. By symmetrical transformation of an object, we mean any *rigid* geometric transformation under which the object remains invariant. The three types of rigid transformations are *translations, reflections* and *rotations*. Translations are relevant to the study of symmetries of crystals which is not considered here. For objects of finite size, e.g. a molecule, a translation of the object as a whole definitely does not change its shape and size, but the final position of the object does not exactly overlap its initial position. For this reason, a translation is not an *element of symmetry* of a molecule. However, rotations and reflections or any combinations of the two are elements of symmetry of a molecule. A rotation is a *proper* transformation because it preserves handedness. On the other hand, reflection is *an improper* transformation. We will present symmetry operations and their resemblance to finite group elements discussed in the previous chapter.

2.1 Elements of Molecular Symmetry

All the possible symmetry transformations of a molecule can be described in terms of some basic transformations. Of these transformations, the simplest is the *identity transformation* E, which leaves the molecule untouched. This transformation should remind the reader of the identity element of a group.

A molecule may have an *axis of symmetry* about which, if the molecule is rotated by a certain minimum angle (say $\frac{2\pi}{n}$), then it appears just as before the rotation. This transformation is symbolically represented as C_n, and the axis is a n-fold axis. It is obvious that rotation by the same angle for n consecutive times would bring the

molecule to the exact same configuration as it was before the rotations were carried out. The order of the transformation C_n is n.

$$C_n^n = E. \tag{2.1.1}$$

Because $C_n^k C_n^{n-k} = E$, C_n^{n-k} may be regarded as the inverse operation of C_n^k. It may so happen that a molecule has more than one axis of symmetry. In such a case the axis with maximum n may be called the *principal axis of symmetry*, though this nomenclature is not absolutely necessary. It is conventional to identify the principal axis with the z-axis of the coordinate system. In the special case when there is a two-fold axis of symmetry perpendicular to the principal axis, the two-fold axis would be symbolically represented by U_2.

A certain plane through a molecule may exist such that reflection of the molecule in it leaves the molecule indistinguishable from the original. Such a plane is called a *plane of symmetry* A molecule may have more than one such plane. In case the plane contains the principal axis, it is the vertical plane and the transformation corresponding to reflection through this plane is denoted by σ_v. Reflections in a plane of symmetry perpendicular to the principal axis are denoted by σ_h (horizontal). Occasionally, as in case of symmetries of a cube, diagonal planes of symmetry exist, denoted by σ_d. Order of all the reflection operations is clearly 2.

$$\sigma_v^2 = \sigma_h^2 = \sigma_d^2 = E. \tag{2.1.2}$$

A molecule may have a *roto-reflection symmetry*. This happens if there is a σ_h plane perpendicular to a C_n axis. A roto-reflection transformation, S_n, can be visualized as a C_n rotation followed by a σ_h reflection.

$$S_n = C_n \sigma_h = \sigma_h C_n. \tag{2.1.3}$$

It is obvious from Figure 2.1.1 that the order in which C_n and σ_h are carried out is immaterial. If n is an odd integer, then n consecutive roto-reflections on the molecule would merely be equivalent to a reflection in the horizontal plane, for $S_n^n = (C_n \sigma_h)^n = C_n^n \sigma_h^n = \sigma_h$. It follows that S_n is a truly distinct element of symmetry only if n is an even integer, the order of S_n in this case being n.

Lastly, a molecule may have *inversion symmetry*, C_i. Such a symmetry occurs if the molecule has a *point of symmetry*. The property of such a point is that all the atoms of the molecule lie on lines passing through the point and for every atom lying on some line, there exists another identical atom at the same distance behind the point of symmetry as the first atom is in front of it. Clearly $C_i^2 = E$. Figure 2.1.2 illustrates inversion symmetry.

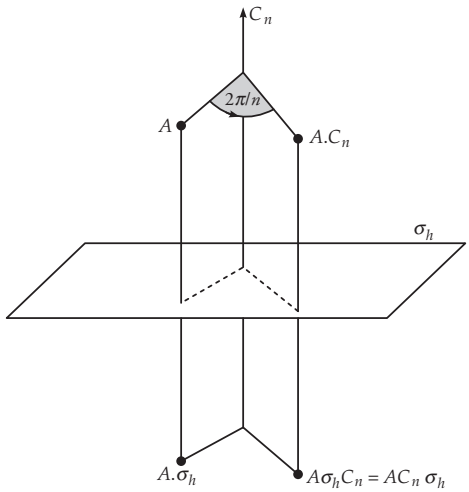


Figure 2.1.1 Roto-Reflection Symmetry.
The figure shows the action of $C_n\sigma_h$ and $\sigma_h C_n$ on an atom A of some molecule

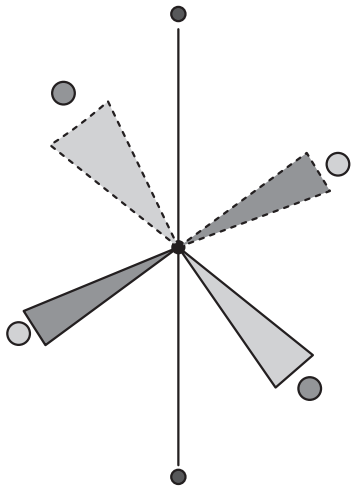


Figure 2.1.2 Inversion Symmetry.
The central dark sphere is the point of symmetry of this hypothetical molecule

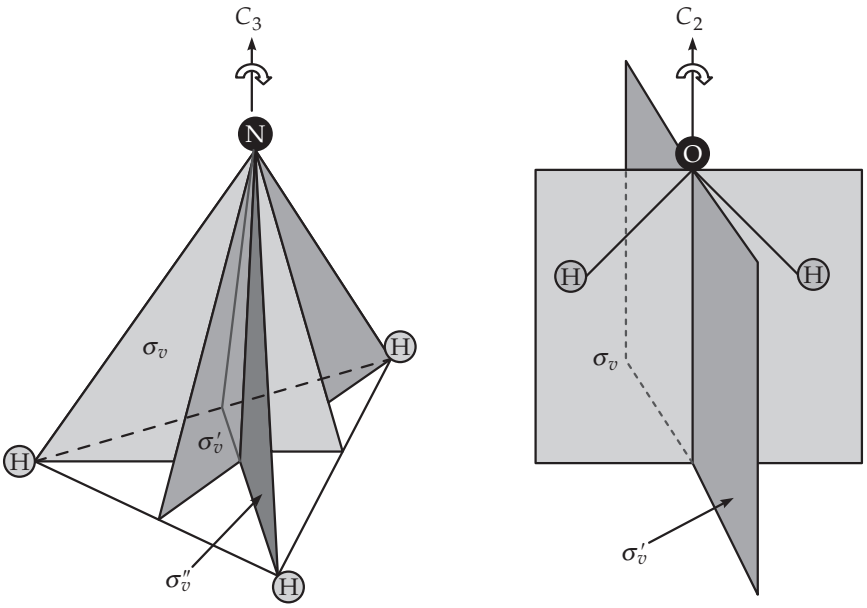
2.2 The Symmetry Group of a Molecule

A molecule may possess one or more of the symmetry elements depending upon its structure. Once the symmetry elements of the molecule are identified, one may compose them (in other words, form their products) in various ways and

generate all possible symmetry transformations of the molecule. The manner of composition of symmetries is to perform each transformation in the prescribed sequence. For example, if a molecule has a five-fold symmetry axis and a horizontal plane of symmetry, then the operation $C_5^3\sigma_h$ would mean 3 consecutive rotations of 72° about the principal axis followed by a reflection in the horizontal plane. As each elementary transformation leaves the molecule invariant, it is clear that any transformations composed of elementary transformations are also symmetry transformations. This shows that the set of symmetry transformations is closed under product operation. Equivalently, these transformations imply that all the symmetry axes and symmetry planes of a molecule must coincide at one point.

Note that every elementary symmetry transformation or composed transformation on a molecule permutes all the identical atoms in the molecule (bijection of space points). It is evident that the set of all elementary as well as composed symmetry transformations form a group. The set contains identity element E which corresponds to no symmetry operation. For every elementary symmetry operation A, we can show that their inverse operation A^{-1} is in the set. If C and B are elementary symmetry operations, then for the symmetry operation CB, the inverse can be defined to be $B^{-1}C^{-1}$. Such a group is an example of a *point group* as there is at least one point in the molecule which remains fixed in all the symmetry transformations.

The number of elements in a point group is finite except for the special case of linear molecules. This follows from the Cayley's Theorem since the point group of a non-linear molecule will be isomorphic to a subgroup of some symmetric group $\mathfrak{S}(n)$. Just like any abstract group, a point group can be decomposed into its conjugacy classes. The conjugacy classes are of importance in the study of *group representations* as will be seen in the next chapter. It is therefore necessary to figure out the conjugacy classes of a given point group. Having identified the various symmetry axes (planes), those axes (planes) are labeled as *equivalent* which can be brought to coincide in direction by a symmetry transformation of the molecule. Symmetry axes of different orders cannot be equivalent. Consider the ammonia molecule shown in Figure 2.2.1. All the σ_v planes are equivalent as the alternate planes can be made to coincide with each other after rotation by an angle of $\frac{2\pi}{3}$ about the C_3 axis ($\sigma_v \overset{C_3}{\to} \sigma_v'' \overset{C_3}{\to} \sigma_v' \overset{C_3}{\to} \sigma_v$). However, the σ_v planes in the water molecule are not equivalent. In the Figure 2.2.2 are shown the symmetry axes of a cube. There are 3 C_4 axes, 4 C_3 axes and 6 C_2 axes. It is easy to verify that all the C_4 axes are equivalent, so are all the C_3 axes as well as all the C_2 axes.



(a) NH_3 (C_{3v} symmetry) (b) H_2O (C_{2v} symmetry)

Figure 2.2.1 Equivalent and Non-equivalent Reflection Planes

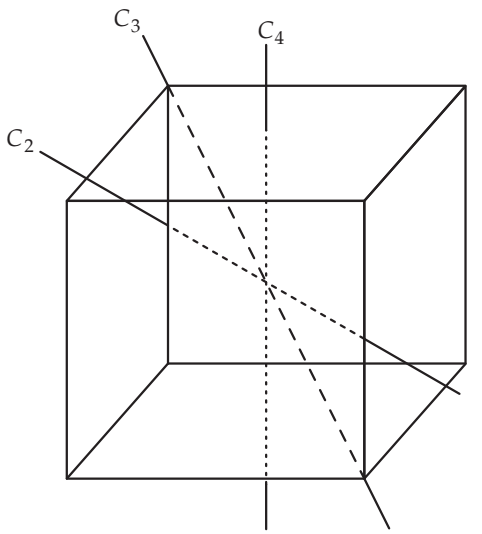


Figure 2.2.2 Symmetry Axes of a Cube

Equal rotations about equivalent axes are conjugate transformations in the symmetry group of a molecule. In order to see this, suppose A_1 and A_2 are two equivalent symmetry axes (C_n) of a molecule. Then there exists some symmetry transformation S of the molecule which carries A_1 to A_2. Then the transformation

$SC_n^k S^{-1}$ carries A_1 to A_2, performs a C_n^k rotation about A_2 and bring A_2 axis back to A_1. This is clearly equivalent to performing a C_n^k rotation about A_1 itself. If an axis C_n lies in a symmetry plane σ, then it is called the *bilateral axis*. For such an axis C_n^k and C_n^{-k} are conjugate. With reference to Figure 2.2.3, the following equalities can be noted:

$$\begin{aligned} A\sigma &= A, \quad A\sigma C_n^{-k} = A', \\ &\Rightarrow \quad A\sigma C_n^{-k}\sigma^{-1} = A\sigma C_n^{-k}\sigma = A'' = AC_n^k \\ &\Rightarrow \quad \sigma C_n^{-k}\sigma^{-1} = C_n^k. \end{aligned}$$

By a similar construction it is easy to see that an axis is bilateral also when there is a U_2 axis (two-fold axis) perpendicular to it (see Exercise 1).

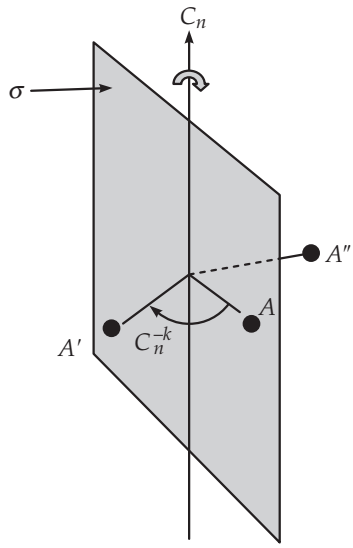


Figure 2.2.3 Bilateral Axis

2.3 Symmetry Point Groups

Finite point groups that describe the symmetries of molecules are considered here. The standard *Schoenflies notation* is used to designate the various groups. The graphical depiction of the groups is done by means of *stereographic projections*. Consider a unit sphere which is divided by the plane of the diagram into two equal parts. In order to form the stereographic projections, we project on the plane of the diagram any general point of the sphere and all its transformed positions obtained by application of the various symmetry transformations of the concerned group. Projections of the points of the upper hemisphere are indicated with a + sign while those of the lower hemisphere are indicated with ◯. Further details on stereographic projections are provided as we consider specific groups.

C_n **Group**. A molecule of C_n symmetry has an n-fold symmetry axis as its only element of symmetry. This group is clearly cyclic, has n elements and each conjugacy class consists of a single element. The special case of $n = 1$, i.e., C_1 corresponds to no symmetry. Figure 2.3.1(a) shows the stereographic projection for a C_3 group. Note that the diagram plane cuts the unit sphere along the dotted circle. The central triangle indicates that the axis of symmetry (perpendicular to the diagram plane) is three-fold. A + is taken into the next in the anticlockwise direction upon a C_3 operation, and then to the second next upon a C_3^2 operation.

S_{2n} **Group**. This is the symmetry group of a molecule having a rotary reflection axis of order $2n$. It is a cyclic group as is evident from the nature of a rotary reflection operation. Thus every element of S_{2n} is the unique member of its conjugacy class. In the Figure 2.3.1(b) is shown the projection diagram for S_6. The 6–order rotary reflection axis is indicated by a hollow hexagon. Note that $S_6^2 = C_6\sigma_h C_6\sigma_h = (C_6)^2(\sigma_h)^2 = C_3$, implying the presence of a three-fold axis of symmetry which is indicated by a solid triangle in the diagram.

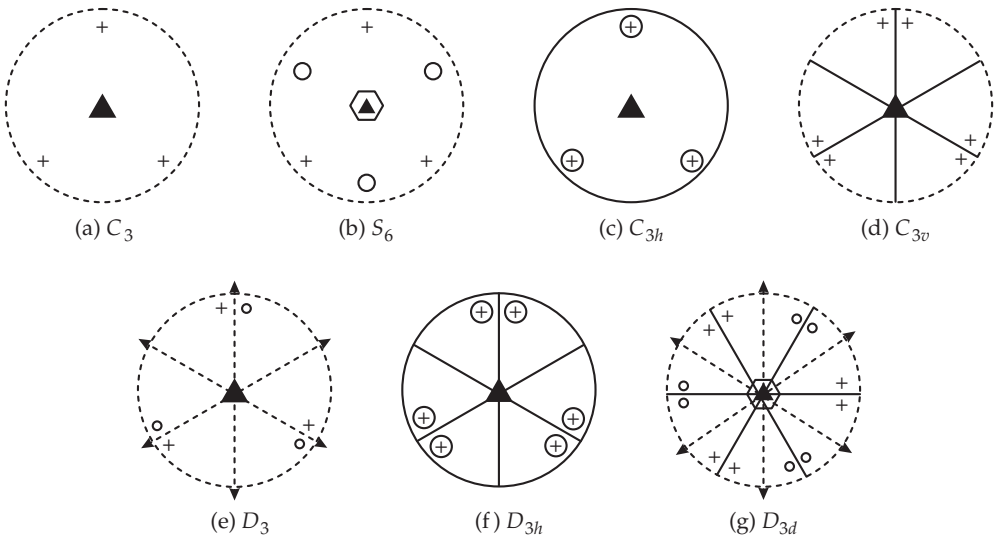


Figure 2.3.1 Stereographic Projections

C_{nh} **Group**. If to an n-fold axis is added a horizontal plane of symmetry σ_h, then the C_{nh} group is obtained. This group has n elements of the C_n group and in addition, further n elements of the type $C_n^k\sigma_h$. It is easy to check that the reflection in a horizontal plane and rotation about the principal axis are commuting operations. Therefore C_{nh} is a cyclic group. Consequently every element of C_{nh} is the unique member of its conjugacy class. In the special case of $n = 1$, i.e., C_{1h} contains only the elements E and σ_h; this group is designated C_s. In the stereographic projection for the C_{3h} group, the solid circle indicates a horizontal symmetry plane.

The aforementioned groups C_n, S_{2n} and C_{nh} are all cyclic groups. For odd $n = 2p+1$ the groups S_{2p+1} and $C_{(2p+1)h}$ are the same. As abstract groups, it may be noted that two cyclic groups of same order are isomorphic.

C_{nv} **Group**. The C_{nv} group is obtained by adding a σ_v plane to a C_n axis. Consequently, a total of n vertical reflection planes appear corresponding to operations σ_v, $\sigma_v C_n^1$, $\sigma_v C_n^2, \ldots \sigma_v C_n^{n-1}$. The total number of elements in the C_{nv} group is therefore $2n$. The number of conjugacy classes depends upon whether n is odd or even. For $n = 2p$, the vertical planes divide into two sets of equivalent planes. This gives two equivalent classes:

$$\left\{\sigma_v,\ \sigma_v C_{2p}^2,\ \ldots\ \sigma_v C_{2p}^{2p-2}\right\}\ \&\ \left\{\sigma C_{2p}^1,\ \ldots\ \sigma_v C_{2p}^{2p-1}\right\},$$

containing p reflections each. The C_{2p} axis is bilateral and thus C_{2p}^k and C_{2p}^{2p-k} are conjugate. This further gives $p-1$ classes, each containing two rotations and one class containing the rotation $C_{2p}^p = C_2$. Then, there is one class containing the identity E. Thus for even $n = 2p$, C_{nv} has $p+3$ equivalence classes. In a similar manner it may be seen that for odd $n = 2p+1$, all the reflection planes are equivalent and the number of equivalence classes is $p+2$. In the stereographic projection for C_{3v}, the solid diametrical lines indicate the vertical reflection planes (Figure 2.3.1(d)).

D_n **Group**. The D_n group is obtained by adding a U_2 axis to the principal C_n axis. As a result a total of n such U_2 axes appear corresponding to operations U_2, $U_2 C_n^1$, $\ldots U_2 C_n^{n-1}$. The total number of elements in D_n is therefore $2n$. The decomposition of the group D_n in conjugacy classes is similar to that of C_{nv} group for both the even and odd n. In fact, in may be noted that D_n and C_{nv} are both isomorphic to the abstract dihedral group discussed in Section 1.4. The stereographic projection for D_3 shows the U_2 axes marked as the double arrowed dotted diametrical lines (Figure 2.3.1(e)).

D_{nh} **Group**. To the group D_n, if a plane σ_h is added as an element of symmetry, then n vertical planes, σ_v appear automatically. Besides the $2n$ elements of group D_n, the group D_{nh} contains $n\sigma_v$ reflections as well as n rotary reflections $\sigma_h C_n^k$. Each σ_v plane contains the principal axis and a U_2 axis. Since σ_h commutes with all the other group elements, $D_{nh} = D_n \times C_s$. The number of classes in D_{nh} is twice the number in D_n enumerated as follows: Half of them are same as those of the group D_n, while the remainder are obtained by multiplying these by σ_h. Note that the reflections in σ_v planes belong to the same class if n is odd or forms two classes if n is even. Also, the rotary reflection elements $\sigma_h C_n^k$ and $\sigma_h C_n^{n-k}$ are conjugate pairwise.

D_{nd} **Group**. If a diagonal plane σ_d bisecting the angle between two adjacent U_2 axes of the D_n is added as a symmetry element, then a further $n-1$ such planes appear. The resultant group is the D_{nd} group containing $4n$ elements. To the $2n$ elements of the D_n group are added n reflections in the diagonal planes and further n transformations of the type $\sigma_d U_2$. The angle between a U_2 axis and the adjacent σ_d planes is clearly $\pi/2n$.

Figure 2.3.2 illustrates the action of the transformation $\sigma_d U_2$ which is nothing but a rotary reflection. That is, $\sigma_d U_2 = S_{2n}$. All the diagonal reflection planes do contain the C_n axis and hence the principal axis is bilateral. For $n = 2p$, the group $D_{2p,d}$ has $2p + 3$ conjugacy classes: E, C_2, $(p-1)$ classes of conjugate rotations about principal axis, a single class of $2pU_2$ rotations, a single class of $2p$ reflections σ_d and p classes of two rotary reflection transformations S_{4p}^{2k+1} and S_{4p}^{-2k-1} where k can take values 0 to $p-1$. For odd $n = 2p+1$, inversion is an element of the group and $D_{2p+1,d} = D_{2p+1} \times C_i$.

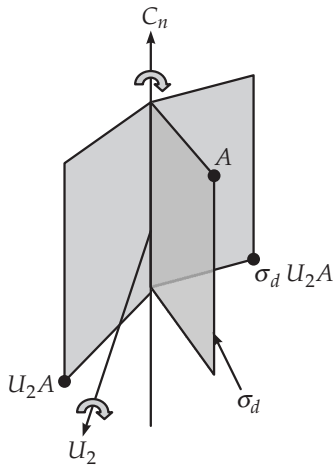


Figure 2.3.2 $\sigma_d U_2$ Transformation in D_{nd} Group

T **Group**. The group T consists of all the rotational symmetries of a regular tetrahedron (Figure 2.3.3). A regular tetrahedron is a flat sided solid with 4 triangular faces, all the faces being same. Through each vertex of the tetrahedron, passes a C_3 axis. All these axes are equivalent. Additionally there are C_2 axes going through midpoints of opposite edges of the tetrahedron. These axes are also equivalent. Hence, the classes of the group T are: E, 4 C_3 rotations, 4 C_3^2 rotations and 3 C_2 rotations.

T_d **Group**. This is the full symmetry group of the tetrahedron. Apart from the proper transformations of the group T, T_d contains the improper transformations as well. These transformations are obtained by adding 6 diagonal reflection planes. One such plane is shown in Figure 2.3.3. As is evident from the diagram, the plane contains the C_3 and C_2 axes. Consequently, the C_3 axes are bilateral as they contain the mirror planes. Another important feature is that the C_2 axes now become S_4 axes. This can be seen by rotating the tetrahedron by $\pi/2$ about the C_2 axis and reflecting in a perpendicular plane that is midway through the C_2 axis. Also S_4 axes are bilateral as they are all contained in diagonal planes. Thus the class structure is: E, all 8 C_3 rotations, all 6 σ_d reflections, 3 $C_2(S_4^2)$ rotations, 6 (S_4 and S_4^3 are conjugate) rotary reflections.

T_h **Group**. To the group T_d, if an inversion operation is added, the T_h group is obtained, $T_h = C_i \times T_d$. Consequently the number of conjugacy classes in T_h is twice as many as in T_d (see Exercise 2).

O **Group**. The O group or the octahedral group is the group of all the rotational symmetries of the cube (Figure 2.2.2). The 4 body diagonals are the C_3 axes. Then there are 3 C_4 axes and 6 C_2 axes. Thus the total number of elements of this group is equal to 24 $(4 \times 2 + 3 \times 3 + 6 + 1)$. All the C_4 axes are equivalent, and so are all the C_3 axes and the C_2 axes. The C_4 axes are bilateral as the C_2 axes are perpendicular to them. For the same reason C_3 axes are also bilateral. The class structure is: E, 6 C_2 rotations, 8 rotations of the type C_3 and C_3^2 6 rotations of the type C_4 and C_4^3 and 3 $C_2 (= C_4^2)$ rotations.

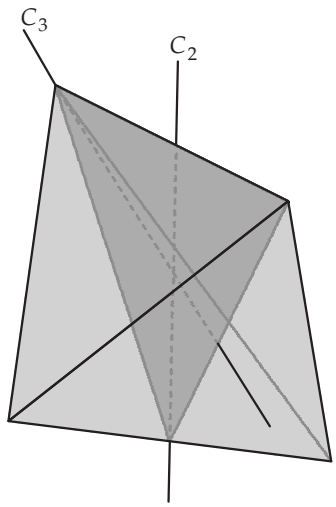


Figure 2.3.3 Symmetry Axes of the Tetrahedron

O_h **Group**. O_h is the full octahedral group and contains all the possible symmetry transformations of the cube. These include the rotational symmetries contained in the O group as well as those symmetries arising from the fact that the center of the cube is a point of symmetry. Consequently, it can be stated that $O_h = C_i \times O$.O_h has 48 elements and twice as many conjugacy classes as the group O.

Y **and** Y_h **Groups**. These are the symmetries of a regular icosahedron. An icosahedron is a convex polyhedron with twenty triangular faces arranged so that at each vertex of the icosahedron 5 triangular faces meet. The group Y is the group of 60 rotational symmetries of the icosahedron and $Y_h = C_i \times Y$. These symmetries occur rather rarely in molecules.

Example 17. Consider the group C_{3v}, the symmetry group of the ammonia molecule (Figure 2.2.1). Label the hydrogen atoms by the numbers 1, 2 and 3. Now a C_3 rotation sends the atom 1 to atom 2, atom 2 to atom 3 and the atom 3 to atom 1. Thus it is correct to represent the C_3 operation by a 3–cycle (1, 2, 3). Now consider the σ_v plane

that contains the nitrogen atom and the hydrogen atom 3. A reflection in this plane switches the positions of 1 and 2, therefore the operation σ_v can be represented by the transposition (1, 2). With this notation, the following equalities are easily verified:

$$\begin{aligned} C_3 &\equiv (1,2,3),\ \sigma_v \equiv (1,2),\ C_3^2 \equiv (1,3,2), \\ \sigma_v C_3 &\equiv (1,3),\ \sigma_v C_3^2 \equiv (2,3). \end{aligned}$$

This way the *permutation representation* of the group C_{3v} is obtained. In fact, it must be noted that the group C_{3v} is isomorphic to the group $\mathfrak{S}(3)$. □

Exercises

1. Show that an axis of symmetry C_n is bilateral if there exists a U_2 axis perpendicular to C_n. Find the conjugate rotations about C_n for both cases of n being even and odd.
2. Show that the inversion operation commutes with all other symmetry elements. If G is a point group then show that the group $G \times C_i$ contains twice as many classes as G; to each class A of G there correspond two classes A and $C_i A$ in the group $G \times C_i$.
3. Draw the stereographic projection for the group D_{4h}. Determine all the conjugacy classes.
4. Find the permutation representation for the Tetrahedral Group T. Identify a permutation group that is isomorphic to T.
5. Determine the permutation representation for the group T_d. Show that C_{3v} is a subgroup of T_d.
6. What is the symmetry group of the hypothetical molecule shown in Figure 2.3.4?
7. What could be the Schoenflies notation for designating the symmetry group of the O_2 molecule? What could it be for the CO molecule? Are these groups finite?

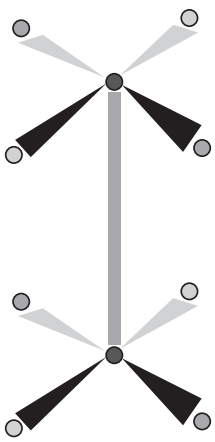


Figure 2.3.4 Hypothetical Molecule

3

Representations of Finite Groups

In the previous chapter, we observed that group multiplication tables of elements of point groups like C_{3v} and T also apply to the corresponding elements of an appropriate permutation group. In fact, the one to one and onto correspondence between these groups were referred to as isomorphism. Such alternative descriptions of the multiplication table of an abstract group G can also be called as *representations* denoted by $\Gamma(g)$ for every element $g \in G$.

One of the extensively studied approaches towards generating representations of a group G is through the familiar matrices. One associates with each element g $\in$ G a matrix $\Gamma(g)$ such that the group multiplication table is obeyed by the matrices under matrix multiplication. Such representations are particularly useful as they are convenient for performing calculations. We present the necessary aspects of the theory of representations combined with examples. In this chapter our emphasis is on the statements of theorems and the results obtained from their application. Readers interested in detailed proofs are advised to refer to the many available standard texts on group theory. For continuity and clarity, we will now begin with vectors and vector spaces which leads to the construction of matrices acting on such vectors.

3.1 Vector Spaces

An abstract *vector space* is an important mathematical structure which is frequently encountered in physics. The elements of a vector space are called *vectors*. The set of vectors forms an abelian group under the addition operation. The identity of this abelian structure is called the *null vector*, denoted usually by 0. Apart from the

operation of addition, the vector space is also closed under the operation of *scalar multiplication*. A scalar, for the purposes of this chapter, is simply a complex number. It is natural to assume that for any vector x in a vector space V, the complex number 1 times x is same as x, i.e., $1x = x$. For scalars α, β and vectors x, y : $(\alpha + \beta)x = \alpha x + \beta x$ as well as $\alpha(x + y) = \alpha x + \alpha y$. Consequently $0x = 0$. The same symbol is used to represent the scalar 0 and the null vector as there is no chance of confusion here. Also, if x, y are any two vectors and α, β are any two complex numbers then the *linear combination* $\alpha x + \beta y$ is also a vector in V. A linear combination of any finite number of vectors can be formed in this way. It may be noted that the scalars themselves need not be members of V. As described, V is a *complex vector space* since all the scalars belong to the set of complex numbers.

A set of non-null vectors $\{x_i\}_{i=1}^n$ in V is said to be a *linearly independent set* if the only possible linear combination of these vectors that is equal to 0 is the one in which all the multiplicative scalars are themselves 0. The set of all possible linear combinations of the linearly independent vectors $\{x_i\}_{i=1}^n$ is the *linear span* of the linearly independent set. Denote the linear span of $\{x_i\}_{i=1}^n$ by $\mathcal{L}(\{x_i\}_{i=1}^n)$. Clearly $\mathcal{L}(\{x_i\}_{i=1}^n)$ is itself a vector space contained in V, and hence is called a subspace of V. When $\mathcal{L}(\{x_i\}_{i=1}^n)$ is equal to V, then V is said to be of *dimension* n and $\{x_i\}_{i=1}^n$ are said to constitute a *basis* for V. Note that $\mathcal{L}(S)$ is defined for any set S of vectors but here the set $\{x_i\}_{i=1}^n$ is assumed to be linearly independent.

Any general vector x in V can be uniquely expressed as a linear combination of the basis vectors. For, if the same vector x could be expressed as $\sum_{i=1}^{n} \alpha_i x_i$ as well as $\sum_{i=1}^{n} \beta_i x_i$ where at least one $\alpha_i \neq \beta_i$, then

$$\sum_{i=1}^{n} (\alpha_i - \beta_i) x_i = 0$$

and it would follow that the basis vectors are not linearly independent. The scalars α_i are called the *components* of the vector x in the basis $\{x_i\}_{i=1}^n$.

From here onwards, it would be assumed that V is of finite dimension, though infinite dimensional vector spaces are quite relevant as well. As the number of vectors in V is infinite (unless of course V contains only the null vector), it may be possible to choose a different set of linearly independent vectors $\{y_j\}_{j=1}^m$ as a basis for V. For the concept of dimension of V to be well defined, it is necessary that both the basis sets contain same number of elements, i.e., $m = n$. In order to see this, suppose $\{x_i\}_{i=1}^n$ and $\{y_j\}_{j=1}^m$ are both basis sets and $m > n$. Since x_1 can be expressed as a linear combination of y_j's, some y_k can be expressed as a linear combination of x_1 and the remaining y_j's. This would mean that the set $B_1 = \{y_1, \ldots, y_{k-1}, x_1, y_{k+1}, \ldots y_m\}$ is a basis set. x_2 can be expressed as a linear combination of vectors in B_1, and because x_2 and x_1 are linearly independent, it would follow that some y_l can be expressed as a linear combination of x_2 and the remaining elements of B_1. Now y_l can be replaced by x_2 and a new basis set is obtained to be $B_2 = \{y_1, \ldots, y_{k-1}, x_1, y_{k+1}, \ldots, y_{l-1}, x_2, y_{l+1}, \ldots, y_m\}$. Continuing in this

manner, the basis set B_n would contain all the $\{x_i\}_{i=1}^n$ and some y_j's. But because $\{x_i\}_{i=1}^n$ is itself a complete basis for V, B_n would no longer be linearly independent which is a contradiction. Thus the conclusion is $m \leq n$. By the same argument, it follows the $n \leq m$ and hence $m = n$.

The subspace $\{0\}$ and the subspace V are the *trivial subspaces* of the vector space V. All other subspaces are non-trivial. The dimension of a subspace of V is clearly less than or equal to the dimension of V. If there exist subspaces W_1 and W_2 of V such that every vector v in V can be uniquely expressed as the sum $w_1 + w_2$ where $w_i \in W_i$, then V is said to be a *direct sum* of the subspaces W_1 and W_2.

$$V = W_1 \oplus W_2. \tag{3.1.1}$$

A *Linear Operator* on a vector space V is a mapping T of V into V such that for all x and y in $V : T(\alpha x + \beta y) = \alpha Tx + \beta Ty$. A consequence of this definition is that $T0 = 0$. Suppose $\{x_i\}_{i=1}^n$ is a basis set for V and x is any element of V. By linearity of T it follows that

$$Tx = T\left(\sum_{j=1}^{n} \alpha_j x_j\right) = \sum_{j=1}^{n} \alpha_j T x_j,$$

i.e., the action of T on any vector is determined completely if the action of T is known on the basis set. Suppose now that

$$Tx_j = \sum_{i=1}^{n} t_{ij} x_i,$$

where t_{ij} are some scalars. Combining the above two

$$Tx = \sum_{i=1}^{n} \left(\sum_{j=1}^{n} t_{ij}\alpha_j\right) x_i.$$

Thus the action of T on the vector $x = (\alpha_1, \ldots \alpha_j, \ldots \alpha_n)$ is to transform it into the vector $Tx = (\beta_1, \ldots, \beta_i, \ldots \beta_n)$ whose component $\beta_i = (\sum_{j=1}^n t_{ij}\alpha_j)$. This is most conveniently represented as the matrix product

$$\begin{pmatrix} \beta_1 \\ \vdots \\ \beta_n \end{pmatrix} = \begin{pmatrix} t_{11} & \cdots & t_{1n} \\ \vdots & \ddots & \vdots \\ t_{n1} & \cdots & t_{nn} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix}.$$

The matrix $\{t_{ij}\}$ is identified with the operator T. It may be noted that the j^{th} column of the operator matrix contains the components of the vector Tx_j. However, the matrix associated with a linear operator is not unique in the sense that the same operator would be represented by a different matrix for a different choice of basis vectors. If T is such that $Tx = Ty \Rightarrow x = y$, then T is a one to one map of V onto V. In such a case

the matrix of T is an invertible $n \times n$ matrix. It is a fact that the set of all invertible square $n \times n$ matrices form a non-abelian group under matrix multiplication.

It is sometimes necessary to relate the matrix representations of a linear operator T in two different basis sets $\{x_i\}_{i=1}^n$ and $\{y_i\}_{i=1}^n$ of a vector space V. Suppose T_x and T_y are the matrices of the operator T in the two bases. The basis vectors $\{x_i\}_{i=1}^n$ themselves must be linearly dependent on the vectors $\{y_i\}_{i=1}^n$ by relations of the form

$$x_i = \sum_{j=1}^{n} s_{ji} y_j,$$

where $\{s_{ji}\}$ are some scalars. The scalars s_{ji} can be thought of as entries of a matrix S. It is clear that S is an invertible matrix, for $\{x_i\}_{i=1}^n$ and $\{y_i\}_{i=1}^n$ form a complete basis. If $x = \sum_{i=1}^n \alpha_i x_i$ is any general vector in V, then the representation of x in the basis $\{y_i\}_{i=1}^n$ can now be obtained as

$$x = \sum_{i=1}^{n} \alpha_i \left(\sum_{j=1}^{n} s_{ji} y_j \right) = \sum_{j=1}^{n} \left(\sum_{i=1}^{n} s_{ji} \alpha_i \right) y_j.$$

It follows that Sx is the representation of x in $\{y_i\}_{i=1}^n$ basis. Because a change of basis should not change the end result of a linear transformation $ST_x x = T_y S x$. In matrix form, this condition can be written as a *similarity transformation*

$$T_x = S^{-1} T_y S. \tag{3.1.2}$$

It may as well be pointed out that the traces (sum of diagonal elements) of matrices that are related by a similarity transformation are equal.

Given an invertible linear operator T on a vector space V, the *Eigenvalue Equation* of the operator is

$$Tx = \lambda x.$$

The non-null vectors x satisfying the above equation are called the *eigenvectors* of T and the scalars λ, the corresponding *eigenvalues*. An important example of an eigenvalue equation is the Schrödinger equation $H\psi = E\psi$ for calculating the stationary states of a closed quantum mechanical system. An operator T which has the same eigenvalue for all $x \in V$ is called a *scaling transformation*.

A vector space V is a *normed space* if for every vector x in V is defined a non-negative real number called the *norm* (or length) of x denoted by $\|x\|$ such that the following properties are satisfied:

1. $\|x + y\| \leq \|x\| + \|y\|$ for all x and y in V.
2. $\|\alpha x\| = |\alpha| \|x\|$ for all x in V and all scalars α.
3. $\|x\| = 0$ if and only if $x = 0$.

A vector of unit norm is called a *unit vector*.

A vector space V is an *inner product space* (or a *unitary space*) if for all $x,\ y$ in V is defined a complex number $(x,\ y)$, called their inner product such that the following properties are satisfied:

1. $(x,\ y) = \overline{(y,\ x)}$ where the overbar means complex conjugation.
2. $(x,\ \alpha y + \beta z) = \alpha(x,\ y) + \beta(x,\ z)$ for all scalars α and β.
3. $(x,\ x) \geq 0$ for all x in V.
4. $(x,\ x) = 0$ if and only if $x = 0$.

Notice that it follows from Property 1 and Property 2 that $(\alpha x,\ y) = \overline{\alpha}(x,\ y)$ and also that $(0,\ x) = (x,\ 0) = 0$. Two non-null vectors x and y are said to be *orthogonal* if $(x,\ y) = 0$. Clearly if $(x,\ y) = 0$ then $(y,\ x) = 0$. It can be proven that if x and y are orthogonal then they are linearly independent.

A unitary space is naturally a normed space if for a vector x, the norm $\|x\| = \sqrt{(x,x)}$. It is easy to check that Property 2 and Property 3 for the norm are satisfied with this definition. In order to verify Property 1, one may note

$$\begin{aligned} \|x+y\|^2 &= (x+y,\ x+y) = (x,\ x) + (y,\ y) + 2\text{Re}\ (x,\ y) \\ &\Rightarrow \quad \|x+y\|^2 \leq \|x\|^2 + \|y\|^2 + 2|(x,\ y)|. \end{aligned}$$

It follows from above that $\|x+y\| \leq \|x\| + \|y\|$ will be true if the following, well known *Cauchy–Schwartz inequality* is satisfied:

$$|(x,\ y)| \leq \|x\|\|y\|. \tag{3.1.3}$$

The Cauchy–Schwartz inequality can be proved as follows. For some scalar α and vectors x and y,

$$\|x + \alpha y\|^2 = \|x\|^2 + 2\text{Re}\ [\alpha(x,\ y)] + |\alpha|^2\|y\|^2 \geq 0.$$

Since the above inequality is true for any arbitrary scalar α, it should as well be true in the special case $\alpha = -\frac{(y,x)}{||y||^2}$ (assuming $y \neq 0$, otherwise the inequality is trivially true). On substituting this value of α, inequality 3.1.3 follows.

The basis set for a unitary space can be chosen in such a way that all the basis vectors are of unit length and are mutually orthogonal. Such a basis is called an *orthonormal basis*. Suppose that $\{x_i\}_{i=1}^n$ is a basis for the unitary space V, which is not necessarily orthonormal. From this basis one may construct an orthonormal basis $\{e_i\}_{i=1}^n$ by the *Gram–Schmidt orthogonalisation* process. It can be checked that with the following definitions for e_i's, the basis $\{e_i\}_{i=1}^n$ is indeed orthonormal.

$$e_1 = \frac{x_1}{\|x_1\|},\ e_2 = \frac{x_2 - (e_1, x_2)e_1}{\|x_2 - (e_1, x_2)e_1\|},\ e_3 = \frac{x_3 - (e_1, x_3)e_1 - (e_2, x_3)e_2}{\|x_3 - (e_1, x_3)e_1 - (e_2,)e_2\|}, \ldots \tag{3.1.4}$$
$$(e_i,\ e_j) = \delta_{ij},$$

where δ_{ij} is the Kronecker delta which assumes the value 1 if $i = j$ and 0 otherwise.

Suppose that T is a linear operator on a unitary space V and $\{e_i\}_{i=1}^n$ an orthonormal basis of V. It is then possible to define another operator $T^\dagger$ related to T, called the *adjoint* of T by the following relation:

$$t_{ij}^\dagger = \overline{t_{ji}}. \tag{3.1.5}$$

Thus the entries of the adjoint $T^\dagger$ are complex conjugates of the corresponding entries of the transpose of the operator T. For this reason the terms *adjoint* and *transpose conjugate* are used interchangeably. The following chains of equalities follow from the definition of the adjoint.

$$(e_i,\ Te_j) = \left(e_i, \sum_{k=1}^n t_{kj}e_k\right) = \sum_{k=1}^n t_{kj}(e_i,\ e_k) = \sum_{k=1}^n t_{kj}\delta_{ik} = t_{ij}.$$

$$(T^\dagger e_i,\ e_j) = \left(\sum_{k=1}^n t_{ki}^\dagger e_k, e_j\right) = \sum_{k=1}^n \overline{t_{ki}^\dagger}(e_k,\ e_j) = \sum_{k=1}^n \overline{t_{ki}^\dagger}\delta_{kj} = \overline{t_{ji}^\dagger} = t_{ij}.$$

Consequently, $(e_i,\ Te_j) = (T^\dagger e_i, e_j)$. In general, for any two vectors x and y

$$(x,\ Ty) = (T^\dagger x,\ y). \tag{3.1.6}$$

An operator is *self-adjoint* if it is equal to its adjoint. In other words $(x,\ Ty) = (Tx,\ y)$ for all x and y in V. Self-adjoint operators are indeed special as their eigenvalues are real. Let T be self-adjoint and x be an eigenvector with eigenvalue λ. Then

$$(x,\ Tx) = (Tx,\ x)$$
$$\Rightarrow (x,\ \lambda x) = (\lambda x,\ x)$$
$$\Rightarrow \lambda(x,\ x) = \overline{\lambda}(x,\ x)$$
$$\Rightarrow (\lambda - \overline{\lambda})\|x\|^2 = 0.$$

As x is not a null vector it follows λ is real. Self-adjoint operators are particularly important for this reason. In fact, operators corresponding to physical quantities in quantum mechanics are necessarily self-adjoint.

The notion of a *unitary operator* is an important one in physical applications. Such an operator is an invertible linear operator with additional conditions. If U is a unitary operator then its inverse operator is the adjoint of U.

$$UU^\dagger = U^\dagger U = 1. \tag{3.1.7}$$

Some of the important properties of unitary operators are worth noting. The norm of a vector remains invariant under a unitary transformation, for $\|Ux\|^2 = (Ux,\ Ux) = (U^\dagger Ux, x) = (x,\ x) = \|x\|^2$. If x is an eigenvector of U with eigenvalue λ, then it follows from the same chain of equalities that $|\lambda|^2 = 1$, i.e., the eigenvalues of a unitary operator are of unit modulus. The rows of a unitary matrix are orthonormal, and so are the columns. The product of two unitary operators (matrix multiplication) is again a unitary operator. Also, the unit matrix is indeed a unitary operator. These properties show that the set of all unitary operators on the vector space V forms a group under matrix multiplication. If V has dimension n, then this group is designated as $U(n)$, also referred to as the unitary group of degree n. The unitary group and its subgroups will be studied in Chapter 5, *Lie Groups*.

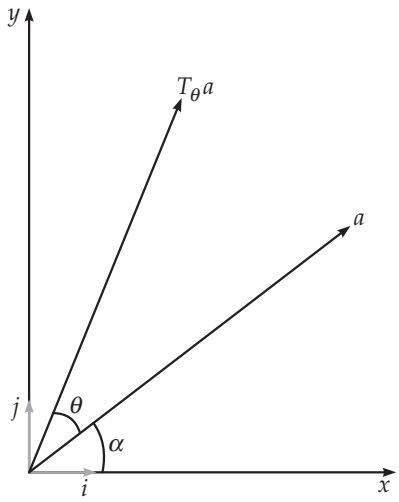


Figure 3.1.1 R^2

The vector space V that is considered here is of the finite dimension. For applications in quantum mechanics, the specialized vector space called *Hilbert space* is sufficient. The Hilbert space is a unitary space with the additional condition of *completeness*. The completeness condition will not be of concern in this text, though it may be implicitly in use. Let it be said that the notions of linear transformations, inverse transformations, eigenvalue equations, adjoints, self-adjoint transformations and unitary operators continue to remain relevant whether the Hilbert space under consideration is finitely dimensional or infinitely dimensional. Also, all the numbered formulae in this section continue to remain valid irrespective.

Example 18. Consider the two-dimensional Euclidean plane endowed with a coordinate system consisting of mutually perpendicular x-y axes. Then the set of radius vectors of all points in the plane is a two-dimensional *real vector space* R^2. A real vector space is one whose multiplicative scalars are chosen from the set of real numbers instead of complex numbers. The reader should be familiar with the *parallelogram law of vector addition* and scaling of vectors via multiplication by real numbers. The unit vectors i and j (Figure 3.1.1) together form an orthonormal basis.

The linear transformation R_θ rotates any general radius vector a by an angle of θ about the origin without changing the length of a. If $\|a\|$ is the length of a then in the chosen basis

$$\begin{aligned} a &= \|a\|(i\cos\alpha + j\sin\alpha), \\ R_\theta a &= \|a\|(i\cos(\alpha+\theta) + j\sin(\alpha+\theta)). \end{aligned}$$

On eliminating α, the transformation matrix is obtained to be

$$R_\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

It can be verified that indeed $R_\theta(\alpha a + \beta b) = \alpha R_\theta a + \beta R_\theta b$ for any two vectors a and b in R^2 and reals α and β. The inverse transformation of R_θ is $R_{-\theta}$ which is also equal to the transpose of R_θ as is evident from the matrix form of R_θ. A transformation whose inverse is the transpose of the transformation is called an *orthogonal transformation*.

R^2 is an inner product space if the inner product of a and b, $(a,\ b) = a.b$, where the right hand side is the usual dot product of vectors one learns about in elementary vector algebra. With this definition it follows that $(R_{-\theta}a,\ b) = (a,\ R_\theta b)$. Hence $R_{-\theta}$ is the adjoint of R_θ in the sense of Equation 3.1.6. □

Example 19. All homogeneous polynomials of degree two in the variables x and y form a three-dimensional vector space. The basis set for this vector space can be chosen to be $\{x^2,\ y^2,\ xy\}$. A general element of this vector space is $\alpha x^2 + \beta y^2 + \gamma xy$ where $\alpha,\ \beta,\ \gamma$ are some complex numbers. If the basis set is chosen to be $\{x^2+y^2,\ x^2 - y^2,\ xy\}$, then the same general element can be written as $\frac{\alpha+\beta}{2}(x^2+y^2) + \frac{\alpha-\beta}{2}(x^2 - y^2) + \gamma xy$. □

3.2 Group Action on Vector Spaces

Given an abstract group G and a vector space V, it is often possible to regard the elements of the group as invertible linear operators on the vector space. Once this is done, every element of G can be associated with the matrix of the operator in a fixed basis for V. Let Γ be a function that maps an element g of G to the matrix $\Gamma(g)$. Then the totality of matrices $\Gamma(g)$ is called a *representation* of G if Γ is a homomorphism, i.e.,

$$\Gamma(g_1 g_2) = \Gamma(g_1)\Gamma(g_2). \tag{3.2.1}$$

Notice that the product on the right hand side is a matrix product, while that on the left hand side is the product defined in the group. If the dimension of V is n then the representation Γ is said to be of degree n. For a given group element g, the entries of $\Gamma(g)$ are easily ascertained from the fact that g acts as an invertible linear operator on V. Thus the j^{th} column of $\Gamma(g)$ are the coordinates of the transformation of the basis vector x_j of V by the group element g in accordance with the map

$$gx_j \to \sum_{i=1}^{n} [\Gamma(g)]_{ij} x_i.$$

A representation of Γ is said to be *faithful* if $\Gamma(g_1) \neq \Gamma(g_2)$ for $g_1 \neq g_2$.

Example 20. Consider the point group C_{3v} and the three-dimensional real vector space $\mathbb{R}^3$ spanned by the unit vectors $\{i,\ j,\ k\}$ (using the conventional notation). The symmetry axis of C_{3v} points along k. The objective is to generate a matrix representation of C_{3v} by letting its elements operate on-$\mathbb{R}^3$. Under the C_3 operation (rotation by $\frac{2\pi}{3}$ in the counterclockwise sense about the *z-axis*), the unit vectors are clearly transformed as follows:

$$\begin{aligned} i &\to -\frac{1}{2}i + \frac{\sqrt{3}}{2}j + 0k, \\ j &\to -\frac{\sqrt{3}}{2}i - \frac{1}{2}j + 0k, \\ k &\to 0i + 0j + k. \end{aligned}$$

It is therefore plausible to make following associations

$$C_3 \equiv \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix},\ C_3^2 \equiv \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

Now consider the σ_v plane to be the z-x plane. Then a σ_v reflection leaves i and k invariant and reverses j.

$$\sigma_v \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The matrix forms of $C_3\sigma_v$ and $C_3^2\sigma_v$ can be found from above matrices. The identity element is the 3×3 identity matrix.

$$E \equiv \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix},\ C_3\sigma_v \equiv \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$C_3^2\sigma_v \equiv \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \qquad \square$$

If $\Gamma(g)$ is the matrix corresponding to group element g in some given basis of V, then under a change of basis effected by an invertible matrix S, the matrix of g becomes $S^{-1}\Gamma(g)S$ in accordance with Equation 3.1.2.

Definition 4. Let Γ be a representation of degree n of a group G. Then the *character* of an element g of G under the representation Γ is the trace of the matrix $\Gamma(g)$.

$$\chi^{\Gamma}(g) = \mathrm{tr}\Gamma(g) = \sum_{i=1}^{n} [\Gamma(g)]_{ii}. \tag{3.2.2}$$

The symbol $\chi^{\Gamma}(g)$ would from now onwards stand for the character of the group element g under the representation Γ.

A consequence of this definition is that if Γ and Θ are two different representations of G related by a similarity transformation, then the character of any element of G has the same value in both the representations. Such representations are *equivalent representations* and are fundamentally not distinguished from each other. A further consequence is that all the group elements which belong to the same conjugacy class have the same character. For if $g_1 = ag_2a^{-1}$, then $\Gamma(g_1) = \Gamma(a)\Gamma(g_2)\Gamma(a)^{-1}$, thereby $\Gamma(g_1)$ and $\Gamma(g_2)$ have the same character. The group character is therefore a *class function*. In the example of the matrix representation of group C_{3v}, $\chi(E) = 3$, $\chi(C_3) = \chi(C_3^2) = 0$ and $\chi(\sigma_v) = \chi(C_3\sigma_v) = \chi(C_3^2\sigma_v) = 1$.

3.3 Reducible and Irreducible Representations

In a representation Γ of a group G over a vector space V, it may so happen that some non-trivial subspace V_1 of V remains invariant under the group action. By this it is meant that the group elements transform V_1 onto V_1, however the vectors outside of V_1 are transformed to vectors outside V_1. When this happens, then Γ is also a representation of G on V_1 and in the context of V, a *subrepresentation* of G. With an appropriate choice and ordering of basis vectors, the representing matrix for any general element g of G takes the form

$$\Gamma(g) = \left(\begin{array}{c|c} \Theta(g) & \Pi(g) \\ \hline 0 & \triangle(g) \end{array}\right),$$

where $\Theta(g)$, $\Pi(g)$ and $\triangle(g)$ are fixed size matrix blocks whose entries vary with g. The bottom left block has 0 as all entries. A representation such as Γ which has a subrepresentation is called a *reducible representation*. A representation with no subrepresentations is called an *irreducible representation*.

A reducible representation is *completely reducible* if it can be decomposed into irreducible representations. If Γ were a completely reducible representation then for every g

$$\Gamma(g) = \begin{pmatrix} \Gamma^1(g) & 0 & 0 \\ 0 & \ddots & 0 \\ 0 & 0 & \Gamma^k(g) \end{pmatrix}.$$

In other words, the representation matrices of all the group elements can be simultaneously put in a block diagonal form of identical structure, with each block being an irreducible subrepresentation. Γ is then a direct sum of the irreducible representations.

$$\Gamma = \bigoplus_{i=1}^{k} \Gamma^i. \tag{3.3.1}$$

It is also obvious from the above decomposition that

$$\chi^{\Gamma}(g) = \sum_{i=1}^{k} \chi^{\Gamma^i}(g). \tag{3.3.2}$$

It is a theorem that all reducible representations of a finite group obtained via group action on complex or real vector spaces are completely reducible. The interested reader is encouraged to study *Maschke's Theorem* (see Appendix A) in this regard. It may as well be noted that every representation of a finite group over a real or a complex vector space is equivalent to a unitary representation, i.e., the matrices of all the group elements are unitary.

It is fairly obvious from the foregoing that the irreducible representations are the building blocks for all possible representations of a finite group. Therefore a study of the irreducible representations of a group is essential. To begin with, a group has the trivial irreducible representation of degree 1 which is generated when every group element maps the unit vector of a one-dimensional vector space to itself. This representation is also called the *unit representation* and is designated by the symbol A. The character of every group element in this representation is equal to 1. It is clear that

$$\sum_{g \epsilon G} \chi^A(g) = |G|, \tag{3.3.3}$$

where summation is over all the elements of the group.

We may recall that the degree of a representation is the dimensionality of the vector space on which the group acts. It may be possible for a group to have non-equivalent irreducible representations of the same degree, and these representations would be treated as distinct. It is a theorem that the degree of an irreducible representation divides the order of the group. Even the number of distinct irreducible representations

of a finite group is finite and is equal to the number of conjugacy classes in the group. It has already been noted that group elements in a conjugacy class have the same character under a given representation. Suppose that the finite group G has r conjugacy classes. If $\Gamma_1,\ \Gamma_2\ , \ldots\ \Gamma_r$ are distinct irreducible representations of a group G whose degrees are $\ell_1,\ \ell_2, \ldots \ell_r$ respectively then

$$\sum_{i=1}^{r} \ell_i^2 = |G|. \tag{3.3.4}$$

The criteria that G has at least one representation of degree 1, that each ℓ_i divides $|G|$ and that together the ℓ_i's satisfy the above equation put stringent constraints on the possible values of ℓ_i's. In most cases, these conditions are sufficient to ascertain the values of ℓ_i's.

Let Γ and Θ be two irreducible unitary representations of a finite group G. Then the following orthogonality relation holds (read *Schur's Lemma* in this connection which we have briefly discussed in Appendix B) between the entries of the matrices of group elements under the two representations.

$$\sum_{g\epsilon G} [\Gamma(g)]_{ik} \overline{[\Theta(g)]}_{lm} = \frac{|G|}{\ell_\Gamma} \delta_{\Gamma\Theta} \delta_{il} \delta_{km}. \tag{3.3.5}$$

The group characters also follow an orthogonality relation given by

$$\sum_{g\epsilon G} \chi^\Gamma(g) . \overline{\chi^\Theta(g)} = |G| \delta_{\Gamma\Theta}. \tag{3.3.6}$$

As the identity or unit representation A is always an irreducible representation of any group, it follows from Equation 3.3.6 that for any irreducible representation Γ other than A

$$\sum_{g\epsilon G} \chi^\Gamma(g) = 0. \tag{3.3.7}$$

If $\Gamma = \Theta$ in Equation 3.3.6, then we have

$$\sum_{g\epsilon G} |\chi^\Gamma(g)|^2 = |G|. \tag{3.3.8}$$

Another fact to bear in mind is that the character of the identity element of a group is always equal to the degree of the representation. If $c_1,\ c_2 \ldots c_r$ represent the classes of G and n_i the number of elements in the conjugacy class c_i, then Equation 3.3.6 may once again be written as

$$\sum_{i=1}^{r} \frac{n_i}{|G|} \chi^\Gamma(c_i) \overline{\chi^\Theta(c_i)} = \delta_{\Gamma\Theta}. \tag{3.3.9}$$

As the number of distinct irreducible representations is also equal to number of classes in G, one may construct a $r \times r$ matrix whose k^{th} row contains that characters of the classes multiplied by $\sqrt{\frac{n_i}{|G|}}$ in the k^{th} representation. Then the orthogonality of group characters is equivalent to stating that the row vectors of this matrix are orthonormal. Since the columns of such a matrix would also be orthonormal, it immediately follows that

$$\sum_{l=1}^{r} \frac{n_i}{|G|} \chi^{\Gamma_l}(c_i) \overline{\chi^{\Gamma_l}(c_j)} = \delta_{ij}. \tag{3.3.10}$$

3.4 Irreducible Representations of Point Groups

In physical applications of the representation theory, it is often only the group characters that are of relevance as against the actual matrices corresponding to the group elements. Equations 3.3.6, 3.3.7 and 3.3.8 prove very useful in the calculation of these characters. The characters of the group classes under various representations are arranged to create a *character table* for the group. A typical character table for representations of a finite group G formally looks like

G	$n_1 g_1$	$\dots$	$n_r g_r$	basis
Γ_1	$\chi^{\Gamma_1}(C_1)$	$\dots$	$\chi^{\Gamma_1}(C_r)$	
$\vdots$		$\ddots$		
Γ_r	$\chi^{\Gamma_r}(C_1)$		$\chi^{\Gamma_r}(C_r)$	

where the symbols have their usual meanings. $n_i g_i$ in the top row states that there are n_i group elements in the conjugacy class c_i, and g_i is a representative element of c_i. The columns to the right of the character entries contain the basis states of the corresponding representations.

While working with point groups, it is conventional to adopt the *Mulliken symbols* for naming irreducible representations. The principal symmetry axis is taken along the *z-axis*. Representations of degree 1 are identified by symbols A and B, degree 2 representations are identified by the symbol E (not to be confused with the identity element) and degree 3 representations by the symbols F or T. Given a symmetry operation g in the group G, the basis vectors of a representation Γ get transformed by $\Gamma(g)$. For certain operations, it may happen that the basis vectors are transformed onto themselves, in which case the representation is symmetric. If on the other hand, the basis vectors are reversed, then the representation is antisymmetric. In case of representations A, the base functions are symmetric with respect to rotation about principal axis, while they are antisymmetric with respect to rotations about principal axis in case of representations B. For representations which are symmetric or antisymmetric with respect to reflections σ_h, their symbols are marked with one prime or two primes respectively. Representations which are symmetric or antisymmetric

with respect to inversions are marked with the letter g (gerade) or u (ungerade) respectively in the subscript to the representation symbol. Following are some examples which illustrate how character tables may be constructed in simple cases.

Example 21. Consider the group C_{2h} (Chapter 2, Section 2.3). The number of classes in C_{2h} is 4. Since $1^2 + 1^2 + 1^2 + 1^2 = 4$, all the irreducible representations are of degree 1. The character of identity element of C_{2h} is 1 in all the representations. However, since the order of every other element of C_{2h} is 2, and that each representation is of degree 1, it follows that the character of every element can be either $+1$ or -1. The character table follows:

C_{2h}	E	C_2	σ_h	I		
A_g	1	1	1	1	R_z	$x^2; y^2; z^2; xy$
A_u	1	1	-1	-1	z	
B_g	1	-1	-1	1	$R_x; R_y$	$xz; yz$
B_u	1	-1	1	-1	$x; y$	

Particular attention should be paid to the names of the irreducible representations. Observe that the character of the inversion operation (I) is $+1$ in the gerade representations and -1 in the ungerade ones. Similarly the character of C_2 operation is $+1$ in A representations and -1 in B representations. Two choice of bases have been shown, linear bases in second last column and quadratic bases in the last column. In case of the linear bases, x, y, z are the polar vectors along the axes and R_x, R_y, R_z are the axial vectors along the axes. The reflection and inversion properties of these vectors are well known from elementary vector algebra and it is left for the reader to verify that indeed the group operations produce the indicated effects: For example, $C_2 R_x = -R_x$ but $C_2 R_z = R_z$ and so on. In case of quadratic bases it is the signs of the expressions that get affected: For example, $C_2 x^2 = x^2$ but $C_2 xz = -xz$ and so on. Notice that C_2 (a rotation by π about *z-axis*) changes the sign of x but leaves that of z unchanged. □

Example 22. Consider the group D_{2d}. This is a group of 8 elements. The 5 conjugacy classes in D_{2d} are: one class containing E, one class containing C_2 rotation, one containing two rotary reflection transformations S_4, one class containing 2 reflections in the diagonal planes σ_d and finally one class containing two rotations about the U_2 axes. There are therefore 5 irreducible representations of D_{2d}. From the equation $1^2 + 1^2 + 1^2 + 1^2 + 2^2 = 8$, it follows that 4 of these representations are of degree 1 and one representation is of degree 2.

D_{2d}	E	C_2	$2S_4$	$2U_2$	$2\sigma_d$		
A_1	1	1	1	1	1		x^2+y^2, z^2
A_2	1	1	1	-1	-1	R_z	
B_1	1	1	-1	1	-1		x^2-y^2
B_2	1	1	-1	1	1	z	xy
E	2	-2	0	0	0	$(x,y);$ (R_x,R_y)	xz, yz

In the unit representation A_1, all the group characters are 1 as usual. In any of the representations, the group characters satisfy Equations 3.3.7 and 3.3.8. From these it follows that

$$\chi(E)+\chi(C_2)+2\chi(S_4)+2\chi(U_2)+2\chi(\sigma_d)=0,$$

$$|\chi(E)|^2+|\chi(C_2)|^2+2|\chi(S_4)|^2+2|\chi(U_2)|^2+2|\chi(\sigma_d)|^2=8.$$

The character of identity is 1 in all the other representations of degree 1. Since the orders of C_2, U_2 and σ_d are two, their character values in a one-dimensional representation can be $+1$ or -1. The second of the above equations then forces the $|\chi(S_4)| = 1$ and the first of the above equations forces it to be real. The only possible combinations of characters satisfying the above equations for representations of degree 1 are then as shown in the character table. In the representation of degree 2 (i.e., the representation E), the character of identity is clearly 2. The characters of other elements in this representation can now be ascertained easily using orthogonality of the columns of the character table (Equation 3.3.10). For example, the columns of the group elements E and C_2 are orthogonal.

$$\overline{\chi^{A_1}(E)}\chi^{A_1}(C_2)+\overline{\chi^{A_2}(E)}\chi^{A_2}(C_2)+\overline{\chi^{B_1}(E)}\chi^{B_1}(C_2)+$$

$$+\overline{\chi^{B_2}(E)}\chi^{B_2}(C_2)+\overline{\chi^{E}(E)}\chi^{E}(C_2)=0.$$

It follows then that $\chi^{E}(C_2)=-2$. In the same manner the characters of other elements in the representation E can be easily checked to be 0. Lastly, it may be noted that the principal axis of symmetry in the group is the S_4 axis. In accordance with this fact, the symmetric representations A_1 and A_2 are the ones in which the $\chi(S_4)=1$, while in the antisymmetric representations B_1 and B_2, $\chi(S_4)=-1$. □

Example 23. Consider the cyclic group C_3. Since there are three conjugacy classes in C_3, there are 3 irreducible representations of C_3. All the representations are of degree 1, as follows from the equation $1^2+1^2+1^2=3$. In the unit representation, all elements have character 1. In a representation of degree 1 (not the unit representation), let the character of rotation C_3 be ω.

C_3	E	C_3	C_3^2		
A	1	1	1	$z; R_z$	$x^2+y^2; z^2$
E	1	$e^{\frac{2\pi i}{3}}$	$e^{-\frac{2\pi i}{3}}$	$(x,y);$	$(x^2-y^2, xy);$
	1	$e^{-\frac{2\pi i}{3}}$	$e^{\frac{2\pi i}{3}}$	(R_x, R_y)	$(yz,\ xz)$

Suppose the basis vector for this representation is ψ. The action of C_3 rotation on ψ is in accordance with $C_3\psi = \omega\psi$. Then

$$C_3^2\psi = C_3(C_3\psi) = C_3(\omega\psi) = \omega C_3\psi = \omega^2\psi.$$

Thus the character of C_3^2 in the same representation is ω^2. It follows from Equation 3.3.9 that $1+\omega+\omega^2 = 0$. Hence ω is the complex cube root of unity. These representations are shown in the last two rows of the character table. However, instead of identifying them as two separate 1 degree representations, these representations are combined into a single 2 degree representation, identified as E in the first column. The reason for doing so will be made clear when applications are considered. □

Example 24. Consider the group C_{3v}. The group is non-abelian with 6 members in 3 conjugacy classes. Since $1^2+1^2+2^2 = 6$, C_{3v} has three irreducible representations, two of which are of degree 1, and one is of degree 2. The calculations in this case are straightforward and the reader can easily verify that indeed the following characters are obtained:

C_{3v}	E	$2C_3$	$3\sigma_v$		
$\mathbf{A_1}$	1	1	1	z	$x^2+y^2; z^2$
$\mathbf{A_2}$	1	1	-1	R_z	
E	2	-1	0	$(x,y); (R_xR_y)$	$xz; yz$

□

3.5 The Regular Representation

Consider a finite group G of order n whose elements are $g_1(=E)$, $g_2, \ldots g_n$. Let $\{x_i\}_{i=1}^n$ be a linearly independent set of unit vectors spanning an n-dimensional vector space. The group elements can be put in a one to one correspondence with the basis vectors clearly by associating g_i with x_i. Then the action of the group element g on this vector space can be formally defined by $x_k = x_i g$ if $g_k = g_i g$. If $g = E$, clearly $x_k = x_i$, i.e., action of the identity element fixes every basis vector. For this reason, E can be associated with the $n \times n$ identity matrix. For any other group element g, right multiplication of G with g is a mere permutation of elements of G in which none of the elements of G are fixed. Correspondingly, g transforms any given unit vector in the basis to another distinct unit vector in the basis. It follows that the matrix

representation of g would be a $n \times n$ matrix in which each row and each column would contain exactly one non-zero entry which will be equal to 1. This particular representation of G is called the *right regular representation*, which we denote by the symbol Γ^R. It is clear the degree of Γ^R is n, $\chi^{\Gamma^R}(E) = n$ and $\chi^{\Gamma^R}(g) = 0$ for $g \neq E$. From orthogonality relations, it follows that Γ^R cannot be an irreducible representation.

The immediate task is to decompose Γ^R as a direct sum of the irreducible representations of G. In order to do this, assume more generally that Γ is some reducible representation of G. Suppose now that

$$\Gamma = \bigoplus_{i=1}^{r} m_i \Gamma^i,$$

where m_i is the multiplicity with which the irreducible representation Γ^i appears in Γ and r is the number of distinct irreducible representations of G. It follows from above that for any group element g

$$\begin{aligned}
\chi^{\Gamma}(g) &= \sum_{i=1}^{r} m_i \chi^{\Gamma^i}(g) \\
&\Rightarrow \chi^{\Gamma}(g)\overline{\chi^{\Gamma^k}(g)} = \sum_{i=1}^{r} m_i \chi^{\Gamma^i}(g)\overline{\chi^{\Gamma^k}(g)} \\
&\Rightarrow \sum_{g \epsilon G} \chi^{\Gamma}(g)\overline{\chi^{\Gamma^k}(g)} = \sum_{i=1}^{r} m_i \sum_{g \epsilon G} \chi^{\Gamma^i}(g)\overline{\chi^{\Gamma^k}(g)}.
\end{aligned}$$

Using Equation 3.3.6, it now easily follows that

$$m_k = \frac{1}{|G|} \sum_{g \epsilon G} \chi^{\Gamma}(g)\overline{\chi^{\Gamma^k}(g)}.$$

The equation above can be used to obtain the multiplicity m_k with which any irreducible representation Γ^k appears in a given reducible representation Γ. In the specific case of $\Gamma = \Gamma^R$, it was earlier noted that $\chi^{\Gamma^R}(E) = n$ and $\chi^{\Gamma^R}(g) = 0$ for $g \neq E$. Since $\chi^{\Gamma^k}(E) = \ell_k$, one has $m_k = \ell_k$ from the above equation. Each irreducible representation of G appears as many times as its degree in the right regular representation of G. Additionally, since $\chi^{\Gamma^R}(E) = \sum_{i=1}^{r} m_i \chi^{\Gamma^i}(E)$, Equation 3.3.4 follows as a consequence. Finally it may be noted that the trivial representation (of degree 1) occurs once in Γ^R.

3.6 Tensor Product of Representations

It is possible to generate reducible representations of a group from its irreducible ones. This can be done by forming what is called the *tensor product* of the

irreducible representations. Let G be a finite group which has Γ_1 and Γ_2 as irreducible representations. Γ_1 is a representation of G on a unitary space V spanned by the basis $\{x_i\}_{i=1}^{n_1}$ whereas Γ_2 is a representation of G on a unitary space W spanned by the basis $\{y_i\}_{i=1}^{n_2}$. The tensor product of V and W, denoted by $V \otimes W$, is another vector space spanned by the basis $\{x_i \otimes y_j\}_{i=1,j=1}^{n_1,n_2}$. The dimension of $V \otimes W$ is clearly equal to the product of the dimensions of V and W. Once the product space has been defined, it remains to construct a representation Γ of G on $V \otimes W$. The representation Γ is called the tensor product of the representations Γ_1 and Γ_2 and symbolically $\Gamma = \Gamma_1 \otimes \Gamma_2$. For completing the definition, $\Gamma(g)$ should be simply related to $\Gamma_1(g)$ and $\Gamma_2(g)$ for all g in G. This essentially requires the specification of action of g on every basis vector of $V \otimes W$. For the basis vector $x_i \otimes y_j$ in $V \otimes W$ let

$$
\begin{aligned}
& g(x_i \otimes y_j) \to g(x_i) \otimes g(y_j) \\
& g(x_i \otimes y_j) \to \left(\sum_{k=1}^{n_1} [\Gamma_1(g)]_{ki} x_k \right) \otimes \left(\sum_{l=1}^{n_2} [\Gamma_2(g)]_{lj} y_l \right) \\
& g(x_i \otimes y_j) \to \sum_{k=1}^{n_1} \sum_{l=1}^{n_2} [\Gamma_1(g)]_{ki} [\Gamma_2(g)]_{lj} x_k \otimes y_l. \qquad (3.6.1)
\end{aligned}
$$

The above mapping defines the action of g on a basis state $x_i \otimes y_j$ of $V \otimes W$. It remains to be shown that with such a definition, Γ is indeed a representation of G on $V \otimes W$, or in other words, Equation 3.2.1 is satisfied. The rows and columns of the matrix $\Gamma(g)$ can be indexed by the basis states $x_i \otimes y_j$. Equation 3.2.1 is true if

$$
[\Gamma(g_1 g_2)]_{x_u \otimes y_v,\, x_s \otimes y_i} = [\Gamma(g_1)\Gamma(g_2)]_{x_u \otimes y_v, x_s \otimes y_i}.
$$

The verification of the above equality is trivial after noticing

$$
[\Gamma(g)]_{x_u \otimes y_v,\, x_s \otimes y_i} = [\Gamma_1(g)]_{us} [\Gamma_2(g)]_{vi}, \qquad (3.6.2)
$$

which follows from the mapping defined in 3.6.1. The character of g can be easily obtained by summing the diagonal elements. A direct consequence of the above is that

$$
\chi^{\Gamma = \Gamma_1 \otimes \Gamma_2}(g) = \chi^{\Gamma_1}(g) \chi^{\Gamma_2}(g). \qquad (3.6.3)
$$

3.7 Decomposition of Reducible Representations

A reducible representation Γ of a group G over a unitary space V can be expressed as a direct sum of the irreducible representations Γ^α of G in which each irreducible representation appears with a certain multiplicity m_α.

$$\Gamma = \bigoplus_{\alpha=1}^{r} m_\alpha \Gamma^\alpha. \tag{3.7.1}$$

In Section 3.5, the formula for m_α was obtained which is restated below for emphasis.

$$m_\alpha = \frac{1}{|G|} \sum_{g \in G} \chi^\Gamma(g) \overline{\chi^{\Gamma^\alpha}(g)}. \tag{3.7.2}$$

It may be desirable sometimes to not only know the multiplicities of the various irreducible representations in Γ but also the subspace of V which is left invariant by the irreducible representation Γ^α (i.e., the subspace of V on which Γ^α is an irreducible representation of G).

Let V be a unitary space of which U and W are proper subspaces such that $V = U \oplus W$. Then any vector v in V can be expressed uniquely as a sum of vectors u and w which belong to U and W respectively. The projection operator P_U is a linear operator on V with values in the subspace U such that

$$P_U v = u.$$

Similarly P_W may be defined so that $P_W v = w$. Since the projection operator is a mapping onto a proper subspace, it is not invertible. The projection operator essentially projects a vector in V on a subspace (for which the operator is defined). As a trivial example, the projection operators that project out the x, y and z components of a vector in $\mathbb{R}^3$ are

$$P_x = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad P_y = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}; \quad P_z = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The problem of finding the subspace of V which is left invariant by the irreducible representation Γ^α (Equation 3.7.1) reduces to constructing the project operator P_{Γ^α}. In the orthogonality relation (Equation 3.3.5)

$$\sum_{g \epsilon G} \overline{[\Gamma^\alpha(g)]}_{ik} [\Gamma^\beta(g)]_{lm} = \frac{|G|}{\ell_{\Gamma^\alpha}} \delta_{\Gamma^\alpha \Gamma^\beta} \delta_{il} \delta_{km},$$

if i is set equal to k and summation over all i is performed, then the relation reduces to

$$\frac{\ell_{\Gamma^\alpha}}{|G|} \sum_{g \epsilon G} \overline{\chi^\alpha(g)} [\Gamma^\beta(g)]_{lm} = \delta_{\Gamma^\alpha \Gamma^\beta} \delta_{lm}.$$

It is evident that when Γ^α and Γ^β are the same representations then the right hand side of the above is the identity matrix of order $\ell_\alpha \times \ell_\alpha$ and in other cases the right

hand side is the null matrix. This important property motivates the following definition of the projection operator P_{Γ^α} on the reducible representation Γ.

$$P_{\Gamma^\alpha} = \frac{\ell_{\Gamma^\alpha}}{|G|} \sum_{g \epsilon G} \overline{\chi^{\Gamma^\alpha}(g)} \Gamma(g). \tag{3.7.3}$$

In the direct sum in Equation 3.7.1, upon action of P_{Γ^α} only those blocks in the matrix $\Gamma(g)$ will be non-zero which correspond to subspaces on which Γ^α gives a representation of G.

Example 25. Consider the group C_{3v}. In an earlier example (Section 3.2, Example 20), the explicit form of the matrices for various group elements was calculated by considering the group's action on $\mathbb{R}^3$. The k vector was left invariant under all transformations and in fact, the representation generated was of degree 2. For reference, the representing matrices of various group elements of C_{3v} in the irreducible representation E are given below:

$$E(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \qquad E(C_3) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix};$$

$$E\left(C_3^2\right) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}; \quad E(\sigma_v) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};$$

$$E(C_3\sigma_v) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}; \quad E\left(C_3^2\sigma_v\right) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}.$$

Let $\Gamma = E \otimes E$ be the tensor product of the irreducible representation of degree 2 with itself. From Equation 3.6.3, it follows that $\chi^\Gamma(E) = 4$, $\chi^\Gamma(C_3) = \chi^\Gamma(C_3^2) = 1$ and $\chi^\Gamma(\sigma_v) = \chi^\Gamma(\sigma_v C_3) = \chi^\Gamma(\sigma_v C_3^2) = 0$. It is now possible to decompose Γ. The multiplicity of various irreducible representations in Γ can be calculated by application of Equation 3.7.2.

$$\text{Multiplicity of } A_1 = \frac{1}{6}[1 \times 4 \times 1 + 2 \times 1 \times 1 + 3 \times 0 \times 1] = 1.$$

$$\text{Multiplicity of } A_2 = \frac{1}{6}[1 \times 4 \times 1 + 2 \times 1 \times 1 + 3 \times 0 \times 0] = 1.$$

$$\text{Multiplicity of } E = \frac{1}{6}[1 \times 4 \times 2 + 2 \times 1 \times -1 + 3 \times 0 \times 0] = 1.$$

It may be noted that $\Gamma = A_1 \oplus A_2 \oplus E$. Each of the irreducible representations of C_{3v} occur only once in Γ. From the matrices of the representation E, the matrices of the representation Γ can be calculated by using Equation 3.6.2. The basis for the tensor product space in this case can be taken as $i_1 \otimes i_2$, $i_1 \otimes j_2$, $j_1 \otimes i_2$ and $j_1 \otimes j_2$ where

$\{i_1,\ j_1\}$ is the basis of one Γ^E and $\{i_2,\ j_2\}$ is the basis for the other. The rows and columns of the matrices in Γ representation are indexed in the order of the basis states of the tensor product space as mentioned in the previous line. With this convention, following matrices in Γ representation are obtained:

$$\Gamma(E) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\Gamma(C_3) = \begin{pmatrix} \frac{1}{4} & \frac{\sqrt{3}}{4} & \frac{\sqrt{3}}{4} & \frac{3}{4} \\ -\frac{\sqrt{3}}{4} & \frac{1}{4} & -\frac{3}{4} & \frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{4} & -\frac{3}{4} & \frac{1}{4} & \frac{\sqrt{3}}{4} \\ \frac{3}{4} & -\frac{\sqrt{3}}{4} & -\frac{\sqrt{3}}{4} & \frac{1}{4} \end{pmatrix},$$

$$\Gamma(C_3^2) = \begin{pmatrix} \frac{1}{4} & -\frac{\sqrt{3}}{4} & -\frac{\sqrt{3}}{4} & \frac{3}{4} \\ \frac{\sqrt{3}}{4} & \frac{1}{4} & -\frac{3}{4} & -\frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & -\frac{3}{4} & \frac{1}{4} & -\frac{\sqrt{3}}{4} \\ \frac{3}{4} & \frac{\sqrt{3}}{4} & \frac{\sqrt{3}}{4} & -\frac{1}{4} \end{pmatrix},$$

$$\Gamma(\sigma_v) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

$$\Gamma(C_3\sigma_v) = \begin{pmatrix} \frac{1}{4} & -\frac{\sqrt{3}}{4} & -\frac{\sqrt{3}}{4} & \frac{3}{4} \\ -\frac{\sqrt{3}}{4} & -\frac{1}{4} & \frac{3}{4} & \frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{4} & \frac{3}{4} & -\frac{1}{4} & \frac{\sqrt{3}}{4} \\ \frac{3}{4} & \frac{\sqrt{3}}{4} & \frac{\sqrt{3}}{4} & \frac{1}{4} \end{pmatrix},$$

$$\Gamma(C_3^2\sigma_v) = \begin{pmatrix} \frac{1}{4} & \frac{\sqrt{3}}{4} & \frac{\sqrt{3}}{4} & \frac{3}{4} \\ \frac{\sqrt{3}}{4} & -\frac{1}{4} & \frac{3}{4} & -\frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{4} & \frac{3}{4} & -\frac{1}{4} & -\frac{\sqrt{3}}{4} \\ \frac{3}{4} & -\frac{\sqrt{3}}{4} & -\frac{\sqrt{3}}{4} & \frac{1}{4} \end{pmatrix}.$$

Finally the projection operators for the irreducible representations in Γ may be calculated from these matrices, the characters of irreducible representations and Equation 3.7.3. For example, all the characters in A_1 are unit, and Equation 3.7.3 takes the form

$$P_{A_1} = \frac{1}{6}\left[\Gamma(E) + \Gamma(C_3) + \Gamma(C_3^2) + \Gamma(\sigma_v) + \Gamma(C_3\sigma_v) + \Gamma(C_3^2\sigma_v)\right].$$

In a similar fashion, the projection operators for other irreducible representations may be obtained. The results follow:

$$P_{A_1} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & \frac{1}{2} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \frac{1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix}, \quad P_E = \begin{pmatrix} \frac{1}{2} & 0 & 0 & -\frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix},$$

$$P_{A_2} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & -\frac{1}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

By letting these projection operators act on any general vector in the tensor product space spanned by $i_1 \otimes i_2$, $i_1 \otimes j_2$, $j_1 \otimes i_2$ and $j_1 \otimes j_2$, the subspace on which the corresponding representation exists is easily found. Let $v = \alpha(i_1 \otimes i_2) + \beta(i_1 \otimes j_2) + \Gamma(j_1 \otimes i_2) + \delta(j_1 \otimes j_2)$ be a typical vector. Then

$$P_E v = \begin{pmatrix} \frac{1}{2} & 0 & 0 & -\frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ 0 & \frac{1}{2} & \frac{1}{2} & 0 \\ -\frac{1}{2} & 0 & 0 & \frac{1}{2} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \\ \Gamma \\ \delta \end{pmatrix} = \frac{1}{2}\begin{pmatrix} \alpha - \delta \\ \beta + \gamma \\ \beta + \gamma \\ -(\alpha - \delta) \end{pmatrix}$$

$$\Rightarrow P_E = \frac{\alpha - \delta}{2}(i_1 \otimes i_2 - j_1 \otimes j_2) + \frac{\beta + \gamma}{2}(i_1 \otimes j_2 + j_1 \otimes i_2).$$

Thus P_E projects onto the two-dimensional subspace spanned by $(i_1 \otimes i_2 - j_1 \otimes j_2)$ and $(i_1 \otimes j_2 + j_1 \otimes i_2)$. Likewise, one may show that P_{A_1} projects onto the one-dimensional subspace spanned by

$$(i_1 \otimes i_2 + j_1 \otimes j_2)$$

and P_{A_2} projects onto the one-dimensional subspace spanned by

$$(i_1 \otimes j_2 - j_1 \otimes i_2).$$ □

The preceding development illustrated the method by which a reducible representation can be decomposed into irreducible parts. In the remainder of this section, decomposition of tensor product of two irreducible representations is considered. Let Γ^1 and Γ^2 be two irreducible representations of a group G and $\Gamma^1 \otimes \Gamma^2$ be their tensor product. The multiplicity of the unit representation of G in $\Gamma^1 \otimes \Gamma^2$ may be calculated by using Equations 3.6.3 and 3.7.2. Since every group element has a unit character in the unit representation, the multiplicity of the unit representation is given by

$$\frac{1}{|G|}\sum_{g\epsilon G}\chi^{\mathrm{A}}(g)\overline{\chi^{\Gamma^1\otimes\Gamma^2}(g)} = \frac{1}{|G|}\sum_{g\epsilon G}\overline{\chi^{\Gamma^1}\chi^{\Gamma^2}}.$$

The right hand side of the above equation is equal to 1 if Γ^1 and Γ^2 are conjugate representations and 0 in all other cases (Equation 3.3.6). If the characters of the representation are real, then the unit representation is present only in the tensor product of the representation with itself. For now suppose Γ is an irreducible representation of G on a unitary space V which is spanned by the basis $\{x_i\}_{i=1}^n$. Then the tensor product space $V \otimes V$ is of dimension n^2 and is spanned by basis states $\{x_i \otimes x_j\}_{i=1,j=1}^{n,n}$. Note that $x_i \otimes x_j$ is distinguished from $x_j \otimes x_i$. Apart from this particular choice of basis, another choice is sometimes useful. Consider the subspaces $(V \otimes V)^\sigma$ and $(V \otimes V)^\alpha$ (read symmetric and antisymmetric subspaces respectively). The symmetric space $(V \otimes V)^\sigma$ is spanned by basis states $x_i \otimes x_j + x_j \otimes x_i$ when $i \neq j$ and the states $x_i \otimes x_i$. Clearly the dimension of $(V \otimes V)^\sigma$ is $\dfrac{n(n+1)}{2}$. In a similar manner, the antisymmetric subspace $(V \otimes V)^\alpha$ spanned by basis states $x_i \otimes x_j - x_j \otimes x_i$ for $i \neq j$ is of dimension $\dfrac{n(n-1)}{2}$. Note that the dimensions of the symmetric and the antisymmetric subspaces add up to n^2 as they should. Let g be some transformation in G. Consider the action of g on a basis state in the antisymmetric subspace. In accordance with Equation 3.6.1, one has

$$g\left(x_i \otimes x_j - x_j \otimes x_i\right) \to g\left(x_i\right) \otimes g\left(x_j\right) - g\left(x_j\right) \otimes g\left(x_i\right)$$

$$g\left(x_i \otimes x_j - x_j \otimes x_i\right) \to \left(\sum_{k=1}^{n}\left[\Gamma(g)\right]_{ki} x_k\right) \otimes \left(\sum_{l=1}^{n}\left[\Gamma(g)\right]_{lj} x_l\right)$$

$$- \left(\sum_{l=1}^{n}\left[\Gamma(g)\right]_{lj} x_l\right) \otimes \left(\sum_{k=1}^{n}\left[\Gamma(g)\right]_{ki} x_k\right)$$

$$g\left(x_i \otimes x_j - x_j \otimes x_i\right) \to \sum_{k,l=1}^{n}\left[\Gamma(g)\right]_{ki}\left[\Gamma(g)\right]_{lj}\left(x_k \otimes x_l - x_l \otimes x_k\right)$$

$$g\left(x_i \otimes x_j - x_j \otimes x_i\right) \to \frac{1}{2}\sum_{k,l=1}^{n}\left(\left[\Gamma(g)\right]_{ki}\left[\Gamma(g)\right]_{lj} - \left[\Gamma\left(g\right)\right]_{li}\left[\Gamma(g)\right]_{kj}\right)\left(x_k \otimes x_l - x_l \otimes x_k\right)$$

As is evident from the above map, the antisymmetric subspace gives a subrepresentation $(\Gamma \otimes \Gamma)^{\alpha}$ of the group G. The characters χ^2_{α} of the antisymmetric representation can be easily obtained from the above map to be

$$\chi^2_{\alpha}(g) = \frac{1}{2}\sum_{i,j=1}^{n}\left([\Gamma(g)]_{ii}\,[\Gamma(g)]_{jj} - [\Gamma(g)]_{ji}\,[\Gamma(g)]_{ij}\right)$$

$$\Rightarrow \quad \chi^2_{\alpha}(g) = \frac{1}{2}\left((\chi(g))^2 - \chi\left(g^2\right)\right). \tag{3.7.4}$$

The reader will do well to convince themselves that the symmetric subspace also gives a subrepresentation $(\Gamma \otimes \Gamma)^{\sigma}$ of G. The characters $\chi^2_{\sigma}(g)$ of the symmetric representation can be shown to be

$$\chi^2_{\sigma}(g) = \frac{1}{2}\left((\chi(g))^2 + \chi\left(g^2\right)\right). \tag{3.7.5}$$

Finally, it may be noted that in the decomposition of the representation $\Gamma \otimes \Gamma$ as $(\Gamma \otimes \Gamma)^{\sigma} \oplus (\Gamma \otimes \Gamma)^{\alpha}$, the symmetric as well as the antisymmetric component may be a reducible representation of Γ.

3.8 Irreducible Representations of Direct Products

As has been noted previously, it is sometimes possible that a group is isomorphic to a direct product of two of its subgroups (e.g. $D_{nh} = D_n \times C_s$). The tensor product described in Section 3.6 allows the construction of all the irreducible representations of the direct product from the irreducible representations of the component groups. Let G be isomorphic to the the direct product $H \times K$ of two groups H and K. Then any element g of G can be expressed uniquely as

$$g = hk,$$

where h is in H and k is in K. It is also known that H and K are normal subgroups in G and elements of H commute with elements of K. Let it be assumed that h_1 and h_2 are conjugate in H and similarly for k_1 and k_2 in K. Then $h_1k_1 = hh_2h^{-1}kk_2k^{-1}$ for some h in H and some k in K. Because of the commutation it follows that $h_1k_1 = (hk)h_2k_2(hk)^{-1}$, i.e., h_1k_1 is conjugate to h_2k_2 and by the same reasoning h_1k_1, h_1k_2, h_2k_1 and h_2k_2 are all conjugates in G. A conjugacy class of G consists of all elements of the form hk in which h's come from one conjugacy class of H and the k's come from one conjugacy class of K. It follows that the number of conjugacy classes in G is equal to the product of the number of conjugacy classes in H and the number of conjugacy classes in K. For this reason the number of irreducible representations of G is equal to the number of irreducible representations of H times the number of irreducible representations of K. It is natural to expect that an irreducible representation of G could be obtained by forming a tensor product of the an irreducible representation of H with an irreducible representation of K. If Γ_H is

an irreducible representation of H on a unitary space V spanned by the basis $\{x_i\}_{i=1}^{n_1}$ whereas Γ_K is an irreducible representation of K on a unitary space W spanned by the basis $\{y_i\}_{i=1}^{n_2}$, then a representation of G on $V \otimes W$ is obtained from the map

$$(hk)(x_i \otimes y_j) \to h(x_i) \otimes k(y_j),$$

where hk is an element of G. Proceeding as before, with maps such as above, it is not very difficult to show that the representations so obtained indeed satisfy Equations 3.3.6, 3.3.7, 3.3.8 and 3.3.9. Additionally, in analogy with Equation 3.6.3, in the current case one has

$$\chi^{\Gamma_H \otimes \Gamma_K}(hk) = \chi^{\Gamma_H}(h)\chi^{\Gamma_K}(k). \tag{3.8.1}$$

Example 26. The group D_{2h} is a direct product of D_2 and C_s. The character tables for D_2 and C_s follow:

D_2	E	$C_2(z)$	$C_2(y)$	$C_2(x)$		
A_1	1	1	1	1		x^2, y^2, z^2
B_1	1	1	-1	-1	z, R_z	xy
B_2	1	-1	1	-1	y, R_y	zx
B_3	1	-1	-1	1	x, R_x	yz

C_S	E	σ_h		
A'	1	1	x, y, R_z	x^2, y^2, z^2
A''	1	-1	z, R_x, R_y	yz, xz

It is evident now that D_{2h} has 8 conjugacy classes and 8 irreducible representations. Apart from all the conjugacy classes in D_2, there are other classes in D_{2h}. For example, $C_2(z)$ in D_2 multiplied with σ_h in C_s gives a class containing a single operation of inversion in D_{2h}, denoted by I. Similarly, multiplication of $C_2(y)$ with σ_h is a class containing the single element corresponding to reflection in the xz plane, and so on. The characters are various classes in D_{2h} and are obtained from those of D_2 and C_s by use of Equation 3.8.1. The names of various irreducible representations of D_{2h}, in accordance with the discussion in Section 3.4, are as mentioned in the character table:

D_{2h}	E	$C_2(z)$	$C_2(y)$	$C_2(x)$	I	σ_{xy}	σ_{xz}	σ_{yz}		
A_g	1	1	1	1	1	1	1	1		x^2, y^2, z^2
B_{1g}	1	1	−1	−1	1	1	−1	−1	R_z	xy
B_{2g}	1	−1	1	−1	1	−1	1	−1	R_y	zx
B_{3g}	1	−1	−1	1	1	−1	−1	1	R_x	yz
A_u	1	1	1	1	−1	−1	−1	−1		
B_{1u}	1	1	−1	−1	−1	−1	1	1	z	
B_{2u}	1	−1	1	−1	−1	1	−1	1	y	
B_{3u}	1	−1	−1	1	−1	1	1	−1	x	

.

□

3.9 Induced Representations

Let G be a group and Γ a representation of G on a vector space V. For a subgroup H of G, the matrices $\Gamma(h)$ for all $h \in H$ together form a representation of H on V. A representation of H obtained by restricting a representation of G to H is denoted by Γ_* in this section. The reverse problem of obtaining a representation of G from a representation Θ of H is considered here. Such a representation of G is said to be induced by the representation Θ of H and is denoted by Θ^* in this section.

The first step in the construction of Θ^* is to realize a representation of G on the set of cosets of H in G. Let $\{x_i\}_{i=1}^n$ be a set of representatives, one from each of the distinct cosets of H in G. Then one has $G = \cup x_i H$. If $g \in G$, then gx_iH is again a coset and therefore equal to x_kH for some x_k. Because $\{x_i\}_{i=1}^n$ are representatives of distinct cosets, $gx_iH \neq gx_jH$ unless $i = j$. In other words, left multiplication by g permutes the cosets of H among themselves. Every $g \in G$ in this way can be identified with a permutation τ_g in $\mathfrak{S}(n)$, the symmetric group on the n letters $\{x_i\}_{i=1}^n$. It follows from

$$\begin{aligned} \tau_{g_1g_2}(x_iH) &= g_1g_2(x_iH) = g_1(g_2x_iH) \\ &\Rightarrow \quad \tau_{g_1g_2}(x_iH) = \tau_{g_1}\tau_{g_2}(x_iH) \end{aligned}$$

that τ is a representation of G into $\mathfrak{S}(n)$, i.e., $\tau : G \to \mathfrak{S}(n)$ is a homomorphism. One notices that the regular representation described in the Section 3.5 corresponds to the case when H is the trivial subgroup $\{E\}$ of G.

Example 27. Consider the group $\mathfrak{S}(3)$ of Example 10 in Chapter 1. The subgroup $H = \{e,\ a\}$ has 3 cosets $eH = \{e,\ a\}$, $bH = \{b,\ ba\}$ and $b^2H = \{b^2,\ b^2a\}$. Consider the action of the element $ab \in \mathfrak{S}(3)$ on the cosets. Evidently

$$ab:\ eH \to b^2H,\ ab:\ bH \to bH,\ ab:\ b^2H \to eH.$$

In matrix form, the above action can be written as

$$\tau_{ab} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

The representation for other elements can be similarly worked out.

$$\tau_e = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tau_a = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \tau_b = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix},$$

$$\tau_{b^2} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \tau_{ab^2} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}. \qquad \square$$

As previously, let Θ be a representation of the subgroup H over a vector space W of dimension m. Θ is extended to Θ^* by τ action of G on the coset space of H. The τ representation of G consists of permutation matrices. Such matrices have a single 1 as the only non-zero entry in each row and each column as is evident from the above example. For $g \in G$, the $(i, j)'$th entry in τ_g is equal to 1 if and only if $x_i^{-1} g x_j \in H$. Define matrices g^{ij} as

$$g^{ij} = \begin{cases} \Theta(x_i^{-1} g x_j) & \text{if } x_i^{-1} g x_j \in H \\ 0_{m\times m} & \text{otherwise.} \end{cases} \tag{3.9.1}$$

Here $0_{m\times m}$ is the $m \times m$ matrix all of whose entries are equal to 0. The matrix $\Theta^*(g)$ in the induced representation is now given in terms of matrix blocks g^{ij} as

$$\Theta^*(g) = \begin{pmatrix} g^{11} & \cdots & g^{1n} \\ \vdots & \ddots & \vdots \\ g^{n1} & \cdots & g^{nn} \end{pmatrix}. \tag{3.9.2}$$

Evidently, the order of $\Theta^*(g)$ is $mn \times mn$. Because of the form of τ, only one matrix block is non-zero in any row or any column of matrix blocks in $\Theta^*(g)$. It remains to be verified that Θ^* is a representation of G. For $g_1, g_2 \in G$ the $(i, j)'$th matrix block of the product matrix $\Theta^*(g_1)\Theta^*(g_2)$ is given by

$$[\Theta^*(g_1)\Theta^*(g_2)]^{ij} = \sum_{k=1}^{n} (g_1)^{ik}(g_2)^{kj}.$$

The matrix in the right hand side of the above can be non-zero only when $(g_1)^{ik}$ and $(g_2)^{kj}$ are non-zero for the same $k = k_0$. This happens when both $x_i^{-1} g_1 x_{k_0}$ and $x_{k_0}^{-1} g_2 x_j$

are in H. Then $(g_1)^{ik_0} = \Theta(x_i^{-1} g_1 x_{k_0})$, $(g_2)^{k_0 j} = \Theta(x_{k_0}^{-1} g_2 x_j)$ and one has

$$\begin{aligned} [\Theta^*(g_1)\Theta^*(g_2)]^{ij} &= \Theta(x_i^{-1} g_1 x_{k_0})\Theta(x_{k_0}^{-1} g_2 x_j) \\ &\Rightarrow \quad [\Theta^*(g_1)\Theta^*(g_2)]^{ij} = [\Theta^*(g_1 g_2)]^{ij}. \end{aligned} \tag{3.9.3}$$

Also note that $g_2 x_j \in x_k H$ for some x_k and if $x_i^{-1} g_1 g_2 x_j \in H$, then both $x_i^{-1} g_1 x_k$ and $x_k^{-1} g_2 x_j$ are in H. Hence the corresponding non-zero blocks of $\Theta^*(g_1)\Theta^*(g_2)$ and $\Theta^*(g_1 g_2)$ are equal. It is similarly shown that the same holds for the zero blocks and Equation 3.9.3 holds generally. It follows that Θ^* is indeed a representation of G.

Example 28. Continuing with the previous example, a representation of H of degree 2 is

$$\Theta(e) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \; \Theta(a) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

The reader should follow the above description to obtain Θ^*. A couple of representing matrices are

$$\Theta^*(ab) = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}; \quad \Theta^*(b^2) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{pmatrix}. \qquad \square$$

If χ is the character of Θ and χ^* that of Θ^*, then it follows from Equation 3.9.2 that $\chi^*(g) = \sum_{i=1}^{n} \text{tr } g^{ii}$. By use of Equation 3.9.1, one has

$$\chi^*(g) = \sum_{i=1,\, x_i^{-1} g x_i \in H}^{n} \chi(x_i^{-1} g x_i). \tag{3.9.4}$$

For $x_i^{-1} g x_i \in H$, one also has $\chi(x_i^{-1} g x_i) = \chi(h^{-1} x_i^{-1} g x_i h) \; \forall \; h \in H$. Employing this fact, the reader can easily establish

$$\chi^*(g) = \frac{1}{|H|} \sum_{t \in G, t^{-1} g t \in H} \chi(t^{-1} g t). \tag{3.9.5}$$

Suppose now that Γ is an irreducible representation of G and Θ an irreducible representation of H, a subgroup of G. In general, Γ_* and Θ^* are reducible representations of H and G respectively. The multiplicity m_* of Θ in Γ_* is given by

$$m_* = \frac{1}{|H|} \sum_{h \in H} \chi^{\Gamma}(h) \chi^{\Theta}(h^{-1}),$$

where use has been made of the facts $\Gamma_*(h) = \Gamma(h)\ \forall\ h \in H$ and $\overline{\chi^{\Theta}(h)} = \chi^{\Theta}(h^{-1})$. The multiplicity m^* of Γ in Θ^* is given by

$$\begin{aligned} m^* &= \frac{1}{|G|}\sum_{g\in G}\chi^{\Theta^*}(g^{-1})\chi^{\Gamma}(g) \\ \Rightarrow\quad m^* &= \frac{1}{|G|}\sum_{g\in G}\chi^{\Gamma}(g)\left(\sum_{i=1, x_i^{-1}g^{-1}x_i\in H}^{n}\chi^{\Theta}(x_i^{-1}g^{-1}x_i)\right). \end{aligned}$$

Rearranging the summations and using the fact that $\chi^{\Gamma}(g) = \chi^{\Gamma}(x_i^{-1}gx_i)$, one has

$$m^* = \frac{1}{|G|}\sum_{i=1}^{n}\sum_{g\in G,\ x_i^{-1}g^{-1}x_i\in H}\chi^{\Gamma}\left(x_i^{-1}gx_i\right)\chi^{\Theta}\left(x_i^{-1}g^{-1}x_i\right).$$

The conjugation $x_i^{-1}Gx_i$ is an automorphism of G. The second summation is therefore over exactly all the elements of H. Since there are $|G|/|H|$ representatives, it follows that

$$m^* = \frac{1}{|G|}\frac{|G|}{|H|}\sum_{h\in H}\chi^{\Gamma}(h)\chi^{\Theta}(h^{-1}) = m_*. \tag{3.9.6}$$

The above result is called the *Frobenius reciprocity theorem*.

Assuming again H to be a subgroup of G, let Θ_1 and Θ_2 be representations of H over vector spaces of W_1 and W_2. Let the degrees of these representations be n_1 and n_2. Then in the representation $\Theta_1 \oplus \Theta_2$ over $W_1 \oplus W_2$, one has for $h \in H$

$$(\Theta_1 \oplus \Theta_2)(h) = \begin{pmatrix} \Theta_1(h) & 0_{n_1\times n_2} \\ 0_{n_2\times n_1} & \Theta_2(h) \end{pmatrix}.$$

The matrices in the representation $(\Theta_1 \oplus \Theta_2)^*$ would have blocks such as above in places where 1 appears in the permutation representation of G on the coset space of H and $0_{(n_1+n_2)\times(n_1+n_2)}$ blocks elsewhere. Such a matrix can be written as a sum of two matrices which operate on complimentary space isomorphic to W_1 and W_2. Therefore, one has

$$(\Theta_1 \oplus \Theta_2)^* = \Theta_1^* \oplus \Theta_2^*. \tag{3.9.7}$$

Exercises

1. Show that all invertible $n \times n$ matrices with complex entries form a group. Also show that the set of matrices whose determinant is of unit modulus is a subgroup.
2. Show that two matrices related by a similarity transformation have the same trace.

3. Using the orthogonality relations, write the character table of the group C_4 and indicate the irreducible representations using Mulliken's symbols. Write down the matrix form of the regular representation of C_4.
4. Show that the characters of a finite cyclic group in any irreducible unitary representation are unimodular.
5. In a certain representation Γ of C_{3v}, it is known that $\chi^{\Gamma}(E) = 7$, $\chi^{\Gamma}(C_3) = 1$ and $\chi^{\Gamma}(\sigma_v) = -3$. Determine the multiplicities of various irreducible representations of C_{3v} in Γ.
6. Obtain the maximal point group symmetry for a particle in a two-dimensional box. Write down the character table for this group along with the basis elements (consider the action of group elements on the coordinate space). Further figure out which stationary states of the particle give the irreducible representations of the group.
7. Construct the character table of the group C_{4v}. Determine the irreducible representations present in the tensor product $E \otimes E$ where E is the two-dimensional irreducible representation of C_{4v}.
8. For the symmetric group $\mathfrak{S}(3)$, determine the characters of all the irreducible representations. Give a complete reducible 3×3 representation Γ of $\mathfrak{S}(3)$ on a three-dimensional vector space V spanned by $(1,\ 0,0)$, $(0,1,0)$ and $(0,0,1)$. Determine the multiplicity of all the irreducible representations in Γ. Using the projection operator on Γ, project out the subspaces of V on which Γ is irreducible.
9. Prove Equation 3.7.5.
10. Construct the character table for the point group D_{3d}. Consider D_{3d} as a direct product of two of its subgroups.
11. Complete the proof of Equation 3.9.5.
12. Let G be a finite group and H a subgroup of G. Show that the regular representation of H induces the regular representation G.
13. If H is a subgroup of G, then show that any irreducible representation of G is a component in the representation induced by some irreducible representation of H. The result of the previous exercise is useful.
14. In the notation of the last section of the chapter, show that $\Gamma \otimes \Theta^* = (\Gamma_* \otimes \Theta)^*$.

4

Elementary Applications

In this chapter, we will focus on solving problems in physics using the group theory representations extensively discussed in the previous chapter. The character tables for any discrete group will be the primary tool to apply in these physical problems. Particular attention will be on atomic and nuclear systems obeying the postulates of quantum mechanics.

For instance, a physical system possessing a discrete group symmetry like C_{4v} may get disturbed by impurities or defects. Such a disturbance could result in a system with a residual symmetry like C_2. In fact, we will see how these effects are reflected in energy spectrum observed experimentally which can be validated using the group representation theory tools.

We hope the readers will appreciate how the formal mathematical steps provide meaning to results observed in the physical systems. We plan to present several examples in atomic, nuclear and particle physics which will highlight the elegance of group theory tools.

4.1 General Considerations

We will briefly review the salient features of quantum mechanics which describe the symmetries possessed by microscopic systems. In fact, this review will be useful for validating these quantum mechanical results applying group theory tools.

For a closed quantum mechanical system, the eigenstates ψ of the system are solutions of the time independent Schrödinger's equation:

$$\mathbf{H}\psi = E\psi, \tag{4.1.1}$$

where H denotes Hamiltonian of the system and E is the energy when the system is in the stationary state ψ. The Hamiltonian H of the system is a self-adjoint operator that acts on the Hilbert space of system states. Equation 4.1.1 essentially states that the action of the Hamiltonian on a stationary state leaves the state invariant apart from a constant factor of E. The eigenstate ψ can be always taken to be a unit vector in the Hilbert space. All vectors which are complex multiples of the same unit vector are assumed to be physically equivalent. In this sense, ψ represents that normalized state of the system. In the notation of Section 3.1, this fact is represented by

$$(\psi,\ \psi) = 1. \tag{4.1.2}$$

Let O be a unitary operator which commutes with H. By the fact that O and H commute, it is implied that the order in which O and H act on a state ψ is immaterial, i.e., $\mathrm{HO}\ \psi = \mathrm{OH}\psi$. If ψ is a stationary state of the system satisfying Equation 4.1.1, then one has

$$\mathbf{H}(\mathbf{O}\psi) = E\mathbf{O}\psi.$$

In other words, if ψ is a stationary state of the system, then so is $\mathrm{O}\psi$. In general, $\mathrm{O}\psi$ would differ from ψ not merely by a constant complex multiple. In this circumstance, the energy level E is said to be *degenerate*.

There can be a set of unitary operators $\{\mathrm{O}_1, \mathrm{O}_2,\ \cdots\}$ commuting with H. By a similar application of these operators to the Schrödinger equation 4.1.1, we deduce energy E to be same for states $\{O_i\psi\}$ which may be linearly independent to ψ. Suppose this set of unitary operators form a group G. Then we interpret such a quantum mechanical system to possess the group symmetry G.

In Section 3.2, it was noted how the elements of a group G may act on a vector space and give a representation of G on that vector space. Suppose that the group G is a symmetrical group of the system under consideration. Such symmetry transformations would leave the form of the Schrödinger equation invariant. We denote the representation of unitary operator O_i as $\Gamma(g_i)$, corresponding to any group element $g_i \in G$, acting on the Hilbert space. Particularly the elements of the set $\{\Gamma(g_i)\}$ commutes with the Hamiltonian of the system possessing group symmetry G. The energy of a stationary state cannot change due to action of $\Gamma(g_i)$. Thus the subspace of degenerate states corresponding to some energy level E gives a representation of G. As this subrepresentation is unitary, it is completely reducible. It is then possible to choose the degenerate eigenstates corresponding to an energy level E so that they transform according to irreducible representations of G. If a particular irreducible representation occurs only once in the representation of G on the full Hilbert space, then all the basis states of this representation are also all the degenerate eigenstates corresponding to some energy E. It may so happen that the degenerate levels of another energy E' give a reducible representation of G. This happens if the Hamiltonian of the system has a higher order symmetry than G, a circumstance we will assume does not occur in the subsequent discussion. To sum up, it would be assumed that the degenerate states corresponding to an energy level can be so chosen that they give an irreducible representation of the symmetry group of the system.

Example 29. For a one-dimensional harmonic oscillator given by the Hamiltonian

$$\mathbf{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2,$$

determine the group symmetry and deduce whether the energy eigenstates are degenerate or non-degenerate.

Observe that the inversion transformation $g : x \to -x$, where $g \in C_i$, commutes with $\mathbf{H}$. Hence C_i is the group symmetry. Recall that the character table of abelian groups contain only one-dimensional irreducible representations. Hence, the energy eigenstates of the harmonic oscillator possessing C_i group symmetry must be non-degenerate.

We have illustrated the power of the group theory tool to deduce the non-degenerate nature of energy eigenstates without solving the Schrödinger equation. Further, the stationary states

$$\psi(x) \propto \Gamma(g)\psi(x),$$

where $\Gamma(g)$ denotes the representation of the group element acting on the Hibert space. By using the projection method (see Section.3.7), the basis states of group C_i can be shown to be either

$$\text{odd} : \psi_0(x) = -\psi_0(-x) \quad \text{or even} : \psi_e(x) = \psi_e(-x).$$

Thus group theory arguments have justified that the stationary states are non-degenerate states which are either $\psi_0(x)$ or $\psi_e(x)$. However, to determine the explicit form of stationary states and the energy eigenvalues, we have to solve the Schrödinger equation. □

We will now look at another system with degenerate energy levels.

Example 30. Consider a particle of mass m moving in two dimensions subjected to potential $\mathrm{V}(x,\ y)$ which is zero inside a square region $-a \leq (x,\ y) \leq a$ and ∞ elsewhere. This is the familiar example in quantum mechanics known as particle in a square box whose energy eigenstates are either non-degenerate or two-fold degenerate. Can we explain the degenerate energy level using the discrete symmetry possessed by the system ?

The Hamiltonian describing such a system is

$$\mathbf{H} = -\frac{\hbar^2}{2\mathrm{m}}\left(\frac{\partial^2}{\partial \mathrm{x}^2} + \frac{\partial^2}{\partial \mathrm{y}^2}\right) + \mathrm{V(x,\ y)},$$

whose stationary states can be determined by solving the Schrodinger Equation 4.1.1. We quote the result which is extensively discussed in any quantum mechanics textbook. The energy eigenstates and eigenvalues are

$$\psi_{(n_1,n_2)}(x,\ y) = \left(\frac{1}{a}\right)\sin\left(\frac{n_1\pi x}{2a}\right)\sin\left(\frac{n_2\pi y}{2a}\right);\ E_{(n_1,n_2)} = \left(n_1^2 + n_2^2\right)\frac{\pi^2\hbar^2}{8ma^2}.$$

Clearly, $\psi_{(n_1,n_2)}(x,\ y)$ and $\psi_{(n_2,n_1)}(x,\ y)$ are linearly independent states sharing the same energy eigenvalues.

The rotation operation by angle $\pi/2$ about z-axis, which transforms $(x,\ y) \rightarrow (y,\ -x)$, as well as mirror reflection σ_v commutes with the Hamiltonian. Hence, the group symmetry possessed by this system is C_{4v}. We observe the character table of C_{4v} has one-dimensional as well as two-dimensional irreducible representations. Hence, we can claim that the energy states are either non-degenerate or two-fold degenerate. It is appropriate to mention that besides the group symmetry accounting for degenerate energy levels, there could be accidental degeneracy. For example, the stationary states with $(n_1, n_2) =$ (5,5), (7, 1), (1, 7) share the same energy eigenvalues where the accidental degenerate state $\psi_{(5,5)}(x,\ y)$ cannot be deduced using group theory tools.

Suppose the square region, where potential is $V(x, y) = 0$, gets slightly modified to a rectangular region due to mild disturbance. We know from quantum mechanics that the two-fold degenerate levels in a square box split into two non-degenerate levels in such a rectangular box of arbitrary length and breath (we neglect accidental degeneracy which can arise due to suitable ratio of the sides of the rectangle). From the group theory point of view, we can say that the two-fold degenerate energy levels show splitting due to disturbance. In the following section, we will understand how disturbance or perturbation can split the degenerate energy levels using group theory tools. □

4.2 Level Splitting under Perturbation

For a system described by H possessing symmetry group G, Equation 4.1.1 will give the stationary states. Let the degenerate eigenstates $\{\psi_i\}_{i=1}^n$ give an irreducible unitary representation Γ of the symmetry group G of the system. The characters of G in Γ are of course assumed known. On application of a perturbation $\mathbf{H_1}$ to the system, the Schrödinger equation takes the form

$$(\mathbf{H} + \mathbf{H}_1)\psi = E\psi.$$

If the perturbation is assumed to be small, the stationary states and the energy levels of the perturbed system are expected to differ only slightly from those of the unperturbed system. It is known from perturbation theory methods in quantum mechanics that a small perturbation usually lifts the degeneracy in a set of degenerate levels such as $\{\psi_i\}_{i=1}^n$. While a complete calculation of the perturbed levels is made possible only through application of perturbation methods to the known form of H_1, group theory allows one to deduce the extent to which the degeneracy gets lifted from the form of H_1 in some cases.

Suppose K is the maximal group of spatial transformations which commutes with the perturbation. If K is a subgroup of G then the perturbation H_1 has a lower order symmetry than the unperturbed Hamiltonian H. Consequently, the complete Hamiltonian of the perturbed system also has its symmetry group as K. Since Γ is a representation of G, it is also a representation of the subgroup K. As Γ is unitary, it is

now possible to completely reduce Γ as a direct sum of irreducible representations of K. These irreducible representations of K correspond to different energy eigenvalues of the perturbed system in accordance with our assumption. It is immediate that Equations 3.7.1 and 3.7.2 are directly applicable in this case.

Using the above arguments, we can now revisit Example 30 where $V(x,\ y) = 0$ in a rectangular region due to perturbation. The group symmetry possessed by the particle in a rectangular box system is no longer $G = C_{4v}$ but $K = C_{2v}$ which is abelian. Hence, any two-dimensional irreducible representation $\Gamma \in C_{4v}$ will become the direct sum of irreducible representation: $\oplus\Gamma^{\alpha} \in C_{2v}$ which are one-dimensional representations. Therefore all the two-fold degenerate levels of the square box will split into non-degenerate levels (ignoring accidental degeneracy). We will elaborate another example which will illustrate the splitting of energy levels using the group theory tools.

Example 31. Let the unperturbed Hamiltonian of a system have T_d symmetry (Chapter 2, Section 2.3). Suppose a small perturbation breaks the symmetry to the subgroup C_{3v}. For reference, character tables for T_d and C_{3v} are given below. Let us determine the splitting of energy level corresponding to a representation of degree 3 (say F_1) in T_d.

T_d	E	$8C_2$	$3C_2$	$6\sigma_d$	$6S_4$
$\mathbf{A_1}$	1	1	1	1	1
$\mathbf{A_2}$	1	1	1	-1	-1
$\mathbf{E}$	2	-1	2	0	0
$\mathbf{F_1}$	3	0	-1	1	-1
$\mathbf{F_2}$	3	0	-1	-1	1

C_{3v}	E	$2C_3$	$3\sigma_v$
$\mathbf{A_1}$	1	1	1
$\mathbf{A_2}$	1	1	-1
$\mathbf{E}$	2	-1	0

Some observations are in order before calculating the split. The permutation representation of T_d is the symmetric group $\mathfrak{S}(4)$. Similarly, the permutation representation of C_{3v} is the symmetric group $\mathfrak{S}(3)$. Since $\mathfrak{S}(3)$ is a subgroup of $\mathfrak{S}(4)$, it follows that C_{3v} is a subgroup of T_d. It may be recalled here that $\mathfrak{S}(4) = V_N \rtimes \mathfrak{S}(3)$. In the point group T_d, the normal subgroup corresponding to V_N (the Klein-4 normal subgroup in $\mathfrak{S}(4)$) consists of the identity transformation along with the three C_2 rotations which interchange pairs of vertices of the tetrahedron. In the isomorphism

$$\frac{T_d}{V_N} \cong C_{3v},$$

the $8C_3$ class in T_d is mapped to $2C_3$ class in C_{3v}, the classes $6\sigma_d$ and $6S_4$ in T_d are both mapped to the class $3\sigma_v$ in C_{3v} while V_N being the kernel of the homomorphism is mapped to the identity class in C_{3v}. The characters of the representations of C_{3v} can be extended in this case to the characters of representations of the same degrees in T_d by noting the fact that all representations of the kernel V_N are of degree 1 since V_N is an abelian group. For example, consider the representation E. The characters of the identity class and the $3C_2$ class in T_d are both equal to 2, the character of the identity

class of C_{3v} (to which both the classes of T_d are mapped in the homomorphism). Similarly one may obtain the characters of other representations of T_d from those of C_{3v}. However, since C_{3v} has no irreducible representations of degree 3, the characters of the representations F_1 and F_2 of T_d would have to be obtained via application of the orthogonality relations on the characters.

Returning to the splitting of the degeneracy of F_1 under a C_{3v} perturbation, the basis states of the representation F_1 of T_d give a reducible representation of C_{3v}. In this reducible representation, the characters of the various classes of C_{3v} can be read directly from the characters of F_1 by considering the homomorphism mentioned above and orthogonality relations:

C_{3v}	E	$2C_3$	$3\sigma_v$
Γ	3	0	1

.

Now apply Equation 3.7.2 (which we note once again)

$$m_\alpha = \frac{1}{|G|} \sum_{g \epsilon G} \chi^{\Gamma}(g) \overline{\chi^{\Gamma^\alpha}(g)}.$$

In the above, Γ is the reducible representation of C_{3v} effected by the basis states of the F_1 representation of T_d and Γ^α is any of the irreducible representations of C_{3v}. Upon carrying out the routine calculations, it is found that

$$\Gamma = A_1 \oplus E.$$

The above indicates that the perturbation splits the triply degenerate energy level of the original Hamiltonian into two levels, one singlet and the other one doubly degenerate. □

Stationary states are the stable energy levels in which the system stays as long as there is no external interactions. Experimentalists in the laboratory measure the frequencies $\{\nu_i\}'s$ of spectral lines emitted whenever an atom undergoes a transition from one energy level to another energy level due to interactions. The observed frequencies are characteristic of an atom and also depend on the nature of interaction. This brings us to topic of *selection rules* where group theory tools can deduce whether an atomic transition is allowed or disallowed due to such interactions.

4.3 Selection Rules

In quantum mechanics, physical quantities are represented by self-adjoint operators acting on the Hilbert space of system states. The Hamiltonian of the system is itself an example of such an operator which is useful to determine the energy eigenvalues E_i and their corresponding stationary states ψ_i solving Schrödinger equation. The stationary states (indexed by a complete set of quantum numbers) form a basis for the Hilbert space. There are other linear operators corresponding to physical quantities like position, momentum, angular momentum and so forth, which can be expressed

in a matrix form in this basis. Let $\mathcal{O}$ represent a self-adjoint operator corresponding to a physical quantity. The matrix of $\mathcal{O}$ in the basis of stationary states is then given by

$$\mathcal{O}_{mn} = \int \psi_m^* \mathcal{O} \psi_n = (\psi_m,\ \mathcal{O}\psi_n), \tag{4.3.1}$$

where $\{\psi_i\}$ are the stationary states indexed by a complete set of quantum numbers. The integration in the equation above is carried out over the complete configuration space of the system. The non-zero matrix element $\mathcal{O}_{\text{mn}}$ implies that the transition from energy level E_n to another energy level E_m due to interaction represented by operator $\mathcal{O}$ is allowed. Instead of working this matrix element by integrating Equation 4.3.1, we would like to exploit the power of group theory to deduce whether $\mathcal{O}_{\text{mn}}$ is zero or non-zero.

Suppose the system possesses group symmetry G corresponding to spatial transformation. We expect the above matrix element $\mathcal{O}_{\text{mn}}$ to be unchanged when any group element $g \in G$ acts on the states ψ_m, ψ_n as well as on the operator $\mathcal{O}$. In fact, one can deduce which of the matrix elements $\mathcal{O}_{mn}$ vanishes by applying the principal ideas of group theory as follows.

For the system described by Equation 4.1.1 having G as its non-trivial symmetry group, we know from Section 4.1 that the degenerate states of same energy belong to an irreducible representation of G. Consider the integral

$$\int \psi_i^\alpha$$

where ψ_i^α is a basis state in some irreducible representation Γ^α of the G. The action of any group element on ψ_i^α transforms into a linear combination of the basis states of same energy to which ψ_i^α belongs. However, a mere spatial transformation which brings the system to an identical configuration should not change the value of the integral $\int \psi_i^\alpha$. In other words it is expected that

$$\int \psi_i^\alpha = \sum_{k=1}^{d} [\Gamma^\alpha(g)]_{ki} \int \psi_k^\alpha,$$

where d is the degree of the representation Γ^α. Also, the above must be true for any transformation g in G. Adding the expressions for all transformations g in G, one has

$$\int \psi_i^\alpha = \frac{1}{|G|} \sum_{k=1}^{d} \left(\sum_{g \in G} [\Gamma^\alpha(g)]_{ki} \right) \int \psi_k^\alpha.$$

If Γ^α is not the trivial representation, then it is easy to verify using Equation 3.3.5 that $(\sum_{g\in G}[\Gamma^\alpha(g)]_{ki})$ vanishes. Therefore, if ψ_i^α is a basis state in some non-trivial irreducible unitary representation Γ^α of the G then

$$\int \psi_i^\alpha = 0. \tag{4.3.2}$$

Returning to Equation 4.3.1, let ψ_m^f and ψ_n^i be eigenstates in two distinct irreducible representations Γ^f and Γ^i respectively, of the symmetry group G of the system. The operator $\mathcal{O}$ is in general some tensor (for example, a dipole moment or a quadrupole moment) which has a certain number of independent components. It will be assumed that these independent components themselves are transformed into a linear combination of each other under the spatial transformations effected by the elements of G. It is then possible to treat those independent components of $\mathcal{O}$ as a basis for irreducible representation of G. For instance, see Example 32 for electric dipole moment components. Formally for any operator $\mathcal{O}$, its representation of G is denoted as $\Gamma^{\mathcal{O}}$. By suitable linear combinations, it is always possible to choose the eigenfunctions of the stationary states to be real and ψ_m in Equation 4.3.1 can be taken as real. Then the states $\psi_m^{f*}\mathcal{O}i$ would be transformed by G according to the states of the tensor product $\Gamma^f \otimes \Gamma^{\mathcal{O}} \otimes \Gamma^i$. The representation $\Gamma^f \otimes \Gamma^{\mathcal{O}} \otimes \Gamma^i$ can obviously be decomposed into a direct sum of irreducible representations of G and the multiplicities of these irreducible representations can be found by using Equation 3.7.2. The evaluation of $\mathcal{O}_{mn}$ reduces to the calculation of the sum of integrals of the form $\int \psi_k^\alpha$ where the ψ_k^α's transform in accordance with some irreducible representation of G. That all such integrals vanish has already been established unless of course some of the ψ_k^α's transform in accordance with the trivial representation. Therefore, the matrix elements of $\mathcal{O}$ vanish unless the trivial representation is present in the decomposition of $\Gamma^j \otimes \Gamma^{\mathcal{O}} \otimes \Gamma^i$. Alternatively, when the tensor product $\Gamma^{\mathcal{O}} \otimes \Gamma^i$ is decomposed into irreducible components, then these irreducible components are the possible values of Γ^f for which the transition elements may be non-zero. This is a very convenient way to decide which matrix elements vanish as against a full-fledged evaluation of the integral. The exact values of the non-vanishing matrix elements would of course have to be calculated by integration. The implementation of this formalism is detailed in Examples 32 and 33.

The aforementioned method for calculation of $\mathcal{O}_{mn}$ works when ψ_m and ψ_n belong to different energy levels of the system. In order to consider transition elements which are diagonal with respect to energy, we make a small digression to recall an important fact related to the solution of the time dependent Schrödinger equation

$$i\frac{\partial}{\partial t}\Psi = \mathrm{H}\Psi.$$

Let the Hamiltonian H of the system described by the time dependent wave function Ψ be a time independent real operator. If the state Ψ of the system develops in accordance with the above equation, then the conjugates of quantities on both sides of the equation should be always equal, i.e.,

$$-i\frac{\partial}{\partial t}\overline{\Psi} = \mathrm{H}\overline{\Psi}$$

$$\Rightarrow i\frac{\partial}{\partial(-t)}\overline{\Psi} = \mathrm{H}\overline{\Psi}. \tag{4.3.3}$$

Equation 4.3.3 is identical to the time dependent Schrödinger equation. In fact, the above equation states that under time reversal, the system that was described by state Ψ would become $\overline{\Psi}$. In this sense $\overline{\Psi}$ is the time reversed state of the system. Under time reversal, various physical quantities related to the system may behave differently (as a simple example, for a particle moving in space-time, under time reversal, assuming there are no spatial transformations involved, the coordinates of the particle remain the same no matter how its velocity vector reverses in direction). The physical quantity $\mathcal{O}$ itself may remain invariant or change sign upon time reversal. This behaviour is important in determining the selection rules for transitions among states that are diagonal with respect to energy. Let the closed system under consideration be in a stationary state whose basis states transform according to the irreducible representation Γ. If the degree of the representation Γ is d, then the energy level is d-fold degenerate with $\{\psi_1, \cdots, \psi_d\}$ serving as a basis. It is of course assumed that all the basis states are real. If ψ is the state of the system belonging to irreducible representation Γ, then in general ψ is a linear combination of the basis states:

$$\psi = \sum_{m=1}^{d} c_m \psi_m.$$

The average value of the quantity $\mathcal{O}$ in this state is obtained according to the usual rules of quantum mechanics. If $\langle \mathcal{O} \rangle$ represents the average value then

$$\langle \mathcal{O} \rangle = \int \overline{\psi} \mathcal{O} \psi = \sum_{m,n=1}^{d} \overline{c_m} c_n \mathcal{O}_{mn}.$$

In the time reversed state $\overline{\psi}$, the average value of $\mathcal{O}$ would be obtained to be

$$\langle \mathcal{O} \rangle_{\text{rev}} = \int \overline{\overline{\psi}} \mathcal{O} \overline{\psi} = \sum_{m,n=1}^{d} \overline{c_m} c_n \mathcal{O}_{nm}.$$

If the physical quantity represented by the operator $\mathcal{O}$ was such that it remained invariant under time reversal, then its average value would remain unchanged under such a transformation. The value $\langle \mathcal{O} \rangle$ and $\langle \mathcal{O} \rangle_{\text{rev}}$ would then be equal. As the coefficients c_i can be complex, it follows that

$$\mathcal{O}_{mn} = \mathcal{O}_{nm}$$

$$\Rightarrow \int \psi_m \mathcal{O} \psi_n = \int \psi_n \mathcal{O} \psi_m.$$

The transition matrix elements would therefore be non-zero when $\Gamma^{\mathcal{O}}$ is present in $(\Gamma \otimes \Gamma)^{\sigma}$, the symmetric component of the tensor product. For a physical quantity

that changes its sign under time reversal, the matrix elements would be non-zero if the antisymmetric component $(\Gamma \otimes \Gamma)^{\alpha}$ contained $\Gamma^{\mathcal{O}}$. This detour on time reversal action leading to the complex conjugation of wavefunction is generally known as *antilinear* property within the linear algebra context.

Example 32. Consider the character table for C_{4v}.

C_{4v}	E	$2C_4$	C_2	$2\sigma_v$	$2\sigma_d$		
$\mathbf{A_1}$	1	1	1	1	1	z	$x^2+y^2; z^2$
$\mathbf{A_2}$	1	1	1	-1	-1	R_z	
$\mathbf{B_1}$	1	-1	1	1	-1		x^2-y^2
$\mathbf{B_2}$	1	-1	1	-1	1		xy
$\mathbf{E}$	2	0	-2	0	0	$(x,y);\ (R_xR_y)$	$xz; yz$

The electric dipole moment $\mathbf{p}$ for a system of charges is defined to be $\sum q_i \mathbf{r}_i$. For a single charge, the x-component of the dipole moment vector (p_x) clearly has transformation properties of the x coordinate which belongs to the E representation of C_{4v}. Hence $\Gamma^{p_x} \in \Gamma^{\mathrm{E}}$. Consider a transition from an initial state corresponding E representation to a final state corresponding to the A_2 representation due to x-component dipole moment interaction. The matrix element of p_x corresponding to this transition would be non-zero only if the tensor product $A_2 \otimes E$ contained the representation E (the representation transforming p_x). It can be observed from the table given above that in fact $A_2 \otimes E = E$. Thus $\langle A_2|q\hat{x}|E\rangle$ is non-zero and the dipole transition is possible. This selection rule of non-zero matrix element will also be valid for the p_y operator because the y-component dipole moment belongs to the irreducible representation E as well. However, p_z belongs to trivial representation and hence $\langle A_2|q\hat{z}|E\rangle = 0$. □

Example 33. Consider the electric quadrupole moment tensor defined as

$$Q_{ik} = e(3x_i x_k - r^2\delta_{ik}), \tag{4.3.4}$$

where the indices i and k take values 1, 2 and 3. In the coordinate notation used in the text, $x_1 = x,\ x_2 = y,\ x_3 = z$ and $r^2 = x^2 + y^2 + z^2$. The tensor is clearly symmetric. Explicitly, the nine components of the quadrupole tensor for unit charge e are

$$Q_{xx} \sim 3x^2 - r^2,\ Q_{yy} \sim 3y^2 - r^2,\ Q_{zz} \sim 3z^2 - r^2,$$

$$Q_{xx} + Q_{yy} + Q_{zz} = 0,$$

$$(Q_{xy} = Q_{yx}) \sim 3xy,\ (Q_{xz} = Q_{zx}) \sim 3xz,\ (Q_{yz} = Q_{zy}) \sim 3yz.$$

From above relationships, it follows that Q_{ik} has 5 independent quantities. It is our purpose to study quadrupole moment selection rules in a system having the octahedral (O) symmetry. The character table for O symmetry group follows:

O	E	$8C_3$	$3C_2$	$6C_4$	$6C_2$		
$\mathbf{A_1}$	1	1	1	1	1		$x^2+y^2+z^2$
$\mathbf{A_2}$	1	1	1	-1	-1		
$\mathbf{E}$	2	-1	2	0	0	0	$(2z^2-x^2-y^2, x^2-y^2)$
$\mathbf{T_1}$	3	0	-1	1	-1	(x,y,z) (R_x,R_y,R_z)	
$\mathbf{T_2}$	3	0	-1	-1	1		(xy, xz, yz)

Comparing the bases of the representation T_2, it is clear that the triplet $(Q_{xy},\ Q_{xz},\ Q_{yz})$ transforms according to the T_2 representation of O. Also notice that $Q_{zz} \sim 2z^2 - x^2 - y^2$ and $Q_{xx} - Q_{yy} \sim x^2 - y^2$. Therefore pair $(Q_{zz},\ Q_{xx} - Q_{yy})$ transforms according to the E representation of O.

Let us first find which matrix elements of $(Q_{xy},\ Q_{xz},\ Q_{yz})$ are non zero for transitions between states of different representations. For this purpose one needs to find which irreducible representations are present in the tensor product of T_2 representation with various other irreducible representations of the group. This is accomplished, as has already been shown through previous examples, by use of Equation 3.7.2. We will leave it to the readers to verify the following:

$$\mathrm{T}_2 \otimes \mathrm{A}_1 = \mathrm{T}_2,$$

$$\mathrm{T}_2 \otimes \mathrm{A}_2 = \mathrm{T}_1,$$

$$\mathrm{T}_2 \otimes \mathrm{E} = \mathrm{T}_1 \oplus \mathrm{T}_2,$$

$$\mathrm{T}_2 \otimes \mathrm{T}_1 = \mathrm{A}_2 \oplus \mathrm{E} \oplus \mathrm{T}_1 \oplus \mathrm{T}_2,$$

$$\mathrm{T}_2 \otimes \mathrm{T}_2 = \mathrm{A}_1 \oplus \mathrm{E} \oplus \mathrm{T}_1 \oplus \mathrm{T}_2.$$

From the above decomposition, it is obvious that $Q_{xy},\ Q_{xz},\ Q_{yz}$ have non-zero matrix elements for transitions

$$\mathrm{A}_1 \leftrightarrow \mathrm{T}_2; \mathrm{A}_2 \leftrightarrow \mathrm{T}_1; \mathrm{E} \leftrightarrow \mathrm{T}_1,\ \mathrm{T}_2; \mathrm{T}_1 \leftrightarrow \mathrm{T}_2.$$

To calculate the non-zero matrix elements for $Q_{xx},\ Q_{yy},\ Q_{zz}$, proceeding as above, the following decompositions of the tensor product of the E representation with various other representations of the group are obtained.

$$\mathrm{E} \otimes \mathrm{A}_1 = \mathrm{E},$$

$$\mathrm{E} \otimes \mathrm{A}_2 = \mathrm{E},$$

$$\mathrm{E} \otimes \mathrm{E} = \mathrm{A}_1 \oplus \mathrm{A}_2 \oplus \mathrm{E},$$

$$E \otimes T_1 = T_1 \oplus T_2,$$

$$E \otimes T_2 = T_1 \oplus T_2.$$

Once again it follows from the above decomposition that Q_{xx}, Q_{yy}, Q_{zz} have non zero matrix elements for transitions

$$E \leftrightarrow A_1,\ A_2; T_1 \leftrightarrow T_2.$$

Till now, the transition matrix elements between states of different representations have been considered. In order to consider matrix elements that are diagonal with respect to energy, the first thing to note is that electric quadrupole moment tensor remains invariant under time reversal. This follows directly from the form of Q_{ik} which is itself defined in terms of quantities that remain unaffected under time reversal. Therefore the symmetric component of the tensor product of an irreducible representation with itself needs to be considered. As an example, consider the symmetric component of the tensor product $T_2 \otimes T_2$, and let this component be represented $(T_2 \otimes T_2)^\sigma$ (in the notation of Chapter 3, Section 3.7). The class characters in the representation $(T_2 \otimes T_2)^\sigma$ are easily found using Equation 3.7.5.

$$\chi^2_\sigma(E) = 6,\ \chi^2_\sigma(8C_3) = 0,\ \chi^2_\sigma(3C_2) = 2,\ \chi^2_\sigma(6C_4) = 0,\ \chi^2_\sigma(6C_2) = 2.$$

From the above character values, the decomposition of $(T_2 \otimes T_2)^\sigma$ is obtained to be

$$(T_2 \otimes T_2)^\sigma = A_1 \oplus E \oplus T_2.$$

In a similar manner, the symmetric components of the tensor products of the other irreducible representations may be obtained.

$$(A_1 \otimes A_1)^\sigma = A_1,$$

$$(A_2 \otimes A_2)^\sigma = A_1,$$

$$(E \otimes E)^\sigma = A_1 \oplus E,$$

$$(T_1 \otimes T_1)^\sigma = A_1 \oplus E \oplus T_2,$$

$$(T_2 \otimes T_2)^\sigma = A_1 \oplus E \oplus T_2.$$

The matrix elements of Q_{xx}, Q_{yy}, Q_{zz} that are diagonal with respect to energy are non-zero for transitions in E, T_1 and T_2. Similarly, the matrix elements of Q_{xy}, Q_{xz}, Q_{yz} that are diagonal with respect to energy are non-zero for transitions in T_1 and T_2. □

The above two examples indicate the power of group theory concepts in deducing selection rules. We have clearly demonstrated that the group representation theory can determine whether any matrix elements of self-adjoint operators between stationary

states is zero or non-zero. In the following section, we will exploit group theory tools to determine the independent vibrational modes of molecules possessing discrete group symmetry. These are well known as normal modes which characterize the molecules.

4.4 Molecular Vibrations

We will first briefly review the concepts of normal modes of vibrations of simple systems which are well known in classical mechanics. Then we will elaborate the elegant group theory approach in reproducing those normal modes of molecules.

Consider the classical problem of two masses m_1 and m_2 connected by a Hooke's spring of stiffness $\varkappa$. It is well known that a small disturbance/displacement leads to oscillations/vibration of the system with a unique frequency ω given by

$$\omega = \sqrt{\frac{\varkappa}{\mu}}.$$

In the above expression for ω, $\mu\left(= \frac{m_1 m_2}{m_1+m_2}\right)$ is the reduced mass of the system. When the number of participating masses and springs is increased, the number of degrees of freedom also increases and as a result the oscillatory motion of the system becomes more complicated. Consider a system consisting of n mass points. Such a system of mass points has in general $3n$ degrees of freedom of movement. Of these, 3 degrees of freedom correspond to an overall motion of the system in the three space directions. Additionally, the system will have rotational degrees of freedom. If the distribution of the mass points in the equilibrium state is in three-dimensional space, then the system has 3 rotational degrees of freedom. All the other degrees correspond to the vibrational motion and therefore such a system has a total of $3n-6$ vibrational degrees of freedom. In case the mass points were distributed along a straight line, the rotational degree of freedom associated with rotation about the axis of the system would have to be discounted since here it is assumed that the masses have negligible physical dimensions. For such an arrangement of mass points, there will be then a total of $3n-5$ vibrational degrees of freedom.

Let us recall the basic theory of small oscillations from classical mechanics. Consider a system with s vibrational degrees of freedom. Let $x_i (i = 1, 2, \cdots, s)$ denote small excursions of the mass points from their mean positions. Let x be a $s \times 1$ column vector such that $\{\mathrm{x}\}_{i1} = x_i$. In general, the kinetic energy T of the system is a quadratic function of $\dot{x}_i$ (time derivative of x_i). The most general form of T is then given by

$$T = \frac{1}{2}\sum_{j,\,k}^{s} m_{jk}\dot{x}_j\dot{x}_k,$$

where m_{jk} are symmetric constants $(m_{jk} = m_{kj})$. It is expected that the system will exhibit oscillatory motion when disturbed from its mean position. In this circumstance, the potential energy of the system can be taken to be minimum (and equal to 0) in the undisturbed state. When the excursions x_i are small, then the potential energy U may be written as,

$$U = \frac{1}{2}\sum_{j,\,k}^{s} \varkappa_{jk} x_j x_k,$$

where $\varkappa_{jk} (= (\frac{\partial^2}{\partial x_j \partial x_k} U)_{x_{j=0}, x_{k=0}})$ are some other symmetric constants. Let M and K be symmetric matrices such that $\{\mathrm{M}\}_{jk} = m_{jk}$ and $\{\mathrm{K}\}_{jk} = \varkappa_{jk}$. The Lagrangian L of the system can therefore be written as

$$L = T - U = \frac{1}{2}\sum_{j,k}^{s} m_{jk}\dot{x}_j\dot{x}_k - \frac{1}{2}\sum_{j,k}^{s} \varkappa_{jk} x_j x_k$$

$$\Rightarrow L = \frac{1}{2}\left[\dot{\mathrm{x}}^{\mathrm{T}}\mathrm{M}\dot{\mathrm{x}} - \mathrm{x}^{\mathrm{T}}\mathrm{K}\mathrm{x}\right]. \tag{4.4.1}$$

We note the Euler–Lagrange equation for convenience here.

$$\frac{d}{dt}\left(\frac{\partial}{\partial \dot{x}_i} L\right) = \frac{\partial}{\partial x_i} L.$$

The equations of motion are obtained by substituting the form of L in the Euler–Lagrange equation. It may be noted that

$$\frac{\partial}{\partial \dot{x}_i} L = \frac{1}{2}\sum_{k=1}^{s} (m_{ik} + m_{ki})\dot{x}_k = \sum_{k=1}^{s} m_{ik}\dot{x}_k,$$

because of symmetry of m_{ik}. In a similar manner $\frac{\partial}{\partial x_i} L$ can be obtained. The equations of motion in their final form are

$$\sum_{k=1}^{s} (m_{ik}\ddot{x}_k + \varkappa_{ik} x_k) = 0; \qquad i = (1, 2 \cdots, s). \tag{4.4.2}$$

Equation 4.4.2 admits simple harmonic solutions of the form $x_k = a_k \exp(i\omega t)$. Substituting for x_k in the above system of equations, we obtain a homogeneous system of equations in complex quantities a_k.

$$\sum_{k=1}^{s} \left(-m_{ik}\omega^2 + \varkappa_{ik}\right) a_k = 0; \qquad i = (1, 2 \cdots, s). \tag{4.4.3}$$

The above system has non-trivial solutions for complex quantities a_k if the determinant of the coefficient matrix vanishes.

$$\begin{vmatrix} \varkappa_{11} - \omega^2 m_{11} & \cdots & \varkappa_{1n} - \omega^2 m_{1n} \\ \vdots & \ddots & \vdots \\ \varkappa_{n1} - \omega^2 m_{n1} & \cdots & \varkappa_{nn} - \omega^2 m_{nn} \end{vmatrix} = 0. \tag{4.4.4}$$

Equation 4.4.4 is called the *secular equation* while the determinant in the left hand side is called the *secular determinant*. Upon explicitly expanding the secular determinant, a polynomial of degree n in ω^2 is obtained. All the values of ω^2 obtained from solving this polynomial equation can be shown to be positive, but we do not prove this here. The positive roots of the various values of ω^2 are called the *eigenfrequencies* of the system. For a system with s vibrational degrees of motion, there are s possible eigenfrequencies. It may so happen that some of the eigenfrequencies coincide, in which case they are called *degenerate*. Suppose that the system has no degenerate frequencies. Upon substituting each of the values of ω, say ω_l in Equation 4.4.3, the values for a_k are obtained up to the same constant complex multiplier c_l for all a_k. Let this value of a_k be denoted by $a_{kl}c_l$ so that $x_k^{(l)} = a_{kl}c_l \exp(i\omega_l t)$ where a_{kl} are all real. Noting that Equation 4.4.2 is homogeneous and linear, the general solution may now be obtained as a linear combination of solutions corresponding to each eigenfrequency.

$$x_k = \Re \sum_{l=1}^{s} a_{kl}[c_l \exp(i\omega_l t)], \tag{4.4.5}$$

where $\Re$ indicates the real part. With the definition $\eta_l = \Re c_l \exp(i\omega_l t)$, and representing the excursion x_k's and η_l's as $s \times 1$ column vectors x and η respectively, the above equation may be written as a matrix equation

$$\mathrm{x} = \mathrm{A}\eta, \tag{4.4.6}$$

where A is the coefficient matrix such that $[\mathrm{A}]_{kl} = a_{kl}$. As the x_k's are independent and so are η_l's, the above equation can be inverted to express η_l in terms of x_k's. This allows us to choose a different set of generalized coordinates, namely η_l to describe the motion of the system. The important property which makes this choice of generalized coordinates more convenient is that

$$\ddot{\eta}_l + \omega_l^2 \eta_l = 0; \;\; l = (1, 2, \cdots, s).$$

Thus the description of the motion of the system is much simpler in terms of the coordinates η_l. These coordinates are called the *normal coordinates*. A normal coordinate is essentially a linear combination of the original coordinates that oscillates at a unique eigenfrequency. The motion of the system corresponding to a normal coordinate is called a *normal mode*. It may be noted that if some particular eigenfrequency ω_l was degenerate with a multiplicity ν_l, then there would be ν_l normal coordinates associated with that frequency. More generally

$$\ddot{\eta}_{lp} + \omega_l^2 \eta_{lp} = 0, \quad \sum_l \nu_l = s, \tag{4.4.7}$$

where the index l ranges over the number of distinct eigen frequencies and the index p ranges from 1 to ν_l. Note that the range of p varies with l. Applying the transformation

in Equation 4.4.6, it is now possible to express the Lagrangian and the total energy H of the vibrating system in a matrix form.

$$L = \frac{1}{2}\left[\dot{\eta}^{\mathrm{T}}\left(\mathrm{A}^{\mathrm{T}}\mathrm{MA}\right)\dot{\eta} - \eta^{\mathrm{T}}\left(\mathrm{A}^{\mathrm{T}}\mathrm{KA}\right)\eta\right], \tag{4.4.8}$$

$$H = \frac{1}{2}\left[\dot{\eta}^{\mathrm{T}}\left(\mathrm{A}^{\mathrm{T}}\mathrm{MA}\right)\dot{\eta} + \eta^{\mathrm{T}}\left(\mathrm{A}^{\mathrm{T}}\mathrm{KA}\right)\eta\right].$$

The important consequence of the transformation to normal coordinates is that the symmetric matrices M and K are simultaneously diagonalized, whereby leading to an expression of the energy of the vibrating system as a sum of energies associated with each of the normal vibrational modes. As a result, one has

$$H = \frac{1}{2}\left[\sum_{l}\sum_{p=1}^{v_l}\mathfrak{m}_{l,p}\dot{\eta}_{l,p}^2 + \sum_{l}\omega_l^2\sum_{p=1}^{v_l}\mathfrak{m}_{l,p}\eta_{l,p}^2\right],$$

where $\mathfrak{m}_{l,p}$ are positive constants. It is conventional to redefine the normal coordinates as $\Theta_{l,p} = \sqrt{\mathfrak{m}_{lp}}\eta_{l,p}$ so that the total energy can be written simply as

$$H = \frac{1}{2}\left[\sum_{l}\sum_{p=1}^{v_l}\dot{\Theta}_{l,p}^2 + \sum_{l}\omega_l^2\sum_{p=1}^{v_l}\Theta_{l,p}^2\right]. \tag{4.4.9}$$

We will apply the classical mechanics approach on a triatomic molecule example and obtain the normal modes.

Example 34. (Landau and Lifshitz, *Mechanics*) Consider a non-linear triatomic molecule such as the one shown in Figure 4.4.1(a). The three mass point m, M and m are nothing but the nuclei of the atoms constituting the molecule. The size of the nuclei is negligible compared to the size of the molecule itself. As the three mass points will always lie in a plane, we need to consider motions that occur only in the x-z plane. For motions restricted to the plane, there are a total of 6 degrees of freedom, out of which 2 are translational and 1 rotational (about an axis perpendicular to the plane of motion). This leaves a total of $6 - 3 = 3$ vibrational degrees of freedom. Let the displacements of the atoms of mass m from their mean positions be $(x_1,\ z_1)$ and $(x_2,\ z_2)$ and that of M be (X, Z). The overall translation of the molecule may be eliminated by imposing the condition that the center of mass of the molecule does not get displaced.

$$m(x_1 + x_2) + MX = 0,$$

$$m(z_1 + z_2) + MZ = 0. \tag{4.4.10}$$

As is obvious from the Figure 4.4.1(a), the location of the center of mass is $(0, \frac{2ml\cos\alpha}{2m+M})$ where l is the bond length between M and m in the undisturbed state and α is the

bond angle. The rotational motion of the molecule may be eliminated by equating the angular momentum of the molecule (with respect to the center of mass of the molecule) to zero. In case of small oscillations, the instantaneous positions of the atoms from the center of mass can always be approximated by their positions with respect to the center of mass in the undisturbed state.

$$\left(-\frac{2ml\cos\alpha}{2m+M}\hat{\mathrm{k}}\right)\times M\left(\dot{Z}\hat{\mathrm{k}}+\dot{X}\hat{\mathrm{i}}\right)+$$
$$\left(l\sin\alpha\hat{\mathrm{i}}+\frac{Ml\cos\alpha}{2m+M}\hat{\mathrm{k}}\right)\times m\left(\dot{x}_1\hat{\mathrm{i}}+\dot{z}_1\hat{\mathrm{k}}\right)+$$
$$\left(-l\sin\alpha\hat{\mathrm{i}}+\frac{Ml\cos\alpha}{2m+M}\hat{\mathrm{k}}\right)\times m\left(\dot{z}_2\hat{\mathrm{k}}+\dot{x}_2\hat{\mathrm{i}}\right)=0.$$

Simplifying the above by use of the first of Equation 4.4.10, the angular motion is eliminated completely by the condition

$$(z_1-z_2)\sin\alpha-(x_1+x_2)\cos\alpha=0. \tag{4.4.11}$$

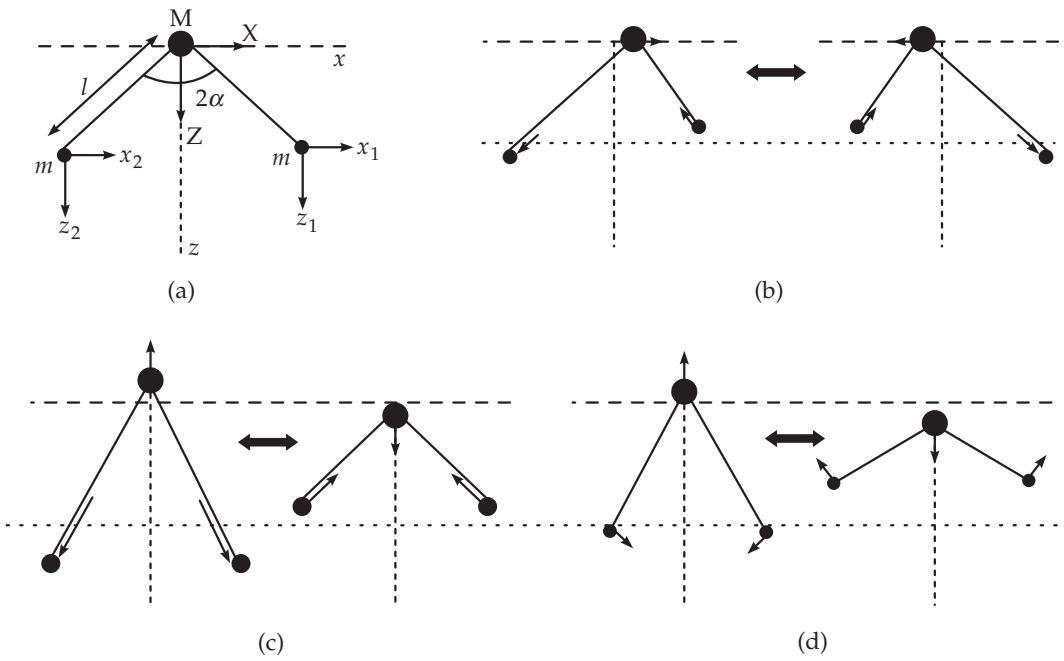


Figure 4.4.1 Normal Modes (Non-linear Tri-atomic Molecule)

As long as displacements of the masses satisfy Equations 4.4.10 and 4.4.11, the motion will be purely vibrational. As the molecule vibrates, it will generally get deformed. There are essentially two types of deformations possible in the current case:

(1) The bond length l changes for either or both the bonds

(2) The bond angle 2α changes.

With both such deformations, we can associate springs of stiffness $\varkappa_l$ and $\varkappa_\alpha$. It is easily seen that the associated deformations are

$$\delta l_1 = (x_1 - X)\sin\alpha + (z_1 - Z)\cos\alpha,$$

$$\delta l_2 = (X - x_2)\sin\alpha + (z_2 - Z)\cos\alpha, \tag{4.4.12}$$

by considering the components of the displacements of atoms along the bond lengths. Likewise, considering the displacements perpendicular to the bond length, the change in the bond angle is obtained to be

$$l\delta(2\alpha) = (x_1 - X)\cos\alpha + (Z - z_1)\sin\alpha$$

$$-(x_2 - X)\cos\alpha - (z_2 - Z)\sin\alpha. \tag{4.4.13}$$

It is possible to eliminate three of the variables from Equations 4.4.10 and 4.4.11. A convenient change of variable is effected by the transformations

$$q_1 = x_1 + x_2,$$

$$q_2 = x_1 - x_2,$$

$$q_3 = z_1 + z_2,$$

$$q_1\cot\alpha = z_1 - z_2. \tag{4.4.14}$$

Note that the last equation in the above is a consequence of the first three and Equation 4.4.11. The coordinates q_1, q_2 and q_3 are three coordinates corresponding to the three vibrational degrees of freedom of the molecule. The above equations can be inverted to obtain z_1, z_2, Z, x_1, x_2, X in terms of q_i's. Upon carrying out the relevant substitutions, one has

$$\delta l_1 = \frac{q_1}{2}\left[\frac{2m}{M} + \frac{1}{\sin^2\alpha}\right]\sin\alpha + \frac{q_2}{2}\sin\alpha + \frac{q_3}{2}\left[1 + \frac{2m}{M}\right]\cos\alpha,$$

$$\delta l_2 = -\frac{q_1}{2}\left[\frac{2m}{M} + \frac{1}{\sin^2\alpha}\right]\sin\alpha + \frac{q_2}{2}\sin\alpha + \frac{q_3}{2}\left[1 + \frac{2m}{M}\right]\cos\alpha,$$

$$l\delta(2\alpha) = q_2\cos\alpha - q_3\left[1 + \frac{2m}{M}\right]\sin\alpha. \tag{4.4.15}$$

The potential energy U of the deformed molecule is calculated from $U = \frac{\varkappa_l}{2}[(\delta l_1)^2 + (\delta l_2)^2] + \frac{\varkappa_\alpha (l\delta(2\alpha))^2}{2}$. The reader is advised to carry out rather straightforward calculations leading to the following form of the Lagrangian.

$$
\begin{aligned}
&L = \frac{m}{4}\left[\frac{2m}{M} + \frac{1}{\sin^2\alpha}\right]\dot{q}_1^2 - \frac{\varkappa_l}{4}\left[\frac{2m}{M} + \frac{1}{\sin^2\alpha}\right]_2^2 q_1^2 \sin^2\alpha + \\
&\frac{m}{4}\dot{q}_2^2 - \left[\varkappa_l \sin^2\alpha + 2\varkappa_\alpha \cos^2\alpha\right]\frac{q_2}{4} + \\
&\frac{m}{4}\left[1 + \frac{2m}{M}\right]\dot{q}_3^2 - \left[1 + \frac{2m}{M}\right]^2\left[\varkappa_l \cos^2\alpha + 2\varkappa_\alpha \sin^2\alpha\right]\frac{q_3^2}{4} + \\
&\left[1 + \frac{2m}{M}\right][\varkappa_l - 2\varkappa_\alpha]\frac{q_2 q_3}{2}\sin\alpha\cos\alpha.
\end{aligned}
\tag{4.4.16}
$$

Finally, the equations of motion obtained from the above form of the Lagrangian are

$$
\begin{aligned}
&m\ddot{q}_1 + \left[1 + \frac{2m}{M}\sin^2\alpha\right]\varkappa_l q_1 = 0, \\
&m\ddot{q}_2 + \left[\varkappa_l \sin^2\alpha + 2\varkappa_\alpha \cos^2\alpha\right] q_2 + \\
&+ \left[1 + \frac{2m}{M}\right][\varkappa_l - 2\varkappa_\alpha](\sin\alpha\cos\alpha) q_3 = 0, \\
&m\ddot{q}_3 + \left[1 + \frac{2m}{M}\right]\left[\varkappa_l \cos^2\alpha + 2\varkappa_\alpha \sin^2\alpha\right] q_3 + \\
&+ [\varkappa_l - 2\varkappa_\alpha](\sin\alpha\cos\alpha) q_2 = 0.
\end{aligned}
\tag{4.4.17}
$$

It is clear that the coordinate $q_1 = x_1 + x_2$ oscillates normally with a frequency $\sqrt{\frac{\varkappa_l}{m}[1 + \frac{2m}{M}\sin^2\alpha]}$. When only this particular mode is excited in the molecule, then $q_2 = q_3 = 0$, or in other words $x_1 = x_2$ and $z_1 = -z_2$. During such an oscillation, the central atom of mass M does not get displaced in the z-direction. This mode is depicted in Figure 4.4.1 (b).

The other coordinates q_2 and q_3 are coupled. The secular equation for the eigenfrequencies of the normal modes associated with q_2 and q_3 is

$$
\begin{vmatrix}
[\varkappa_l \sin^2\alpha + 2\varkappa_\alpha \cos^2\alpha] - \omega^2 m & \left[1 + \frac{2m}{M}\right][\varkappa_l - 2\varkappa_\alpha] \times (\sin\alpha\cos\alpha) \\
[\varkappa_l - 2\varkappa_\alpha] \times (\sin\alpha\cos\alpha)\nu_2 & \left[1 + \frac{2m}{M}\right]\left[\varkappa_l \cos^2\alpha + 2\varkappa_\alpha \sin^2\alpha\right] - \omega^2 m
\end{vmatrix} = 0.
$$

The solution of the secular equation gives 2 more eigenfrequencies corresponding to distinct normal modes. These modes would in general be some linear combinations of q_2 and q_3. When only one of these modes is excited then $q_1 = 0$, i.e., $x_1 = -x_2$. The central atom of mass M cannot get displaced in the x-direction now. Figure 4.4.1 (c), (d) depicts the two modes. □

It will be interesting to obtain all the three non-degenerate normal modes depicted in Figure 4.4.1 (b), (c), (d) using group theory. Clearly, this molecule has C_{2v} symmetry. We revisit this triatomic molecule (see Example 36) where we reproduce these normal modes by exploiting the group symmetry. We will elaborate another example using the conventional classical mechanics procedure to emphasize that the methodology is tedious but systematic. Then, the readers will be able to appreciate the results when we discuss elegant group theory approaches towards deriving normal modes.

Example 35. Consider a hypothetical equilateral molecule of three identical atoms shown in Figure 4.4.2. The Lagrangian of the system is given by

$$L = \frac{m}{2}\left[\dot{x}_1^2 + \dot{y}_1^2 + \dot{x}_2^2 + \dot{y}_2^2 + \dot{x}_3^2 + \dot{y}_3^2\right] - \frac{\varkappa}{2}\left[\Delta l_{12}^2 + \Delta l_{23}^2 + \Delta l_{13}^2\right],$$

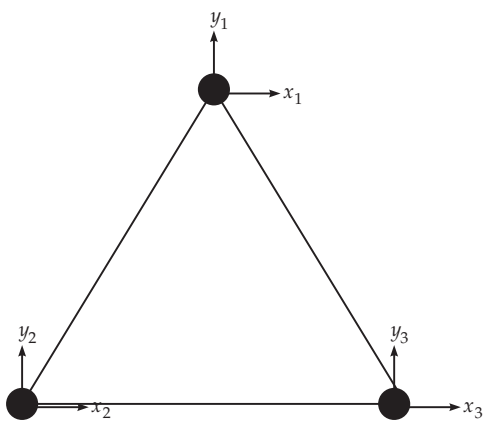


Figure 4.4.2 Hypothetical Equilateral Molecule

where Δl_{12} is the extension in the bond between nuclei 1 and 2 etc. The extensions are easily calculated to be

$$\Delta l_{12} = \frac{x_1 - x_2}{2} + \sqrt{3}\frac{y_1 - y_2}{2},$$
$$\Delta l_{13} = \frac{x_3 - x_1}{2} + \sqrt{3}\frac{y_1 - y_3}{2},$$
$$\Delta l_{23} = x_3 - x_2.$$

The conditions for zero momentum of the molecule and zero angular momentum are given by

$$x_1 + x_2 + x_3 = 0,$$

$$y_1 + y_2 + y_3 = 0,$$

$$-x_1 + \frac{x_2 + x_3}{2} + \sqrt{3}\frac{y_3 - y_2}{2} = 0.$$

With a choice of $q_1 = x_1$, $q_2 = x_3 - x_2$ and $q_3 = y_1 - y_3$ and from above equations, three coordinates can be eliminated. From here the Lagrangian can be expressed completely in terms of the three vibrational coordinates q_1, q_2, q_3 and their time derivatives. The intervening steps are left as an exercise for the reader who shall eventually obtain the following equations of motion:

$$\ddot{q}_1 + \frac{3\varkappa}{2m}q_1 = 0,$$

$$\frac{3\varkappa}{4m}q_1 + \left(\ddot{q}_2 + \frac{9\varkappa}{4m}q_2\right) + \frac{\sqrt{3}\varkappa}{2m}q_3 = 0,$$

$$\frac{3\sqrt{3}\varkappa}{8m}q_1 + \frac{3\sqrt{3}\varkappa}{8m}q_2 + \left(\ddot{q}_3 + \frac{9\varkappa}{4m}q_3\right) = 0.$$

The secular equation of this system gives a doubly degenerate mode of frequency $\sqrt{\frac{3\varkappa}{2m}}$ and another mode of frequency $\sqrt{\frac{3\varkappa}{m}}$. □

The technique illustrated in Examples 34 and 35 for calculating eigenfrequencies of molecular vibrations is generalizable for molecules with more atoms. A thorough calculation as performed in the previous examples is desirable for all these polyatomic molecules. However, the computation becomes very tedious. In many situations, it is not the exact values of these eigenfrequencies that are needed but rather a classification of the normal modes. In the case of the non-linear triatomic molecule, this classification could have been done without actually going through the full calculations. With reference to Figure 4.4.1, one may note that the three normal modes of the motion are quite obvious from mere inspection of the structure of the molecule. The symmetry of the molecule allows one to guess the simplest possible ways in which the molecule can be vibrating. While such intuitive guesswork might work in the simplest of cases, a more formal approach is necessary when one needs to classify the normal modes of polyatomic molecules. Group theory provides an elegant solution to this classification problem.

In a vibrating molecule, the atomic nuclei do not remain in their mean positions. If the nuclei were assumed fixed in their mean positions, then a given molecule would

possess a certain point group symmetry. For small vibrations of the molecule, the symmetry is amply retained so as to be useful in classification of the normal modes.

If the molecule is vibrating in some specific normal mode, upon a symmetry transformation the frequency of the oscillation should remain unchanged but the coordinate designations change for various nuclei. The vibration in the transformed state of the molecule can at best be a linear combination of the degenerate normal modes associated with this particular frequency. The degenerate normal coordinates of the molecule are transformed into linear combinations of each other upon action of the symmetry group and therefore they give a representation of the symmetry group. That this representation is always irreducible is ensured by the fact that the quadratic form $\sum_{p=1}^{v_l} \Theta_{l,p}^2$ (Equation 4.4.9) remains invariant under every symmetry transformation. For, if the representation of the symmetry group given by the normal coordinates of a degenerate frequency were reducible, then the cancellation of the cross terms in the transformed value of $\sum_{p=1}^{v_l} \Theta_{l,p}^2$ could no more be guaranteed. The conclusion may now be stated that the degenerate normal modes of vibration give an irreducible representation of the symmetry group of the molecule.

If the normal coordinates are known at the outset, it would be a simple matter to calculate the symmetry group action on them and thereby construct a representation of the same. Such a representation is called the *full vibrational representation* of the symmetry group of the molecule. The vibrational representation is a reducible representation. From the characters of the vibrational representation it is possible to decompose the representation into irreducible parts using a projection operator. Since the knowledge of the normal coordinates is not assumed to begin with, the characters of the vibrational representation would have to be calculated by other means. In Equation 4.4.6, it was noted that the transformation A is an invertible transformation. It follows that the representation of the symmetry group over the normal coordinates and the representation of the symmetry group over any other basis for the vibrational degrees of freedom are equivalent, and hence have the same characters. Once a basis for the vibrational degrees of freedom is obtained, the symmetry group action on the basis yields a representation of the symmetry group. The characters of the group elements can be easily calculated from the representing matrices.

Example 36. The non-linear triatomic molecule is considered here again. The symmetry group of the molecule is clearly C_{2v}. With reference to Figure 4.4.1(a), the C_2 axis is along the *z-axis*, the $\sigma_v(\sigma_v')$ planes are the x-z plane and the y-z plane. To each of the molecules is attached a basis of its excursions from the mean position, namely (x_1, z_1), (x_2, z_2) and (X, Z). Upon eliminating the translational and rotational motion of the molecule it was shown in the previous example that coordinates $q_1 = x_1 + x_2$, $q_2 = x_1 - x_2$ and $q_3 = z_1 + z_2$ correspond to the three vibrational degrees of freedom, though not all of them are the normal coordinates. Consider the basis set (q_1, q_2, q_3) and let the symmetry group C_{2v} act on this basis. The representation of C_{2v} on this basis is the full vibrational representation Γ^V. The reader should have no difficulty in verifying that the representing matrices for various group elements are

$$\Gamma^V(E) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \Gamma^V(C_2) = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

$$\Gamma^V(\sigma_v) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad \Gamma^V(\sigma_v') = \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

Note that the action of C_2 is such that $x_1 \mapsto -x_2, x_2 \mapsto -x_1, z_1 \mapsto z_1$ and $z_2 \mapsto z_2$; consequently $q_1 \mapsto -q_1, q_2 \mapsto q_2$ and $q_3 \mapsto q_3$. Likewise the whole group action can be worked out. The character table for C_{2v} that includes the characters for the representation Γ^V is

C_{2v}	E	C_2	σ_v	σ_v'	
$\mathbf{A_1}$	1	1	1	1	z
$\mathbf{A_2}$	1	1	−1	−1	R_z
$\mathbf{B_1}$	1	−1	1	−1	x, R_y
$\mathbf{B_2}$	1	−1	−1	1	y, R_x
$\Gamma^{\mathbf{V}}$	3	1	3	1	(q_1, q_2, q_3)

.

From the character table, it is easily seen that $\Gamma^{\mathrm{V}} = \mathrm{A}_1 \oplus \mathrm{A}_1 \oplus \mathrm{B}_1$. Since all the irreducible representations present in Γ^{V} are of degree 1, all the eigenfrequencies are non-degenerate. Two of the eigenfrequencies transform according to the symmetric representation A_1, the ones depicted in Figures 4.4.1(c) and (d). Then there is one frequency corresponding to the antisymmetrical representation B_1 of Figure 4.4.1(b). □

Instead of generating the vibrational representation of the molecule, it is often more convenient to generate the representation on a basis consisting of excursions. We do this in the following example.

Example 37. Continuing from the previous example, let the excursions be labeled $(x_1,\ z_1)$, $(x_2,\ z_2)$ and $(X,\ Z)$. Consider the group action on the basis $(x_1,\ z_1,\ x_2,\ z_2,\ X,\ Z)$. In this case, identify the degree 6 reducible representation as Γ^M. The following representing matrices are obtained for Γ^M:

$$\Gamma^M(E) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\Gamma^M(C_2) = \begin{bmatrix} 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\Gamma^M(\sigma_v) = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix},$$

$$\Gamma^M(\sigma_v') = \begin{bmatrix} 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

As for the characters of Γ^M, one has

C_{2v}	E	C_2	σ_v	σ_v'
Γ^M	6	0	6	0

Upon decomposition, it is found that $\Gamma^{\mathrm{M}} = 3\mathrm{A}_1 \oplus 3\mathrm{B}_1$. Now consider the representations of pure translations and rotations that keep the molecule in the x-z plane. Translations in z and x directions correspond to the representations A_1 and B_1 respectively, while the rotation about the y-axis corresponds to another instance of the irreducible representation B_1. The vibrational representation Γ^{V} is therefore equal to $\Gamma^{\mathrm{M}} - (\mathrm{A}_1 \oplus 2\mathrm{B}_1)$ which is same as $\mathrm{A}_1 \oplus \mathrm{A}_1 \oplus \mathrm{B}_1$, as was found before for vibrational representation.

Thus having determined the irreducible representations representing the normal modes of the triatomic molecule possessing C_{2v} symmetry, we can extract the three non-degenerate normal coordinates in the following manner: Construct the projection operators $\mathrm{P}_{\mathrm{A}_1}$ and subtract the translation operator T_z denoting the translation along the z direction which belongs to A_1 basis. The explicit matrix form of the two operators in the excursion basis is

$$\mathbf{P}^M_{\mathbf{A_1}} = \frac{1}{4} = \begin{bmatrix} 2 & 0 & -2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 2 & 0 & 0 \\ -2 & 0 & 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 2 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 4 \end{bmatrix}, \quad \mathbf{T}^M_{\mathbf{z}} = \frac{1}{3} \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix}.$$

In fact, the rank of $\mathbf{P}_{\mathbf{A_1}} - \mathbf{T}_{\mathbf{z}}$ is two whose non-trivial eigenvectors

$$\begin{pmatrix} -1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix} = x_2 - x_1, \quad \begin{pmatrix} 0 \\ -1/2 \\ 0 \\ -1/2 \\ 0 \\ 1 \end{pmatrix} = Z - \frac{z_1 + z_2}{2},$$

which are proportional to q_2 and q_3 in the center of the mass frame.

The projection operator eigenvectors are not in general the frequency eigenbasis. However, this group theory approach will assert that the frequency basis (normal modes) belonging to the A_1 irreducible representation will involve only linear superposition of q_2 and q_3. Similarly, we can obtain the projection operator for irreducible representation P_{B_1} and subtract translation operator T_x. The rank of $P_{B_1} - T_x$ is again two whose the non-trivial eigenvectors are $q_1 = x_1 + x_2$ (vibrational mode) and $z_1 - z_2$ (rotational mode) consistent with the classical mechanics approach discussed in Example 34. □

The above two examples illustrate how the representation of the symmetry group of a molecule on the basis of excursions can be utilized to infer the normal modes of the vibrations of the molecule. Also, the matrix representation in the excursion basis is useful to infer the normal coordinates. However, the characters of the vibrational representation can be inferred directly in all cases without actually determining the representing matrices.

Consider a molecule with point group symmetry G in a coordinate system oriented in the usual way so that z-axis is the symmetry axis of the molecule. With each nucleus of the molecule as an origin, construct coordinate systems of excursions such that their axes are parallel to the original coordinate system (Figure 4.4.1(a)). We consider the group action on the excursions. There are $3n$ coordinates in general for an n-atomic molecule. If a symmetry transformation displaces a nucleus into another identical one, then the representing matrix of the transformation cannot have diagonal elements corresponding to coordinates of the first nucleus. Thus the character of the transformation will depend on the action of the transformation on the coordinates of the nuclei which are unmoved from their positions by the transformation. Suppose the symmetry transformation C_θ is a rotation of the molecule about z-axis by an angle θ.

Let the molecule whose excursion coordinates are (x_a, y_a, z_a) remain unmoved by the C_θ transformation. The excursion coordinates are transformed due to rotation as

$$x_a \mapsto x_a \cos\theta + y_a \sin\theta,$$
$$y_a \mapsto -x_a \sin\theta + y_a \cos\theta,$$
$$z_a \to z_a.$$

The contribution to the character of the rotation C_θ from one such nucleus is $(1 + 2\cos\theta)$ If there are N_C nuclei which are unmoved, then the total contribution to the character is $N_C(1 + 2\cos\theta)$. However, in the process of calculating the character, one has to keep track of the translational motion of the molecule as a whole as well as its rotation about the symmetry axis. Under pure rotation, both the vectors corresponding to small displacements of the center of mass as well as small angular displacements behave as polar vectors and consequently contribute 2 $(1 + 2\cos\theta)$ to the character of C_θ. Therefore the character of C_θ in the vibrational representation Γ^V is given by

$$\chi^{\Gamma^V}(C_\theta) = (N_C - 2)(1 + 2\cos\theta). \tag{4.4.18}$$

For calculating the character of the rotary reflection transformation S_θ, it may be noted first of all that under such a transformation the coordinates x_a and y_a transform as indicated above, however $z_a \mapsto -z_a$. If there are N_S nuclei which are unmoved by S_θ, then the total contribution to the character of S_θ is $N_S(-1 + 2\cos\theta)$. The polar vector corresponding to the overall translational motion transforms in the same manner and has a contribution of $(-1 + 2\cos\theta)$. The vector corresponding to small angular displacement no more transforms as a polar vector since there is reflection involved in S_θ. Under reflection, the angular displacement transforms are an axial vector. For such a vector, it is well known that the components of the vector parallel to the plane of reflection reverse direction while the component of the vector perpendicular to the plane remains unchanged. After carrying out a rotation by θ, the components of the angular displacement transform as above. Since the plane of reflection is the x-y plane after reflection in this plane the final transformations are given by

$$x_a \mapsto -x_a \cos\theta - y_a \sin\theta,$$
$$y_a \mapsto x_a \sin\theta - y_a \cos\theta,$$
$$z_a \mapsto z_a.$$

The contribution to the character from the transformation of a small angular displacement of the molecule by S_θ is therefore $(1–2\cos\theta)$. Adding this contribution to the contribution from the translational motion, and subtracting from the overall, the character of S_θ in the vibrational representation Γ^V is obtained to be

$$\chi^{\Gamma^V}(S_\theta) = N_S(-1 + 2\cos\theta). \tag{4.4.19}$$

It is also clear that N_S can be either 0 or 1. A reflection in the x-y plane σ is simply a rotary reflection transformation with $\theta = 0$. Its character is therefore

$$\chi^{\Gamma^V} = N_\sigma, \tag{4.4.20}$$

where N_σ is the number of the nuclei in the reflection plane. The same formula holds for σ_v reflections. For inversions, take $\theta = \pi$ in Equation 4.4.19.

Example 38. Consider the methane molecule (CH_4). In the equilibrium state of the molecule, the hydrogen atoms are at the vertices of a regular tetrahedron and the carbon is at the geometrical center. Clearly this molecule has T_d point group symmetry. The reader may refer to the character table for the T_d group given in Section 4.2.The molecule has 9 vibrational degrees of freedom. The character of the identity element E is therefore 9. On a C_3 axis, there are two nuclei (one hydrogen and the central carbon) which are therefore unmoved by C_3 rotations. In accordance with Equation 4.4.18, the character of C_3 rotations is zero. The C_2 and the S_4 axes leave only the central carbon unmoved and the respective characters are 1 and -1 (Equation 4.4.19). The characters of σ_d reflections are 3 as the σ_d planes contain two hydrogen atoms and the central carbon. To summarize

T_d	E	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$
$\Gamma^{\mathbf{V}}$	9	0	1	-1	3

.

Decomposing the vibrational representation, one has

$$\Gamma^{\mathbf{V}} = \mathbf{A_1} \oplus \mathbf{E} \oplus \mathbf{F_2} \oplus \mathbf{F_2}.$$

There are a total of 4 distinct vibrational frequencies,[1] two of which $(\mathbf{F_2})$ are triply degenerate, one is doubly degenerate $(\mathbf{E})$ and one is non-degenerate $(\mathbf{A_1})$. □

Exercises

1. Suppose we confine a particle to move in two dimensions where the potential is $U(x,\ y) = 0$ in a region enclosing an equilateral triangle and zero elsewhere. Purely from group theory, deduce whether the stationary states are non-degenerate or degenerate.
2. Suppose the C_{3v} symmetry of a molecule breaks down to a subgroup $C_s = \{E,\ \sigma_v\}$ due to external perturbation. How does the degree 2 degenerate level of C_{3v} split with respect to the C_s group.

[1] https://www.youtube.com/watch?v=3RqEIr8NtMI& index=29& list=PLEB476ECA0DA9481C.

3. Determine the irreducible representations corresponding to the normal modes of the ammonia molecule.
4. Write down the decompositions of all possible tensor products of two irreducible representations of C_{3v}. Show that the electric and magnetic dipole transitions between states of representations $\mathbf{A_1}$ and $\mathbf{A_2}$ are forbidden.
5. From Equation 4.4.19, calculate the character of the inversion operation I.
6. For the symmetry group D_{3d}, find all the allowed electric and magnetic dipole transitions. The character table for D_{3d} is produced below for reference.

D_{3d}	E	$2C_3$	$3C_2$	I	$2S_6$	$3\sigma_d$		
$\mathbf{A_{1g}}$	1	1	1	1	1	1		x^2+y^2, z^2
$\mathbf{A_{2g}}$	1	1	−1	1	1	−1	R_z	
$\mathbf{E_g}$	2	−1	0	2	−1	0	$(R_x\ R_y)$	(x^2-y^2, xy) .
$\mathbf{A_{1u}}$	1	1	1	−1	−1	−1		
$\mathbf{A_{2u}}$	1	1	−1	−1	−1	1	z	
$\mathbf{E_u}$	2	−1	0	−2	1	0	(x, y)	

7. Find the allowed electric quadrupole transitions for the symmetry group D_{3d}.
8. Exploiting the C_{3v} symmetry of an equilateral molecule made of three identical nuclei, determine the degree of degeneracy of the eigenfrequencies. Calculate the eigenfrequencies of small oscillations of the molecule by utilizing the symmetry of the normal modes. Verify that the frequencies are the same as those obtained in Example 35. The bonds connecting the nuclei, all have same spring constant $\varkappa$.
9. Using discrete group symmetry, analyze the normal modes of a square system of four identical masses. Identical springs connect two masses along the edges of the square. The mass points are constrained to move in a plane.

5

Lie Groups and Lie Algebras

The previous chapters dealt with some systems whose symmetry could be described by finite groups. Such systems possess *discrete symmetry*. One does not need to go too far afield to find an example of a system whose symmetry is not discrete. Consider a sphere which appears the same when viewed from all orientations. If the sphere were to be rotated by any angle whatsoever about an axis that passes through the sphere's center, it would still appear the same. Any diametrical plane is also a reflection plane of symmetry. Therefore, there are an infinite number of symmetrical transformations of the sphere. Apart from this fact, it is possible to develop the notion of *closeness* between certain symmetry transformations. If C_α is the symmetry transformation corresponding to a rotation by α about the axis C passing through the sphere's center, then $C_{\alpha+\epsilon}$ is also a symmetry transformation for the sphere where ϵ could be made arbitrarily small in magnitude. This is an instance of *continuous symmetry*. The theory of Lie groups is the suitable tool for study of such symmetries. It is the purpose of this chapter to introduce the basic concepts of the theory of Lie groups and their associated Lie algebras so as to be able to quickly apply these for problem solving.

5.1 The Circle Group U(1)

Consider the group of complex numbers of unit modulus with the group operation being the usual multiplication. All such numbers lie on the unit circle centered at the origin in the complex plane (Figure 5.1.1). This group is called the $\mathbf{U}(\mathbf{1})$ group. Apart from satisfying the group axioms, $\mathbf{U}(\mathbf{1})$ has a richer structure owing to the fact that it is a subset of the complex plane. For any two complex numbers z_1 and z_2,

their product $z_1 z_2$ is uniquely defined. Additionally, for small variations in z_1 or z_2 or both, the value of the product varies by a small amount. More precisely, the map $(z_1,\ z_2) \to z_1 z_2$ is continuous. The inversion operation $z \to \frac{1}{z}$ for $z \neq 0$ can be shown to be a continuous map. As $\mathbf{U}(\mathbf{1})$ is a subset of the complex plane, these properties are inherited in $\mathbf{U}(\mathbf{1})$. The product and inversion operations in $\mathbf{U}(\mathbf{1})$ are continuous operations and this makes $\mathbf{U}(\mathbf{1})$ a *continuous group*.

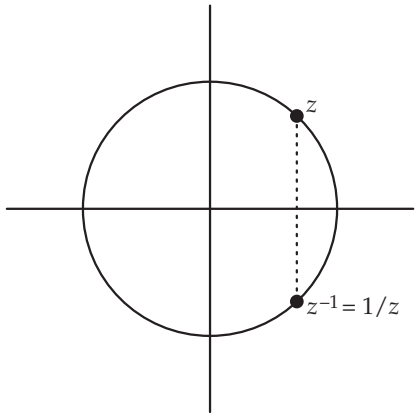


Figure 5.1.1 The Circle Group U(1)

Another important feature of $\mathbf{U}(\mathbf{1})$ is that there is a homomorphism from the additive group of real numbers onto $\mathbf{U}(\mathbf{1})$. This homomorphism is clearly given by the map

$$t \to \exp(i\omega t)$$

where ω is any non-zero real constant, and t varies over the real line $\mathbb{R}$. Thus $\mathbf{U}(\mathbf{1})$ is a *one-parameter group* in the sense that all the group elements are parametrized using a single real parameter t. It may be noticed that such a parametrization is not unique and depends on the choice of the value of ω. The identity of $\mathbf{U}(\mathbf{1})$ is prametrized by all integral multiples of $2\pi/\omega$. For group elements z_1 and z_2 parametrized by t_1 and t_2, their product is parametrized by $t_1 + t_2$. If $z(t) = z_1 z_2$ and t is assumed to be functionally related to t_1 and t_2 such as $t = f(t_1,\ t_2)$, then it is clear that in case of $\mathbf{U}(\mathbf{1})$ this functional dependence is given by

$$f(t_1,\ t_2) = t_1 + t_2.$$

Likewise, if the parameters of z and z^{-1} are assumed to be related by the function $g(t)$, then in case of $\mathbf{U}(\mathbf{1})$

$$g(t) = -t.$$

Both f and g are not merely continuous but are in fact *analytic functions* (i.e., they can be expanded as a Taylor Series about any point in their domains of definition). $\mathbf{U}(\mathbf{1})$ is an almost trivial example of a class of groups called *Lie groups*.

5.2 The Matrix Exponential

It is clear from the above discussion that any given parametrization $\exp(i\omega t)$ of $\mathbf{U}(\mathbf{1})$ is a one-dimensional unitary representation of the group $\mathbf{U}(\mathbf{1})$. The generalisation of such a parametrization and exponentiation for other Lie group elements involving higher dimensional matrices will be

$$g(\{t^a\}) = \exp(i\sum_{a=1}^{s} X_a t^a) \equiv \exp(\Omega) \text{ where } g(\{t^a = 0\}) = \mathbb{I}, \tag{5.2.1}$$

and t^a's are the parameters. Note that the number of parameters depends on the group properties of the Lie group. For instance, a set of 2×2 unitary matrices forms a group $U(2)$. Though there are 8 real entries (4 complex entries) in these matrices, the unitarity property imposes four real constraints. Hence, the number of independent real parameters to describe these matrices reduces from 8 to 4. Associated with every real parameter, there is a corresponding matrix X_a. Hence there will be four linearly independent X_a's for $U(2)$ group. The role of X_a's is to take group elements away from identity $\mathbb{I}$ and hence they are called **generators** of the Lie group.

5.2.1 Generators of the Lie group

Suppose u is a real parameter and $\Omega \equiv i\sum_a X_a t^a$ a square matrix. Let $f(u) = \exp(\Omega u)$ be a matrix valued function of u. Following the usual rules of differentiation of functions of a real variable, one has

$$\frac{d}{du} f(u) = \exp(\Omega u)\Omega = \Omega \exp(\Omega u). \tag{5.2.2}$$

Such a differentiation cannot determine each of the generators separately. In order to determine the generators, we need to take the parameters δt^a's to be infinitesimal so that differentiation with respect to δt^a is meaningful; leading to:

$$X_a = -i\frac{\partial}{\partial \delta t^a} \exp\left(i\sum_b \delta t^b X_b\right) |_{\delta t^a = 0}. \tag{5.2.3}$$

Using the group multiplication law, $g(\{t^a\})g(\{u^b\}) = g(\{v^c(t^a,\ u^b)\})$, it is a straightforward exercise (as discussed in Section 5.5) to show that the generators X^a's satisfy

$$X_a X_b - X_b X_a = i C^c_{ab} X_c \tag{5.2.4}$$

where coefficients C^c_{ab} are known as structure constants and the above relation is called Lie algebra $\mathfrak{g}$ whose formal definitions and properties are elaborated in Section 5.3.

5.2.2 Convergence property of matrix exponentials

It is not at all clear whether the exponential of the square matrix which can also be formally written as the power series expansion

$$\exp \Omega = \sum_{k=0}^{\infty} \frac{\Omega^k}{k!}, \tag{5.2.5}$$

is a convergent series. In the case of $\mathbf{U}(\mathbf{1})$, $\Omega = [i\omega t]$ is a 1×1 matrix, and the above expansion is same as that of $\exp(i\omega t)$. However, for a general square matrix Ω, Equation 5.2.5 is meaningful only if the infinite series in its right hand side converges. Noting that all the summands are matrices of same order, the critierion for convergence can be set simply to be that all the series of corresponding matrix entries in the summands converge. We will now illustrate this convergence property through a simple example.

Example 39. Consider the matrix

$$\Omega \equiv i\omega\theta = \begin{pmatrix} 0 & -\theta \\ \theta & 0 \end{pmatrix}.$$

It is easily seen that

$$\Omega^{2s} = \begin{pmatrix} (-1)^s\theta^{2s} & 0 \\ 0 & (-1)^s\theta^{2s} \end{pmatrix}$$

$$\Omega^{2s+1} = \begin{pmatrix} 0 & (-1)^{s+1}\theta^{2s+1} \\ (-1)^s\theta^{2s+1} & 0 \end{pmatrix} \qquad s = \{0, 1, 2, \ldots\}.$$

With the definition $\exp \Omega \equiv \exp i\omega\theta$ as in Equation 5.2.5, one has

$$\exp \Omega \equiv \exp i\omega\theta = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}.$$

The reader should immediately recognize $\exp \Omega$ as the familiar rotation matrix $\mathbf{R}_\theta$ about an axis perpendicular to the x-y plane. □

The inverse of such a matrix will be given by $\mathbf{R}^{-1}_\theta \equiv \mathbf{R}_{-\theta} = R^T_\theta$ implying that the matrix $\mathbf{R}_\theta$ denotes an orthogonal matrix with the corresponding Ω matrix being the

antisymmetric matrix $\Omega^T = -\Omega$. Note that the equivalent expression in terms of the ω matrix will imply that the matrices $\exp(i\omega\theta)$ are unitary with ω being self-adjoint as illustrated below.

The adjoint of a linear transformation was defined in Section 3.1. If $\Omega \equiv i\omega\theta$ is a square antisymmetric matrix, then it follows from the definition of adjoint that $[(i\omega)^\dagger]_{jk} = \overline{[(i\omega)_{kj}]} = -i\overline{[\omega_{kj}]}$. Further, if ω itself was self-adjoint then

$$[(i\omega)^\dagger]_{jk} = -i\omega_{jk}$$

$$\Rightarrow (i\omega)^\dagger = -i\omega.$$

Assuming that the matrix exponential $\exp(i\omega\theta)$ converges for some self-adjoint ω, upon taking the adjoint of Equation 5.2.5 one has

$$[\exp(i\omega\theta)]^\dagger = \sum_{k=0}^{\infty} \frac{\theta^k}{k!}[(i\omega)^k]^\dagger = \sum_{k=0}^{\infty} \frac{\theta^k}{k!}(-i\omega)^k$$

$$\Rightarrow [\exp(i\omega\theta)]^\dagger = \exp(-i\omega\theta).$$

From the definition of the matrix exponential, it can be shown that

$$\exp(-i\omega\theta)\exp(i\omega\theta) = \exp(i\omega\theta)\exp(-i\omega\theta) = \mathbb{I}. \tag{5.2.6}$$

In other words, $\exp(i\omega\theta)$ is a unitary matrix if ω is self-adjoint. This property has several applications in quantum mechanics as will be seen in the next chapter. It is important to bear in mind that for two square matrices Ω_1 and Ω_2 of same order, the equality $\exp\Omega_1 \exp\Omega_2 = \exp(\Omega_1 + \Omega_2)$ holds only if the Ω_1 and Ω_2 commute. Such a property is obeyed by the set of rotation matrices $\{\mathbf{R}_\theta\}$ which are orthogonal 2×2 matrices. Incidentally, these 2×2 matrices, involving four real entries, are dependent only on one parameter θ. This is because the orthogonality property gives three constraints reducing four real entries of 2×2 matrices to one. Hence this set R_θ forms a group $SO(2)$ where the letter O denotes the matrices are orthogonal and S implies that their determinants are unity. Like $U(1)$, the one parameter group $SO(2)$ is also abelian group:

$$R_{\theta_1}R_{\theta_2} = R_{\theta_2}R_{\theta_1} \tag{5.2.7}$$

The *commutator* of Ω_1 and Ω_2, denoted by the symbol $[\Omega_1,\ \Omega_2]$, is defined as

$$[\Omega_1,\ \Omega_2] = \Omega_1\Omega_2 - \Omega_2\Omega_1. \tag{5.2.8}$$

Thus the condition for $\exp\Omega_1 \exp\Omega_2 = \exp(\Omega_1 + \Omega_2)$ to be true is that $[\Omega_1,\ \Omega_2] = 0$. The following properties of the commutator are directly obtained from its definition.

(1) $[\lambda\Omega_1 + \mu\Omega_2,\ \Omega_3] = \lambda[\Omega_1,\ \Omega_3] + \mu[\Omega_2,\ \Omega_3]$ for any complex λ and μ.

(2) $[\Omega_1,\ \Omega_2] = -[\Omega_2,\ \Omega_1]$.

(3) $[\Omega_1,\ [\Omega_2,\ \Omega_3]] + [\Omega_2,\ [\Omega_3,\ \Omega_1]] + [\Omega_3,\ [\Omega_1,\ \Omega_2]] = 0$.

The last equality is called the *Jacobi identity*. All the three aforementioned properties of the commutator are also properties of the *Poisson bracket* if Ω_i were dynamical quantities of a Hamiltonian describing classical system. The generators of a Lie group (5.2.4) indeed have such non-trivial commutators. We will formally introduce the algebra obeyed by the generators X_a's in the following section.

5.3 Finite Dimensional Lie Algebras

Definition 5. A *Lie Algebra* $\mathfrak{g}$ is a vector space on which is defined a binary operation $[\ ,\ ]$ having following properties:

(1) For all x and y in $\mathfrak{g}$, $[x,\ y]$ is in $\mathfrak{g}$.

(2) For all $x,\ y$ and z in $\mathfrak{g}$, and scalars λ and μ, $[\lambda x + \mu y,\ z] = \lambda[x,\ z] + \mu[y,\ z]$.

(3) $[x,\ y] = -[y,\ x]$.

(4) $[x,\ [y,\ z]] + [y,\ [z,\ x]] + [z,\ [x,\ y]] = 0$. [Jacobi identity]

If the scalars are chosen from the set of real numbers, then the Lie algebra is called a *real Lie algebra*. In case the scalars come from the set of complex numbers, one has a *complex Lie algebra*. The properties of the composition $[\ ,\ ]$ are identical to the properties of the commutator discussed in the last section. The composition $[x,\ y]$ of $x,\ y \in \mathfrak{g}$ would be refered to as the *Lie bracket* of x and y. A Lie algebra $\mathfrak{g}$ in which the Lie bracket vanishes identically over $\mathfrak{g}$ is an *abelian algebra*. Being a vector space, $\mathfrak{g}$ has a basis. It will be assumed throughout that $\mathfrak{g}$ is finite dimensional. If $\{x_i\}_{i=1}^n$ is a basis for $\mathfrak{g}$ then for any x_s and x_t in the basis it must be true that

$$[x_s,\ x_t] = \sum_{k=1}^{n} c_{st}^k x_k \tag{5.3.1}$$

since $[x_s,\ x_t]$ is after all yet another vector in $\mathfrak{g}$. The coefficients c_{st}^k are called the *structure constants* of the Lie algebra. The obvious relation $[x_s,\ x_t] + [x_t,\ x_s] = 0$ for commutator bracket puts the following restriction on the structure constants:

$$\sum_{k=1}^{n} (c_{st}^k + c_{ts}^k) x_k = 0.$$

From linear independence of $\{x_i\}_{i=1}^n$, it follows that $c_{st}^k = -c_{ts}^k$. In a Lie algebra, it can be shown further that

$$\sum_{k=1}^{n} [c_{sk}^l c_{tu}^k + c_{tk}^l c_{us}^k + c_{uk}^l c_{st}^k] = 0$$

The following definitions of Lie algebra and the properties of the structure functions are essential and will henceforth be assumed for the rest of the chapter. We will now present two familiar examples where the structure constants and Lie algebra appear.

Example 40. The cross product of vectors in the three-dimensional space $\mathbb{R}^3$ turns into a three-dimensional Lie algebra. If the basis vectors are taken to be the standard **i**, **j** and **k**, then all the four properties of Definition 5 are easily seen to be satisfied. The non-zero structure constants are

$$c^i_{jk} = c^j_{ki} = c^k_{ij} = +1$$

$$c^i_{kj} = c^j_{ik} = c^k_{ji} = -1,$$

and the other structure constants are all equal to zero. □

Example 41. In quantum mechanics, the operators of position $\hat{x}$ and the corresponding component of momentum $\hat{p}_x$ of a particle do not commute and the identities

$$[\hat{x}, \hat{p}_x] = [\hat{y}, \hat{p}_y] = [\hat{z}, \hat{p}_z] = i\hbar \tag{5.3.2}$$

are well known. For simplicity, let us set $\hbar$ (proportional to Planck constant) to be 1. The position components and the momentum components commute amongst themselves. Also, position components commute with any orthogonal momentum component. The components of the orbital angular momentum operators $\hat{\ell} = \hat{\mathbf{r}} \times \hat{\mathbf{p}}$ of the particle

$$\hat{\ell}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y$$

$$\hat{l}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z$$

$$\hat{l}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x,$$

generate a three-dimensional Lie algebra. Using the position-momentum algebra (5.3.2) and the definitions of the commutator, the readers can verify that the Lie algebra amongst the angular momentum components become:

$$[\hat{l}_x, \hat{l}_y] = i\hat{l}_z$$

$$[\hat{l}_y, \hat{l}_z] = i\hat{l}_x \tag{5.3.3}$$

$$[\hat{l}_z, \hat{l}_x] = i\hat{l}_y$$ □

We will now focus on rotation operations in three-dimensional space and apply the above algebra. We can consider three independent rotations depending on the choice

of perpendicular axis. Let $R(\boldsymbol{\theta} \equiv \theta\hat{\mathbf{n}})$ denote 3×3 matrix representation of proper rotations θ about $\hat{\mathbf{n}}$ axis, acting on any position vector $\vec{r_1}$ as follows:

$$R(\boldsymbol{\theta}) : \vec{r_1} \to \vec{r_2},$$

where rotations keeps the norm of vectors $\vec{r_1}.\vec{r_1} = \vec{r_2}.\vec{r_2}$ same. This implies that the rotation $R(\theta)$ must obey the orthogonal property

$$R(\boldsymbol{\theta})R^T(\boldsymbol{\theta}) = \mathbb{I}.$$

The determinant of these proper rotations matrices must be one. Depending on the axis of rotation, there will be an appropriate $\Omega \equiv -i\boldsymbol{L}.\boldsymbol{\theta}$ in the exponential map: $R(\theta) = \exp(-i\boldsymbol{\theta}.\boldsymbol{L})$. Just like the collection of one parameter elements $\{\exp(i\omega t)\}$ of $U(1)$ group and $\{\exp(i\omega\theta)\}$ of $SO(2)$ group, the set of orthogonal 3×3 matrices $R(\boldsymbol{\theta}) = \exp(\Omega) = \exp(-i\boldsymbol{\theta}.\boldsymbol{L})$, involving three parameters $\boldsymbol{\theta}$ and three generators $\mathbf{L}$, forms a group $SO(3)$. We leave it to the readers to verify that orthogonal 3×3 matrices will require only three independent entries. Unlike the $SO(2)$ group (5.2.7) where the elements commute, the $SO(3)$ group elements do not obey

$$\exp(i\Omega_{1)} \exp i\Omega_2 \neq \exp[i(\Omega_{1+}\Omega_2)]$$

and hence the group is non-abelian. For infinitesimal angle $\boldsymbol{\delta\theta}$, the exponential map of $SO(3)$ elements can be approximated as

$$R(\boldsymbol{\delta\theta}) = \mathbb{I} - i\delta\theta\hat{\mathbf{n}}.\boldsymbol{L}, \tag{5.3.4}$$

where we have denoted the magnitude of the rotation angle about an axis $\hat{n}$

Example 42. It is straightforward to check that the infinitesimal rotations of magnitude $\delta\theta$ about x-axis $\mathrm{R}(\delta\theta\hat{\mathbf{i}})$ and the infinitesimal rotations of same magnitude $\delta\theta$ about y-axis $\mathrm{R}(\delta\theta\hat{\mathbf{j}})$ obey the following relation:

$$\mathrm{R}(\delta\theta\hat{\mathbf{i}})\mathrm{R}(\delta\theta\hat{\mathbf{j}}) - \mathrm{R}(\delta\theta\hat{\mathbf{j}})\mathrm{R}(\delta\theta\hat{\mathbf{i}}) = \mathrm{R}(\delta\theta^2\hat{\mathbf{k}}) - \mathbb{I}. \tag{5.3.5}$$

Using the definition (5.3.4) in the above equation, verify that the 3×3 matrices L_x, L_y, L_z obey angular momentum algebra (5.3.3):

$$[L_x,\ L_y] = iL_z.$$

Using $R(\delta\theta\hat{\mathbf{i}}) \equiv I - i\delta\theta L_x$ and $R(\delta\theta\hat{\mathbf{j}}) \equiv I - i\delta\theta L_y$, the LHS (5.3.5) simplifies to $(-i)^2\delta\theta^2[L_x, L_y]$ whereas the RHS (5.3.5) gives $-i\delta\theta^2 L_z$ leading to the conventional angular momentum algebra (5.3.3). □

Thus $L_x,\ L_y,\ L_z$, which are the generators of the rotation group $SO(3)$, constitute the Lie algebra $\mathfrak{g}$ of the rotation group $SO(3)$ denoted as $\mathfrak{g} \equiv \mathfrak{so}(3)$ which is isomorphic

to the angular momentum algebra (5.3.3). Incidentally, the range of the magnitude of the parameter $\boldsymbol{\theta} = \theta\hat{\mathbf{n}}$ must be $-\pi \leq \theta < \pi$. Hence the parameter space describing the group $SO(3)$ will be a solid sphere of radius π. The groups with such bounded parameters are referred to as *compact groups*.

Every point inside the solid sphere corresponds to a distinct group element of $SO(3)$. However, the diametrically opposite points on the boundary of the solid sphere of radius π will denote the same group element $(R[\pi\hat{\mathbf{n}}] = R[\pi(-\hat{\mathbf{n}})]$. Hence, this identification of diametrically opposite points allows two topologically distinct closed curves inside the sphere as shown in Figure 5.3.1. In the literature, such a parameter space is called *doubly-connected space*.

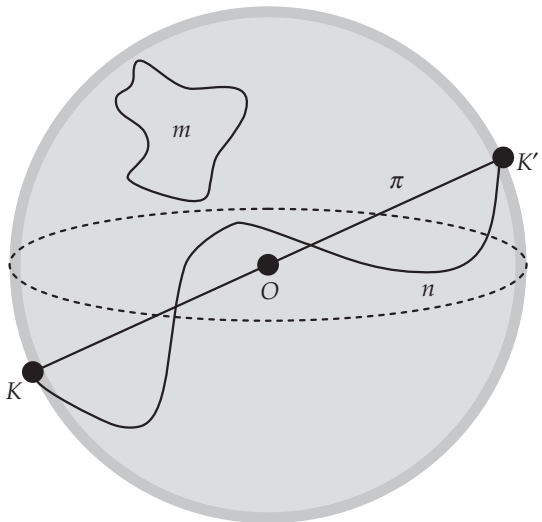


Figure 5.3.1 Group Manifold of the $SO(3)$ (doubly-connected space)

Definition 6. If $\mathfrak{g}$ is a Lie algebra and $\mathfrak{h}$ is a subset of it such that the elements of $\mathfrak{h}$ form a Lie algebra under the Lie bracket of $\mathfrak{g}$, then $\mathfrak{h}$ is called a *subalgebra*. The subalgebra $\mathfrak{h}$ is an *invariant subalgebra* if $[g,\ h] \in \mathfrak{h}$ for all $g \in \mathfrak{g}$ and $h \in \mathfrak{h}$.

Example 43. Suppose $g \in \mathfrak{g}$ and $h \in \mathfrak{h}$ where $\mathfrak{h}$ is an invariant subalgebra of $\mathfrak{g}$. Show that the set of elements $\{\exp(ih)\}$ forms an invariant subgroup $H \subset G$ where the set $\{\exp(ig)\}$ belongs to Lie group G. In other words, show that

$$\exp(ig)\exp(ih)\exp(-ig) = \exp(ih_1)$$

where $h_1 \in \mathfrak{h}$.

Using the well-known properties of matrices and the fact that $h \in \mathfrak{h}$, we can deduce

$$\exp(ig)h\exp(-ig) = h + i[g,\ h] - \frac{1}{2!}[g,\ [g,\ h]] + \ldots = h_1,$$

as $[g, h]$, $[g, [g, h]]$, $\ldots \in \mathfrak{h}$. Hence, for any exponential form of h in LHS of the above equation, we will get RHS as $\exp(ih_1)$. □

In Chapter 3, linear representations of finite groups were studied in some length. Analogously, representations of a Lie algebra may be defined. To begin with, let V be a complex (or real) vector space of dimension n. Let $\mathfrak{gl}(V)$ be the set of all linear operators on V. For $T_1,\ T_2 \in \mathfrak{gl}(V)$ and scalars $\alpha,\ \beta$ one may define a linear combination $\alpha T_1 + \beta T_2$ to be the linear operator which acts on V in accordance with

$$(\alpha T_1 + \beta T_2)x = \alpha T_1(x) + \beta T_2(x),$$

for all x in V. With the above definition, $\mathfrak{gl}(V)$ itself is a vector space. If $\{x_i\}_{i=1}^n$ is a basis for V, then define linear operators X_{ij} which act on the basis of V such that $X_{ij}(x_k) = \delta_{ik}x_j$. Any linear operator in $\mathfrak{gl}(V)$ may be expressed as a linear combination of X_{ij}'s. It is left to the reader to verify that X_{ij} are in fact linearly independent. It follows that the dimension of the space $\mathfrak{gl}(V)$ is n^2. Apart from being a vector space, $\mathfrak{gl}(V)$ has an additional important structure. Two linear operators can be composed according to the usual rules of function composition, $(T_1T_2)(x) = T_1(T_2(x))$. Linearity of T_1 and T_2 immediately leads to linearity of T_1T_2 so that T_1T_2 is also in $\mathfrak{gl}(V)$. One can now employ the vector space structure of $\mathfrak{gl}(V)$ along with this property to define the Lie bracket $[T_1,\ T_2] = T_1T_2 - T_2T_1$. The conclusion that, for a given finite dimensional vector space V, the space $\mathfrak{gl}(V)$ of all linear operators on V can be turned into Lie algebra is obvious.

Example 44. It is trivial that the set of real numbers $\mathbb{R}$ is a one-dimensional real vector space. The linear operators are the real numbers themselves and the commutator identically vanishes. The Lie algebra is abelian. □

Example 45. Consider the two-dimensional complex vector space. In any basis, the linear operators on this space can be represented by 2×2 matrices with complex entries. The Lie algebra of this four-dimensional complex vector space of linear operators is denoted $\mathfrak{gl}(2,\ \mathbb{C})$. $\mathfrak{gl}(2,\ \mathbb{C})$ is clearly non-abelian which is spanned by four 2×2 matrices such as

$$E_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix},\ E_2 = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix},$$

$$E_3 = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix},\ E_4 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$

Example 46. There are several important subalgebras of $\mathfrak{gl}(2,\ \mathbb{C})$. For instance, consider matrices of the form

$$X = \begin{bmatrix} a & z \\ z^* & -a \end{bmatrix},$$

where a is a real number and z a complex number. The important properties of such matrices are that they are traceless and Hermitian. The complex subspace of $\mathfrak{gl}(2,\ \mathbb{C})$ spanned by matrices of this type is a subalgebra denoted by $\mathfrak{sl}(2,\ \mathbb{C})$. If $\{X_i\}_{i=1}^n$ are traceless Hermitian matrices and $\{\alpha_i\}_{i=1}^n$ complex numbers, then $X = \sum_{i=1}^n \alpha_i X_i$ is in $\mathfrak{sl}(2,\ \mathbb{C})$. Similarly, for $Y = \sum_{j=1}^m \beta_j Y_j$ in $\mathfrak{sl}(2,\ \mathbb{C})$, by linearity of the Lie bracket, one has

$$[X,\ Y] = \sum_{i,j} \alpha_i \beta_j [X_i,\ Y_j] \equiv Z.$$

The reader can verify that the brackets $[X_i,\ Y_j]$ are all equal to the imaginary unit times Z_{ij}, where Z_{ij} is again a traceless Hermitian matrix. Then the above equality shows that $[X,\ Y] \in \mathfrak{sl}(2,\ \mathbb{C})$. Hence, $\mathfrak{sl}(2,\ \mathbb{C})$ is indeed a subalgebra of $\mathfrak{gl}(2,\ \mathbb{C})$. Since $\mathfrak{sl}(2,\ \mathbb{C})$ is a proper subspace of $\mathfrak{gl}(2,\ \mathbb{C})$, its dimension is less than 4. Notice that a traceless Hermitian matrix is completely specified if the 3 independent quantities a, z and z^* are known. Therefore the dimension of $\mathfrak{sl}(2,\ \mathbb{C})$ must be 3. This can be seen more explicitly by considering the matrices

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},\ \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix},\ \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

σ_x, σ_y and σ_z are traceless Hermitian matrices which are also linearly independent. Their linear span is definitely a subset of $\mathfrak{sl}(2,\ \mathbb{C})$. It follows that their linear span is all of $\mathfrak{sl}(2,\ \mathbb{C})$. The matrices σ_x, σ_y and σ_z are the familiar Pauli matrices.

Complex numbers z in $\mathbb{C}$ are pairs of independent real numbers $(\Re(z),\ \Im(z))$. Similarly, an n-tuple of complex numbers is a $2n$-tuple of real numbers. Thus a complex vector space of dimension n can be regarded as a real vector space of dimension $2n$. In the above discussion, $\mathfrak{gl}(2,\ \mathbb{C})$ was regarded as a complex vector space of dimension 4. As a real vector space, $\mathfrak{gl}(2,\ \mathbb{C})$ has dimension 8 spanned by the basis consisting of E_1, E_2, E_3 and E_4 and the matrices

$$\begin{bmatrix} i & 0 \\ 0 & 0 \end{bmatrix},\ \begin{bmatrix} 0 & i \\ 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 \\ i & 0 \end{bmatrix},\ \begin{bmatrix} 0 & 0 \\ 0 & i \end{bmatrix}.$$

Likewise, $\mathfrak{sl}(2,\ \mathbb{C})$ is a six-dimensional real Lie algebra spanned by a basis consisting of σ_x, σ_y, σ_z and the matrices

$$S_x = \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix},\ S_y = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},\ S_z = \begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}.$$

The following Lie brackets are easily computed from the above *representations* of the basis elements of $\mathfrak{sl}(2,\ \mathbb{C})$.

$$[\sigma_x,\ \sigma_y] = 2i\sigma_z\ [\sigma_y,\ \sigma_z] = 2i\sigma_x\ [\sigma_z,\ \sigma_x] = 2i\sigma_y \qquad (5.3.6)$$
$$[S_x,\ S_y] = -2S_z\ [S_y,\ S_z] = -2S_x\ [S_z,\ S_x] = -2S_y.$$

The lower set of 3 equations is completely equivalent to the upper 3 equations since $S_x = i\sigma_x$, etc. The three-dimensional real subalgebra of $\mathfrak{sl}(2,\ \mathbb{C})$ spanned by $S_x,\ S_y$ and S_z is called the $\mathfrak{su}(2)$ algebra. Notice that $S_x,\ S_y$ and S_z are skew-Hermitian ($S_x^\dagger = -S_x$ etc.) traceless matrices. □

Definition 7. Let $\mathfrak{g}$ be a Lie algebra and $\mathfrak{gl}(V)$ the Lie algebra of operators on the vector space V. A linear map π from $\mathfrak{g}$ into $\mathfrak{gl}(V)$ is said to be a representation of $\mathfrak{g}$ on the vector space V if

$$\pi([x,\ y]) = [\pi(x),\ \pi(y)] \qquad (5.3.7)$$

for all x, y in $\mathfrak{g}$. The dimension of V is the degree of the representation π.

Since a Lie algebra $\mathfrak{g}$ is also a vector space, the above definition of representation allows one to represent $\mathfrak{g}$ over itself. For some $x \in \mathfrak{g}$, consider a mapping ad_x from $\mathfrak{g}$ into $\mathfrak{g}$ defined by $\mathrm{ad}_x(y) = [x,\ y]$ for all $y \in \mathfrak{g}$. It is clear that ad_x is a linear operator on the vector space $\mathfrak{g}$ since the Lie bracket is linear in y by definition. Therefore $\mathrm{ad}_x \in \mathfrak{gl}(\mathfrak{g})$ and one has a mapping ad from $\mathfrak{g}$ into $\mathfrak{gl}(\mathfrak{g})$ defined as ad $(x) = \mathrm{ad}_x$ for all x in $\mathfrak{g}$. This mapping is a representation if ad $([x,\ y]) = [\mathrm{ad}(x), \mathrm{ad(y)}\ ]$. Let $z \in \mathfrak{g}$ so that one has

$$\mathrm{ad}_{[x,y]}(z) = [[x,\ y],\ z] = [x,\ [y,\ z]] + [y,\ [z,\ x]]$$

$$\Rightarrow \mathrm{ad}_{[x,y]}(z) = [x,\ [y,\ z]] - [y,\ [x,\ z]]$$

$$\Rightarrow\ \mathrm{ad}_{[x,y]} =\ \mathrm{ad}_x\,\mathrm{ad}_y -\ \mathrm{ad}_y\,\mathrm{ad}_x \qquad (5.3.8)$$

and one has shown that ad is indeed a representation. Such a representation of a Lie algebra is called an *adjoint representation*. From Equation 5.3.1 it immediately follows that the representing matrices of the bases $\{x_s\}_{i=1}^n$ of $\mathfrak{g}$ are given by

$$[\mathrm{ad}_{x_s}]_{kt} = c_{st}^k. \qquad (5.3.9)$$

Example 47. The $\mathfrak{su}(2)$ algebra was described in the previous example (Equation 5.3.6). If one takes $S_x/2,\ S_y/2$ and $S_z/2$ as the basis for the algebra then in the adjoint representation, the matrices are easily found to be

$$S_x/2 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix},\ S_y/2 = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

$$S_z/2 = \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$ □

5.3.1 $\mathfrak{su}(2)$ algebra

In quantum mechanics, we define generators of $su(2)$ Lie algebra as J_i's obeying

$$[J_i, J_j] = i\epsilon_{ijk}J_k.$$

The representation for $J_i = \frac{1}{2}\sigma_i$ is known as the fundamental matrix representation which act on a two-dimensional complex vector space V. Using the redefinition $(J_1 \pm iJ_2)/\sqrt{2} = J_\pm$ where $J_\pm$ are known as raising and lowering operators, the algebra becomes

$$[J_+,\ J_-] = J_3\ ;\ [J_3,\ J_\pm] = \pm J_\pm. \tag{5.3.10}$$

In fact such a redefinition naturally appears in the formal discussion of Cartan classification of semi-simple Lie algebras. We will briefly present such ladder operators in Section 5.7.

As the $\mathfrak{su}(2)$ algebra has no abelian subalgebra, it is always possible to choose one of the generators to have a diagonal matrix representation. Following the convention in many books, we take the representation of J_3 as diagonal matrix and work with its eigenvectors as basis $\{|j,m\rangle\} \in V$. That is,

$$J_3|j,m\rangle = m|j,m\rangle,$$

where m can be either integers or half-odd integers. We refer to maximum eigenvalue of J_3 as j and the corresponding highest value state is $|j,j\rangle$.

Applying $J_\pm$ on the states $|j,m\rangle$ we observe

$$J_3\{J_\pm|jm\rangle\} = J_\pm\{J_3|j,m\rangle\} \pm J_\pm|j,m\rangle = (m \pm 1)\{J_\pm|j,m\rangle\}.$$

From this relation, it is clear that the J_3 eigenvalue of states $J_\pm|jm\rangle$ is $m \pm 1$. For highest value state $|j,\ j\rangle$, we cannot get J_3 eigenvalue as $j+1$ for $J_+|j,j\rangle$ which implies

$$J_+|j,j\rangle = 0.$$

The other eigenbasis of J_3 can be obtained by applying lowering operator J_- on the highest value state $|j,j\rangle$:

$$J_-|j,j\rangle = N_{j,j}|j,j-1\rangle.$$

Taking inner product of the above state with its dual state $\langle j,j|J_+$, we get

$$\langle j,j|J_+J_-|j,j\rangle = |N_{j,j}|^2 = \langle j,j|J_3 + J_-J_+|j,j\rangle = \langle j,j|J_3|j,j\rangle = j,$$

implying $N_{j,j} = \sqrt{j}$. We can now determine

$$J_+|j,j-1\rangle = \frac{1}{N_{j,j}}J_+J_-|j,j\rangle = \frac{1}{N_{j,j}}\{J_3 + J_-J_+\}|j,j\rangle = \sqrt{j}|j,j\rangle = N_{j,j}|j,j\rangle.$$

This application of J_- can be continued to obtain the basis states $|j,j-2\rangle,\ |j,j-3\rangle,\ldots$ belonging to the vector space V:

$$J_-|j,j-r\rangle = N_{j,j-r}|j,j-r-1\rangle\ ;\ J_+|j,j-r-1\rangle = N_{j,j-r}|j,j-r\rangle.$$

Using the $\mathfrak{su}(2)$ algebra involving ladder operators, it is easy to deduce

$$N^2_{j,j-r} = \langle j,j-r|J_+J_-|j,j-r\rangle = N^2_{j,j-r+1} + j - r,$$

giving a recursion relation amongst the coefficients whose solution turns out to be

$$N_{j,m} = \frac{1}{\sqrt{2}}\sqrt{(j+m)(j-m+1)}.$$

As the vector space is finite dimensional, we will also have a lowest eigenvalue state $|j,j-k\rangle$ such that

$$J_-|j,j-k\rangle = 0.$$

Clearly, $N_{j,m} = 0$ when $m = j+1$ (highest value state $|j,j\rangle$) and $m = j-k = -j$ (lowest value state $|j,j-k\rangle$) which means $k = 2j$. The highest value j can be also determined by acting $\boldsymbol{J}.\boldsymbol{J} = J_3^2 + J_+J_- + J_-J_+on|j,m\rangle$:

$$\boldsymbol{J}.\boldsymbol{J}|j,m\rangle = (J_3^2 + J_+J_- + J_-J_+)|j,m\rangle = j(j+1)|j,m\rangle.$$

Notice that $\boldsymbol{J}.\boldsymbol{J}$ commutes with the all the three $su(2)$ generators.

$$[\boldsymbol{J}.\boldsymbol{J},\ J_3] = \ [\boldsymbol{J}.\boldsymbol{J},\ J_+] = [\boldsymbol{J}.\boldsymbol{J},\ J_3] = 0.$$

Such quantities are called *Casimir operators.*

We will see that the above discussion on $\mathfrak{su}(2)$ algebra and their action on basis states of finite dimensional vector space V will be useful when we formally introduce root vectors and study $\mathfrak{su}(2)$ subalgebras constituting compact semi-simple Lie algebras in Section 5.7.

By exponential mapping, the special unitary group $SU(2)$ group elements will be

$$g(\boldsymbol{\theta}) = \exp(i\boldsymbol{\theta}.\boldsymbol{J}),$$

whose parameters are similar to that of group $SO(3)$ but there is a subtle difference. For the fundamental representation $\boldsymbol{J} = \boldsymbol{\sigma}/2$, using the properties of the Pauli matrices, these group elements can be written as

$$g(\theta\hat{\mathbf{n}}) = \cos(\theta/2)\mathbb{I} + i\hat{\mathbf{n}}.\boldsymbol{\sigma}\sin(\theta/2),$$

which implies $g(2\pi) \neq g(0)$, suggesting that the parameter space will not be a solid sphere of radius π. Instead, the $SU(2)$ parameter space is a solid sphere of radius 2π. Further, all points on the boundary of the solid sphere are identified making this $SU(2)$ parameter space *simply connected*. In other words, there will be only one class of closed curves in the parameter space. This subtle difference in the parameter space also indicates that the group $SO(3)$ (Figure 5.3.1) is not isomorphic to group $SU(2)$. That is, $g(\theta\hat{\mathbf{n}})$ and $g((\theta + \pi)\hat{\mathbf{n}})$ are mapped to $R(\theta\hat{\mathbf{n}}) \in SO(3)$ giving *two to one* mapping (homomorphism). In the literature, $SU(2)$ is refered to as a *double cover* of $SO(3)$ because of the above properties.

5.4 Semi-simple Lie Algebras

The explicit construction of the adjoint representation of a Lie algebra allows for introduction of the *Killing form* on it. The advantage of the Killing form lies in that it bears some resemblance to the concept of inner product on an inner product space. One should bear in mind that this resemblance is exact only for a certain type of Lie algebras. It is very convenient that such Lie algebras turn out to be quite useful in physical applications.

Let $\mathfrak{g}$ be a Lie algebra and ad its adjoint representation. For $x,\ y \in \mathfrak{g}$, the Killing form $\kappa(x,\ y)$ is given by

$$\kappa(x,\ y) = -\mathbf{tr}(\mathrm{ad}(x)\ \mathrm{ad}(y)), \tag{5.4.1}$$

where **tr** stands for trace of the matrix products. Evidently $\kappa(x,\ y) = \kappa(y,\ x)$. The linearity of the map ad gives $\kappa(\alpha x + \beta y,\ z) = \alpha\kappa(x,\ z) + \beta\kappa(y,\ z)$ for scalars $\alpha,\ \beta$ and $x,\ y,\ z \in \mathfrak{g}$. Killing form is therefore a symmetric bilinear form. If either x or y is 0, then $\kappa(x,\ y) = 0$.

Consider the set $\mathfrak{g}^{\perp} = \{x \in \mathfrak{g}\ |\kappa(x,\ y) = 0\ \forall\ y \in \mathfrak{g}\}$. $\mathfrak{g}^{\perp}$ is clearly a subspace of $\mathfrak{g}$ as follows from linearity of κ. The notation seems to suggest that $\mathfrak{g}^{\perp}$ consists of vectors orthogonal to the linear space $\mathfrak{g}$. However, this orthogonality is with respect to the Killing form (5.4.1) and not in the usual sense of orthogonality in an inner product space. It very well might be that $\mathfrak{g}^{\perp}$ is not merely the null space and $\mathfrak{g}^{\perp} \subset \mathfrak{g}$. When this is true, the Killing form κ is said to be *degenerate*.

Definition 8. A Lie algebra whose Killing form is non-degenerate is called *semi-simple*.

Let $\mathfrak{h}$ be an invariant subalgebra (Definition 6) of a semi-simple Lie algebra $\mathfrak{g}$. $\mathfrak{h}^\perp = \{x \in \mathfrak{g} \,|\kappa(x,\, y) = 0 \;\forall\; y \in \mathfrak{h}\}$ is the orthogonal subspace of $\mathfrak{h}$ in $\mathfrak{g}$. Also suppose $g \in \mathfrak{g}$, $h \in \mathfrak{h}$ and $x \in \mathfrak{h}^\perp$ so that $[g,\, h] \in \mathfrak{h}$ and $\kappa(x,\, h) = 0$. Then one has $\kappa([x,\, g],\, h) = \mathbf{tr}\,(\mathrm{ad}([x,\, g])\mathrm{ad}(h))$ and from the property of trace and Equation 5.3.8, $\kappa([x,\, g],\, h) = \kappa(x,\, [g,\, h]) = 0$. It follows that $[x,\, g] \in \mathfrak{h}^\perp$ and since g is arbitrary in $\mathfrak{g}$, $\mathfrak{h}^\perp$ is an invariant subagebra in $\mathfrak{g}$. The reader can easily verify that $\mathfrak{h} \cap \mathfrak{h}^\perp$ is also an invariant subalgebra in $\mathfrak{g}$. Since $\kappa(x,\, y) = 0$ for $x,\, y \in \mathfrak{h}^\perp \cap \mathfrak{h}$, it follows that for any $g \in \mathfrak{g}$, $\kappa(g,\, [x,\, y]) = \kappa(x,\, [y,\, g]) = 0$ requires $\mathfrak{h}^\perp \cap \mathfrak{h}$ is an abelian subalgebra because κ is non-degenerate for $\mathfrak{g}$.

A basis $\{x_i\}_{i=1}^{k}$ for the subspace $\mathfrak{h} \cap \mathfrak{h}^\perp$ can be chosen which can be extended to a complete basis $\{x_i\}_{i=1}^{k+l}$ for $\mathfrak{g}$. $\{x_j\}_{j=k+1}^{k+l}$is then a basis for the complement of the subspace $\mathfrak{h} \cap \mathfrak{h}^\perp$ in $\mathfrak{g}$. As $\mathfrak{h} \cap \mathfrak{h}^\perp$ is an abelian subalgebra, it immediately follows that the matrix of the operator ad (g) ad (x) is of the form

$$\begin{bmatrix} 0_{k\times k} & B_{k\times l} \\ 0_{l\times k} & 0_{l\times l} \end{bmatrix}$$

for any $x \in \mathfrak{h} \cap \mathfrak{h}^\perp$ and $g \in \mathfrak{g}$. The size of the various 0-blocks and the matrix B has been indicated by subscripts. From the above it follows that $\mathbf{tr}\,(\mathrm{ad}(g)\mathrm{ad}(x)) = \kappa(g,\, x) = 0$ for all $g \in \mathfrak{g}$. Because κ is non-degenerate by assumption, the only possible conclusion is $x = 0$ and one has $\mathfrak{h} \cap \mathfrak{h}^\perp = \{0\}$. Hence, for semi-simple Lie algebra, it can be shown that $\mathfrak{g} = \mathfrak{h} \oplus \mathfrak{h}^\perp$.

Suppose $\{h_i\}_{i=1}^{m}$ is a basis of the subspace $\mathfrak{h}$. Any $x \in \mathfrak{h}$ can be expressed $x = \sum_{i=1}^{m} c_i h_i$ where c_i are real or complex (depending upon whether $\mathfrak{g}$ is a real or complex vector space). Thus every $x \in \mathfrak{h}$ corresponds to an m-tuple of numbers. Let the collection of all such m-tuples be called F^m. Here F stands for the *field* $\mathbb{R}$ or C. With component wise addition and scalar multiplication of the m-tuples, F^m is a vector space which has the same dimension as the subspace $\mathfrak{h}$. Consider a map T (Section 3.1) from $\mathfrak{g}$ into F^m such that for $g \in \mathfrak{g}$,

$$T(g) = (\kappa(g,\, h_1),\, \ldots,\, \kappa(g,\, h_m)).$$

T is then a linear transformation which is also a group homomorphism (Section 1.5) between the abelian group structures on $\mathfrak{g}$ and F^m. The kernel of this homomorphism, $\mathrm{Ker}(T)$ consists of $g \in \mathfrak{h}$ such that $\kappa(g,\, h_i) = 0$ for all $i \in \{1,\, \ldots,\, m\}$. In other words, $\mathrm{Ker}(T) = \mathfrak{h}^\perp$. Therefore the quotient group $\mathfrak{g}/\mathfrak{h}^\perp$ is isomorphic to the image of $\mathfrak{g}$ in F^m under the mapping T. The reader can easily infer that the group $\mathfrak{g}/\mathfrak{h}^\perp$ is a vector space of dimension equal to dim g–dim $\mathfrak{h}^\perp$. Since $\mathfrak{g}/\mathfrak{h}^\perp$ is a subspace in F^m, it's dimension can be no more than m. Thus one has the inequality

$$\dim \mathfrak{g} \;\leq \dim \mathfrak{h} \;+ \dim \mathfrak{h}^\perp.$$

Since the only common subspace of $\mathfrak{h}$ and $\mathfrak{h}^\perp$ is the null space, $\dim \mathfrak{g} = \dim \mathfrak{h} + \dim \mathfrak{h}^\perp$ and one has $\mathfrak{g} = \mathfrak{h} \oplus \mathfrak{h}^\perp$. Also, the restriction of κ to $\mathfrak{h}$ is non-degenerate and $\mathfrak{h}$ is semi-simple. For emphasis, we sum up the arguments of this paragraph as the following:

Theorem. *If $\mathfrak{h}$ is an invariant subalgebra of a finitely dimensional semi-simple Lie algebra $\mathfrak{g}$ and $\mathfrak{h}^\perp$is the orthogonal complement of $\mathfrak{h}$ with respect to the Killing form on $\mathfrak{g}$, then $\mathfrak{g} = \mathfrak{h} \oplus \mathfrak{h}^\perp$. Additionally, $\mathfrak{h}$ is semi-simple and $\mathfrak{h}^\perp$is an invariant subalgebra.*

It is clear from the above that a semi-simple Lie algebra can have no non-trivial invariant abelian subalgebras. Also note the following

Definition 9. A *simple Lie algebra* that has no non-trivial invariant subalgebras is a semi-simple Lie algebra.

It is an obvious consequence of the above theorem that a semi-simple Lie algebra is a direct sum of simple Lie algebras.

5.5 Lie Algebra of a Lie Group

Definition 10. A Lie group is a group with the structure of an *analytic manifold* in which group multiplication and inversion are analytic functions of their arguments.

The precise concept of an analytic manifold will not be made here. The analytic nature of the group product will be central in subsequent development. The fact that a Lie group is an analytic manifold leads to the consequence that any small neighborhood of the identity of the group has the structure of a vector space. In the example of the circle group, this vector space is one-dimensional and in the exponential representation $\exp(i\omega t)$, it is spanned by the basis $[\omega]$. Generally, the number of parameters needed to span the local vector space near the group identity may be more than one. It is assumed that this number is always finite. Let G be a Lie group whose elements in the vicinity of identity can be parametrized by n real numbers t^α[†]. Then G is said to be of dimension n. The identity itself is parametrized so that each of t^α is set to zero. For two group elements g_1 and g_2 parametrized by the sets of real quantities t_1^α and t_2^α respectively, the parameters t^α of their product $g = g_1 g_2$ are analytic functions of t_1^α and t_2^α. Suppose

$$t^\alpha = f^\alpha(t_1,\, t_2),$$

where t_1 and t_2 represent the complete sets of n parameters of g_1 and g_2 respectively. Letting $t_1 = 0$ or $t_2 = 0$ to be parameters for the identity element, the condition on f^α obtained is

$$t^\alpha = f^\alpha(t,\, 0) = f^\alpha(0,\, t).$$

[†]The superscript α should not be confused as an exponent.

With this condition, and the fact that the functions f^α are analytic functions of t_1 and t_2, a Taylor series for f^α may be written as

$$t^\alpha = f^\alpha(t_1,\ t_2) = t_1^\alpha + t_2^\alpha + \frac{1}{2}\sum_{\gamma.\delta} f^\alpha_{\gamma\delta} t_1^\gamma t_2^\delta + \ldots \tag{5.5.1}$$

where $f^\alpha_{\gamma\delta}$ are derivatives of f^α at $t_1 = t_2 = 0$. If Γ is a unitary representation of G (assuming such a representation exists) and g an element of G close to identity then the representing matrix $\Gamma(g)$ of g is an analytic function of the parameters t^α for g.

$$\Gamma(g) = I + i\sum_\alpha t^\alpha X_\alpha - \frac{1}{2}\sum_{\alpha,\beta} t^\alpha t^\beta X_{\alpha\beta} + \ldots \tag{5.5.2}$$

where $X_\alpha,\ X_\alpha X_\beta$ etc are matrices of the same order and do not depend on the value of the real parameters t^α. Suppose $g = g_1 g_2$, one has $\Gamma(g_1)\Gamma(g_2) = \Gamma(g)$. The parameters of g are given by Equation 5.5.1. Similar expressions for $\Gamma(g_1)$ and $\Gamma(g_2)$ in combination with $\Gamma(g_1)\Gamma(g_2) = \Gamma(g)$ give

$$\begin{aligned}
&\left[I + i\sum_\alpha t_1^\alpha X_\alpha - \frac{1}{2}\sum_{\alpha,\beta} t_1^\alpha t_1^\beta X_{\alpha\beta} + \cdots\cdots\right] \times \\
&\quad\left[I + i\sum_\alpha t_2^\alpha X_\alpha - \frac{1}{2}\sum_{\alpha,\beta} t_2^\alpha t_2^\beta X_{\alpha\beta} + \cdots\right] = \\
&I\ + i\sum_\alpha \left[t_1^\alpha + t_2^\alpha + \frac{1}{2}\sum_{\gamma,\delta} f^\alpha_{\gamma,\delta} t_1^\gamma t_2^\delta \ldots\right] X_\alpha - \\
&\qquad\frac{1}{2}\sum_{\alpha,\beta}\left[t_1^\alpha + t_2^\alpha + \frac{1}{2}\sum_{\gamma,\delta} f^\alpha_{\gamma,\delta} t_1^\gamma t_2^\delta \ldots\right] \times \\
&\qquad\left[t_1^\beta + t_2^\beta + \frac{1}{2}\sum_{\gamma,\delta} f^\beta_{\gamma,\delta} t_1^\gamma t_2^\delta \ldots\right] X_{\alpha\beta} + \ldots
\end{aligned}$$

Expanding the above equation, the reader should observe that the leading terms remaining after cancellations are quadratic in \$. For reference, an intermediate step is

$$-\sum_{\alpha,\beta} t_1^\alpha t_2^\beta X_\alpha X_\beta = \frac{i}{2}\sum_{\alpha,\gamma,\delta} t_1^\gamma t_2^\delta f^\alpha_{\gamma,\delta} X_\alpha - \frac{1}{2}\sum_{\alpha,\beta}[t_1^\alpha t_2^\beta + t_2^\alpha t_1^\beta] X_{\alpha\beta}.$$

Here one may notice that the $X_{\alpha\beta} = X_{\beta\alpha}$ since these are coefficients in the Taylor expansion Equation. 5.5.2. After relabelling the indices in the first term in the right hand side of above and using the fact that t_i^α are independent, one has

$$-X_\alpha X_\beta = \frac{i}{2}\sum_\gamma f^\gamma_{\alpha\beta} X_\gamma - X_{\alpha\beta}. \tag{5.5.3}$$

Interchanging α and β in above equation and subtracting gives

$$[X_\alpha,\ X_\beta] = \frac{i}{2}\sum_\gamma (f^\gamma_{\beta\alpha} - f^\gamma_{\alpha\beta}) X_\gamma, \tag{5.5.4}$$

where the $[X_\alpha,\ X_\beta]$ stands for the commutator of X_α and X_β. The reader will immediately recognize the above equation as the commutation relation in a Lie algebra (Equation 5.3.1) with the structure constants $c^\gamma_{\alpha\beta} = \frac{1}{2}\sum_\gamma (f^\gamma_{\beta\alpha} - f^\gamma_{\alpha\beta})$. The structure constant $c^\gamma_{\alpha\beta}$ is clearly antisymmetric with respect to interchange of indices α and β. In the other direction, if the structure constant of this Lie algebra are known, then Equation 5.5.3 allows us to calculate $X_{\alpha\beta}$ and consequently, the representing matrix for any group element near the identity up to a precision of second order by use of Equation 5.5.2.

A more general result is that in fact, all the matrices in the infinite series in the right hand side of Equation 5.5.2 are known from the commutations in Equation 5.5.4. This result will not be proven here. An immediate consequence is that knowledge of X_α and its commutations are sufficient to calculate $\Gamma(g)$ for all g in a finite neighborhood of the identity. For this reason all the constituents of X_α are called the *generators* of the group and the vector space spanned by generators is the Lie algebra $\mathfrak{g}$ associated with the group G. A Lie group whose Lie algebra is real is called a *real Lie group* and similarly for *complex Lie group* corresponds to Lie algebra which is complex. In the following section, we will discuss examples of Lie groups.

5.6 Examples of Lie Groups

Important examples of Lie groups are the *general linear groups* and some of their subgroups. These are Lie groups which can be faithfully represented by matrices of finite size, and so are called *matrix Lie groups*.

The general linear group of degree n is the group of invertible $n \times n$ matrices with the group operation being the usual multiplication of matrices. The general linear group of degree n whose representing matrices have only real entries is denoted by $GL(n,\ \mathfrak{R})$. In the complex case the notation is $GL(n,\ \mathfrak{C})$. The group $GL(n,\ \mathfrak{R})$ is itself a subgroup of $GL(n,\ \mathfrak{C})$. Regarded as Lie groups on their own, there is an important difference between $GL(n,\ \mathfrak{R})$ and $GL(n,\ \mathfrak{C})$. $GL(n,\ \mathfrak{R})$ consists of invertible matrices whose determinants are non vanishing. Therefore these determinants can be either positive valued or negative valued.

For $\mathbf{M_1}$ and $\mathbf{M_2}$ in $GL(n,\ \mathfrak{R})$ such that $\det \mathbf{M_1} > 0$ and $\det \mathbf{M_2} < 0$, there cannot then exist a continuous real parameter smoothly connecting $\mathbf{M_1}$ to $\mathbf{M_2}$. On the otherhand, $GL(n,\ \mathfrak{C})$ does not suffer from this discontinuity as it is always possible to find a path in the complex plane. $GL(n,\ \mathfrak{C})$ is therefore an example of a *connected Lie*

group. $GL(n, \mathfrak{R})$ can be decomposed into two components. One component consists of matrices with positive determinant while the other of matrices with negative determinant. Each component is connected in itself but disconnected from the other. The identity matrix of $GL(n, \mathfrak{R})$ lies in the positive component.

Special linear groups are subgroups of general linear groups. The corresponding notations are $SL(n, \mathfrak{R})$ and $SL(n, \mathfrak{C})$. These groups consist of matrices whose determinants equal unity. As before, $SL(n, \mathfrak{R})$ is a subgroup of $SL(n, \mathfrak{C})$. Both the groups are connected Lie groups.

The *orthogonal group* $O(n)$ is a subgroup of $GL(n, \mathfrak{R})$. The defining condition for a matrix $\mathbf{M} = [m_{ij}]_{n\times n}$ to be in $O(n)$ is that

$$\mathbf{M}^{\mathrm{T}}\mathrm{M} = \mathrm{M}\mathrm{M}^{\mathrm{T}} = \mathrm{I}. \tag{5.6.1}$$

Upon explicitly writing out the product $\mathbf{M}^{\mathrm{T}}\mathbf{M}$, the above condition reduces to $\sum_{i=1}^{n} m_{ij}m_{ik} = \delta_{jk}$. In other words, the columns of any matrix in $O(n)$ are orthonormal. The same can be inferred about the rows. From the defining Equation 5.6.1 it also follows that the determinant of the matrices in $O(n)$ can be either $+1$ or -1. The subgroup of $O(n)$ consisting of matrices whose determinants equal unity is called the *special orthogonal group* $SO(n)$. The group $SO(n)$ essentially consists of transformations that preserve handedness (rotations), while in $O(n)$ there are also improper transformations like reflections which do not preserve handedness.

The *generalized orthogonal group* $O(m, n)$ is another subgroup of $GL(m + n, \mathfrak{R})$. Define $\mathbf{g}$ to be a $(m + n) \times (m + n)$ matrix in which the the first m entries in the principal diagonal are $+1$, the last n entries in the principal diagonal are -1 while all the other entries are 0. A real matrix $\mathbf{M}$ is in $O(m, n)$ if and only if

$$\mathbf{M}^{\mathrm{T}}\mathrm{g}\mathrm{M} = \mathrm{M}\mathrm{g}\mathrm{M}^{\mathrm{T}} = \mathrm{g}. \tag{5.6.2}$$

It is obvious from the above definition that $\det \mathbf{M} = \pm 1$. The subgroup of $O(m, n)$ which contains only matrices of unit determinant is the *generalized special orthogonal group* $SO(m, n)$. In fact, the *Lorentz group* is the group $SO(1,3)$. As this group is the symmetry group of physical systems respecting the laws of special theory of relativity, we will elaborate the representations of Lorentz group in the next chapter.

The *symplectic group* $Sp(2n, \mathfrak{R})$ is another subgroup of $SL(2n, \mathfrak{R})$. The defining equation of a symplectic matrix $M_{2n\times 2n} \in Sp(2n, \mathfrak{R})$ is

$$\mathbf{M}^{\mathrm{T}}\mathrm{J}\mathrm{M} = \mathrm{J},$$

where

$$J = \begin{bmatrix} 0_{n\times n} & I_{n\times n} \\ -I_{n\times n} & 0_{n\times n} \end{bmatrix}.$$

Symplectic groups find applications in the transformation properties of the position and velocity variables describing classical systems. Now turning to $GL(n,\ \mathfrak{C})$, the subgroup consisting of such matrices $\mathbf{M}$ for which

$$\mathbf{M}^{\dagger}\mathbf{M} = \mathbf{M}\mathbf{M}^{\dagger} = \mathbf{I} \tag{5.6.3}$$

is called the *unitary group* $U(n)$. The circle group $U(1)$ was the first example of this type. It is obvious from the above definition that determinants of matrices in $U(n)$ are unimodular complex numbers. The subgroup of $U(n)$ containing matrices whose determinants equal unity is call the *special unitary group* $SU(n)$. The group $SU(2)$ plays an important role in description of particle spin in quantum mechanics. Hence their applications in quantum mechanics and particle physics will be discussed in the following chapter.

We will now discuss the classification of semi-simple Lie algebras known in the literature as *Cartan classification*.

5.7 Compact Simple Lie Algebras

In Section 5.5, we came across the fact that the Lie algebra of a Lie group can reveal the structure of the group in a finite neighborhood of the identity element. Here, we will focus on the broad classification of simple Lie algebras.

The works of Killing and Cartan led to the classification of simple Lie algebras $\mathfrak{g}$ to be of four infinite types and five exceptional types. We will now present the definitions that govern operations followed by the n basis elements of Lie algebra $\mathfrak{g}$ without proofs.

Let ℓ independent elements $\{H_i\} \in \mathfrak{g}$ obey abelian subalgebra:

$$[H_i, H_j] = 0;\ \ i,\ j = 1, \ldots \ell$$

which is known in the literature as *Cartan subalgebra*. The number of commuting elements (ℓ) of the algebra $\mathfrak{g}$ is called the *rank* of the algebra.

The remaining $n - \ell$ elements $E_{\pm\boldsymbol{\alpha}} \in \mathfrak{g}$ are even in number. Note that the subscript $\pm\boldsymbol{\alpha}$ are ℓ-component vectors which are referred to as positive and negative *root vectors* of the algebra. Hence, there will be $n - \ell$ non-zero root vectors associated with the Lie algebra $\mathfrak{g}$. The algebra involving $E_{\pm\boldsymbol{\alpha}}$ will yield

$$[E_{\boldsymbol{\alpha}},\ E_{-\boldsymbol{\alpha}}] = \sum_{i=1}^{\ell} \alpha_i H_i,$$

where α_i refers to the i-th component of the root vector $\boldsymbol{\alpha}$. If $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ are two different root vectors of $\mathfrak{g}$ then

$$[E_{\boldsymbol{\alpha}},\ E_{\boldsymbol{\beta}}] = \mathcal{N}_{\alpha,\beta} E_{\boldsymbol{\alpha}+\boldsymbol{\beta}},$$

where $\mathcal{N}_{\alpha,\beta} = -\mathcal{N}_{\beta,\alpha} \neq 0$ if and only if $\boldsymbol{\alpha} + \boldsymbol{\beta}$ is also a root vector of $\mathfrak{g}$. Further, for complete definition of the algebra $\mathfrak{g}$, we need the following commutator as well:

$$[H_i, E_{\boldsymbol{\alpha}}] = \alpha_i E_{\boldsymbol{\alpha}};\ [H_i, E_{-\boldsymbol{\alpha}}] = -\alpha_i E_{-\boldsymbol{\alpha}}\,.$$

Note that the above commutator bracket resembles ladder operators and J_3 of $\mathfrak{su}(2)$ algebra (5.3.10). As $\mathfrak{su}(2)$ algebra has only one diagonal generator, the rank of the $\mathfrak{su}(2)$ algebra is $\ell = 1$ leading to one-component root vectors (numbers). The comparison of the formal $\mathfrak{g}$ algebra with $\mathfrak{su}(2)$ implies that there are two non-zero roots $\pm\alpha = \pm 1$ and hence the corresponding generators $E_{\pm 1} \equiv J_{\pm}$.

For a general Lie algebra $\mathfrak{g}$, we can construct many $\mathfrak{su}(2)$ subalgebras in the following way:

$$J_{\pm}^{(\boldsymbol{\alpha})} = |\boldsymbol{\alpha}|^{-1} E_{\pm\boldsymbol{\alpha}};\ J_3^{(\boldsymbol{\alpha})} = |\boldsymbol{\alpha}|^{-2}\boldsymbol{\alpha}.\boldsymbol{H}.$$

Similar to the $\mathfrak{su}(2)$ eigenbasis $|jm\rangle$ of J_3 with half integer values m, we have eigenbasis $|\boldsymbol{\Lambda}, \boldsymbol{\mu}\rangle \in V$ of $J_3^{(\boldsymbol{\alpha})}$ where $\boldsymbol{\Lambda}$ is the highest weight vector and $\boldsymbol{\mu}$ denotes ℓ component weight vector with the following properties:

$$J_3^{(\boldsymbol{\alpha})}|\boldsymbol{\Lambda}, \boldsymbol{\mu}\rangle = \frac{\boldsymbol{\alpha}.\boldsymbol{\mu}}{|\boldsymbol{\alpha}|^2}|\boldsymbol{\Lambda}, \boldsymbol{\mu}\rangle\ ;\ J_{\pm}^{(\boldsymbol{\alpha})}|\boldsymbol{\Lambda}, \boldsymbol{\mu}\rangle \propto |\boldsymbol{\Lambda}, \boldsymbol{\mu} \pm \boldsymbol{\alpha}\rangle$$

where the eigenvalues of $J_3^{(\boldsymbol{\alpha})}$ are half integers. Hence,

$$\frac{2\boldsymbol{\alpha}.\boldsymbol{\mu}}{|\boldsymbol{\alpha}|^2} = \text{integer.}$$

This integer can be determined by finding $p,\ q$ such that

$$(J_+^{(\boldsymbol{\alpha})})^{p+1}|\boldsymbol{\Lambda}, \boldsymbol{\mu}\rangle = 0\ ;\ (J_-^{(\boldsymbol{\alpha})})^{q+1}|\boldsymbol{\Lambda}, \boldsymbol{\mu}\rangle = 0, \tag{5.7.1}$$

implying that the eigenvalue of $J_3^{(\boldsymbol{\alpha})}$ is maximum $(+j)$ for state $|\boldsymbol{\Lambda}, \boldsymbol{\mu} + p\boldsymbol{\alpha}\rangle$ and minimum $(-j)$ for state $|\boldsymbol{\Lambda}, \boldsymbol{\mu} - q\boldsymbol{\alpha}\rangle$. That is,

$$\frac{\boldsymbol{\alpha}.(\boldsymbol{\mu} + p\boldsymbol{\alpha})}{|\boldsymbol{\alpha}|^2} = j = -\frac{\boldsymbol{\alpha}.(\boldsymbol{\mu} - q\boldsymbol{\alpha})}{|\boldsymbol{\alpha}|^2},$$

which implies

$$\frac{2\boldsymbol{\alpha}.\boldsymbol{\mu}}{|\boldsymbol{\alpha}|^2} = (q - p). \tag{5.7.2}$$

Comparing with the $\mathfrak{su}(2)$ ladder operations, we can say highest weight state $|\mathbf{\Lambda}, \mathbf{\Lambda}\rangle$ is defined as

$$J_+^{(\boldsymbol{\alpha})}|\mathbf{\Lambda}, \boldsymbol{\mu} = \mathbf{\Lambda}\rangle = 0 \; \forall \; \boldsymbol{\alpha}.$$

Suppose we choose the vector space $V = \mathfrak{g}$ (adjoint representation), then the eigenbasis of the $J_3^{(\boldsymbol{\alpha})}$ can be represented by $\{|H_i\rangle\}$, $\{|E_{\pm\boldsymbol{\beta}}\rangle\}$. In fact, for adjoint representation, the weight vector of states are root vectors. Applying $J_3^{(\boldsymbol{\alpha})}$, $J_3^{(\boldsymbol{\beta})}$ on such states will give the following eigenvalue equations:

$$J_3^{(\boldsymbol{\alpha})}|\mathbf{\Lambda}, E_{+\beta}\rangle = \frac{\boldsymbol{\alpha}.\boldsymbol{\beta}}{|\boldsymbol{\alpha}|^2}|\Lambda, E_{+\beta}\rangle \; ; \; J_3^{(\boldsymbol{\beta})}|\mathbf{\Lambda}, E_{+\boldsymbol{\alpha}}\rangle = \frac{\boldsymbol{\alpha}.\boldsymbol{\beta}}{|\boldsymbol{\beta}|^2}|\mathbf{\Lambda}, E_{+\boldsymbol{\alpha}}\rangle.$$

Using the two equations (Equation 5.7.1 and 5.7.2) for the above states, we can infer:

$$\frac{2\boldsymbol{\alpha}.\boldsymbol{\beta}}{|\boldsymbol{\alpha}|^2} = (q-p), \; \frac{2\boldsymbol{\beta}.\boldsymbol{\alpha}}{|\boldsymbol{\beta}|^2} = (q'-p'),$$

suggesting that the angle between two root vectors must obey:

$$\cos^2\theta_{\boldsymbol{\alpha},\boldsymbol{\beta}} = \frac{(q-p)(q'-p')}{4},$$

where p, q, p', q' are integers. This forces the non-trivial angle between two root vectors to assume values of $90^0, 60^0$ or $120^0, 45^0$ or $135^0, 30^0$ or 150^0.

If the rank of the Lie algebra $\mathfrak{g}$ is ℓ, then there are ℓ *simple roots*. The remaining positive and negative roots can be obtained from linear combination of the simple roots.There is a neat concise way of classifying simple Lie algebras $\mathfrak{g}$ using connected graphs called Dynkin diagrams. Suppose we denote the ℓ simple root vectors by ℓ filled circles. We connect these ℓ filled circles by single bond or double bond or triple bond depending on the angle between any two simple roots $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$. In fact,

$$4\cos^2\theta_{\boldsymbol{\alpha},\boldsymbol{\beta}} = m,$$

where m is the number of bonds connecting the simple roots $\boldsymbol{\alpha}$, $\boldsymbol{\beta}$. For instance, the Lie algebra $A_\ell \equiv su(\ell+1)$ has ℓ simple roots of equal length $(\boldsymbol{\alpha}^{(1)}, \boldsymbol{\alpha}^{(2)}, \ldots \boldsymbol{\alpha}^{(\ell)})$ and has a single bond connecting adjacent simple roots as shown in Figure 5.7.1. That is,

$$4\cos^2\theta_{\boldsymbol{\alpha}^{(i)},\boldsymbol{\alpha}^{(i\pm1)}} = 1.$$

Besides the A_ℓ infinite series Dynkin diagram depicting unitary algebras $\mathfrak{su}(\ell+1)$ of arbitrary ranks, we have other connected graphs corresponding to orthogonal algebras $so(n)$ which belong to infinite series Dynkin diagrams $B_{\ell\geq3}$ for $n = 2\ell+1$

and $D_{\ell\geq 4}$ for $n = 2\ell$ as shown in Figure 5.7.1. Note that the last two simple roots in B_ℓ are connected by double bond and the orientation of the arrow indicates that the length of the root vectors obey $|\alpha^{(i)}| > |\alpha^{(\ell)}|$ for all $i < \ell$. The Dynkin diagram of the symplectic algebra $C_{\ell\geq 2} \equiv sp(2\ell)$ has a reversed orientation implying $|\alpha^{(i)}| < |\alpha^{(\ell)}|$ for all $i < \ell$. Besides these connected graphs of arbitrary ranks (see Figure 5.7.1(a)), we can have finite rank Dynkin diagrams which are known in the literature as five exceptional Lie algebras (as shown in Figure 5.7.1(b)). Basically, these four infinite series and five exceptional series are the only allowed connected graphs for linearly independent simple roots which can represent simple Lie algebras $\mathfrak{g}$.

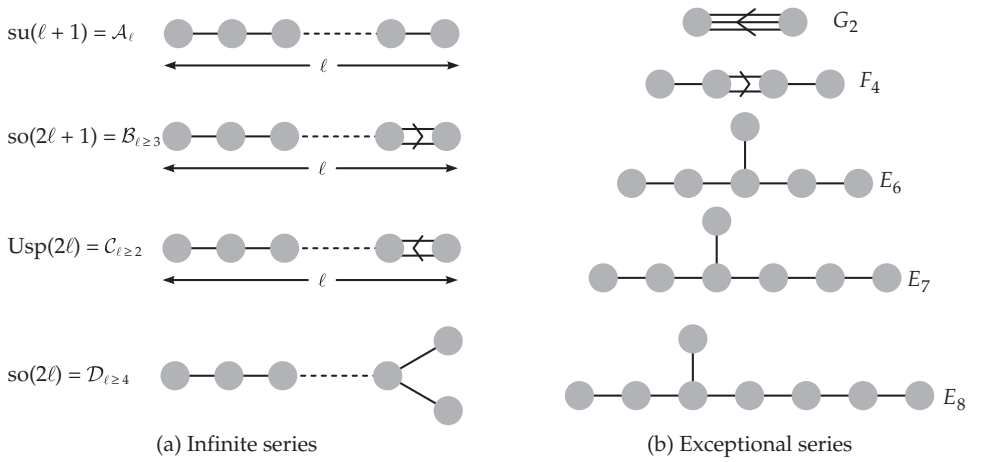


Figure 5.7.1 Dynkin Diagrams

With the formal definition of simple Lie algebras where we introduced root and weight vectors, we will now extensively discuss $A_{\ell=2} \equiv \mathfrak{su}(3)$ algebra.

5.7.1 $\mathfrak{su}(3)$ algebra

Just like the 2×2 σ matrices are the fundamental representation of $\mathfrak{su}(2)$ acting on a two-dimensional complex vector space V, we have 3×3 Gell-Mann matrices $\{\lambda_a\}$'s which are referred to as the defining representation of $\mathfrak{su}(3)$ acting on three-dimensional complex vector space V. These Gell-Mann matrices are Hermitian and traceless. Hence, there will be 8 λ_a's denoting the basis elements of $\mathfrak{su}(3)$ algebra because hermiticity and traceless conditions reduce the nine complex entries of these 3×3 matrices to eight independent real entries. The explicit form of the Gell-Mann matrices are

$$\lambda_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \lambda_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\lambda_4 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix},\ \lambda_5 = \begin{pmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{pmatrix},\ \lambda_6 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix},\ \lambda_8 = \frac{1}{\sqrt{3}} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{pmatrix}.$$

Note that there are two diagonal matrices $\lambda_3,\ \lambda_8$ which constitute the Cartan subalgebra of rank $\ell = 2$. Hence the three basis states

$$|\mathbf{\Lambda}\boldsymbol{\mu}_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix},\ |\mathbf{\Lambda}\boldsymbol{\mu}_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},\ |\mathbf{\Lambda}\boldsymbol{\mu}_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}.$$

of the fundamental three-dimensional complex vector space V are simultaneous eigenstates of both $H_1 = \lambda_3/2$ and $H_2 = \lambda_8/2$. We have indicated both the eigenvalues in the two-dimensional $H_1 - H_2$ diagram (Figure 5.7.2) for the three basis states. Hence, we can equivalently represent the basis state as two-component weight vectors:

$$|\mathbf{\Lambda}\boldsymbol{\mu}_1\rangle \equiv (1/2,\ \sqrt{3}/6); |\mathbf{\Lambda}\boldsymbol{\mu}_2\rangle \equiv (-1/2,\ \sqrt{3}/6); |\mathbf{\Lambda}\boldsymbol{\mu}_3\rangle \equiv (0,\ -\sqrt{3}/3).$$

The weight vectors are called negative weight vectors if the first non-zero component is negative. In the above set of weight vectors, $\boldsymbol{\mu}_1$ is positive weight vector whereas $\boldsymbol{\mu}_2, \boldsymbol{\mu}_3$ are negative weight vectors.

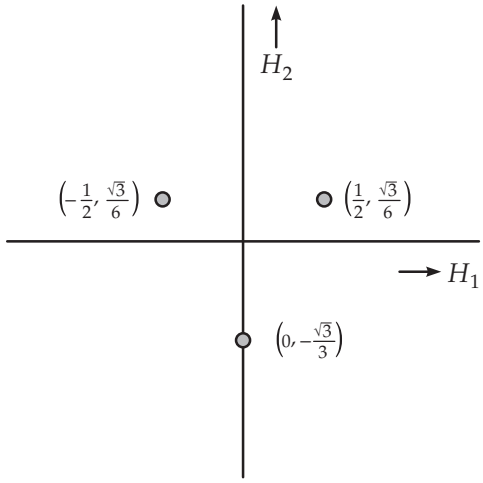


Figure 5.7.2 $\mathfrak{su}(3)$ Weight Diagram for Defining Representation

The raising and lowering operators will take one basis state to another basis state. The explicit form of such operators will involve the remaining six Gell-Mann matrices in the following way:

$$E_{\pm\boldsymbol{\alpha}^{(3)}} = \frac{1}{2\sqrt{2}}(\lambda_1 \pm i\lambda_2)\ ;\ E_{\pm\boldsymbol{\alpha}^{(1)}} = \frac{1}{2\sqrt{2}}(\lambda_4 \pm i\lambda_5);$$

$$E_{\mp\boldsymbol{\alpha}^{(2)}} = \frac{1}{2\sqrt{2}}(\lambda_6 \pm i\lambda_7),$$

where

$$E_{-\boldsymbol{\alpha}^{(3)}}|\boldsymbol{\Lambda}, \boldsymbol{\mu}_1\rangle \propto |\boldsymbol{\Lambda}, \boldsymbol{\mu}_1 - \boldsymbol{\alpha}^{(3)}\rangle = |\boldsymbol{\Lambda}, \boldsymbol{\mu}_2\rangle\ ;\ E_{+\boldsymbol{\alpha}^{(i)}}|\boldsymbol{\Lambda}, \boldsymbol{\mu}_1\rangle = |\boldsymbol{\Lambda}, \boldsymbol{\mu}_1 + \boldsymbol{\alpha}^{(i)}\rangle = 0\,\forall\, i, \quad (5.7.3)$$

implying that the weight vector $|\boldsymbol{\Lambda}, \boldsymbol{\mu}_1\rangle$ is the *highest weight state* (that is., $\boldsymbol{\Lambda} = \boldsymbol{\mu}_1$ and the root vector

$$\boldsymbol{\alpha}^{(3)} = \boldsymbol{\mu}_1 - \boldsymbol{\mu}_2 = (1, 0).$$

In the similar fashion, you can check that

$$\boldsymbol{\alpha}^{(1)} = \boldsymbol{\mu}_1 - \boldsymbol{\mu}_3 = (1/2,\ \sqrt{3}/2),\ \boldsymbol{\alpha}^{(2)} = \boldsymbol{\mu}_3 - \boldsymbol{\mu}_2 = (1/2,\ -\sqrt{3}/2). \quad (5.7.4)$$

Note that $\boldsymbol{\alpha}^{(3)} = (1, 0) = \boldsymbol{\alpha}^{(1)} + \boldsymbol{\alpha}^{(2)}$ indicating that the two simple roots of the $\mathfrak{su}(3) \equiv A_2$ algebra are $\boldsymbol{\alpha}^{(1)}$, $\boldsymbol{\alpha}^{(2)}$ whereas $\boldsymbol{\alpha}^{(3)}$ is not a simple root vector. These non-zero root vectors can be plotted in the $H_1 - H_2$ graph (see Figure 5.7.3 where the right side of the graph has positive roots and left side of the graph has negative roots) which are the non-zero weight vector states of the adjoint representation which also represent the raising and lowering operators of $\mathfrak{su}(3)$ algebra. The origin of the graph are the null root vectors denoting the Cartan subalgebra operators H_1, H_2.

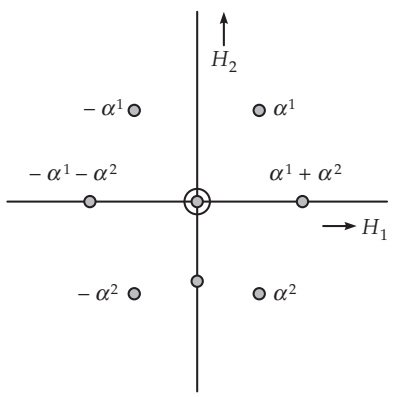


Figure 5.7.3 $\mathfrak{su}(3)$ Root Diagram

5.7.2 Cartan matrix

For a Lie algebra of rank ℓ, there will be ℓ simple roots. One can construct the Cartan matrix

$$A_{ij} = \frac{2\boldsymbol{\alpha}^{(i)}.\boldsymbol{\alpha}^{(j)}}{|\boldsymbol{\alpha}^{(i)}|^2}$$

from the Dynkin diagram. For $A_2 \equiv su(3)$, the Cartan matrix elements using the simple root vectors (5.7.4):

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

5.7.3 Fundamental weights

We will have ℓ fundamental highest weight vectors $\mu^{(i)}$'s such that

$$\frac{2\boldsymbol{\alpha}^{(i)}.\boldsymbol{\mu}^{(j)}}{|\boldsymbol{\alpha}^{(i)}|^2} = \delta_{ij}. \tag{5.7.5}$$

Example 48. For su(3) algebra, determine the two fundamental highest weight vectors.

Let us take the 2-component fundamental highest weight vector as $(u,\ v)$, Using the orthogonality property (5.7.5) with simple roots (5.7.4), we get $u = \pm\sqrt{3}v$. The normalized form of the two fundamental highest weight vectors are

$$\boldsymbol{\mu}^{(1)} = (1/2,\ \sqrt{3}/6)\ ;\ \boldsymbol{\mu}^{(2)} = (1/2,\ -\sqrt{3}/6). \qquad \square$$

Recall $\boldsymbol{\mu}^{(1)}$ (5.7.3) is the highest weight vector of the defining representation which we discussed using Gell-Mann matrices. For arbitrary representation of su(3), the highest weight vector will be

$$\boldsymbol{\Lambda} \equiv \boldsymbol{\mu} = a\boldsymbol{\mu}^{(1)} + b\boldsymbol{\mu}^{(2)}$$

where $a,\ b$ are positive integers. For example, the highest weight vector of the adjoint representation is $\boldsymbol{\alpha}^{(1)} + \boldsymbol{\alpha}^{(2)} = \boldsymbol{\mu}^{(1)} + \boldsymbol{\mu}^{(2)} = (1, 0)$.

Armed with the formal aspects of Lie groups and Lie algebras discussed in this chapter, we will focus on their applications in the following chapter. Also, the tensor product of irreducible representations of su(2) and su(3) algebra will be discussed in detail.

Exercises

1. We have discussed that the group $U(2)$ has four independent parameters. Suppose we impose that the determinant of these unitary matrices to be $+1$, then we call the group as $SU(2)$. What will be the number of independent parameters for $SU(2)$ group.
2. Determine the number of independent parameters (equal to number of generators) for a general $U(N)$ group and $SU(N)$ group.
3. For a Lie algebra $\mathfrak{g}$ in which the structure constants are c_{st}^{k} as in Equation 5.3.1, show that

$$\sum_{k=1}^{n}[c_{sk}^{l}c_{tu}^{k}+c_{tk}^{l}c_{us}^{k}+c_{uk}^{l}c_{st}^{k}]=0$$

   [*Hint*: Jacobi identity]
4. Let $\mathfrak{g}$ be a semi-simple Lie algebra and $\mathfrak{h}$ an invariant subalgebra in $\mathfrak{g}$. Show that $(\mathfrak{h}^{\perp})^{\perp}=\mathfrak{h}$.
5. For vectors x and y in $\mathfrak{R}^{n}$, define the product of x and y as

$$x.y=\sum_{i=1}^{n}x_{i}y_{i}.$$

   Show that under a transformation $\mathbf{M}$ in $O(n)$, the value of the product is invariant, i.e.,

$$x.y{=}Mx.My.$$

6. For vectors x and y in $\mathfrak{R}^{m+n}$, define the product of x and y as

$$\mathrm{x.y}\ =\sum_{i=1}^{m}x_{i}y_{i}-\sum_{j=1}^{n}x_{m+j}y_{m+j}.$$

   Show that under a transformation $\mathbf{M}$ in $O(m,\ n)$, the value of the product is invariant.
7. For vectors x and y in an n-dimensional complex vector space, define the product of x and y as

$$xy=\sum_{i=1}^{n}\overline{x_{i}}y_{i}$$

   where $\overline{x_{i}}$ represents the complex conjugate of x_{i}. Show that under the transformations in $U(n)$, the value of the product is invariant.
8. Given a Lie algebra $\mathfrak{g}$ having two simple roots

$$\boldsymbol{\alpha}^{(1)}=(0,1),\ \boldsymbol{\alpha}^{(2)}=(\sqrt{3}/2,\ -3/2),$$

   work out the Cartan matrix and the corresponding Dynkin diagram. Also determine their fundamental highest weight vectors.

6

Further Applications

With the formal aspects of Lie algebra and Lie groups discussed in the previous chapter, it is now possible to apply the power of continuous symmetry to physics of many simple and complex systems. This chapter will focus upon the applications of Lie algebra and groups to physical systems possessing orthogonal group or unitary group symmetry. For completeness, note that the symplectic group $sp(2n)$ is nothing but the canonical transformation of $2n$ phase space variables (position and velocity variables). Readers are advised to look up canonical transformations in any classical mechanics textbooks such as Goldstein for further appreciation of the natural emergence of symplectic group symmetry in classical systems.

Many classical systems in three-dimensional space respect spherical symmetry. Such systems remain unchanged under proper rotations. Noether's theorem states that 'associated with any continuous group symmetry, there is always a constant of motion'. In Section 6.1, we will briefly discuss classical systems possessing translational symmetry and show that the constant of motion is linear momentum $\mathbf{p}$.

We have extensively discussed, in the previous chapter, the rotation group $SO(3)$ and its Lie algebra $\mathfrak{so}(3)$ whose generators are the three components of orbital angular momentum $\mathbf{L}$. Thus the generators of the group are nothing but constants of motion in the classical system respecting rotational symmetry. The rotational invariance of quantum mechanical systems leads to a natural emergence of group $SU(2)$ extensively presented in the previous chapter. Particularly, the Lie algebra generators are the components of the total angular momentum operator $\hat{\mathbf{J}} = \hat{\mathbf{L}} + \hat{\mathbf{S}}$ incorporating the intrinsic spin $\hat{\mathbf{S}}$ in accordance with the famous Stern–Gerlach experiment. Any basic course on the quantum mechanics of rotational invariant systems is based on the theory of angular momentum algebra which is isomorphic to $\mathfrak{su}(2)$.

In the previous chapter, we have discussed the actions of Lie algebra generators $E_{\pm\boldsymbol{\alpha}}$, associated with a root vector $\boldsymbol{\alpha}$, on the highest weight vector $\boldsymbol{\Lambda}$ leading to weight vectors $\boldsymbol{\Lambda} \pm \boldsymbol{\alpha}$. Through $\mathfrak{su}(2)$ as an example (Chapter 5, Section 5.3.1), we showed that angular momentum corresponds to the highest weights in the Lie group context and the the range of z–components of angular momentum are the weights. In Section 6.2, we will construct the tensor product of two or more angular momentum states using the Young tableau approach. In quantum mechanics literature, they are known as *addition of angular momentum*. In Subsection 6.2.1, we have a small digression on Young Tableau approach for both symmetry group of degree n and $SU(N)$ group. Then, we will discuss *selection rules* for the quantum mechanical transition from initial state to final state due to interactions. The important theorem known as *Wigner–Eckart theorem* will be dealt with proof. Through examples, readers will come to appreciate the power and elegance of $SU(2)$ group theory tools in validating experimentally observed allowed and forbidden transitions in quantum systems possessing rotational symmetry. We also remind the readers to compare the selection rules due to discrete symmetry discussed in Chapter 4 to the Wigner–Eckart theorem rules discussed here.

This theorem is applicable to many other systems possesing $SU(2)$ symmetry. For instance, theoretical validation of (i) almost same mass $\mathrm{m_p} \approx \mathrm{m_n}$ of proton and neutron (ii) experimentally observed strong interaction processes (scattering and decay) involving such elementary particles (broadly classified as *baryons* and *mesons*) are deduced invoking $SU(2)$ Lie group symmetry. For baryons and mesons, $SU(2)$ represents rotational symmetry in an abstract internal space called *isospin* space whose algebra is same as $\mathfrak{su}(2)$. We discuss these features in elementary particle physics in Section 6.3.

Interestingly, these elementary particles with same angular momentum $\mathbf{J}$ but with different isospin $\mathbf{I}$ and charge Q can be plotted on a two-dimensional diagram which appears identical to the $\mathfrak{su}(3)$ weight diagrams discussed in the previous chapter. Historically, Gell-Mann introduced a simple model called the *quark model* to theoretically predict the baryons and mesons observed in the laboratory. According to the quark model, particles like protons, neutrons and other baryons must be composed of three quarks. Assuming that there are three flavors of quarks: u, d, s (up, down and strange), Gell-Mann applied the unitary group $SU(3)$ and tensor product of quarks to account for baryons observed in experiments. Interestingly, he predicted that the $SU(3)$ symmetry requires the presence of a baryon Ω^- which was detected experimentally three years later. This is one of the instances where an abstract theory was validated by the experiment after some years. We discuss the quark model in Section 6.4. Similar to the symmetry breaking discussed in the discrete group context, we will briefly present symmetry breaking in the context of continuous groups. The $SU(3)$ quark model can be generalized to $SU(N)$ assuming quarks come in N flavors using Young diagrams and their tensor product discussed in Subsection 6.2.1.

Besides compact groups, there exist non-compact groups whose Lie algebra can be systematically deduced. In Section 6.5, we will elaborate on one such group called Lorentz group : $SO(3,1)$. One of the reasons for focussing on this Lorentz group is because it is the symmetry possessed by relativistic particles in the $3+1$ dimensional

Minkowski space-time. We will briefly discuss Poincare algebra and Poincare groups which serve as a underlying symmetry of many physical systems. Many systems near criticality (near phase transition point) are invariant under scale transformation. The group symmetry possessed by such systems are known as *conformal groups*. We will give an overview of the conformal group symmetry and their generators. Finally, the readers can see through the exercise problem, the resemblence between the Lorentz algebra $\mathfrak{so}(3,1)$ and $\mathfrak{so}(4)$ associated with rotations in four-dimensional space.

Even though four-dimensional space is not physical, we will show in Section 6.6 that the abstract group $SO(4)$ has an elegant way of reproducing familiar hydrogen atom energy levels without solving the Schrödinger equation. Besides angular momentum $\mathbf{L}$, the hydrogen atom has another constant of motion called Runge–Lenz vector $\mathbf{M}$. The abstract group $SO(4)$ generators and their algebra turns out to be isomorphic to the algebra involving $\mathbf{L}$ and $\mathbf{M}$. Unlike angular momentum $\mathbf{L}$ which can be attributed to geometrical transformation of rotations, $\mathbf{M}$ has no such geometrical interpretation. Such a symmetry which has no geometrical interpretation is known as *dynamical symmetry*.

6.1 Continuous Symmetry and Constant of Motion

We will focus on the familiar translation symmetry to formally understand the corresponding constant of motion (Noether theorem). Further, we will also examine representations of these translation group elements and deduce the generators of such transformation. This detailed description will show that the constants of motion act as generators of the corresponding group transformation.

6.1.1 Translational symmetry in three-dimensional space

At the start, we will take the simplest symmetry of a system under the space translation operation. Consider a free particle moving in our three-dimensional space. The classical Hamiltonian $H = p^2/(2m)$ is unchanged under translation $\mathbf{x} \to \mathbf{x} + \boldsymbol{a}$ for any constant shift vector $\mathbf{a}$. For such a translationally invariant classical system, it is easy to show that the Hamilton's equation of motion involving Poisson bracket $\{,\}$ (see *Classical Mechanics* by Goldstein) is

$$\frac{d\mathbf{p}}{dt} = \{H,\ \mathbf{p}\} = 0,$$

which implies linear momentum $\mathbf{p}$ is a constant of motion for translationally invariant systems.

In quantum mechanics, the free particle wavefunction $\psi(\mathbf{x})$ under translation operation $\hat{\mathbf{T}}(\mathbf{a})$ transforms as follows:

$$\hat{\mathbf{T}}(\mathbf{a})\psi(\mathbf{x}) = \psi'(\mathbf{x}),$$

where wavefunctions obey $\psi(\mathbf{x}) = \psi'(\mathbf{x}+\mathbf{a})$ for translation invariant systems. This implies $\psi'(\mathbf{x}) = \psi(\mathbf{x}-\mathbf{a})$. Substituting this functional form in the above equation and writing as a Taylor series expansion, we can deduce the form of the operator from

$$\hat{\mathrm{T}}(\mathbf{a})\psi(\mathbf{x}) = \exp(-\mathbf{a}.\nabla)\psi(\mathbf{x}).$$

The differential operator is related to the well-known momentum operator, $\hat{\mathbf{p}} = -\mathrm{i}\hbar\nabla$, leading to the explicit form of the translation operator as

$$\hat{\mathrm{T}}(\mathbf{a}) = \exp\left(\frac{-i\mathbf{a}.\hat{\mathbf{p}}}{\hbar}\right).$$

For an infinitesimal translation (**a** small), for the above operator the expansion up to $\mathcal{O}(\mathrm{a})$ will be

$$\hat{\mathbf{T}}(\mathrm{a}) \approx \mathbb{I} - i\mathbf{a}.\hat{\mathbf{p}}/\hbar + \mathcal{O}(\mathrm{a}^2).$$

In fact, as discussed in the previous chapter on Lie groups, the deviation from identity $\mathbb{I}$ operator generates the infinitesimal translation operation. Thus for spatial translations, linear momentum $\hat{\mathbf{p}}$ is the generator and $\mathbf{a} \in \mathbb{R}^3$ is the parameter in three-dimensional space. We have explicitly shown that the constant of motion is indeed the linear momentum generating translational symmetry. This methodology can be applied to time translations as well where the generator turns out to be the Hamiltonian H and the corresponding time translation parameter $\tau \in \mathbb{R}$ belongs to a real line. We have already seen rotational symmetry groups $SO(3)$ and their Lie algebra $\mathfrak{so}(3)$ whose generators are the orbital angular momentum **L** in the three-dimensional space. For completeness, rotational symmetry and corresponding constant of motion is presented through the following example.

Example 49. For a rotationally invariant system described by the Hamiltonian

$$H = \frac{p^2}{2m} + \frac{k}{r^2},$$

where r is the radial coordinate and constant k is a dimensionful constant. Show that $d\mathbf{L}/\mathrm{dt} = 0$, confirming that the generators **L** are constants of motion of such rotational invariant systems.

The Poisson bracket

$$\{H,\ \mathrm{L_i}\} = \sum_j \frac{\partial H}{\partial x_j}\frac{\partial L_i}{\partial p_j} - \frac{\partial H}{\partial p_j}\frac{\partial L_i}{\partial x_j} = \sum_{j,l} \in_{ilj} \left(\frac{k}{r^3}x_j x_l - \frac{1}{m}p_j p_l\right) = 0.$$

Hence the Poisson equation of motion for $d\mathbf{L}/\mathrm{dt}$ is zero indicating that the angular momentum is a constant of motion for rotational invariant systems. □

In the context of discrete groups, the tensor product of two or more polar vectors and their decomposition as binary basis, tertiary basis and so on, were dealt with using character tables and projection operators. Interestingly, there is an equivalent systematic procedure to deal with the tensor product of vectors and higher rank tensors, leading to irreducible tensors of $SO(3)$. As the algebra $\mathfrak{so}(3)$ is same as $\mathfrak{su}(2)$ algebra, the construction of a tensor product in the $SU(2)$ context turns out to be applicable to $SO(3)$ as well. Hence in the following section, we will elaborate on this tensor product aspect using the irreducible angular momentum states $|j,\, m\rangle \in V^j$ (vector space whose dimension is $d_j = 2j+1$ as $m \in [-j, -j+1, \ldots j]$) and the action of $\mathfrak{su}(2)$ generators $J_\pm, J_z$ discussed in the previous chapter. This is the main core of the addition of angular momentum and the construction of irreducible states in quantum mechanics.

6.2 Tensor Product Rule for $SU(2)$ Irreducible Representations

Let us take the tensor product of two vector spaces $V^{j_1} \otimes V^{j_2}$ whose decomposition into irreducible components can be formally written as

$$V^{j_1} \otimes V^{j_2} = \sum_j N^j_{j_1,j_2} V^j, \tag{6.2.1}$$

where it can be shown that $N^j_{j_1,j_2} = 1$ when $|j_1 - j_2| \leq j \leq j_1 + j_2$ and $N^j_{j_1,j_2} = 0$ for the other j's. Basically, the proof for the allowed range of j and minimum value of $j = j_{\min}$ is based on taking maximum $j = j_{\max} = j_1 + j_2$ and constraining the dimension of the vector space to obey

$$d_{j_1}.d_{j_2} = \sum_{j=j_{\min}}^{j_{\max}} N^j_{j_1,j_2} d_j.$$

There is an equivalent elegant Young tableau approach of obtaining such a tensor product decomposition. We present this diagrammatic method where we can directly determine d_j as well as visualize decomposition.

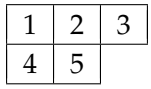
6.2.1 Digression on the Young tableau approach

Symmetric Group $\mathfrak{S}(n)$

Recall the definition of the Young tableau diagram which we reviewed in the context of cycle structure of the elements of the symmetric group $\mathfrak{S}(n)$. We can also use the set of integers $\lambda_1 \geq \lambda_2 \ldots$, associated with a Young diagram Y to denote an irreducible representation of $\mathfrak{S}(n)$. Here λ_1 denotes the number of boxes in first row, λ_2 being the number of boxes in second row and so on such that $\sum_i \lambda_i = n$. Note that n entries

in these boxes must be distinct for a permutation group. The diagram implies totally symmetric property along any row and totally antisymmetric along any column.

For instance, an irreducible representation $Y \in \mathfrak{S}(5)$ denoted by

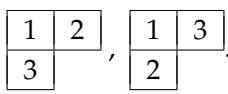


with integer entries inside the boxes indicating that first row boxes are totally symmetric under exchange. Similarly, the boxes on the second row are also totally symmetric. The exchanges of boxes within the first column as well as exchange of boxes within the second column are each totally antisymmetric. Note that there is no symmetry between boxes numbered 3 and boxes numbered 5 belonging to a different row and a different column.

The dimension d_Y of the irreducible representation Y can be determined by counting the possible options of putting integer entries on the boxes such that they are increasing along their row or their column. Such a prescription incorporates the symmetric or antisymmetric or no-symmetry nature of the given Young diagram Y. The following example will illustrate the prescription giving dimension d_Y.

Example 50. Determine the dimensions of the irreducible representation $Y \in \mathfrak{S}(3)$ whose Young tableau is

We can place integers in the boxes following the above mentioned prescription



Thus there are only two possibilities indicating that the dimension $d_Y = 2$.

This procedure can be done for any $Y \in \mathfrak{S}(n)$ but the method may become tedious for large n. There is an alternative formula giving the dimensions d_Y:

$$d_Y = n! / \prod_{i \in Y} h_i, \tag{6.2.2}$$

where h_i denotes the hook length of a box i in the Young diagram Y. Basically, h_i counts the number of boxes to the right of the box i along the same row plus the number of boxes below the box i along the column plus one (for the box i).

In the above example, the three hook lengths associated with the three boxes of Y will be $h_1 = 3$, $h_2 = 1$, $h_3 = 1$ resulting in $d_Y = 3!/(3 \times 1 \times 1) = 2$ in agreement with Example 50.

The irreducible representations Y of $\mathfrak{S}(n)$ has a close resemblance to the irreducible representation of $SU(n)$ but there are also differences. This naturally leads us to discuss $SU(N)$ group derived from the Young diagram approach.

$SU(N)$ Young tableau

We will now briefly review the Young diagrams Y depicting irreducible $SU(N)$ representations. Here N denotes the number of possible states which we can place in every box of Y. Remember that the entry in each box of a Young diagram can be any of the N values (with or without repetition) such that the properties of symmetric nature along the horizontal direction and antisymmetric nature along the vertical direction are maintained.

Suppose we try to place these states in a vertical column of N boxes, we have only one possibility as the states along a column must be antisymmetric. Hence, one or more vertical columns of N boxes denote a singlet or trivial representation. Unlike the $\sum_i \lambda_i = n$ constraint in the Young diagram Y of the permutation group $\mathfrak{S}(n)$, there is no such restriction on the total number of boxes of Y denoting non-trivial irreducible representation of $SU(N)$. However, the number of rows must not exceed $N-1$ for non-trivial irreducible representation. The dimension d_Y for any $SU(N)$ Young diagram can be determined through combinatorial consideration of symmetric, antisymmetric and mixed symmetry properties of N variables.

Example 51. Obtain the dimension of the irreducible representation $Y \in SU(3)$ whose Young diagram is $\begin{array}{|c|c|}\hline & \\ \hline \\ \cline{1-1} \end{array}$

The $SU(N=3)$ rule here is to put three states u, d, s in the boxes such that repetition along the row is allowed but forbidden along the column. Hence the possible states are

$$\begin{array}{|c|c|}\hline u & u \\ \hline d \\ \cline{1-1} \end{array}\ ,\ \begin{array}{|c|c|}\hline u & u \\ \hline s \\ \cline{1-1} \end{array}\ ,\ \begin{array}{|c|c|}\hline d & d \\ \hline u \\ \cline{1-1} \end{array}\ ,\ \begin{array}{|c|c|}\hline d & d \\ \hline s \\ \cline{1-1} \end{array}\ ,\ \begin{array}{|c|c|}\hline s & s \\ \hline u \\ \cline{1-1} \end{array}\ ,\ \begin{array}{|c|c|}\hline s & s \\ \hline d \\ \cline{1-1} \end{array}\ ,\ \begin{array}{|c|c|}\hline u & d \\ \hline s \\ \cline{1-1} \end{array}\ ,\ \begin{array}{|c|c|}\hline u & s \\ \hline d \\ \cline{1-1} \end{array}$$

giving dimension $d_Y = 8$.

Alternatively, there is a formula involving hook number

$$d_Y = Nr_Y / \prod_{i \in Y} h_i, \tag{6.2.3}$$

where the numerator Nr_Y is calculated as follows: place N, $N+1$, along the boxes in the first row and decreasing those integers in steps of one along the vertical columns. Then Nr_Y is the product of all the integers in the boxes of Y.

The integer entries for the above example will be $\begin{array}{|c|c|}\hline 3 & 4 \\ \hline 2 \\ \cline{1-1} \end{array}$, giving $Nr_Y = 3 \times 4 \times 2 = 24$ and its hook length as discussed in Example 50 is 3. Hence, we get dimension $d_Y = 24/3 = 8$ which is in agreement with that obtained in Example 51.

Example 52. Deduce the Young diagram $Y \in SU(2)$ corresponding to the irreducible representation V^j whose dimension is $2j+1$.

Recall that the non-trivial irreducible representation of $SU(2)$ can be shown by a single row Young diagram $\begin{array}{|c|c|c|c|c|c|}\hline a_1 & a_2 & . & . & . & a_m \\ \hline \end{array}$ where a_i's can be either u

or d. Note that diagrams with one or more columns of two boxes $\begin{array}{|c|}\hline a_1 \\ \hline b_1 \\ \hline \end{array}$ are trivial one-dimensional representations because if a_1 is chosen as u then b_1 is necessarily d. Hence, for an irreducible representation $Y = \begin{array}{|c|c|c|c|c|c|}\hline a_1 & a_2 & . & . & . & a_m \\ \hline \end{array}$ of $SU(2)$, the dimension can be calculated using formula (6.2.3). Placing integers $N = 2$ in the first box and increasing them one by one along the row, we can determine the dimension to be

$$d_Y = Nr_Y / \prod_{i \in Y} h_i = (2 \times 3 \times \ldots m+1)/(m)! = m+1.$$

This implies that the irreducible representation V^j, corresponding to angular momentum j, whose dimension is $2j+1$ can be presented as the following Young tableau: $\begin{array}{|c|c|c|c|c|c|}\hline a_1 & a_2 & . & . & . & a_{2j} \\ \hline \end{array}$. □

This has been a quick overview of Young tableau presentation of irreducible representation of $SU(N)$. We can now understand the diagrammatic construction of tensor product $Y_1 \otimes Y_2$ of two irreducible representations and their decomposition $\oplus Y$.

Highest weight associated with $SU(N)$ Young diagrams

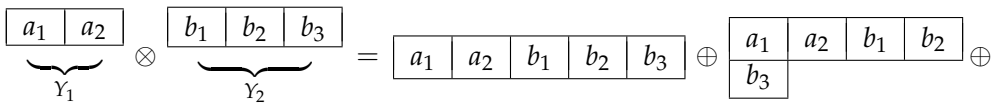
In the previous chapter, we deduced the two $SU(3)$ fundamental weight vectors from the two simple root vectors. The fundamental weight vector $\boldsymbol{\mu}^{(1)}$ is the highest weight state
of representation $\begin{array}{|c|}\hline \\ \hline \end{array}$ and the fundamental weight $\boldsymbol{\mu}^{(2)}$ vector is the highest weight state of representation $\begin{array}{|c|}\hline \\ \hline \\ \hline \end{array}$. Any arbitrary representation of $SU(3)$ will have a_1 single boxes and a_2 double vertical boxes. For example, the Young diagram $\begin{array}{|c|c|c|c|c|c|c|}\hline \\ \hline \\ \hline \end{array}\!\!\begin{array}{|c|c|}\hline \\ \hline \end{array}$ has $a_1 = 5$ and $a_2 = 2$. The highest weight vector of such a $SU(3)$ representation will be $\boldsymbol{\Lambda} = a_1\boldsymbol{\mu}^{(1)} + a_2\boldsymbol{\mu}^{(2)}$. The Young diagram can be equivalently denoted as (a_1, a_2).

This procedure can be generalized to $SU(N)$ group as follows: there will be $N-1$ component fundamental weight vectors $\boldsymbol{\mu}^{(i)}$'s where $i = 1, 2, \ldots N-1$ whose corresponding Young diagrams will be $\begin{array}{|c|}\hline \\ \hline \end{array}$, $\begin{array}{|c|}\hline \\ \hline \\ \hline \end{array}$, $\begin{array}{|c|}\hline \\ \hline \\ \hline \\ \hline \end{array}$, ... respectively. Further arbitrary $SU(N)$ representation can be written as $(a_1, a_2, \ldots, a_{N-1})$ whose equivalent Young diagram will have a_1 single boxes, a_2 double vertical boxes and so on, and the corresponding highest weight will be

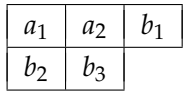
$$\boldsymbol{\Lambda} = a_1\boldsymbol{\mu}^{(1)} + a_2\boldsymbol{\mu}^{(2)} \ldots + a_{N-1}\boldsymbol{\mu}^{(N-1)}.$$

Diagrammatic understanding of tensor product

Let us explain this aspect through the following simple example:



(6.2.4)



where we have placed a_i's in the boxes of Y_1 and b_i's in the boxes of Y_2. This will keep track of decomposition possibilities $\oplus_\alpha Y_\alpha$ as depicted above on the right hand side. Note that the symmetric nature amongst boxes with entries a_i's and amongst boxes with entries b_i's are maintained in the irreducible representations Y. Also observe that the boxes with entries a_i can be symmetric or antisymmetric with respect to boxes with entries b_i in the irreducible representations Y.

Example 53. Work out the dimensions for the above Young diagrams $Y_1, Y_2, Y \in SU(4)$ and verify

$$d_{Y_1} d_{Y_2} = \sum_{Y \in Y_1 \times Y_2} d_Y.$$

The dimensions of representations of $SU(4)$(6.2.3):

d 4 5 $= (4 \times 5)/(1 \times 2) = 10,$

d 4 5 6 $= (4 \times 5 \times 6)/(1 \times 2 \times 3) = 20.$

Hence LHS: $d_{Y_1} d_{Y_2} = 200$. In the similar fashion, we can work out

d 4 5 6 7 8 $= 56,$

d 4 5 6 7 / 3 $= (3 \times 4 \ldots 7)/(1 \times 5 \times 3 \times 2 \times 1) = 84$ and

d 4 5 6 / 3 4 $= 1440/(2 \times 4 \times 3 \times 1) = 60.$

Thus RHS: $\sum_{Y \in Y_1 \times y_2} d_Y = 56 + 84 + 60 = 200.$ □

The tensor product (6.2.4) and $SU(N)$ decomposition can be further simplified for the $SU(2)$ group as vertical column(s) with two boxes are trivial:

$$\boxed{a_1}\boxed{a_2} \otimes \boxed{b_1}\boxed{b_2}\boxed{b_3} = \boxed{a_1}\boxed{a_2}\boxed{b_1}\boxed{b_2}\boxed{b_3} \oplus \boxed{a_2}\boxed{b_1}\boxed{b_2} \oplus \boxed{b_1} \tag{6.2.5}$$

which agrees with the tensor product Equation 6.2.1 $V^1 \otimes V^{3/2} = \oplus_{j=1/2}^{5/2} V^j$ where V^j denotes single row Young tableau with $2j$ boxes. Just like the basis states $|j, m\rangle$ belong to V^j, we could also have rank k irreducible tensors $O(k,\ q)$ whose transformation properties are similar to the state $|k,\ q\rangle$. For example, vector $\vec{A}$ belongs to rank 1 irreducible tensor. Tensor product of two vectors $\vec{A}$ and $\vec{B}$ whose decomposition will be exactly like Equation 6.2.1:

$$\vec{A} \otimes \vec{B} = \oplus_{k=0}^{2} O(k,\ q).$$

Comparing the form of spherical harmonics $Y_m^{\ell=1}(\theta,\ \phi)$ with the components of position vector, the vector $\vec{A}$ can be rewritten in the spherical rank 1 tensor form as

$$A(1,\ 0) = A_z\ ,\ A(1,\ \pm 1) = \mp \frac{A_x \pm i A_y}{\sqrt{2}}. \tag{6.2.6}$$

We had elaborated the projector method of obtaining binary and tertiary basis from tensor product in the discrete group context. In similar fashion, the states $|j, m\rangle$ belonging to the irreducible space $V^j \in V^{j_1} \otimes V^{j_2}$ must be rewritable as the linear combination of tensor product states $|j_1, m_1\rangle|j_2, m_2\rangle$. The projection method for tensor product of $SU(2)$ representations is the focus of the following section.

6.2.2 $SU(2)$ Clebsch–Gordan matrix

The decomposition into irreducible component states $|j, m\rangle \in V^j$ from the tensor product of states $|j_1, m_1\rangle \otimes |j_2, m_2\rangle$ involves a matrix $C^{j,m}_{j_1,m_1;j_2,m_2}$ called Clebsch–Gordan (CG) coefficient matrix:

$$|j, m\rangle = \sum_{m_1 m_2} C^{j,m}_{j_1,m_1;j_2,m_2} |j_1, m_1\rangle \otimes |j_2, m_2\rangle, \tag{6.2.7}$$

where CG coefficients are non-zero if and only if $|j_1 - j_2| \leq j \leq j_1 + j_2$ and $m = m_1 + m_2$. These CG coefficients are available in the form of tables. We can also obtain these coefficients by assuming CG coefficient of the maximum angular momentum state, $|j_{\max} = j_1 + j_2,\ m = j_1 + j_2\rangle$ (also called as highest weight state), as $C^{j_1+j_2, j_1+j_2}_{j_1,j_1;j_2,j_2} = 1$, i.e.,

$$|j_1 + j_2, j_1 + j_2\rangle = |j_1, j_1\rangle|j_2, j_2\rangle. \tag{6.2.8}$$

Recall the action of the $\mathfrak{su}(2)$ generators $J\pm,\ J_z$ on the states discussed in the previous chapter:

$$J_\pm|j,m\rangle = \hbar\sqrt{(j\mp m)(j\pm m+1)}|j,m\pm 1\rangle;\ J_z|j,m\rangle = \hbar m|j,m\rangle. \tag{6.2.9}$$

Incidentally, $\mathfrak{su}(2)$ generators on the tensor product state $|j_1,m_1\rangle|j_2,m_2\rangle$ can be deduced from the tensor product of the infinitesimal group elements : $(\mathbb{I}+\sum_{a=1}^{3} J_a^{(1)}\delta\theta^a)\otimes(\mathbb{I}+\sum_{a=1}^{3} J_a^{(2)}\delta\theta^a)$ where the superscript on the generators keeps track of the angular momentum. Keeping up to order $\mathcal{O}(\delta\theta^2)$, the tensor product simplifies to

$$\mathbb{I}+\left[\left(\sum_{a=1}^{3} J_a^{(1)}\theta^a\right)\otimes\mathbb{I}+\mathbb{I}\otimes\left(\sum_{a=1}^{3} J_a^{(2)}\theta^a\right)\right]+\mathcal{O}(\delta\theta^2),$$

indicating that the generators acting on tensor product state must be

$$[J\otimes\ \mathbb{I}+\ \mathbb{I}\otimes J]\,|j_1,m_1\rangle\otimes|j_2,m_2\rangle.$$

Applying these $\mathfrak{su}(2)$ generators on both the LHS and RHS of Equation 6.2.8 leads to the following:

$$J_-|j_1+j_2,j_1+j_2\rangle = \sqrt{2j_1+2j_2}|j_1+j_2,j_1+j_2-1\rangle. \tag{6.2.10}$$

The action of these generators on the tensor product state of RHS of Equation 6.2.8 will be

$$\{J_-|j_1,j_1\rangle\}|j_2,j_2\rangle+|j_1,j_1\rangle\{J_-|j_2,j_2\rangle\} = \sqrt{2j_1}|j_1,j_1-1\rangle|j_2,j_2\rangle+\sqrt{2j_2}|j_1,j_1\rangle|j_2,j_2-1\rangle. \tag{6.2.11}$$

From the two equations given above (Equations 6.2.10 and 6.2.11), we obtain

$$|j_1+j_2,j_1+j_2-1\rangle = \sqrt{\frac{j_1}{j_1+j_2}}|j_1,j_1-1\rangle|j_2,j_2\rangle+\sqrt{\frac{j_2}{j_1+j_2}}|j_1,j_1\rangle|j_2,j_2-1\rangle. \tag{6.2.12}$$

Comparing the above equation with Equation 6.2.7, we can read off CG coefficients

$$C^{j_1+j_2,j_1+j_2-1}_{j_1,j_1;j_2,j_2-1} = \sqrt{\frac{j_2}{j_1+j_2}},\ C^{j_1+j_2,j_1+j_2-1}_{j_1,j_1-1;j_2,j_2} = \sqrt{\frac{j_1}{j_1+j_2}}. \tag{6.2.13}$$

This procedure can be similarly continued acting J_- on Equation 6.2.12.

Example 54. Work out the CG coefficients $C^{1/2,1/2}_{1/2,1/2;1,0}$, $C^{1/2,1/2}_{1/2,-1/2;1,1}$. From Equation 6.2.12, the state $|3/2,1/2\rangle$ is

$$|3/2,1/2\rangle = \sqrt{\frac{1}{3}}|1/2,\ -1/2\rangle|1,1\rangle + \sqrt{\frac{2}{3}}|1/2,1/2\rangle|1,0\rangle.$$

We need to write the state $|1/2,1/2\rangle$ to obtain the CG coefficients $C^{1/2,1/2}_{1/2,1/2;1,0}$, $C^{1/2,1/2}_{1/2,-1/2;1,1}$. This state must be orthogonal to $|3/2,1/2\rangle$. Hence

$$|1/2,1/2\rangle = \sqrt{\frac{1}{3}}|1/2,\ -1/2\rangle|1,1\rangle - \sqrt{\frac{2}{3}}|1/2,1/2\rangle|1,0\rangle,$$

which leads to the CG coefficients:

$$C^{1/2,1/2}_{1/2,1/2;1,0} = -\sqrt{\frac{2}{3}},\ C^{1/2,1/2}_{1/2,-1/2;1,1} = \sqrt{\frac{1}{3}}.$$ □

The CG method, which we described for the tensor product of any two states, is also applicable to the tensor product of two irreducible rank tensors $O(k_1,\ q_1)$, $O(k_2,\ q_2)$ or the tensor product of $O(k,\ q)$ with state $|j_1,m_1\rangle$. Similar to the action of $\mathfrak{su}(2)$ generators on states $|j,m\rangle$ in Equation 6.2.9, their action on the irreducible tensors can be shown to satisfy:

$$[J_z,\ O(k,\ q)] = \hbar q\, O(k,\ q), \tag{6.2.14}$$

$$[J_\pm,\ O(k,\ q)] = \hbar\sqrt{k(k+1) - (q\pm 1)}O(k,\ q\pm 1). \tag{6.2.15}$$

Example 55. Using the familiar transformation of rank one tensor $\vec{A}$ under infinitesimal rotation R by angle $\delta\theta$ about axis $\hat{n}$ to the quantum mechanical operator transformation

$$\vec{A}' = R\vec{A} = \vec{A} + \delta\theta\hat{\mathbf{n}}\times\vec{A} = U_R\vec{A}U_R^\dagger,$$

prove Equations 6.2.14 and 6.2.15 where $U_R = \left(1 + \frac{i\delta\theta}{\hbar}\hat{\mathbf{n}}.\vec{J}\right)$.

Equating $\mathcal{O}(\delta\theta)$ terms in the above equation, we get

$$\frac{i}{\hbar}[\hat{\mathbf{n}}.\vec{J},\ \vec{A}] = \hat{\mathbf{n}}\times\vec{A},$$

which simplifies for components of $\vec{A}$. For instance, the above equation for A_x turns out to be

$$[A_x,\ J_x] = 0\ ;\ [A_x,\ J_y] = i\hbar A_x\ ;\ [A_x,\ J_z] = -i\hbar A_y,$$

which implies the following compact form

$$[J_i,\ A_j] = \epsilon_{ijk} i\hbar A_k,$$

leading to obtaining the algebra for $A(1,\ q)$(6.2.6):

$$[J_z,\ A(1,\ q)] = \hbar q A(1,\ q)\ ;\ [J\pm,\ A(1,\ q)] = \hbar\sqrt{2 - q(q \pm 1)}A(1,\ q \pm 1). \qquad \square$$

Example 56. Construct the rank 2 tensor component $T(2,1)$ using two rank one tensors $A(1,\ q_1)$ and $B(1,\ q_2)$.

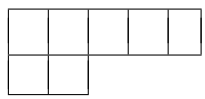
Following the Clebsch–Gordan procedure for states, we start with the maximum q tensor as

$$T(2,2) = A(1,1)B(1,1),$$

and applying J_- on both LHS as well as RHS will give

$$T(2,1) = \frac{1}{\sqrt{2}}[A(1,1)B(1,0) + A(1,0)B(1,1)]. \qquad \square$$

Even though we confined ourselves to the construction of $SU(2)CG$ matrix and angular momentum states, the method can be extended to $SU(N)$ starting with the highest weight vector state $|\mathbf{\Lambda}, \mathbf{\Lambda}\rangle$ and applying $\mathfrak{su}(N)$ generators $E_{\pm\boldsymbol{\alpha}},\ H_i$ associated with simple root vector $\boldsymbol{\alpha}$.

Recall our discussion on highest weight vector states of the irreducible representation of $SU(N)$. For the Young diagram depicted:  $\in SU(3)$, the highest weight vector will be

$$\mathbf{\Lambda} = 3\boldsymbol{\mu}^{(1)} + 2\boldsymbol{\mu}^{(2)},$$

where $\boldsymbol{\mu}^{(1)},\ \boldsymbol{\mu}^{(2)}$ are the two fundamental weights of $SU(3)$ discussed in the previous chapter (see Example 48).

Similar to the $SU(2)$ CG construction, we can take the tensor product of two $SU(3)$ irreducible representations of highest weights $|\mathbf{\Lambda}_1, \mathbf{\Lambda}_1\rangle \otimes |\mathbf{\Lambda}_2, \mathbf{\Lambda}_2\rangle$ to give highest weight vector $\mathbf{\Lambda} = \mathbf{\Lambda}_1 + \mathbf{\Lambda}_2$. The other weight vector states are obtained by applying $E_{-\boldsymbol{\alpha}^{(1)}},\ E_{-\boldsymbol{\alpha}^{(2)}},\ E_{-\boldsymbol{\alpha}^{(3)}}$ on both sides as follows:

$$E_{-\boldsymbol{\alpha}^{(i)}}|\mathbf{\Lambda}, \mathbf{\Lambda}\rangle \propto |\mathbf{\Lambda}, \mathbf{\Lambda} - \boldsymbol{\alpha}^{(i)}\rangle = [E_{-\boldsymbol{\alpha}^{(i)}}|\mathbf{\Lambda}_1, \mathbf{\Lambda}_1\rangle]|\mathbf{\Lambda}_2, \mathbf{\Lambda}_2\rangle + |\mathbf{\Lambda}_1, \mathbf{\Lambda}_1\rangle[E_{-\boldsymbol{\alpha}^{(i)}}|\mathbf{\Lambda}_2, \mathbf{\Lambda}_2\rangle].$$

The proportionality factor can be deduced by the action of the corresponding $\mathfrak{su}(2)$ subalgebra generators $J_3^{(\boldsymbol{\alpha})}$, $J_-^{(\boldsymbol{\alpha})}$ on the highest weight states:

$$J_3^{(\boldsymbol{\alpha})}|\boldsymbol{\Lambda}, \boldsymbol{\Lambda}\rangle = \frac{(\boldsymbol{\Lambda}.\boldsymbol{\alpha})}{|\boldsymbol{\alpha}|^2}|\boldsymbol{\Lambda}, \boldsymbol{\Lambda}\rangle,$$

$$J_-^{(\boldsymbol{\alpha})}|\boldsymbol{\Lambda}, \boldsymbol{\Lambda}\rangle = \frac{\sqrt{[(\boldsymbol{\Lambda}+\boldsymbol{\Lambda}).\boldsymbol{\alpha}][(\boldsymbol{\Lambda}-\boldsymbol{\Lambda}).\boldsymbol{\alpha}+1]}}{|\boldsymbol{\alpha}|}|\boldsymbol{\Lambda}, \boldsymbol{\Lambda}-\boldsymbol{\alpha}\rangle.$$

For the lower weight states $|\boldsymbol{\Lambda}, \boldsymbol{\Lambda} - m(\boldsymbol{\alpha})^{(1)} - n\boldsymbol{\alpha}^{(2)}\rangle$ where m, n are integers, the $J_3^{(\boldsymbol{\alpha})}$, $J_\pm^{(\boldsymbol{\alpha})}$ operator action will be

$$J_3^{(\boldsymbol{\alpha})}|\boldsymbol{\Lambda}, \boldsymbol{\Lambda} - m\boldsymbol{\alpha}^{(1)} - n\boldsymbol{\alpha}^{(2)}\rangle = \frac{\left(\boldsymbol{\Lambda} - m\boldsymbol{\alpha}^{(1)} - n\boldsymbol{\alpha}^{(2)}\right).\boldsymbol{\alpha}}{|\boldsymbol{\alpha}|^2}|\boldsymbol{\Lambda}, \boldsymbol{\Lambda} - m\boldsymbol{\alpha}^{(1)} - n\boldsymbol{\alpha}^{(2)}\rangle, \quad (6.2.16)$$

$$J_\mp^{(\boldsymbol{\alpha})}|\boldsymbol{\Lambda}, \boldsymbol{\Lambda} - m\boldsymbol{\alpha}^{(1)} - n\boldsymbol{\alpha}^{(2)}\rangle = \frac{1}{|\boldsymbol{\alpha}|}\sqrt{[\{\boldsymbol{\Lambda} \pm (\boldsymbol{\Lambda} - m\boldsymbol{\alpha}^{(1)} - n\boldsymbol{\alpha}^{(2)})\}.\boldsymbol{\alpha}]}$$
$$\sqrt{[\{\boldsymbol{\Lambda} \mp (\boldsymbol{\Lambda} - m\boldsymbol{\alpha}^{(1)} - n\boldsymbol{\alpha}^{(2)})\}.\boldsymbol{\alpha}+1]}|\boldsymbol{\Lambda}, \boldsymbol{\Lambda} - m\boldsymbol{\alpha}^{(1)} - n\boldsymbol{\alpha}^{(2)} \mp \boldsymbol{\alpha}\rangle.$$

This CG construction of tensor product of weight vector states will be useful for determining the states of hadrons which are bound states of fundamental quarks. These hadronic states in the continuous group context are similar to the binary or tertiary basis discussed in the discrete group context. We will illustrate in Section 6.4.1 for a bound state when we discuss hadrons in particle physics.

In the following subsection, we will look at the selection rules for transition from the initial state to the final state due to interactions respecting $SU(2)$ symmetry. In Chapter 4, we had deduced that the matrix elements in the discrete symmetry situation would be non-zero if the tensor product of the irreducible representations corresponding to basis states and operators turned out to be trivial representation. In the same fashion, the matrix elements $\langle \beta j_f, m_f | O(k,\ q) | \alpha j_i, m_i\rangle$ between initial state α with angular momentum j_i and final state β angular momentum j_f due to interactions, like electric dipole moment interaction or quadrapole moment interaction and suchlike, denoted by the irreducible rank k tensor operator $O(k,\ q)$ can be deduced to be vanishing or non-vanishing. This is the content of Wigner–Eckart theorem which we will present with proof.

6.2.3 Wigner–Eckart theorem

The theorem states that the matrix elements of the irreducible tensor operator between two angular momentum states consists of product of two terms

$$\langle \beta j_f, m_f | O(k,\ q) | \alpha j_i, m_i\rangle = \langle \beta j_f || O(k) || \alpha j_i\rangle C^{j_f, m_f}_{j_i, m_i; k, q},$$

where the first factor is called reduced matrix element which depends on the quantum states $|\alpha j_i\rangle$, $|\beta j_f\rangle$ and the rank of the tensor operator whereas the second factor is purely geometrical given by the CG coefficient. Even though we need experimental data to determine the reduced matrix element, we can at least rule out (using CG coefficients) whether the process is allowed or forbidden in any system with rotational spherical symmetry: $SU(2)$.

From Equation 6.2.14 we know that

$$\langle \beta j_f, m_f | [j_z, O(k,\ q)] - \hbar q O(k,\ q) | \alpha j_i, m_i \rangle = 0,$$

leading to the constraint $m_f - m_i = q$ for non-zero $\langle \beta j_f, m_f | O(k,\ q) | \alpha j_i, m_i \rangle$ when we expand the commutator. This is one of the properties of the CG coefficient. Similarly, we can impose the following constraint using Equation 6.2.15:

$$\langle \beta j_f, m_f | [j\pm, O(k,\ q)] - \hbar \sqrt{(k \mp q) - (k \pm q + 1)} O(k,\ q \pm 1) | \alpha j_i, m_i \rangle = 0.$$

Again expanding the commutator, the equation resembles the recursion relation obeyed by the Clebsch–Gordan coefficients. Thus we conclude that

$$\langle \beta j_f, m_f | O(k,\ q) | \alpha j_i, m_i \rangle \propto C^{j_f, m_f}_{j_i, m_i; k, q},$$

and the proportionality constant will be independent of m_f, m_i, q proving the Wigner–Eckart Theorem. □

Example 57. Given that the diagonal matrix element of $\langle \alpha j, m' = j | Q(2,0) | \alpha j, m = j \rangle = K$, determine the matrix element of

$$\langle \alpha j, m' | Q(2,\ -2) | \alpha j, m = j \rangle.$$

Using Wigner–Eckart theorem, $\langle \alpha j, m' = j | Q(2,0) | \alpha j, m = j \rangle = K = \langle \alpha j || Q(2) || \alpha j \rangle C^{j,j}_{j,j;2,0}$. This determines the reduced matrix element in terms of K and Clebsch–Gordan coefficient:

$$\langle \alpha j || Q(2) || \alpha j \rangle = K / C^{j,j}_{j,j;2,0}.$$

Once we know the reduced matrix element then

$$\langle \alpha j, m' | Q(2,\ -2) || \alpha j, m = j \rangle = \left(K C^{j, m' = j-2}_{j,j;2,-2} \right) / C^{j,j}_{j,j;2,0}.$$

Thus the theorem is useful in determining the matrix elements of other components of $Q(2,\ q)$ from the experimental result for one component. □

6.3 Elementary Particles in Nuclear and Particle Physics

In this section, we will focus on the applications of $SU(2)$ and $SU(3)$ symmetries in nuclear and particle physics. The periodic table of elementary particles is broadly classified as *hadrons and leptons*. The electromagnetic and nuclear interactions amongst these particles are mediated by *new particles* which are referred to as *force carriers*. For instance, *photon* γ is the mediator of electromagnetic interaction. Similarly, there are eight gluons g_i's which are mediators of strong nuclear interaction and three vector bosons $W\pm$, Z mediating weak nuclear interaction. In order to give masses to these particles, the Higgs particle was theoretically proposed and recently discovered in the Large Hadron Collider experiments at CERN, Geneva.

Hadrons are further subclassified as *baryons* and *mesons*. The protons and neutrons inside the atomic nucleus are examples of baryons. Surprisingly, the nuclear magnetic moment of the proton and neutron are proportional to nuclear magneton but the proportionality constant is a real number and not an integer. Hence the protons and neutrons cannot be elementary but must have a structure. The other massive baryons like $\triangle$, Σ, ... appear in the collision experiments involving high energy proton beams. Similar to the Rutherford scattering experiment which suggested a massive nucleus inside the atom, deep inelastic scattering experiments of baryons indicated that they are bound states of three quarks. Unlike electrons, protons and neutrons, free quarks are not seen in nature.

In the language of group theory, we will say that baryons can be obtained by taking the tensor product of three fundamental representations associated with the quarks. Unlike baryons, mesons are the bound states of quark and antiquark pairs. For example, pions π and ρ particle are mesons.

Murray Gell-Mann was influenced by the pattern diagrams emerging from plotting baryons and mesons based on their mass m and charge Q for a fixed angular momentum $\mathbf{J}$ (some patterns resemble an eight-fold path). Importantly, he proposed the *quark model* to reproduce the observed patterns. The readers can actually visualize that these pattern diagrams are nothing but the weight diagrams discussed in Chapter 5 for $SU(3)$ Lie group.

From the experimentally observed strong nuclear scattering or decay process of hadrons, theoreticians postulated that there must be an additional conservation law (isospin conservation) besides linear momentum, energy and angular momentum conservation laws. Similar to Wigner–Eckart theorem, discussed in the context of $\mathfrak{su}(2)$ angular momentum states and operators, there will be selection rules for such scattering or decay processes obeying isospin conservation.

We will briefly discuss selection rules of strong scattering and decay processes involving hadrons in the following subsection and then elaborate the Gell-Mann quark model, in Section 6.4, to understand the theoretical construction of observed baryons and mesons and the pattern diagrams.

6.3.1 Isospin symmetry

There is a quantity called *isospin* $\vec{I}$ in nuclear and particle physics whose Lie algebra

$$[I_i,\ I_j] = i\epsilon_{ijk}I_k$$

is exactly similar to angular momentum algebra. Interestingly any decay or scattering process involving hadrons $A \to B + C$ must conserve isospin. In other words, isospin symmetry is respected in such strong interaction processes. The tensor operators describing such scattering/decay processes are scalar operators $S(0,\ 0)$. We can now study allowed and forbidden processes using Wigner–Eckart theorem.

The isospin $\mathbf{I}$ and the z-component of isospin I_z for few baryons and mesons which are needed to determine Clebsch–Gordan coefficients are as follows:

delta particles $\triangle$: $\mathbf{I} = 3/2, I_z = +3/2, 1/2, -1/2, -3/2$ for $\triangle^{++},\ \triangle^{+},\ \triangle^{0},\ \triangle^{-}$,

nucleons N: $\mathbf{I} = 1/2,\ I_z = 1/2,\ I_z = -1/2$ for p and n,

pi meson π: $\mathbf{I} = 1, I_z = +1, 0, -1$ for $\pi^{+},\ \pi^{0}$ and π^{-},

rho meson ρ: $\mathbf{I} = 1, I_z = +1, 0, -1$ for $\rho^{+},\ \rho^{0}$ and ρ^{-}.

With this data, let us attempt to figure out the allowed and forbidden processes of strongly interacting baryons and mesons.

Example 58. Show that the the ratio of the decay rate between the two strong decay processes respecting isospin symmetry is

$$\frac{\Gamma[\triangle^{+} \to p\pi^{0}]}{\Gamma[\triangle^{+} \to n\pi^{+}]} = \frac{|\langle p\pi^{0}|S(0,0)|\triangle^{+}\rangle|^2}{|\langle n\pi^{+}|S(0,0)|\triangle^{+}\rangle|^2} = 2.$$

Using the Wigner–Eckart theorem, the decay process $\triangle^{+} \to p\pi^{0}$ is given by the matrix element

$$\langle p\pi^{0}|S(0,0)|\triangle^{+}\rangle \propto \langle p\pi^{0}|3/2, 1/2\rangle = C^{3/2,1/2}_{1/2,1/2;1,0}, \tag{6.3.1}$$

where $|p\pi^{0}\rangle \equiv |1/2, 1/2; 1, 0\rangle = |1/2, 1/2\rangle|1, 0\rangle$. Similarly the decay amplitude of $\triangle^{+} \to n\pi^{+}$ is given by

$$\langle n\pi^{+}|S(0,0)|\triangle^{+}\rangle \propto \langle n\pi^{+}|3/2, 1/2\rangle = C^{3/2,1/2}_{1/2,-1/2;1,1}. \tag{6.3.2}$$

The Clebsch–Gordan decomposition of the state $|3/2, 1/2\rangle$ obtained from the tensor product of $\mathbf{I}_1 = 1/2 \otimes \mathbf{I_2} = 1$ will be

$$|3/2, 1/2\rangle = \sqrt{\frac{2}{3}}\underbrace{|1/2, 1/2; 1, 0\rangle}_{|p,\pi^{0}\rangle} + \sqrt{\frac{1}{3}}\underbrace{|1/2, -1/2; 1, 1\rangle}_{|n\pi^{+}\rangle}.$$

Using the above CG coefficients, the ratio of Equations 6.3.1 and 6.3.2 gives

$$\frac{\Gamma[\triangle^+ \to p\pi^0]}{\Gamma[\triangle^+ \to n\pi^+]} = \frac{\left(\sqrt{\frac{2}{3}}\right)^2}{\left(\sqrt{\frac{1}{3}}\right)^2} = 2.$$

□

6.4 Quark Model

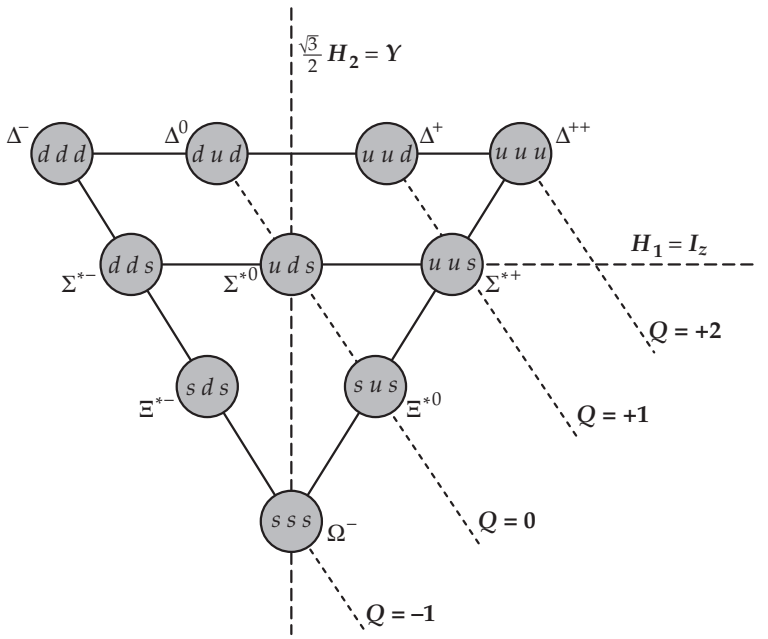
The angular momentum of the baryons are either $\mathbf{J} = 3/2$ or $\mathbf{J} = 1/2$. Further, the observed magnetic moments of protons are not integral multiples of nuclear magneton $\mu_N = e\hbar/(2m_p)$ indicating the baryons are not elementary particles but composites made up of n number of quarks which are spin $1/2$ particles.

The angular momentum state of these spin $1/2$ quarks belong to the two-dimensional space $V^{1/2}$. Baryonic states belong to the irreducible spaces obtained from the tensor product of these n quarks:

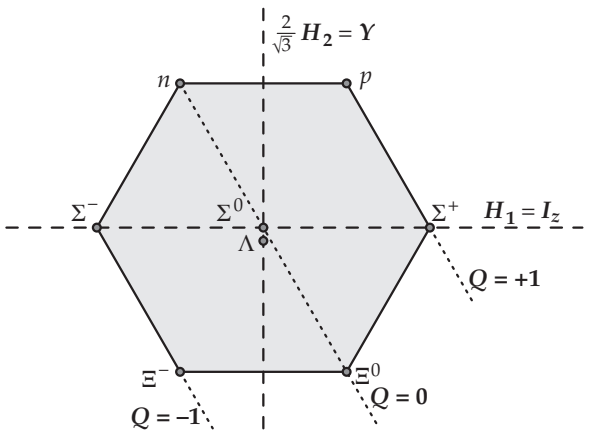
$$\underbrace{V^{1/2} \otimes V^{1/2} \otimes \ldots V^{1/2}}_{n} = V^{n/2} \oplus V^{n/2-1} \oplus \ldots$$

The angular momentum of the irreducible representations, denoting baryonic states, must have either spin $3/2$ or spin $1/2$. Equating highest spin $n/2$ of the irreducible space $V^{n/2}$ to spin $3/2$, we deduce that the baryons must be made up of $n = 3$ quarks.

Even though we have accounted for the observed angular momentum of baryons, we still need a radical idea to explain the reason for eight baryons including nucleons to have $\mathbf{J} = 1/2$ and the rest of the baryons including $\triangle$ particles to have $\mathbf{J} = 3/2$. Figure 6.4.l(b) shows the plots of $\mathbf{J} = 1/2$ baryons resembling eight-fold path diagram and Figure 6.4.l(a) for $\mathbf{J} = 3/2$ baryons. Note that the dotted lines indicate the line of same charge Q and the horizontal lines have same isospin I and decreasing I_z components in steps of one from right to left. Interestingly, Gell-Mann's mathematical formulations used Lie groups to produce the observed plots. This is famously known as Gell-Mann's quark model for which he received the Nobel Prize in the year 1969. We will explain the rescaling of the vertical axis and the definition of Y in the next subsection.



(a) Decimet diagram of spin $J = 3/2$ baryons



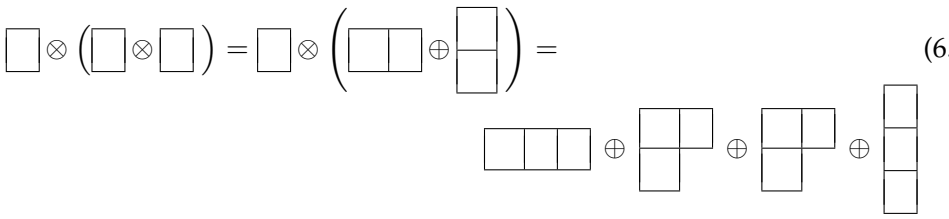
(b) Octet diagram of spin $J = 1/2$ baryons

Figure 6.4.1 Quark Model

6.4.1 $SU(3)$ group approach quark model

Gell-Mann assumed that the quarks come in three flavors u, d, s (up, down, strange quarks). In the flavor space, $(u,\ d)$ are states having isospin $\mathbf{I} = 1/2$ and have the z-component of isospin as $+1/2, -1/2$ respectively, whereas s has isospin $\mathbf{I} = 0$.

We can denote the representation of the quark in flavor space as a Young diagram $\square \in SU(3)$. Its dimension is $d_{\square} = 3$ indicating that we can place any of the three-flavors in the single box which agrees with the dimension in formula (6.2.3) for group $SU(N = 3)$. We have already studied the tensor product of $SU(N)$ representations and their irreducible decomposition through the Young diagram approach. In the present context, we can construct baryon states from the tensor product of three quarks in flavor space as follows:



(6.4.1)

The baryons belonging to irreducible representation $\square\square\square$ refers to all possible totally symmetric three quark states with and without repetition of the three flavors. Hence, the total number of possible states in the above representation will be 10 with the following possible entries in the boxes : *uuu*; *ddd*; *sss*; *uud*; *uus*; *ddu*; *dds*; *ssu*; *ssd*; *uds*. Using the dimension formula (6.2.3), $d_{\square\square\square} = 10$. We would like to emphasize that the pattern of the ten possible states indeed coincides with the observed pattern diagram of baryons with angular momentum **J** = 3/2. When Gell-Mann proposed the $SU(3)$ quark model deducing the decimet states, the baryon Ω^- had not been discovered by experimentalists. They discovered Ω^- three years after the quark model hypothesis, demonstrating the power of group theory prediction.

Note that the highest weight of the decimet representation is $\mathbf{\Lambda} = 3\boldsymbol{\mu}^{(1)} = (3/2, 3\sqrt{3}/6)$. In the decimet diagram 6.4.1a, this highest weight state is the $\triangle^{++}$ baryon whose $I_z = 3/2$ and charge $Q = 2$. The first component of the weight vector is the eigenvalue of Cartan generator H_1 which matches with the $I_z = 3/2$ whereas the second component of the weight vector is the eigenvalue of Cartan generator H_2. Using the Gell-Mann–Nishijima formula $Q = I_z + (B + S)/2$, the following relation to H_2 can be deduced:

$$\frac{2}{\sqrt{3}} H_2 = 2(Q - I_z) \equiv Y = (B + S),$$

where Y is referred to as *hypercharge* whose value can be deduced using the charge Q and z-component of isospin of the particles. Equivalently, all baryons are assigned baryon number $B = +1$. If the baryons have strange quarks as constituents, these baryons have a non-zero strangeness S quantum number. The $\triangle$ particles have $B = 1$, $S = 0$ whereas Σ^{*+} has $B = 1$, $S = -1$. That is, for every s quark, we associate $S = -1$. In terms of B, S, the hypercharge $Y = B + S$ can be obtained. Using the lowering

operators $E_{-\boldsymbol{\alpha}^{(i)}}$ on the highest weight vector state $|\boldsymbol{\Lambda}, \boldsymbol{\Lambda} = 3\boldsymbol{\mu}^{(1)} \equiv \triangle^{++}\rangle$, we can obtain the remaining nine baryons in the deciment diagram. Hence, the deciment diagram is indeed a weight diagram with the $H_1 \equiv I_z$ and $H_2 = \sqrt{3}Y/2$ for the irreducible representation $\begin{array}{|c|c|c|}\hline \ & \ & \ \\ \hline \end{array} \in SU(3)$. Following the relation of H_1 and H_2 to isospin and hypercharge, the $SU(3)$ defining representation weight diagram states discussed in Chapter 5 can be equivalently interpreted as $|\boldsymbol{\mu}_1 \equiv u\rangle$, $|\boldsymbol{\mu}_2 \equiv d\rangle$, $|\boldsymbol{\mu}_3 \equiv s\rangle$.

We leave the readers to compute the dimensions of the other irreducible representation of $SU(3)$ in the tensor product $\square \otimes \square \otimes \square$ and verify that the dimension of Equation 6.4.1 is

$$3 \otimes 3 \otimes 3 = 10 \oplus 8 \oplus 8 \oplus 1.$$

Note that there are two eight-dimensional representations from the group theory tensor product whereas there is only one octet weight diagram for baryons. The weight vector states of each irreducible representation can be obtained using the CG method and shown that they are orthonormal to each other. In fact, the experimental value of the magnetic moment data can be reproduced only for a suitable linear combination of the two eight-dimensional representation. This experimentally stringent requirement justifies one octet diagram of baryons. Interested readers can refer to any elementary particle physics textbook for details.

Let us now work out a simple example to determine $SU(3)$ CG coefficients.

Example 59. For a di-quark bound state, determine the six weight vector states associated with the Young diagram $\begin{array}{|c|c|}\hline \ & \ \\ \hline \end{array} \in SU(3)$ using the CG construction.

The highest weight vector state is $|2\boldsymbol{\mu}^{(1)}, 2\boldsymbol{\mu}^{(1)}\rangle \equiv |\begin{array}{|c|c|}\hline u & u \\ \hline \end{array}\rangle = |uu\rangle$. We can now apply the lowering operators $J_-^{(\boldsymbol{\alpha}^{(1)})}$ on the highest weight state. Before we do that, we know that

$$(2\boldsymbol{\alpha}^{(1)}.2\boldsymbol{\mu}^{(1)})/|\boldsymbol{\alpha}^{(1)}|^2 = q = 2.$$

Thus there will be two weight vector states

$$|2\boldsymbol{\mu}^{(1)}, 2\boldsymbol{\mu}^{(1)} - \boldsymbol{\alpha}^{(1)}\rangle,\ |2\boldsymbol{\mu}^{(1)}, 2\boldsymbol{\mu}^{(1)} - 2\boldsymbol{\alpha}^{(1)}\rangle.$$

Applying the lowering operator (6.2.16):

$$J_-^{(\boldsymbol{\alpha}^{(1)})}|2\boldsymbol{\mu}^{(1)}, 2\boldsymbol{\mu}^{(1)}\rangle = \sqrt{2}|2\boldsymbol{\mu}^{(1)}, 2\boldsymbol{\mu}^{(1)} - \boldsymbol{\alpha}^{(1)}\rangle = |us\rangle + |su\rangle.$$

Thus we get the weight vector state

$$|2\boldsymbol{\mu}^{(1)}, 2\boldsymbol{\mu}^{(1)} - \boldsymbol{\alpha}^{(1)}\rangle = \frac{1}{\sqrt{2}}(|us\rangle + |su\rangle) \equiv |\begin{array}{|c|c|}\hline u & s \\ \hline \end{array}\rangle.$$

Further operating the same lowering operator, we can show that

$$|2\boldsymbol{\mu}^{(1)}, 2\boldsymbol{\mu}^{(1)} - 2\boldsymbol{\alpha}^{(1)}\rangle = |\,\boxed{s}\boxed{s}\,\rangle \equiv |ss\rangle.$$

Remember that $J_{-}^{(\boldsymbol{\alpha}^{(2)})}|2\boldsymbol{\mu}^{(1)}, 2\boldsymbol{\mu}^{(1)}\rangle = 0$ as $\boldsymbol{\alpha}^{(2)}.\boldsymbol{\mu}^{(1)} = 0$. However, we can operate the lowering operator associated with the positive root $\boldsymbol{\alpha}^{(3)} = \boldsymbol{\alpha}^{(1)} + \boldsymbol{\alpha}^{(2)}$ to derive the following two states:

$$|2\boldsymbol{\mu}^{(1)}, 2\boldsymbol{\mu}^{(1)} - \boldsymbol{\alpha}^{(1)} - \boldsymbol{\alpha}^{(2)}\rangle = \frac{1}{\sqrt{2}}(|ud\rangle + |du\rangle) \equiv |\,\boxed{u}\boxed{d}\,\rangle;$$

$$|2\boldsymbol{\mu}^{(1)}, 2\boldsymbol{\mu}^{(1)} - 2\boldsymbol{\alpha}^{(1)} - 2\boldsymbol{\alpha}^{(2)}\rangle = |\,\boxed{d}\boxed{d}\,\rangle \equiv |dd\rangle.$$

On the state $|\,\boxed{d}\boxed{d}\,\rangle$, we cannot apply $J_{-}^{(\boldsymbol{\alpha}^{(2)})}$ as the dot product of the root vector with the weight vector being $2\boldsymbol{\alpha}^{(2)}.(2\boldsymbol{\mu}^{(1)} - 2\boldsymbol{\alpha}^{(1)} - 2\boldsymbol{\alpha}^{(2)})/|\boldsymbol{\alpha}^{(2)}|^2 = (q - p) = -2$. Hence, we will try raising the operator twice on the state. Applying once gives

$$|2\boldsymbol{\mu}^{(1)}, 2\boldsymbol{\mu}^{(1)} - 2\boldsymbol{\alpha}^{(1)} - \boldsymbol{\alpha}^{(2)}\rangle = \frac{1}{\sqrt{2}}(|ds\rangle + |sd\rangle) \equiv |\,\boxed{d}\boxed{s}\,\rangle,$$

and applying the raising operator on the $|\,\boxed{d}\boxed{s}\,\rangle$ will give the state $|\,\boxed{s}\boxed{s}\,\rangle$ already obtained. Thus we have derived the six weight vector states and presented the CG coefficient decomposition of the di-quark bound state by applying the $\mathfrak{su}(3)$ raising and lowering operators as briefly mentioned in Section 6.2.2. In the similar way, we can write the highest weight vector state $|3\boldsymbol{\mu}^{(1)}, 3\boldsymbol{\mu}^{(1)}\rangle \equiv \boxed{}\boxed{}\boxed{} = |uuu\rangle$ and determine the weight states corresponding to the remaining nine baryons in the decimet diagram using the CG construction method.

6.4.2 Antiparticles

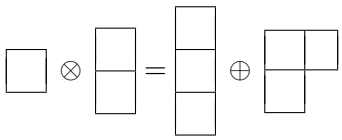
Antiparticles of quarks are called antiquarks. Just as for particles, we can have decimet diagrams and octet diagrams for antibaryons. The values of I_z, Y, Q, S, B of antiparticles are opposite in sign with respect to their corresponding particles. We will now describe the Young diagram for the antiparticle multiplet of the $SU(N)$ group.

Suppose a particle multiplet is $(a_1,\ a_2, \ldots a_{N-1})$ where $a_1,\ a_2, \ldots a_{N-1}$ are the number of single box, number of double vertical boxes, $\cdots$ number of columns of $N-1$ vertical boxes in the corresponding Young diagram presentation. Then the antiparticle multiplet will be given by $(a_{N-1}, a_{N-2}; \ldots a_2, a_1)$. For example, $SU(3)$ decimet baryon multiplet $\boxed{}\boxed{}\boxed{}$ denoted by $(a_1 = 3, a_2 = 0)$. The corresponding antibaryon decimet is $(a_2 = 0, a_1 = 3)$ whose Young diagram is $\begin{array}{|c|c|c|}\hline & & \\ \hline & & \\ \hline \end{array}$. Similarly,

$SU(3)$ antiquark representation is (0, 1) whose Young diagram is  . The highest weight vector of the antiquark state is $\boldsymbol{\mu}^{(2)}$. If we change the signs of x_i's and y_i's of the points $(x_i,\ y_i)$ in the $SU(3)$ fundamental representation weight diagram in the $H_1,\ H_2$ plane (see Figure 5.7.2) denoting u, d, s quarks, we get the weight diagram of $SU(3)$ antiquarks. The readers can verify that the highest weight vector of the antiquark multiplet is $\boldsymbol{\mu}^{(2)}$ (as determined in Example 48). Using these Young diagrams of the antiparticle multiplet, we can study mesons which are bound states of quarks and antiquarks.

Mesons

In group theory language, we say that the $SU(3)$ mesons belong to irreducible representations obtained from tensor products of quark and antiquark representation:



(6.4.2)

where the first irreducible representation (vertical 3 boxes) is a trivial $SU(3)$ representation whose isospin $\vec{I}, I_z$, hypercharge Y are zero. The second irreducible representation whose dimension is 8 is called octet meson multiplet. Notice that the meson bound state multiplet is its own antimeson multiplet. That is, some mesons are their own antimesons and some mesons get mapped to another set of mesons within the octet multiplet.

During the 1974 - 1984 period, new mesons and baryons were discovered which required the introduction of more flavors for quarks besides $u,\ d,\ s$. As of today, there are actually six flavors of quarks indirectly observed through scattering experiments. They are called up (u), down (d), strange (s), charm (c), beauty (b) and top (t) quarks. We could extend Gell-Mann's quark model proposal by including these flavors as well. That is, the Lie group will be $SU(N)$ where N denotes the number of quark flavors. We have given exercise problems to use the Young diagram tensor product tools to understand such new baryons and meson bound states.

We will now discuss in the following subsection as to how the $SU(3)$ irreducible representations like decimet and octet will break if there is a perturbation that breaks the symmetry to a lower rank group. In Chapter 4, we discussed (in the discrete group context) how some degenerate energy levels split into non-degenerate states. In similar fashion, we would like to understand how the ten-dimensional decimet belonging to $SU(3)$ breaks to a lower rank group symmetry by adding perturbations.

6.4.3 Symmetry breaking from $SU(3) \to SU(2)$

In the absence of perturbation, the system described by the Hamiltonian H_0 possesses $SU(3)$ symmetry if and only if the Hamiltonian commutes with all the eight generators

of $\mathfrak{su}(3)$. Suppose we add a perturbation term to the Hamiltonian $H_1 = k\sum_{i=1}^{3}\lambda_i^2$ where k is a constant ($|k| < 1$) and $\lambda_{\{i=1,2,3\}}$ are the first three Gell-Mann matrices, then the total Hamiltonian

$$[H = H_0 + H_1,\ \lambda_i] = 0,$$

where $i = 1, 2, 3$. Note that the first three Gell-Mann matrices satisfy $\mathfrak{su}(2)$ algebra. Suppose the system is the quark system described by defining representation, we see that

$$(\lambda_1 + i\lambda_2)|\mathbf{\Lambda}, \boldsymbol{\mu}_1 \equiv u\rangle \propto |\mathbf{\Lambda}, \boldsymbol{\mu}_2 \equiv d\rangle; (\lambda_1 - i\lambda_2)|\mathbf{\Lambda}, \boldsymbol{\mu}_2 \equiv d\rangle \propto |\mathbf{\Lambda}, \boldsymbol{\mu}_1 \equiv u\rangle,$$

whereas the state $|\mathbf{\Lambda}, \boldsymbol{\mu}_3\rangle \equiv |s\rangle$ remains invariant under the action of $\lambda_{\{i=1,2,3\}}$ which means that the state transforms as a one-dimensional representation of $SU(2)$. That is, the three-dimensional defining representation under the perturbation H_1 breaks as

$$3 \to 2 + 1.$$

The three-dimensional multiplet becomes

$$(u\ d\ s) = (u\ d) \oplus (s).$$

Example 60. Suppose the perturbation breaks the $SU(3)$ symmetry to $SU(2)$ such that s quarks behave like a trivial (singlet) representation of $SU(2)$. How will the $SU(3)$ baryons in the decimet multiplet break under such a perturbation?

Recall, that in the decimet weight diagram Δ particles are made of non-strange quarks. Hence they transform like $\square\square\square \in SU(2)$ which is four-dimensional. The baryons $\sum^*$ have one strange quark and hence will transform as $\square\square \in SU(2)$ as one of the boxes with s quark behaves trivial. Similarly Ξ^* has two s quarks which will transform as $\square \in SU(2)$. The Ω^- has three s quarks and hence will transform as a singlet representation. Therefore

$$10 \to 4 + 3 + 2 + 1$$

is the way in which decimet breaks under the perturbation which reduces the $SU(3)$ symmetry to $SU(2)$ symmetry. □

So far, we have discussed applications in quantum mechanics, particle and nuclear physics in an elaborate fashion. Particularly, we have examined the tensor product of $SU(2)$, $SU(3)$ representations which is generalizable for $SU(N)$ groups and their relevance to selection rules and elementary particle multiplets. In the following section, we will discuss the non-compact group symmetry which forms the backbone of quantum theories in 3+1 dimensional flat space-time (also known as Minkowski space-time).

6.5 Non-compact Groups

We will discuss the non-compact group symmetries like Lorentz group, Poincare groups, conformal groups in this section.

6.5.1 The Lorentz group

The Lorentz group $SO(3,1)$ is a set of $\{\Lambda\}$ 4×4 matrices with real matrix elements and determinant $+1$ satisfying

$$\Lambda^T \eta \Lambda = \eta,$$

where η is a 4×4 diagonal matrix (also known as Minkowski metric):

$$\eta = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}.$$

Using the above condition, we can deduce that the number of independent matrix elements is 6. That is, there must be six Lie algebra generators. These 4×4 matrices Λ act on the four-dimensional space-time coordinates $x^\mu = (x^0, \vec{x}) = (ct,\ x,\ y,\ z)$. Alternatively, the group is a set of transformations

$$x^\mu \to x'^\mu = \Lambda^\mu_\nu x^\nu; \equiv \begin{pmatrix} ct' \\ x' \\ y' \\ z' \end{pmatrix} = \Lambda^\mu_\nu \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix}$$

such that

$$(cdt \quad dx \quad dy \quad dz) \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} cdt \\ dx \\ dy \\ dz \end{pmatrix} =$$

$$(cdt' \quad dx' \quad dy' \quad dz') \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \begin{pmatrix} cdt' \\ dx' \\ dy' \\ dz' \end{pmatrix}.$$

The familiar rotation group $SO(3)$ in the three-dimensional space $(x,\ y,\ z)$ is a subgroup $SO(3,1)$. Besides the rotation operation, we can also consider the following operation called Lorentz transformation by boosting along the x-direction:

$$t' = \frac{t - \frac{v_x x}{c^2}}{\sqrt{1 - \frac{v_x^2}{c^2}}}; \quad x' = \frac{x - v_x t}{\sqrt{1 - \frac{v_x^2}{c^2}}}; \quad y' = y; \quad z' = z, \tag{6.5.1}$$

where v_x is the x-component boost velocity which serves as one of the parameters of the Lorentz group. Thus, the parameters corresponding to three rotations $\theta_x, \theta_y, \theta_z$ about the x, y, z axes plus the three boost parameters v_x, v_y, v_z corresponding to Lorentz transformation along x, y, z directions combine to give six independent parameters. We can determine the matrix form of the corresponding generators associated with the infinitesimal transformations.

Generators of the Lorentz group

The generators of rotation for the Lorentz group along the three coordinate axes (x, y, z) are the same as the generators of the $SO(3)$ group that forms a closed algebra of angular momentum operators L as discussed in Chapter 5. Instead of our earlier notion of rotation about axis, we will state the rotation operation in a plane so that the we can generalize the operation to four-dimensional Minkowski space-time as well as rotations in any higher dimensional space. For example, consider an infinitesimal rotation about z-axis. We will denote the rotation parameter as $\delta\phi_{xy}$ (as a rotation about z-axis which mixes x and y components):

$$R(\delta\theta_z) \equiv R(\delta\phi_{xy}), \tag{6.5.2}$$

$$R(\delta\phi_{xy}) = \begin{pmatrix} \cos\delta\phi_{xy} & -\sin\delta\phi_{xy} & 0 \\ \sin\delta\phi_{xy} & \cos\delta\phi_{xy} & 0 \\ 0 & 0 & 1 \end{pmatrix} = \mathbb{I} + \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \delta\phi_{xy} = \mathbb{I} + L_{xy}\delta\phi_{xy},$$

where $L_{xy} = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ is the generator for rotation in the x-y plane and $\delta\phi_{xy}$ is the corresponding parameter for this transformation. The matrix form of these generators must be 4×4 in the four-dimensional Minkowski space-time. That is we should add an extra first row and a first column associated with the time coordinate with 0 as entries:

$$L_{xy} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{6.5.3}$$

Similarly, the generators for rotation in the y-z plane (about the x-axis) and z-x plane (about the y-axis) respectively are

$$L_{yz} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}; \quad L_{zx} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \tag{6.5.4}$$

These three rotation generators in Equations 6.5.3 and 6.5.4 satisfy the commutation relation

$$[\hat{L}_i, \hat{L}_j] = \epsilon_{ijk}\hat{L}_k, \tag{6.5.5}$$

where $\hat{L}_p = \frac{1}{2}\epsilon_{pqr}L_{qr}$, with the $p,\ q,\ r \in (x,\ y,\ z)$ and ϵ_{pqr} is the Levi–Civita antisymmetric tensor of rank 3 where

$$\epsilon_{xyz} = \epsilon_{yzx} = \epsilon_{zxy} = -\epsilon_{yxz} = -\epsilon_{xzy} = -\epsilon_{zyx} = +1,$$

and zero otherwise. Similar to the matrix form of rotation generators, we will determine the matrix form of boost generators by rewriting the Lorentz transformation (6.5.1) operation using the notation $\beta = \frac{v_x}{c}; \gamma = \frac{1}{\sqrt{1-\beta^2}}$

$$\begin{pmatrix} ct' \\ x' \\ y' \\ z' \end{pmatrix} = \begin{pmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ct \\ x \\ y \\ z \end{pmatrix}. \tag{6.5.6}$$

Implementing the following change of variables:

$$\gamma = \cosh\phi_{xt} \ \text{ and } \ \beta\gamma = \sinh\phi_{xt} \Rightarrow \beta = \tanh\phi_{xt}, \tag{6.5.7}$$

where the quantity ϕ_{xt} is known in literature as 'rapidity' which is related to velocity v_x as $\phi_{xt} = \tanh^{-1}\beta$. The subscript xt on the rapidity parameter keeps track of the boost along x-direction which mixes the $x,\ t$ coordinates. We can now determine the boost generator from the infinitesimal transformation:

$$\Lambda(\delta\phi_{xt}) = \begin{pmatrix} \gamma & -\beta\gamma & 0 & 0 \\ -\beta\gamma & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \mathbb{I} + K_{xt}\delta\phi_{xt}, \tag{6.5.8}$$

where K_{xt} is the generator for Lorentz boost along x-direction and $\delta\phi_{xt}$ is the parameter corresponding to the transformation

$$\Lambda(\delta\phi_{xt}) = \begin{pmatrix} \cosh\delta\phi_{xt} & -\sinh\delta\phi_{xt} & 0 & 0 \\ -sinh\delta\phi_{xt} & cosh\delta\phi_{xt} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \mathbb{I} + \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \delta\phi_{xt}. \tag{6.5.9}$$

So, now, comparing Equations 6.5.8 and 6.5.9, we get the Lorentz boost generator along x-direction:

$$K_{xt} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{6.5.10}$$

Similarly, the generators for boost along the y-direction and z-direction respectively are

$$K_{yt} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \quad K_{zt} = \begin{pmatrix} 0 & 0 & 0 & -1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}. \tag{6.5.11}$$

Rewriting $\hat{K}_i = K_{it}$ where i denotes the $x,\ y,\ z$ coordinates, it is simple to verify that the matrices in Equations 6.5.10, 6.5.11, 6.5.3 and 6.5.4 satisfy the following commutation relations:

$$[\hat{K}_i, \hat{K}_j] = -\epsilon_{ijk}\hat{L}_k, \tag{6.5.12}$$

$$[\hat{L}_i, \hat{K}_j] = \epsilon_{ijk}\hat{K}_k. \tag{6.5.13}$$

So, the six generators of the Lorentz group $(L_{xy},\ L_{yz},\ L_{zx},\ K_{xt},\ K_{yt},\ K_{zt})$ satisfy the three commutation relations given in Equations 6.5.5, 6.5.12 and 6.5.13. The Lie algebra of the Lorentz group is based on these three commutation relationships of the generators.

The rotation group is compact, i.e., the parameter space for rotation, consisting of angles, is bound between 0 and $2\pi (0 \leq \phi_{xy}, \phi_{yz},\ \phi_{zx} \leq 2\pi)$; while the boost operation is non-compact, i.e., the parameter space for boost transformations ranges from $-\infty$ to $\infty (-\infty \leq \phi_{xt}, \phi_{yt},\ \phi_{zt} \leq \infty)$, although the boost velocity is constrained by the special theory of relativity by $-c \leq v_x,\ v_y,\ v_z \leq c$.

Thus the Lorentz group $SO(3,1)$ is a non-compact group whose Lie algebra involves three rotation generators as well as three boost generators.

6.5.2 Poincare group

Besides the Lorentz group symmetry, physical systems can respect space translational and the time translational symmetry. The generators of the space-time translation in relativistic notation is four momentum vector: $p^\mu = (E/c, \vec{p})$. Recall that the linear momentum $\vec{p}$ corresponds to space translation generator and energy E corresponds to the time translational generator. The readers can extend the algebra by including $E,\ p_x,\ p_y, p_z$ along with the six Lorentz generators and thereby construct Poincare algebra.

6.5.3 Scale invariance

All physical systems near their phase transition point are called critical systems. For example, near liquid-vapor phase transition, water molecules of all possible sizes will be present. In other words, the systems at criticality possess scale symmetry: $x'^\mu = \exp(\alpha)x^\mu$.

Example 61. Determine the generator D for the scale transformation:

$$x'^\mu = \exp(\alpha)x^\mu.$$

For infinitesimal scale transformation any function

$$f\left(x'^\mu\right) = f\left(x^\mu + \alpha x^\mu\right) = f(x^\mu) + \alpha x^\mu \frac{\partial}{\partial x^\mu} f(x^\mu),$$

implying that the generator is

$$D = x^\mu \frac{\partial}{\partial x^\mu}.$$

6.5.4 Conformal group

In addition to the scaling symmetry and Poincare symmetry, there is a symmetry called special conformal transformation which is defined as follows:

$$x^\mu \to x'^\mu = \frac{x^\mu}{|x|^2} \to x''^\mu = x'^\mu + b^\mu \to x'''^\mu = \frac{x''^\mu}{|x''|^2}.$$

In words, it is an inversion followed by a translation by vector b^μ and again another inversion. There will be four generators associated with the four parameters. The algebra of $E,\ p_x,\ p_y, p_z,\ \hat{L}_i, \hat{K}_i, D$ plus the four special conformal transformation generators form an algebra called conformal algebra. These symmetries find applications in quantum field theories called conformal field theories, the conformal group symmetries. Interested readers can pursue these areas for research.

6.6 Dynamical Symmetry in Hydrogen Atom

The resemblance between the Kepler problem of planetary motion and the charged particle in Coulombic potential motivates us to understand symmetries possessed by such systems. We can formally write the Hamiltonian as

$$H = \frac{\vec{p}^2}{2\mu} - \frac{\kappa}{r}, \tag{6.6.1}$$

where μ is the reduced mass $[Mm/(M+m)], \kappa = GMm$ (for gravitational potential) and $\kappa = Ze^2$ (for Coulombic potential where Z is the atomic number). These systems possess rotational symmetry and hence the angular momentum $\vec{L} = \vec{r} \times \vec{p}$ (generators of rotations in three-dimensional space) is a conserved quantity. Further, for such a central force potential satisfying the inverse-square law, there is one another conserved quantity known as the *Runge–Lenz* vector:

$$\vec{M} = \frac{\vec{p} \times \vec{L}}{\mu} - \frac{\kappa}{r}\hat{r}. \tag{6.6.2}$$

Unlike the geometrical interpretation for rotation generators, we do not have a geometrical description for the Runge–Lenz vector. Hence we say that $\vec{M}$ represents generators of dynamical (hidden) symmetry. Classically, $\vec{M}$ satisfies the following relations:

$$\vec{L} \cdot \vec{M} = 0 \;\; ; \;\; \vec{M}^2 = \frac{2H}{\mu}\vec{L}^2 + \kappa^2, \tag{6.6.3}$$

where H is the Hamltonian of the system.

The quantum mechanical operator $\hat{M}$ of the classical Runge–Lenz vector $\vec{M}$ will be defined as follows:

$$\hat{M} = \frac{1}{2\mu}(\hat{p} \times \hat{L} - \hat{L} \times \hat{p}) - \frac{\kappa}{r}\hat{r}, \tag{6.6.4}$$

as we require Hermitian operators corresponding to observables in quantum mechanics. This operator (6.6.4) commutes with the Hamiltonian, $[\hat{M},\ H] = 0$, and hence is a conserved quantity. The relations in Equation 6.6.3 become

$$\hat{L} \cdot \hat{M} = \hat{M} \cdot \hat{L} = 0 \;\; ; \;\; \hat{M}^2 = \frac{2H}{\mu}(\hat{L}^2 + \hbar^2) + \kappa^2. \tag{6.6.5}$$

We will now present the Lie algebra determined by working out the commutator brackets amongst the components of $\hat{M}$ as well as the commutator bracket between $\hat{M}$ and $\hat{L}$.

6.6.1 Lie algebra symmetry

The commutation relations satisfied by the components $M_x,\ M_y,\ M_z$ are as follows:

$$[M_i,\ L_i] = 0, \tag{6.6.6}$$

$$[M_i,\ L_j] = i\hbar\epsilon_{ijk}M_k, \tag{6.6.7}$$

$$[M_i,\ M_j] = -\frac{2i\hbar}{\mu}\epsilon_{ijk}HL_k, \tag{6.6.8}$$

where $i,\ j,\ k = x,\ y,\ z = 1, 2, 3$.

Replacing the Hamiltonian operator H by its corresponding energy eigenvalue E, and rescaling M as

$$\hat{M} \to \hat{M}' = a\hat{M},$$

the commutation relation (6.6.8) becomes

$$\frac{1}{a^2}[M'_x,\ M'_y] = \left(-\frac{2i\hbar}{\mu}E\right) L_z. \tag{6.6.9}$$

So, the M_i's and L_i's as generators constitute a closed SO(4) algebra if

$$a^2\left(\frac{-2}{\mu}E\right) = 1 \Rightarrow a = \left(-\frac{\mu}{2E}\right)^{1/2}, \tag{6.6.10}$$

$$\hat{M}' = \left(-\frac{\mu}{2E}\right)^{1/2}\hat{M}. \tag{6.6.11}$$

Using this rescaling factor, Equation 6.6.8 becomes

$$[M'_i,\ M'_j] = i\hbar\epsilon_{ijk}L_k. \tag{6.6.12}$$

Comparing with the exercise problem (14), these generators can be mapped to $SO(4)$ group generators as follows:

$$\hat{M}'_i \equiv L_{i4};\ \hat{L}_i \equiv \frac{1}{2}\epsilon_{ijk}L_{jk},$$

In other words, we have to add a fourth fictitious coordinate ω such that the following operation defines $SO(4)$ group operation:

$$\begin{pmatrix} x' \\ y' \\ z' \\ \omega' \end{pmatrix} = e^{\Sigma_{i<j}\theta_{ij}L_{ij}} \begin{pmatrix} x \\ y \\ z \\ \omega \end{pmatrix}. \tag{6.6.13}$$

Thus the $SO(4)$ group symmetry respected by the hydrogen atom Hamiltonian has no geometric interpretation in the three-dimensional physical space. Hence the $SO(4)$ symmetry is referred to as the dynamical symmetry respected by the hydrogen atom.

In quantum mechanics textbooks, the hydrogen atom energy spectrum $E_n = -13.6eV/n^2$ is determined by solving the time independent Schrödinger equation. In the following subsection, our aim is to highlight the power of SO(4) dynamical symmetry. By exploiting this dynamical symmetry, we obtain the energy levels of the hydrogen atom ($1/n^2$ dependence of energy spectrum) without solving the Schrödinger equation.

6.6.2 Energy levels of hydrogen atom

The SO(4) group (generated by operators $\hat{L}$ and $\hat{M}'$) can be decomposed into two independent SU(2) groups. That is,

$$SO(4) \equiv SU(2) \times SU(2).$$

The generators of the two $SU(2)$ groups are

$$\hat{I} = \frac{1}{2}(\hat{L} + \hat{M}'); \quad K = \frac{1}{2}(\hat{L} - \hat{M}'), \tag{6.6.14}$$

which satisfies the following commutation relations:

$$[I_i,\ I_j] = i\hbar\epsilon_{ijk}I_k,$$

$$[K_i,\ K_j] = i\hbar\epsilon_{ijk}K_k,$$

$$[\hat{I}, \hat{K}] = 0.$$

We observe that the algebra of the operators involving $\hat{I}$ and $\hat{K}$ form two independent $su(2)$ algebra which commutes with the Hamiltonian:

$$[\hat{I},\ H] = 0;\ [\hat{K}, H] = 0.$$

Hence we can construct states $|E,\ i,\ i_z,\ k,\ k_z\rangle$ which are simultaneous eigenstates of $\hat{I}_z, \hat{K}_z, H$ where E is the energy eigenvalue, $i,\ k$ denote highest weights and $i_z,\ k_z$ are the weights obtained by the operation of $\hat{I}_z, \hat{K}_z$ operators:

$$I_z|E,\ i,\ i_z,\ k,\ k_z\rangle = i_z\hbar|E,\ i,\ i_z,\ k,\ k_z\rangle,$$

$$K_z|E,\ i,\ i_z,\ k,\ k_z\rangle = k_z\hbar|E,\ i,\ i_z,\ k,\ k_z\rangle.$$

The highest weight can be obtained by the action of $\hat{I}.\hat{I} = I_z^2 + (I_+I_- + I_-I_+)$ and $\hat{K}.\hat{K} = K_z^2 + (K_+K_- + K_-K_+)$ on the states as follows:

$$\hat{I}.\hat{I}|E,\ i,\ i_z,\ k,\ k_z\rangle = i(i+1)\hbar^2|E,\ i,\ i_z,\ k,\ k_z\rangle,$$

$$\hat{K}.\hat{K}|E,\ i,\ i_z,\ k,\ k_z\rangle = k(k+1)\hbar^2|E,\ ;\ i,\ i_z,\ k,\ k_z\rangle \tag{6.6.15}$$

We now construct two new operators,

$$C_1 = \hat{I}.\hat{I} + \hat{K}.\hat{K}\ \ ; \qquad C_2 = \hat{I}.\hat{I} - \hat{K}.\hat{K}. \tag{6.6.16}$$

Using Equations 6.6.5 and 6.6.14, we can confirm that

$$C_2 = \hat{I}.\hat{I} - \hat{K}.\hat{K} = 0 \Rightarrow \hat{I}.\hat{I} = \hat{K}.\hat{K}. \tag{6.6.17}$$

The above condition forces that the highest weights $i,\ k$ cannot be independent but equal. Further incorporating this condition, the action of C_1 on the states will be

$$C_1|E,\ i,\ i_z,\ k,\ k_z\rangle = 2i(i+1)\hbar^2|E,\ i,\ i_z,\ k,\ k_z\rangle. \tag{6.6.18}$$

Substituting Equations 6.6.5, 6.6.11, 6.6.14, and 6.6.16, the form of the operator C_1 is:

$$C_1 = \frac{1}{2}(\hat{L}^2 + \hat{M}'^2) = -\frac{\hbar^2}{2} - \frac{\mu\kappa^2}{4H}. \tag{6.6.19}$$

Comparing the above equation with Equation 6.6.18, we deduce:

$$C_1|E,\ i,\ i_z,\ k,\ k_z\rangle = 2i(i+1)\hbar^2|E,\ i,\ i_z,\ k,\ k_z\rangle$$

$$= \left(-\frac{\hbar^2}{2} - \frac{\mu\kappa^2}{4E}\right)|E,\ i,\ i_z,\ k,\ k_z\rangle.$$

which implies

$$2i(i+1)\hbar^2 = -\frac{\hbar^2}{2} - \frac{\mu\kappa^2}{4E}, \tag{6.6.20}$$

indicating that the energy eigenvalues are

$$E_i = \frac{-\mu\kappa^2}{2\hbar^2(2i+1)^2}, \tag{6.6.21}$$

where we have put a subscript on the energy E to keep track of the highest weight i. Recall that the highest weights of $\mathfrak{su}(2)$ algebra could be half-odd integers or integers. Hence,

$$2i + 1 = n,$$

where n is always an integer. Substituting the value of κ for hydrogen atom, the energy eigenvalues (6.6.21) in terms of n are exactly same as that obtained from the Schrödinger equation:

$$E_n = -\frac{\mu e^4}{2\hbar^2 n^2}, \tag{6.6.22}$$

indicating that the integer n can be referred to as the principal quantum number. The energy levels in the hydrogen atom are degenerate with degeneracy of n^2. Interestingly, using the $SU(2) \times SU(2)$ symmetry arguments we can reproduce the degeneracy of the energy levels. The physical orbital angular momentum operator $\hat{L} = \hat{I} + \hat{K}$ involves addition of two $su(2)$ generators.

Applying the CG construction method, we can obtain eigenstates $|\ell\ell_z\rangle$ of $\hat{L}_z$ from the simultaneous eigenstates of I_z, K_z In fact, we can show that the the allowed highest weight $\{\ell\}$ corresponding to $\hat{L}$ generators will range from $i + k,\ i + k - 1,\ \ldots |i - k|$. Substituting $i = k$ (6.6.17) will give $\ell = 2i,\ 2i - 1,\ \ldots 0$. In terms of n, the range of $\ell = 0, 1,\ \ldots n - 1$. For each ℓ, the states $|\ell\ell_z\rangle$ allow $2\ell + 1$ states. The energy eigenvalues (6.6.22) are independent of both ℓ and ℓ_z accounting for degeneracy as

$$\text{degeneracy } = \sum_{\ell=0}^{n-1} (2\ell + 1) = n^2.$$

Exercises

1 Quadrapole moment tensor $Q(2,\ q)$ is derivable from the tensor product of $\vec{r} \otimes \vec{r} = \oplus_{q=-2}^{2} Q(2,\ q)$. Show that $Q(2,0) = 2z^2 - r^2$ and $Q(2,2) - Q(2,-2) = x^2 - y^2$.

2 Consider two spin 1/2 particles (proton and neutron) described by the Hamiltonian $H = k\hat{s}_n.\hat{s}_p$ where k is a constant. Find the symmetry possessed by the system and the corresponding conserved quantity. Determine the energy eigenstates and eigenvalues.

3 If $S(k,q)$ and $T(k,q)$ are two irreducuble tensor operators of rank k, prove that $\omega = \sum_{q=-k}^{k} (-1)^q T(k,q) S(k,-q)$ is a scalar operator.

4 A deuteron has spin 1. Use the Wigner–Eckart theorem to find the ratios of the expectation values of the electric quadrupole moment operator $Q(2,0)$ for the three orientations of deutron $(m = 0,\ +1,\ -1)$.

5 Using the Clebsch–Gordan coefficient,

$$\langle j_1 = j,\ j_2 = 2,\ m_1 = j,\ m_2 = 0 | J = j,\ m = j\rangle = \sqrt{\frac{j(2j-1)}{(j+1)(2j+3)}},$$

verify the following statement for quadrupole moment tensor: The static 2^k pole moment of a charge distribution has zero expectation value in any state with angular momentum $j < (k/2)$.

6 Show that the strong decay process $\rho^0 \to \pi^0\pi^0$ is forbidden.

7 The highest weight vector state for decimet irreducible representation belonging to $SU(3)$ group is

$$|3\boldsymbol{\mu}^{(1)}, 3\boldsymbol{\mu}^{(1)}\rangle \equiv |\begin{array}{|c|c|c|}\hline \ \ & \ \ & \ \ \\ \hline \end{array}\rangle = |uuu\rangle.$$

Determine the weight vector states corresponding to the remaining nine baryons in the decimet diagram using the CG construction method on the tensor product of three fundamental quarks $\begin{array}{|c|}\hline \ \ \\ \hline \end{array} \in SU(3)$.

8 Suppose an irreducible representation $\begin{array}{|c|c|c|}\hline \ \ & \ \ & \ \ \\ \hline \ \ \\ \cline{1-1} \end{array} \in SU(3)$ denotes a hypothetical particle multiplet. What will be the Young diagram depicting the corresponding antiparticle multiplet?

9 Suppose we rewrite the Lorentz group $SO(3,1)$ generators as $\mathrm{M_i} = \hat{L}_i + i\hat{\mathrm{K}}_\mathrm{i}$ and $\mathrm{N}_i = \hat{L}_i - i\hat{\mathrm{K}}_\mathrm{i}$. Note that the $M_i,\ N_i$ are complex conjugates of each other. Write the algebra satisfied by these M_i's and N_i's.

10 Suppose we are given a six-dimensional multiplet belonging to a irreducible representation of a unitary group of rank less than 3. How do we check whether the six states $|i\rangle$ belong to spin $5/2$ of $SU(2)$ ($\begin{array}{|c|c|c|c|c|}\hline \ \ & \ \ & \ \ & \ \ & \ \ \\ \hline \end{array}$) or symmetric tensor of rank 2 representation $\begin{array}{|c|c|}\hline \ \ & \ \ \\ \hline \end{array}$ of $SU(3)$? Explain.

11 Assume quarks occur in four flavors. For this case, determine the irreducible representations and their dimensions for baryons and mesons.

12 For quarks belonging to the fundamental representation of $SU(N)$, determine the dimensions of the meson multiplets.

13 Determine the irreducible representations and their dimensions for di-baryon bound states obtained from baryons belonging to the octet multiplet of $SU(3)$.

14 $SO(4)$ denotes the group of orthogonal matrices in four-dimensional space with determinant 1. (i) Using the orthogonality property, show that the number of independent parameters is 6. (ii) We know that $\phi_k (k = 1,2,3)$ denotes rotation

about the k-axis in three dimensions. Similarly, we can give geometrical meaning by choosing the six parameters as $\phi_{ij}(i > j,\ i = 1,2,3,4)$ to denote rotation in the i-j plane. Let $L_{ij} = r_i p_j - r_j p_i$ be the generators of rotation about i-j plane. Show that the generators obey a closed algebra.

Appendix A

Maschke's Theorem

Let V be a finite dimensional vector space (real or complex) and T a linear operator on V. The kernel of the transformation T is the subspace K of V on which T vanishes. The image of T is also a subspace of V, let this subspace be R. One seeks the condition on the operator T so that any given vector $v \in V$ can be expressed uniquely as $v = k + r$ for some $k \in K$ and $r \in R$. Notice that $v = (I - T)v + Tv$ and $Tv \in R$. If this representation of v is unique, then $(I - T)v \in K$. It follows that $T(I - T)v = 0$ for all $v \in V$ and one has the condition

$$T^2 = T \tag{A.0.1}$$

if $V = K \oplus R$. Conversely, suppose the above condition holds for T. If $u \in K \cap R$, then $Tu = 0$ and also there exists a $w \in V$ such that $Tw = u$. Then

$$u = Tw = TTw = Tu = 0.$$

It also follows from here that $v = (I - T)v + Tv$ is the desired unique representation of any given $v \in V$, i.e., $V = K \oplus R$. Any operator T that satisfies the condition A.0.1 is called a projection operator. The reader can easily construct an operator on $\mathbb{R}^2$ which has a non-trivial kernel but is not a projection operator.

Now let Γ_1 and Γ_2 be representations of a group G on vector spaces V and W respectively. A linear transformation T from V to W is said to be *G-linear* if

$$T \circ \Gamma_1(g) \ = \Gamma_2(g) \circ T$$

for all $g \in G$. K be the kernel of T and $L = T(V)$ be the subspace of W. If $l \in L$, then there exists a $v \in V$ such that $l = Tv$. For any $g \in G$, $\Gamma_2(g)l = \Gamma_2(g) \circ Tv = T \circ \Gamma_1(g)v$, i.e., $\Gamma_2(g)l \in L$. Hence, Γ_2 is a subrepresentation of G on L. A similar argument shows that Γ_1 is a subrepresentation of G on K.

THEOREM. *Let Γ be a representation of G on a finite dimensional vector space V (Real or Complex). If Γ is a subrepresentation on a subspace L of V, then Γ is a subrepresentation on another subspace K of V such that $V = K \oplus L$.*

PROOF. A basis of L in V can always be extended to a basis of V. Then the subspace K' spanned by basis vectors required for the extension is such that $V = K' \oplus L$. For every $v \in V$, one has $v = k + l$ uniquely for some $k \in K'$ and $l \in L$. Define the projection operator P on V such that $Pv = l$. Then K' is the kernel of P and L is the image of P. If P was G-linear, then the theorem follows from the discussion prior to the statement of the theorem. However P need not be G-linear. Consider the operator T defined as

$$T = \frac{1}{|G|} \sum_{g \in G} \Gamma(g^{-1}) P \Gamma(g).$$

By construction, T is G-linear (see also the discussion of Equation B.0.2). Also, for every $l \in L$, because L is invariant under $\Gamma(g)$ for all $g \in G$ and P is projection onto L, $Tl = l$. This shows that T a map of V into V whose image is the subspace L. For these same reasons, $T^2 = T$ and it follows that T is a projection. Let the kernel of T be K, so that one has by the property of projection operator T

$$V = K \oplus L$$

and Γ is a subrepresentation of G over the subspace K. □

The Maschke's theorem states that every representation of a finite group over a finite dimensional vector space (real or complex) is completely reducible. This is a direct consequence of the above result.

Appendix B

Schur's Lemma

Schur's Lemma is stated and proved in the following. Some of its consequences, as regards irreducible representations and their characters are also developed. It is assumed that the vector spaces are finite dimensional over real or complex numbers and the groups are finite. The reader should be familiar with the notation and terminology introduced in Sections 3.1 to 3.3.

LEMMA. *(Schur) Let* Γ_1 *and* Γ_2 *be irreducible representations of a group G over vector spaces* V_1 *and* V_2*. If T is a linear transformation of* V_1 *into* V_2 *such that*

$$T\Gamma_1(g) = \Gamma_2(g)T \tag{B.0.1}$$

for all g in G, then either T is an isomorphism of spaces V_1 *and* V_2 *or the kernel of T is* V_1*. In the case T is an isomorphism with* $\Gamma_1(g) = \Gamma_2(g)$ *for all g in G, T is an scaling transformation.*

PROOF. Let the image of T in V_2 be L. If L is a non-trivial proper subspace of V_2, then the condition implies that Γ_2 is a representation on L. This is not possible since Γ_2 is irreducible over V_2. Then L is either the null vector space or all of V_2. Similarly, the kernel K of T is either the null vector space or all of V_1.

In the case K is the null vector space and $L = V_2$, T is evidently an invertible linear transformation satisfying $T\Gamma_1(g)T^{-1} = \Gamma_2(g)$ for all g in G, i.e., Γ_1 and Γ_2 are equivalent. T may now be regarded as an invertible linear operator on the vector space $V(= V_1)$. There then exists a scalar $\lambda \neq 0$ and a vector $v \neq 0$ in V such that

$$Tv = \lambda v.$$

Assuming $\Gamma_1 = \Gamma_2 = \Gamma$, the linear span $\mathcal{L}(\{\Gamma(g)v\}_{g\in G})$ is a representation subspace of V, and by irreducibility of Γ, $\mathcal{L}(\{\Gamma(g)v\}_{g\in G}) = V$. Any vector $v' \in V$, can be expressed in the form $v' = \sum_{g\in G} \alpha_g \Gamma(g)v$ for some choice of scalars α_g. Then one has

$$Tv' = T\left(\sum_{g\in G} \alpha_g \Gamma(g)v\right) = \sum_{g\in G} \alpha_g T\Gamma(g)v = \sum_{g\in G} \alpha_g \Gamma(g)Tv$$

$$\Rightarrow Tv' = \lambda v'. \qquad \square$$

In the general case, a transformation T need not satisfy the condition (B.0.1). In order to successfully apply the Lemma, it is desirable to obtain a suitable transformation T_S from a given T so that T_S fits the condition. Consider the following expression for T_S:

$$T_S = \frac{1}{|G|} \sum_{g\in G} \Gamma_2(g^{-1})T\Gamma_1(g), \tag{B.0.2}$$

where Γ_1 and Γ_2 are irreducible representations of the the group G on vector spaces V_1 and V_2, while T is a linear transformation from V_1 into V_2. Clearly, T_S is also a linear transformation from V_1 into V_2. The form of T_S suggests an averaging of T over the group. For $h \in G$,

$$T_S\Gamma_1(h) = \frac{1}{|G|} \sum_{g\in G} \Gamma_2(g^{-1})T\Gamma_1(g)\Gamma_1(h)$$

$$\Rightarrow T_S\Gamma_1(h) = \frac{1}{|G|} \sum_{g\in G} \Gamma_2(h)\Gamma_2(h^{-1})\Gamma_2(g^{-1})T\Gamma_1(g)\Gamma_1(h)$$

$$\Rightarrow T_S\Gamma_1(h) = \Gamma_2(h)\left[\frac{1}{|G|} \sum_{g\in G} \Gamma_2((gh)^{-1})T\Gamma_1(gh)\right]$$

$$\Rightarrow T_S\Gamma_1(h) = \Gamma_2(h)T_S$$

which is exactly the condition one needs for application of the Lemma. In Equation B.0.2, if $\Gamma_1 = \Gamma_2 = \Gamma$, then T_S is a transformation of scale λ. If the degree of representation Γ is ℓ_Γ, then upon equating the trace of both sides of Equation B.0.2, one obtains

$$\lambda = \frac{tr(T)}{\ell_\Gamma}. \tag{B.0.3}$$

In this case, T_S is diagonal and each entry in the diagonal is equal to λ. Upon explicitly writing, say the element $(T_S)_{ii}$ from Equation B.0.2

$$\frac{\sum_{j=1}^{\ell_\Gamma} T_{jj}}{\ell_\Gamma} = \frac{1}{|G|} \sum_{g \in G} [\Gamma(g)]_{ik} T_{km} [\Gamma(g^{-1})]_{mi} \tag{B.0.3}$$

and because the matrix T is an arbitrary linear transformation, one can equate coefficients of T_{km} on both sides of above to obtain

$$\sum_{g \in G} [\Gamma(g)]_{ik} [\Gamma(g^{-1})]_{ml} = \frac{|G|}{\ell_\Gamma} \delta_{il} \delta_{km}.$$

Similar calculation for $\Gamma_1 \neq \Gamma_2$ readily leads to

$$\sum_{g \in G} [\Gamma_1(g)]_{ik} [\Gamma_2(g^{-1})]_{ml} = 0.$$

If it is further assumed that the representations are unitary, and noting that in such a case $[\Gamma(g^{-1})]_{ml} = \overline{[\Gamma(g)]}_{lm}$, the above two expressions combined give Equation 3.3.5

$$\sum_{g \epsilon G} [\Gamma(g)]_{ik} \overline{[\Theta(g)]}_{lm} = \frac{|G|}{\ell_\Gamma} \delta_{\Gamma\Theta} \delta_{il} \delta_{km}.$$

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