Group Theory

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Chapter 1

Abstract Group Theory

1.1 Group

A group is a set of elements that have the following properties:

1. Closure: if a and b are members of the group, $c = ab$ is also a member of the group.

2. Associativity: $(ab)c = a(bc)$ for all a, b, c in the group.

3. Unit element: there is an element e such that $ea = a$ for every element a in the group.

4. Inverse: to every element a there is a corresponding inverse element a^{-1} in the group such that $a^{-1}a = e$.

The following properties follow from the above definition:

1. Left cancellation: If $ax = ay$ then $x = y$ for all a in the group.
   Proof: $ax = ay \rightarrow a^{-1}(ax) = a^{-1}(ay) \rightarrow (a^{-1}a)x = (a^{-1}a)y \rightarrow ex = ey \rightarrow x = y$.

2. Unit element on the right: $ae = a = ea$.
   Proof: $a^{-1}(ae) = (a^{-1}a)e = ee = e = a^{-1}a$ and using the left cancellation law we have $ae = a$.

3. Inverse element on the right: $aa^{-1} = e = a^{-1}a$.
   Proof: $a^{-1}(aa^{-1}) = (a^{-1}a)a^{-1} = ea^{-1} = a^{-1} = a^{-1}e$. Using the left cancellation law, $aa^{-1} = e$.

4. Right cancellation: If $xa = ya$ then $x = y$ for all a in the group.
   Proof: $xa = ya \rightarrow (xa)a^{-1} = (ya)a^{-1} \rightarrow x(aa^{-1}) = y(aa^{-1}) \rightarrow xe = ye \rightarrow x = y$.

We note the importance of associativity in the above proofs.

The following identity is often useful:

$$(ab)^{-1} = b^{-1}a^{-1}$$

which follows from $(ab)^{-1}(ab) = 1 \rightarrow (ab)^{-1}a = b^{-1} \rightarrow (ab)^{-1} = b^{-1}a^{-1}$.

1.2 Abelian Group

If a group has a further property that $ab = ba$ for all a, b in the group, the group is called Abelian.

1.3 Subgroup

A subgroup is a set of elements within a group which forms a group by itself. Evidently, the unit element forms a subgroup by itself.

We note that the definition of a group does not require all elements to be distinct from one another. However, when two elements are identical, then one of them is redundant so that we usually assume that all elements are different. A group with n identical elements evidently has at least n identical subgroups.

1.4 Examples

1. Integers under addition. The unit element $e = 0$ and the inverse of an element a is $a^{-1} = -a$. This group is Abelian and infinite.

2. A set of all $n \times n$ unitary matrices U ($U^\dagger = U^{-1}$) under matrix multiplication. The unit element is the unit matrix and the inverse of U is $U^\dagger$ by definition. We have to show that a product of two unitary matrices is unitary .

$$\begin{aligned}(U_1U_2)^\dagger &= U_2^\dagger U_1^\dagger \\ &= U_2^{-1}U_1^{-1} \\ &= (U_1U_2)^{-1}\end{aligned}$$

3. The set of permutation operations that take ABC into ABC, ACB, BAC, CAB, BCA, CBA. The elements of the group are

$$e = \begin{pmatrix} A & B & C \\ A & B & C \end{pmatrix} \quad \alpha = \begin{pmatrix} A & B & C \\ B & C & A \end{pmatrix} \quad \beta = \begin{pmatrix} A & B & C \\ C & A & B \end{pmatrix}$$

$$\gamma = \begin{pmatrix} A & B & C \\ A & C & B \end{pmatrix} \quad \mu = \begin{pmatrix} A & B & C \\ C & B & A \end{pmatrix} \quad \nu = \begin{pmatrix} A & B & C \\ B & A & C \end{pmatrix}$$

The operation $\alpha\beta$ means: first do permutation β and then permutation α on the previous result. We show below that every permutation has an inverse permutation and two successive permutations correspond to a single permutation i.e. the permutations form a group.

We see from the above examples that "multiplication" can mean addition, matrix multiplication etc. or simply that one operation is performed on the result of the preceeding operation like in the example 3.

1.5 Multiplication Table

The group multiplication table is a matrix $M_{ab} = ab$, where a and b are elements of the group and the matrix element corresponding to row a and column b is given by the group multiplication ab. We illustrate this definition by constructing the multiplication table of the permutation group in the example 3 above.

	e	α	β	γ	μ	ν
e	e	α	β	γ	μ	ν
α	α	β	e	μ	ν	γ
β	β	e	α	ν	γ	μ
γ	γ	ν	μ	e	β	α
μ	μ	γ	ν	α	e	β
ν	ν	μ	γ	β	α	e

Thus, for example, the inverse of α is β and vice versa. The group is clearly not Abelian because e.g. $\alpha\gamma \neq \gamma\alpha$. The elements (e, γ) form a subgroup, so do (e, μ), (e, ν) and (e, α, β). Obviously, the unit element e forms a subgroup by itself.

The group multiplication table mathematically characterises the group. All groups with the same multiplication table are mathematically identical with respect to their group properties. The multiplication table has the following properties:

1. Rearrangement Theorem: In every row or column, each element must appear once and once only and therefore each row (column) is different from any other row (column).
   Proof: Suppose element b appears twice in the row a. This means that $ac = b$ and $ad = b$ where $c \neq d$. But this implies that $ac = ad \rightarrow c = d$ which is a contradiction. Thus element b cannot appear more than once and since the size of the row or column is the same as the number of elements in the group, it follows that each element must appear once and once only.

2. The multiplication table is symmetric across the diagonal when the group is Abelian because the elements commute with one another.

1.6 Cyclic Groups

A group of n elements is said to be cyclic if it can be generated from one element. The elements of the group must be

$$a, a^2, a^3, \ldots, a^n = e$$

n is called the order of the cyclic group. A cyclic group is evidently Abelian but an Abelian group is not necessarily cyclic. It is shown below that every non-cyclic group has at least a cyclic subgroup.

Examples of cyclic groups are the subgroups of the permutation group in the example 3. The subgroup (e, α, β) is the same as $(\alpha, \alpha^2 = \beta, \alpha^3 = e)$.

1.7 Order of an Element

Let $a \neq e$ be an element of a group. Form the products $a^2, a^3, \ldots$. a^2 must be either e or a different element from a because if $a^2 = a \rightarrow a = e$. If $a^2 \neq e$ we continue forming a^3. By a similar argument, a^3 must be either e or a different element from a and a^2. If $a, a^2, \ldots, a^n$ are distinct from each other and $a^n = e$ then n is called the order of element a. These elements form a cyclic group. Thus every group must have at least one cyclic subgroup. In the example 3 above, α and β are of order 3 and γ, μ, and ν are of order 2.

1.8 Properties of Finite Groups

We summarise below the properties of finite groups.

1. Every element a has a finite order n such that $a^n = e$.
2. Rearrangement Theorem: Multiplying all elements in a group by an arbitrary element reproduces the group. This has been proven above in the properties of the multiplication table.
3. Every non-cyclic group has at least a cyclic subgroup.

1.9 Cosets

If S is a subgroup of G and a is an element of G not in S, then the sets aS and Sa are called the left and right cosets of S respectively. a cannot be a unit element and therefore a coset can never be a group because it has no unit element. It is also evident that aS or Sa have no element in common with S for otherwise, a should be included in S. Morevoer, if b is

an element of G which is neither in S nor in aS, then bS has no element in common with either S or aS.
Proof: Let x and y be in S such that $ax = by$. We have $axy^{-1} = b$, but xy^{-1} is an element in S and therefore b is in aS which is a contradiction.

Consequently, a finite group can be factorised as

$$G = S + aS + bS + \ldots$$

but the factorisation is not unique. It depends on the choice of S, a, b, ..., etc. The number of factors must be finite and the factorisation must exhaust the group. Thus we have the following theorem:
Let h be the number of elements of a group G and g be the number of elements of a subgroup S of G. Then

$$\frac{h}{g} = integer$$

As a consequence, if h is prime then G must be cyclic and it has no subgroup other than the trivial subgroup of e.

1.10 Class

Two elements a and b of a group are conjugate to one another if there is an element g in the group such that

$$a = gbg^{-1} \tag{1.1}$$

(Since every element has an inverse, it also follows that $b = g'ag'^{-1}$ where $g' = g^{-1}$). The transformation gbg^{-1} is often called a similarity transformation. If a and b are conjugate to each other and b and c are conjugate to each other, then a and c are also conjugate to each other. This is because $a = g_1bg_1^{-1}$ and $b = g_2cg_2^{-1}$ $\rightarrow a = g_1g_2cg_2^{-1}g_1^{-1} = g_1g_2c(g_1g_2)^{-1}$.

A class C is a set of elements which are conjugate to each other. The unit element evidently forms a class by itself. If G is Abelian, each element also forms a class by itself. It is clear that a group may be broken up into classes

$$G = C_1 + C_2 + \ldots$$

and an element cannot belong to more than one class.

As an example, we work out one of the classes of the permutation group. In working out the classes, it is obviously not necessary to consider similarity transformations with either the unit element or the element itself. We use the multiplication table that we have constructed previously:

$$\begin{aligned}
\beta\alpha\beta^{-1} &= \beta\alpha\alpha = \beta\beta = \alpha \\
\gamma\alpha\gamma^{-1} &= \gamma\alpha\gamma = \gamma\mu = \beta \\
\mu\alpha\mu^{-1} &= \mu\alpha\mu = \mu\nu = \beta \\
\nu\alpha\nu^{-1} &= \nu\alpha\nu = \nu\gamma = \beta
\end{aligned}$$

Thus α and β belong to the same class. Similarly we can show that (γ, μ, ν) also form a class.

Elements belonging to the same class usually have the same characteristic. In the above example, α and β both correspond to cyclic permutations whereas γ, μ, and ν correspond to permutations with one member fixed.

1.11 Isomorphism and Homomorphism

Two groups are said to be isomorphic if they have the same multiplication table, by reordering the elements if necessary. If F is isomorphic to G then there is a one-to-one correspondence between the elements of F and G, $f_i \rightarrow g_i$, such that if $f_i f_j = f_k$ then $g_i g_j = g_k$. Two groups can only be isomorphic if they have the same number of elements. As an example, the permutation group in the example 3 is isomorphic to the symmetry operations that take an equilateral triangle into itself. This isomorphism can be seen by labelling the corners of the triangle with A, B, C.

Homomorphism is similar to isomorphism except that the relationship is many-to-one. Two groups G and G' are said to be homomorphic if each element of G can be associated with some elements of G': $a \rightarrow a' = (a'_1, a'_2, \ldots)$, $b \rightarrow b' = (b'_1, b'_2, \ldots)$, $c \rightarrow c' = (c'_1, c'_2, \ldots)$, such that if $ab = c$ then $a'_i b'_j = c'_k$ i.e. for every i, j, c'_k lies in c'.

1.12 Invariant Subgroup

We prove the following theorem:

Theorem: If S is a subgroup of G and a is an element of G then $S' = aSa^{-1}$ is also a subgroup and it is isomorphic to S. We assume that the elements of S are distinct.

Proof: We first show that the elements of S' are distinct. Let $as_ia^{-1} = as_ja^{-1}$ and $i \neq j$. Then by the cancellation law, $s_i = s_j$, which is a contradiction. Thus the elements of S' are distinct. We now show that if $s_is_j = s_k$ then $s'_is'_j = s'_k$. Proof: $s'_is'_j = as_ia^{-1}as_ja^{-1} = as_is_ja^{-1} = as_ka^{-1} = s'_k$. Thus S and S' are isomorphic with the same unit element $e' = aea^{-1} = e$ and the inverse of s'_i is $s'^{-1}_i = (as_ia^{-1})^{-1} = as_i^{-1}a^{-1} = (s_i^{-1})'$.

If S' is the same as S for every a in the group then the subgroup S is called an invariant subgroup. This implies that the left coset of S is the same as its right coset, i.e.

$$aS = Sa$$

If we break a group into its cosets,

$$G = S + aS + bS, \ldots$$

with an invariant subgroup S, then these cosets form a group with the unit element equal to S. Thus $aSbS = abSS = abS = cS$ if $ab = c$. This group is called a factor group. It is an example of homomorphism where the invariant subgroup S is associated with the elements of S and the coset aS is associated with the elements of aS.

1.13 Direct Product Group

Let F be a group with elements f_i, $i = 1, \ldots, h_F$, and G be a group with elements g_i, $i = 1, \ldots, h_G$, such that $f_ig_j = g_jf_i$ for all i and j. The direct product group $F \otimes G$ is defined to be the set of all distinct elements f_ig_j. If F and G have no common element, apart from the identity, then the order of the direct product group will be h_Fh_G.

We show that $F \otimes G$ is a group.

1. Closure: $(f_i g_j)(f_k g_l) = (f_i f_k)(g_j g_l) = f_r g_s$. Since f_r is in F and g_s is in G then by definition $f_r g_s$ is in $F \otimes G$.
2. Unit element is $e_F e_G$.
3. Inverse of $f_i g_j$ is $(f_i g_j)^{-1} = g_j^{-1} f_i^{-1} = f_i^{-1} g_j^{-1}$.
4. Associativity: obvious.

We have the following theorem:

Theorem: The classes of the direct product group are given by the direct products of the classes of the individual groups.

Proof: We label the elements of the product group $a_{ij} = f_i g_j$. According to the definition of a class, we have

$$\begin{aligned} C_{ij} &= a_{rs}^{-1} a_{ij} a_{rs}, \quad for \ \ all \ \ r, s \\ &= f_r^{-1} g_s^{-1} f_i g_j f_r g_s \\ &= (f_r^{-1} f_i f_r)(g_s^{-1} g_j g_s) \end{aligned}$$

Chapter 2

Theory of Group Representations

2.1 Definitions

A group $\{A, B, C, ...\}$ may be represented by a set of square matrices $\{T(A),\ T(B),\ T(C),\ \ldots\}$. These matrices are said to form a representation for the group if they satisfy the same group multiplication rule:

$$AB = C \rightarrow T(A)T(B) = T(C) \tag{2.1}$$

The identity element E is represented by a unit matrix and each matrix must have an inverse. Some or all of the matrices may be the same. If the matrices are different, the representation is called faithful (isomorphic). The order of the matrices is called the dimension of the representation.

2.2 Equivalent Representations

If T is a representation then

$$T' = S^{-1}TS \tag{2.2}$$

with an arbitrary but non-singular S is also a representation because

$$T'(A)T'(B) \;\; = \;\; S^{-1}T(A)SS^{-1}T(B)S$$

$$\begin{aligned} &= S^{-1}T(A)T(B)S \\ &= S^{-1}T(AB)S \\ &= T'(AB) \end{aligned}$$

T and T' are equivalent and there are an infinite number of equivalent representations.

2.3 Reducible and Irreducible Representation

A representation T is reducible if there exists a non-singular matrix S such that the equivalent representation $T' = S^{-1}TS$ has the form

$$T' = \begin{pmatrix} T_1 & & & & \\ & T_2 & & & \\ & & T_3 & & \\ & & & . & \\ & & & & . \end{pmatrix}$$

for all elements in the group. T_1, T_2, $T_3, \ldots$ are square matrices and the rest of the elements are zero. The representation is irreducible if it cannot be reduced into the above form.

2.4 Equivalent Unitary Representation

There are an infinite number of equivalent representations but it is possible to find one which is unitary.

Theorem 1:
Given an arbitrary representation T, there is always an equivalent unitary representation.

Proof:
Construct a Hermitian matrix

$$H = \sum_G T(G)T^\dagger(G)$$

According to matrix algebra, we can always diagonalise a Hermitian matrix by a unitary transformation

$$\begin{aligned} D &= U^{-1}HU \\ &= \sum_G U^{-1}T(G)T^\dagger(G)U \\ &= \sum_G U^{-1}T(G)UU^{-1}T^\dagger(G)U \\ &= \sum_G T'(G)T'^\dagger(G) \end{aligned}$$

U is made up of the eigenvectors of H and D is diagonal by definition and its diagonal elements are real and positive.

$$\begin{aligned} D_{jj} &= \sum_G \sum_k T'_{jk}(G)T'^\dagger_{kj}(G) \\ &= \sum_G \sum_k T'_{jk}(G)T'^*_{jk}(G) \\ &= \sum_G \sum_k |T'_{jk}(G)|^2 \geq 0 \end{aligned}$$

In fact, it can never be equal to zero because otherwise $T' = 0$. Since D is diagonal, we may define a diagonal matrix $D^{-1/2}$ with diagonal elements equal to $D_{ii}^{-1/2}$ so that

$$1 = D^{-1/2}\sum_G T'(G)T'^\dagger(G)D^{-1/2}$$

Using the above result, the matrix $T''(G) = D^{-1/2}T'(G)D^{1/2}$ can be shown to be unitary.

$$\begin{aligned} T''(G)T''^\dagger(G) &= D^{-1/2}T'(G)D^{1/2}[D^{-1/2}\sum_{G'} T'(G')T'^\dagger(G')D^{-1/2}] \\ &\times \; D^{1/2}T'^\dagger(G)D^{-1/2} \\ &= D^{-1/2}\sum_{G'} T'(G)T'(G')T'^\dagger(G')T'^\dagger(G)D^{-1/2} \\ &= D^{-1/2}\sum_{G'} T'(G)T'(G')[T'(G)T'(G')]^\dagger D^{-1/2} \\ &= D^{-1/2}\sum_{G'} T'(GG')T'^\dagger(GG')D^{-1/2} \end{aligned}$$

$$\begin{aligned} &= D^{-1/2} \sum_{G''} T'(G'') T'^{\dagger}(G'') D^{-1/2} \\ &= 1 \end{aligned}$$

The second last step has been obtained by using the Rearrangement Theorem. Thus, given an arbitrary representation T, it is always possible to construct a unitary representation by forming

$$T'' = D^{-1/2} U^{-1} T U D^{1/2} \tag{2.3}$$

From now on we assume that we have a unitary representation.

2.5 Schur's Lemma

Schur's lemma is used in proving many of the theorems in group theory.
Theorem 2 (Schur's lemma):
Given that $[M, T] = MT - TM = 0$ for all elements in the group, then
(a) if T is irreducible, $M = cI$ where c is a constant and I is a unit matrix.
(b) if $M \neq cI$ then T is reducible.

Proof: We first show that it is sufficient to prove the theorem for a Hermitian M.

$$\begin{aligned} TM &= MT \\ (TM)^{\dagger} &= (MT)^{\dagger} \\ M^{\dagger} T^{\dagger} &= T^{\dagger} M^{\dagger} \\ T(M^{\dagger} T^{\dagger}) T &= T(T^{\dagger} M^{\dagger}) T \\ TM^{\dagger} &= M^{\dagger} T \end{aligned}$$

since $T^{\dagger} = T^{-1}$ (unitary). Adding and substracting the first and the last equations, we get

$$T(M + M^{\dagger}) = (M + M^{\dagger}) T$$

and

$$T\, i(M - M^{\dagger}) = i(M - M^{\dagger})\, T$$

Let $H_1 = M + M^{\dagger}$ and $H_2 = i(M - M^{\dagger})$ so that $[H_1, T] = [H_2, T] = 0$. H_1 and H_2 are Hermitian and $M = 1/2(H_1 - iH_2)$. Thus, if the theorem is

true for a Hermitian matrix, it must be true for M. We can now assume M to be Hermitian and perform a unitary transformation so that M becomes diagonal, $D = U^{-1}MU$, and define an equivalent representation $T' = U^{-1}TU$. Then

$$\begin{aligned} T'D &= U^{-1}TUU^{-1}MU \\ &= U^{-1}TMU \\ &= U^{-1}MTU \\ &= U^{-1}MUU^{-1}TU \\ &= DT' \end{aligned}$$

We have to show that the diagonal elements of D are all identical if T, or equivalently T', is irreducible. Consider the ij, $i \neq j$, element,

$$\begin{aligned} T'_{ij}D_{jj} &= D_{ii}T'_{ij} \\ T'_{ij}(D_{jj} - D_{ii}) &= 0 \end{aligned} \tag{2.4}$$

Let us order the diagonal elements of D such that $D_{ii} \leq D_{jj}$ for $i < j$ which can always be done by rearranging the columns of U. Suppose $D_{11} = D_{nn}$ and $D_{11} < D_{ii}$ where $n \geq 1$ and $i > n$. Then it follows from Eq. (2.4) that T' must have the form

$$T' = \begin{pmatrix} X & 0 \\ 0 & Y \end{pmatrix}$$

where X is an $n \times n$ matrix, i.e. T' is reducible.

Let us summarise the conclusions: If $M \neq cI$ then T must be reducible. If $M = cI$ then obviously it commutes with T whether it is reducible or irreducible. Hence if T is irreducible then M must be equal to cI for otherwise T would be reducible.

Theorem 3:
Given $T^\alpha M = MT^\beta$, where T^α and T^β are irreducible representations of dimension l_α and l_β respectively and M is a rectangular $l_\alpha \times l_\beta$ matrix, then
(a) if $l_\alpha \neq l_\beta$, $M = 0$ or
(b) if $l_\alpha = l_\beta$ either $M = 0$ or $|M| \neq 0$. In the latter case, M will have an

inverse so that T^α and T^β are equivalent.

Proof:

$$\begin{aligned}
T^\alpha(G)M &= MT^\beta(G) \\
(T^\alpha(G)M)^\dagger &= (MT^\beta(G))^\dagger \\
M^\dagger T^{\alpha\dagger}(G) &= T^{\beta\dagger}(G)M^\dagger \\
M^\dagger T^{\alpha -1}(G) &= T^{\beta -1}(G)M^\dagger \\
MM^\dagger T^{\alpha -1}(G) &= MT^{\beta -1}(G)M^\dagger \\
MM^\dagger T^{\alpha}(G^{-1}) &= MT^{\beta}(G^{-1})M^\dagger \\
MM^\dagger T^{\alpha}(G^{-1}) &= T^{\alpha}(G^{-1})MM^\dagger
\end{aligned}$$

Since T^α is irreducible, it follows from Schur's lemma (Theorem 2) that $MM^\dagger = cI$. Consider the case $l_\alpha = l_\beta$.

$$|MM^\dagger| = |cI|; \;\; |M||M^\dagger| = ||M||^2 = c^{l_\alpha}$$

If $c \neq 0$, then $|M| \neq 0$ i.e. M^{-1} exists. It follows that T^α and T^β are equivalent since

$$M^{-1}(T^\alpha(G)M) = M^{-1}(MT^\beta(G)) = T^\beta(G)$$

If $c = 0$, then $MM^\dagger = 0$. Let us look at the diagonal elements of $MM^\dagger$:

$$\begin{aligned}
\sum_k M_{ik}M^\dagger_{ki} &= 0 \\
\sum_k M_{ik}M^*_{ik} &= 0 \\
\sum_k |M_{ik}|^2 &= 0
\end{aligned}$$

Since this is positive definite, each term must vanish i.e. $M = 0$. Consider now the case $l_\alpha \neq l_\beta$, $l_\alpha > l_\beta$. We enlarge M into a $l_\alpha \times l_\alpha$ square matrix N with the additional elements equal to zero. Then $NN^\dagger = MM^\dagger = cI$. But $|N| = 0$ because one of its columns is zero.

$$NN^\dagger = cI \rightarrow |NN^\dagger| = c^{l_\alpha} \rightarrow |N||N^\dagger| = c^{l_\alpha} \rightarrow c = 0$$

Hence $NN^\dagger = 0$ which implies $N = 0$. Since M is contained in N, then $M = 0$.

2.6 Orthogonality Theorem

We are now in a position to prove the Orthogonality Theorem which is central in representation theory.

Theorem 4: Orthogonality Theorem

$$\sum_G T^\alpha_{ij}(G)^* T^\beta_{kl}(G) = (h/l_\alpha)\delta_{\alpha\beta}\delta_{ik}\delta_{jl} \tag{2.5}$$

α and β label the irreducible representations, l_α and l_β are the dimensions of these irreducible representations, and h is the number of elements in the group.

Proof:
Define a matrix

$$M = \sum_G T^\alpha(G) X T^\beta(G^{-1})$$

where X is an arbitrary matrix and $\alpha \neq \beta$. We want to show that this matrix satisfies the postulates of Theorem 3. Consider

$$\begin{aligned}
T^\alpha(A)M &= \sum_G T^\alpha(A)T^\alpha(G)XT^\beta(G^{-1}) \\
&= \sum_G T^\alpha(A)T^\alpha(G)XT^\beta(G^{-1})T^\beta(A^{-1})T^\beta(A) \\
&= \sum_G T^\alpha(AG)XT^\beta(G^{-1}A^{-1})T^\beta(A) \\
&= \sum_G T^\alpha(AG)XT^\beta((AG)^{-1})T^\beta(A) \\
&= \sum_G T^\alpha(AG)XT^{\beta^{-1}}(AG)T^\beta(A) \\
&= \sum_G [T^\alpha(G)XT^{\beta^{-1}}(G)]T^\beta(A) \\
&= MT^\beta(A)
\end{aligned}$$

We have again made use of the Rearrangement Theorem in the second last step. According to Theorem 3, $M = 0$ since we are considering the case of $\alpha \neq \beta$ so that

$$M_{ij} = 0 = \sum_G \sum_{kl} T^\alpha_{ik}(G) X_{kl} T^\beta_{lj}(G^{-1})$$

Since X is arbitrary, we may set $X_{kl} = \delta_{km}\delta_{ln}$. Then

$$\begin{aligned}\sum_G T^\alpha_{im}(G)T^\beta_{nj}(G^{-1}) &= \sum_G T^\alpha_{im}(G){T^\beta}^{-1}_{nj}(G) \\ &= \sum_G T^\alpha_{im}(G){T^{\beta\dagger}}_{nj}(G) \\ &= \sum_G T^\alpha_{im}(G){T^{\beta *}}_{jn}(G) \\ &= 0\end{aligned}$$

When $\alpha = \beta$, according to Schur's lemma (Theorem 2)

$$\begin{aligned}M_{ij} = c\,\delta_{ij} &= \sum_G\sum_{kl} T^\alpha_{ik}(G)X_{kl}T^\alpha_{lj}(G^{-1}) \\ &= \sum_G T^\alpha_{im}(G)T^\alpha_{nj}(G^{-1})\end{aligned}$$

Putting $i = j$ and summing over i yields

$$\begin{aligned}c\,l_\alpha &= \sum_G\sum_i T^\alpha_{im}(G)T^\alpha_{ni}(G^{-1}) \\ &= \sum_G T^\alpha_{nm}(E) \\ &= h\delta_{nm}\end{aligned}$$

Thus we have

$$\sum_G T^\alpha_{im}(G)T^\alpha_{nj}(G^{-1}) = (h/l_\alpha)\delta_{nm}\delta_{ij}$$

Since T is unitary,

$$\sum_G T^\alpha_{im}(G)T^\alpha_{jn}(G)^* = (h/l_\alpha)\delta_{nm}\delta_{ij}$$

Eqn. (2.5) has the form of a dot product with $T^\alpha_{ij}(G)$ as the G'th component of a vector labelled by α, i and j, in the h dimensional space of the group elements. This means that the number of distinct labels (α, i, j) cannot exceed h, i.e. $\sum_\alpha l^2_\alpha \le h$. It will be proven later that in fact

$$\sum_\alpha l^2_\alpha = h$$

The result is very useful in working out the irreducible representations of a group.

2.7 The Characters of a Representation

We have seen that a representation is not unique. We recall that if T is a representation, so is $T' = S^{-1}TS$. Given T and T', how can we then tell that they are equivalent ? One way will be to figure out if there is a matrix S, such that $T' = S^{-1}TS$. But this is a complicated procedure. What we are looking for are properties of a matrix which are invariant under a similarity transformation. The eigenvalues are one of them but they are too cumbersome to calculate. A simpler quantity is the trace of a matrix or the sum of the diagonal elements:

$$\chi^{\alpha}(G) = Tr\ T^{\alpha}(G) = \sum_i T^{\alpha}_{ii}(G) \tag{2.6}$$

We show that the trace or character of a matrix is invariant under a similarity transformation:

$$\begin{aligned} Tr\ T' &= \sum_i \sum_{jk} S^{-1}_{ij} T_{jk} S_{ki} \\ &= \sum_{jk} (\sum_i S_{ki} S^{-1}_{ij}) T_{jk} \\ &= \sum_{jk} \delta_{kj} T_{jk} \\ &= Tr\ T \end{aligned}$$

The characters of a representation α is a set of h numbers $\{\chi^{\alpha}(G)\}$. It will be shown later that if the representation is irreducible, its characters are unique.

Theorem 5:
If elements A and B of a group belong to the same class, then the characters of their representations are the same.

Proof:
Since A and B belong to the same class, there is an element C such that $A = C^{-1}BC$. Consequently,

$$Tr\ T(A) = Tr\ [T(C^{-1})\ T(B)\ T(C)]$$

$$\begin{aligned} &= Tr\,[T(C)\,T(C^{-1})\,T(B)] \\ &= Tr\,[T(E)\,T(B)] \\ &= Tr\,T(B) \end{aligned}$$

Theorem 6: First Orthogonality Relation

$$\sum_G \chi^\alpha(G)^*\chi^\beta(G) = \sum_k \chi^\alpha(C_k)^*\chi^\beta(C_k)N_k = h\delta_{\alpha\beta} \tag{2.7}$$

C_k labels a class with N_k elements.

Proof:
Setting $i = j$ and $k = l$ in Eqn. (2.5) (Orthogonality Theorem) and summing over i and l we have

$$\begin{aligned} \sum_G \chi^\alpha(G)^*\chi^\beta(G) &= (h/l_\alpha)\delta_{\alpha\beta}\sum_{il}\delta_{il}\delta_{il} \\ \sum_k \chi^\alpha(C_k)^*\chi^\beta(C_k)N_k &= h\delta_{\alpha\beta} \end{aligned}$$

Eqn. (2.7) has the form of a weighted dot product with weight N_k in a space with dimension equal to the number of classes of the group. $\chi^\alpha(C_k)$ is the k'th component of vector α. It follows that the number of irreducible representations must be less than or equal to the number of classes.

2.8 The Regular Representation

We prove the following theorem:
Theorem 7:

$$\sum_\alpha l_\alpha^2 = h \tag{2.8}$$

Proof:

A proof of this theorem is provided by considering the so called regular representation. The regular representation is formed in the following way. We write the multiplication table as follows:

	e	α	β	γ	...
e	e				
α^{-1}		e			
β^{-1}			e		
γ^{-1}				e	

We form the regular representation of an element a by writing 1 wherever the element a occurs in the table and zero otherwise. Let the group elements be $a_i,\ i = 1, 2, \ldots, h$, then the regular representation is given by

$$\begin{aligned} T_{jk}(a_i) &= 1 \ \ if \ \ a_j^{-1} a_k = a_i \\ &= 0 \ \ otherwise \end{aligned}$$

It is clear from the definition that the representation is faithful. To show that it is really a representation, we have to prove that

$$\sum_k T_{jk}(a_i) T_{kl}(a_m) = T_{jl}(a_p)$$

if and only if $a_i a_m = a_p$. By definition, $T_{jk}(a_i) \neq 0$ only when k is such that $a_k = a_j a_i$ and similarly $T_{kl}(a_m) \neq 0$ only when k is such that $a_k = a_l a_m^{-1}$. Therefore $\sum_k T_{jk}(a_i) T_{kl}(a_m) = 1$ if and only if $a_k = a_j a_i = a_l a_m^{-1}$ and zero otherwise. However, $a_j a_i = a_l a_m^{-1}$ implies $a_j^{-1} a_l = a_i a_m = a_p$.

The character is given by

$$\begin{aligned} \chi(a_i) = \sum_{j=1}^{h} T_{jj}(a_i) &= h \ \ if \ \ a_i = e \\ &= 0 \ \ otherwise \end{aligned}$$

This is clear by inspection of the multiplication table. We can now prove Theorem 7 by writing the character of the regular representation as a sum over characters of the irreducible representations:

$$\chi(a_i) = \sum_\alpha m_\alpha \chi^\alpha(a_i)$$

From the orthogonality relation we have

$$m_\alpha = \frac{1}{h}\sum_i \chi^{\alpha *}(a_i)\chi(a_i)$$

Since $\chi^\alpha(e) = l_\alpha$, $\chi(e) = h$, and $\chi(a_i \neq e) = 0$ it follows that $m_\alpha = l_\alpha$. Each irreducible representation occurs in the regular representation a number of times equal to the dimension of the irreducible representation. On the other hand, $h = \sum_\alpha m_\alpha l_\alpha$ so that

$$h = \sum_\alpha l_\alpha^2$$

This result together with the orthogonality theorem show that there are exactly h orthogonal vectors T_{ij}^α.

Theorem 8: Second Orthogonality Relation

$$\sum_\alpha \chi^\alpha(C_k)^* \chi^\alpha(C_l) = (h/N_k)\delta_{kl} \tag{2.9}$$

Proof:
We recall that the matrix representation T_{ij}^α can be regarded as a set of orthogonal vectors in the h- dimensional space of the group elements. $T_{ij}^\alpha(G)$ is the component of the vector T_{ij}^α along the "G-axis". T_{ij}^α themselves can be regarded as a basis in the space of the group elements since the number of α, i, j is precisely h. Any vector in this space can therefore be expanded in T_{ij}^α:

$$\chi = \sum_{\alpha ij} c_{\alpha ij} T_{ij}^\alpha$$

We sum the components of χ along G-axes which belong to a given class C_k,

$$\begin{aligned}
\chi(C_k) &= \sum_{G\in C_k} \chi(G) \\
&= \sum_{G\in C_k}\sum_{\alpha ij} c_{\alpha ij} T_{ij}^\alpha(G) \\
&= \frac{1}{h}\sum_{G_1}\sum_{G\in C_k}\sum_{\alpha ij} c_{\alpha ij} T_{ij}^\alpha(G_1^{-1}GG_1)
\end{aligned}$$

$$\begin{aligned}
&= \frac{1}{h}\sum_{G_1}\sum_{G\in C_k}\sum_{\alpha ij}\sum_{kl} c_{\alpha ij}T^{\alpha}_{ik}(G_1^{-1})T^{\alpha}_{kl}(G)T^{\alpha}_{lj}(G_1)\\
&= \sum_{G\in C_k}\sum_{\alpha ij}\sum_{kl} c_{\alpha ij}\delta_{ij}\delta_{kl}T^{\alpha}_{kl}(G)/l_\alpha\\
&= \sum_{G\in C_k}\sum_{\alpha i} c_{\alpha ii}\chi^{\alpha}(G)/l_\alpha\\
&= \sum_{\alpha} a_\alpha \chi^{\alpha}(C_k)
\end{aligned}$$

where $a_\alpha = (N_k/l_\alpha)\sum_i c_{\alpha ii}$. The third step uses the fact that $G_1^{-1}C_kG_1 = C_k$ for every G_1 in the group, the fifth step uses the orthogonality theorem, and the last step uses the fact that the characters of elements belonging to the same class are identical. Thus the set of vectors $\{\chi(C_k)\}$ are linearly independent because the group elements can be divided uniquely and completely into distinct classes.

Multiplying $\chi(C_k)$ by $\chi^{\beta *}(C_k)N_k$ and summing over the classes k yields

$$\begin{aligned}
\sum_k \chi(C_k)\chi^{\beta *}(C_k)N_k &= \sum_\alpha a_\alpha \sum_k \chi^{\alpha}(C_k)\chi^{\beta *}(C_k)N_k\\
&= \sum_\alpha a_\alpha h\delta_{\alpha\beta}\\
&= ha_\beta
\end{aligned}$$

Consequently,

$$\begin{aligned}
\chi(C_l) &= \sum_\beta a_\beta \chi^{\beta}(C_l)\\
&= (1/h)\sum_\beta\sum_k \chi(C_k)\chi^{\beta *}(C_k)N_k\chi^{\beta}(C_l)\\
0 &= \sum_k \chi(C_k)\left[(N_k/h)\sum_\beta \chi^{\beta *}(C_k)\chi^{\beta}(C_l) - \delta_{kl}\right]
\end{aligned}$$

This is true for an arbitrary $\chi(C_k)$ so that the quantity in the square bracket must vanish which proves the theorem.

Eqn. (2.9) has the form of a dot product in a space with dimension equal to the number of irreducible representations. It follows that the number of classes must be less than or equal to the number of irreducible representations. On the other hand by Theorem 6 the number of irreducible

representations must be less than or equal to the number of classes. Thus we conclude the following corollary:

The number of irreducible representations is equal to the number of classes.

Theorem 6 and 8 imply that the irreducible representations are uniquely characterised by their characters and consequently two distinct irreducible representations cannot have the same set of characters.

2.9 The Character Table

The character table is a square matrix with dimension equal to the number of classes or irreducible representations:

$$Q_{\alpha k} = \chi^{\alpha}(C_k)$$

It has the form

	$C_1 = C_E$	N_2C_2	N_3C_3	...
T^1	1	1	1	
T^2	l_2	...	...	
T^3	l_3	...	...	

The row is labelled by the irreducible representations and the column by the classes.

2.10 Properties of the Character Table

The properties listed below are useful for constructing the character table.

1. The number of irreducible representations is equal to the number of classes.

2. The first column contains the dimension of each representation and the sum of its square is the total number of elements in the group (Theorem 7): $\sum_\alpha l_\alpha^2 = h$.

3. As a convention, the first row is the identity or unit representation consisting of 1.

4. Each row or column can be regarded as a vector. In this sense:

   (a) The rows are orthogonal with weighting factor N_k (Theorem 6) and normalised to h.

   (b) The columns are orthogonal and normalised to h/N_k (Theorem 8).

5. If the character table of a factor group is known, then due to homomorphism, the character of an element aS in the factor group may be assigned to the classes which are contained in aS. We recall that if a group has an invariant subgroup S, then we can form a group $S, aS, bS, \ldots$ where a is not in S, b is not in S and aS etc. This group is a called a factor group with S as the unit element and it is homomorphic with the group itself. An invariant subgroup means that $x^{-1}Sx = S$ for every element x in the group and by Theorem 9 discussed in the next section, S must consist wholly of classes. The homomorphism between the factor group and the group itself means that if $T(aS)$ is a matrix representation of the element aS of the factor group then the same matrix may be used to represent all elements in the coset aS. Thus, the characters of the classes in aS is just the same as the character of $T(aS)$.

   The above five rules are often sufficient to construct the character table but the following rule, which is described in the next section, can be of help.

6. The characters of the α representation are related by

$$N_i\chi^\alpha(C_i)N_j\chi^\alpha(C_j) = l_\alpha \sum_k m_{ijk}N_k\chi^\alpha(C_k) \tag{2.10}$$

   where m_{ijk} is the coefficients of class multiplication, $C_iC_j = \sum_k m_{ijk}C_k$.

2.11 Class Multiplication

Let C be a collection of classes. From the definition of a class we have

$$x^{-1}Cx = C$$

for every element x in the group. This is evident from the fact that all elements in a class are conjugate to one another and if two elements a and b are different then $x^{-1}ax \neq x^{-1}bx$. Moreover, an element cannot belong to more than one class. Thus the elements on the right hand side must be identical to the elements in C.

Theorem 9:
A set of elements C obeying $x^{-1}Cx = C$ for all x in the group must be composed wholly of classes.
Proof:
Suppose R is a set of elements in C which do not form a class. But $x^{-1}Rx$ must be equal to R itself since $(C - R)$ form classes and by definition they will never be conjugate to elements in R. Thus R must be a class.

We now consider a product of two classes and here we do count all resulting elements even when some are the same.

$$\begin{aligned} C_iC_j &= x^{-1}C_ixx^{-1}C_jx \\ &= x^{-1}C_iC_jx \end{aligned}$$

By Theorem 9, it follows that C_iC_j must consist wholly of classes. Therefore it must be possible to write

$$C_iC_j = \sum_k m_{ijk}C_k \tag{2.11}$$

where m_{ijk} are integers telling how often the class C_k appears in the product C_iC_j.

Let us consider the class multiplication in terms of matrix representations. If we let $S(C_i)$ be the sum of matrices of all elements in the class C_i and $T(x)$ be a matrix representation of the element x then we have $T^{-1}(x)S(C_i)T(x) = S(C_i)$ or $S(C_i)T(x) = T(x)S(C_i)$. If the representation T is irreducible, then it follows from Schur's Lemma that $S(C_i) = c_iI$.

Thus

$$c_i c_j = \sum_k m_{ijk} c_k$$

Taking the trace of $S(C_i)$ and assuming we are in the irreducible representation α we get

$$Tr\ S(C_i) = Tr\ c_i I = c_i l_\alpha$$

On the other hand,

$$Tr\ S(C_i) = N_i \chi^\alpha(C_i)$$

Therefore

$$c_i = N_i \chi^\alpha(C_i)/l_\alpha$$

and Eq. (2.10) follows.

2.12 Direct Product Groups

If a group is a direct product of two groups, then the irreducible representations and the character table of the product group can be worked out easily from those of the two individual groups with the help of the following theorem.

Theorem 10:
If $G = G_1 \otimes G_2$ then $T^{\alpha\otimes\beta} = T_1^\alpha \otimes T_2^\beta$ is an irreducible representation of G. Moreover, for all T_1^α and T_2^β these are all possible irreducible representations of the product group.
Proof:
We first show that T is a representation of G. Let $a_1, a_2, \ldots$ and $b_1, b_2, \ldots$ be the elements of G_1 and G_2 respectively and let $c_{ij} = a_i b_j$ be the elements of the direct product group G. Suppose $c_{ij}c_{kl} = c_{mn}$ which implies that $a_i b_j a_k b_l = a_m b_n$ or $a_i a_k b_j b_l = a_m b_n$ since the elements of G_1 and G_2 commute. This means that $a_i a_k = a_m$ and $b_j b_l = b_n$ or $T^\alpha(a_i)T^\alpha(a_k) = T^\alpha(a_m)$ and $T^\beta(b_j)T^\beta(b_l) = T^\beta(b_n)$. Writing the last two matrix equations in component form, multiplying them and using the definition of direct product yield the required result.

Let M be a matrix which commutes with every $T^{\alpha\otimes\beta}$. M may be written in the form $M = M_1 \otimes M_2$ where M_1 and M_2 have the same dimensions as T_1^α and T_2^β respectively. The commutivity of M with $T^{\alpha\otimes\beta}$

implies the commutivity of M_1 with T_1^α and M_2 with T_2^β. By Schur's lemma, $M_1 = k_1 I_1$ and $M_2 = k_2 I_2$ and hence $M = k_1 k_2 I$ and no non-constant matrix M exists so that by Schur's lemma $T^{\alpha\otimes\beta}$ is irreducible.

To show the last part of the theorem, we recall that $\sum_\alpha l_{1\alpha}^2 = h_1$ and $\sum_\beta l_{2\beta}^2 = h_2$. Let $l_{\alpha\beta} = l_1^\alpha l_2^\beta$ be the dimension of the irreducible representation $T^{\alpha\otimes\beta}$. We have

$$\sum_{\alpha\beta} l_{\alpha\beta}^2 = \sum_\alpha l_{1\alpha}^2 \sum_\beta l_{2\beta}^2 = h_1 h_2$$

But $h_1 h_2$ is the order of the direct product group and therefore there are no more possible irreducible representations other than $T^{\alpha\otimes\beta}$ for all T_1^α and T_2^β.

2.13 Examples

1. We construct the character table of the permutation group of three objects which we have considered previously. There are three classes $C_1 = e$, $C_2 = (\alpha, \beta)$, and $C_3 = (\gamma, \mu, \nu)$ and therefore by rule 1 there are three irreducible representations. Rule 2 tells us that $l_1^2 + l_2^2 + l_3^2 = 6$. There is always an identity representation so we may take $l_1 = 1$. Then $l_2 = 1$ and $l_3 = 2$ are the only possible solution and the character table must look like as follows:

	C_1	$2C_2$	$3C_3$
T^1	1	1	1
T^2	1	a	b
T^3	2	c	d

   To determine $a, b, c,$ and d we need to know one of them and we can find the others by orthogonality (rule 4). The subgroup $S = (e, \alpha, \beta) = C_1 + C_2$ is an invariant subgroup and the corresponding factor group has the multiplication table

	S	γS
S	S	γS
γS	γS	S

where $\gamma S = \mu S = \nu S = (\gamma, \mu, \nu) = C_3$. This is a group of two elements and there are evidently two classes, the first class consists of the unit element S and the second class consists of the element γS. The number of irreducible representations is two and both must have dimension one, by rule 2. The irreducible representations of the factor group must be $(1, 1)$ and $(1, -1)$. Then from rule 5 we may assign $a = 1$ and $b = -1$ ($a = 1$ and $b = 1$ gives the identity representation). Note that we have taken a and b and not c and d because the irreducible representations of the factor group are one dimensional and T^2 is also a one dimensional representation. The other two characters c and d can be easily obtained from the orthogonality between columns.

$$\begin{aligned} 1 \cdot 1 + 1 \cdot a + 2 \cdot c &= 0 \rightarrow c = -1 \\ 1 \cdot 1 + 1 \cdot b + 2 \cdot d &= 0 \rightarrow d = 0 \end{aligned}$$

Finally we have

	C_1	$2C_2$	$3C_3$
T^1	1	1	1
T^2	1	1	-1
T^3	2	-1	0

2. Abelian groups: Every element in an Abelian group forms a class by itself. Therefore the number of irreducible representations is simply equal to the number of elements in the group. Moreover, rule 2 implies that all irreducible representations have dimension one. The consequences are

   (a) Unitarity of representations implies that the numbers representing an Abelian group have modulus one.

(b) If the number X represents an element x then X^* represents x^{-1}.

(c) The character table serves also as a representation table.

As an example we consider a non-cyclic group of fourth order with the following multiplication table

	e	a	b	c
e	e	a	b	c
a	a	e	c	b
b	b	c	e	a
c	c	b	a	e

$a^2 = b^2 = c^2 = e$ so a, b, and c are represented either by ± 1. If a is represented by 1 then $b = c = \pm 1$ because $bc = a$. If $a = -1$ then either $b = 1$ and $c = -1$ or $b = -1$ and $c = 1$. Thus we have

	e	a	b	c
T^1	1	1	1	1
T^2	1	1	-1	-1
T^3	1	-1	1	-1
T^4	1	-1	-1	1

3. Cyclic groups: These are Abelian groups which can be generated by a single element: $G = (a, a^2, \ldots, a^h = e)$. If a is represented by a number A_k then a^2 is represented by A_k^2 etc. and $A_k^h = 1$ since e is always represented by 1. Thus, A_k must be one of the h roots of

unity, i.e. $A_k = \exp(i2\pi k/h)$ and the character table is given by

	e	a	a^2	...	a^{h-1}
T^1	1	1	1	...	1
T^2	1	A_1	A_1^2	...	A_1^{h-1}
T^3	1	A_2	A_2^2	...	A_2^{h-1}
.	.	.	.	...	.
.	.	.	.	...	.
T^h	1	A_{h-1}	A_{h-1}^2	...	A_{h-1}^{h-1}

Chapter 3

Group Theory in Quantum Mechanics

3.1 Linear Vector Space

A set $\{\mathbf{r}_1, \mathbf{r}_2, \ldots\}$ is said to form a linear vector space L if $\mathbf{r}_i + \mathbf{r}_j$ is another member in the set for every i, j and $c\mathbf{r}_i$ is also another member in the set where c is a complex constant. The quantities $\{\mathbf{r}_1, \mathbf{r}_2, \ldots\}$ are called vectors and there are an infinite number of them.

A set of vectors $\{\mathbf{v}_1, \mathbf{v}_2, \ldots, \mathbf{v}_p\}$ is said to be linearly independent if none of them can be expressed as a linear combination of the others. If a set of coefficients $\{c_k\}$ can be found such that

$$\sum_{k=1}^{p} c_k \mathbf{v}_k = 0$$

then the vectors are said to be linearly dependent. The largest number of vectors in L which form a linearly independent set is called the dimension of L. This is the same as the smallest number of vectors needed to describe every vector in L and these vectors are said to form a basis. We denote the dimension of L by s and the basis vectors by $\{\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_s\}$ so that any vector $\mathbf{v}$ may be written as

$$\mathbf{v} = \sum_{i=1}^{s} v_i \mathbf{e}_i$$

In order to determine the coefficients v_i from a given vector $\mathbf{v}$ we introduce the concept of scalar or dot product between two vectors $\mathbf{v}_1$ and $\mathbf{v}_2$ which we denote by $(\mathbf{v}_1, \mathbf{v}_2)$. The particular definition of the scalar product is arbitrary but it must satisfy the following general conditions:

1. $(\mathbf{v}_1, \mathbf{v}_2)$ is a complex number
2. $(\mathbf{v}_1, \mathbf{v}_2) = (\mathbf{v}_2, \mathbf{v}_1)^*$
3. $(\mathbf{v}_1, c\mathbf{v}_2) = c(\mathbf{v}_1, \mathbf{v}_2) \rightarrow (c\mathbf{v}_1, \mathbf{v}_2) = (\mathbf{v}_2, c\mathbf{v}_1)^* = c^*(\mathbf{v}_1, \mathbf{v}_2)$
4. $(\mathbf{v}_1 + \mathbf{v}_2, \mathbf{v}_3) = (\mathbf{v}_1, \mathbf{v}_3) + (\mathbf{v}_2, \mathbf{v}_3)$
5. $(\mathbf{v}_1, \mathbf{v}_1) \geq 0$. It is only zero when $\mathbf{v}_1 = 0$.

Examples:

1. Vectors in 3-dimensional space. The dot product is defined as $(\mathbf{v}_1, \mathbf{v}_2) = v_1 v_2 cos\theta$ where v_1 and v_2 are the lengths of the vectors and θ is the angle between the two vectors.
2. Function spaces. The dot product is defined as $(\psi_i, \psi_j) = \int d^3r \; w(\mathbf{r})\psi_i^*(\mathbf{r})\psi_j(\mathbf{r})$ where w is a weight function which is usually real and positive definite so that the last condition is satisfied. We can also define orthonormal basis functions $\{\phi_i\}$ such that any function can be expanded in this basis: $\psi = \sum_{i=1}^{\infty} c_i\phi_i$ The linear space spanned by this basis is called the Hilbert space.

We define an operator $\hat{T}$ by

$$\hat{T}\mathbf{v} = \mathbf{v}'$$

where $\mathbf{v}$ is an arbitrary vector or function which is carried into another vector or function $\mathbf{v}'$. Both $\mathbf{v}$ and $\mathbf{v}'$ are in L. The operator is called linear if

$$\begin{aligned} \hat{T}(\mathbf{v}_1 + \mathbf{v}_2) &= \hat{T}\mathbf{v}_1 + \hat{T}\mathbf{v}_2 \\ \hat{T}c\mathbf{v} &= c\hat{T}\mathbf{v} \end{aligned}$$

We will consider only linear operators.

Since any vector in L can be expanded in the basis vectors, it is only necessary to study the effects of the operator on the basis vectors.

$$\hat{T}\mathbf{e}_j = \sum_i \mathbf{e}_i T_{ij}$$

The matrix T_{ij} is said to form a representation for the operator $\hat{T}$ in the linear vector space L.

It is usually convenient to choose an orthonormal basis, by this we mean $(\phi_i, \phi_j) = \delta_{ij}$. This can always be done by the Gramm-Schmidt orthogonalisation procedure. We illustrate the method for three vectors. The generalisation to an arbitrary number of vectors is straightforward. Let ϕ_1, ϕ_2, ϕ_3 be three linearly independent functions which are not necessarily orthogonal nor normalised. Let $\psi_1 = \phi_1/\sqrt{(\phi_1, \phi_1)}$ and construct $\tilde{\psi}_2 = \phi_2 - \psi_1(\psi_1, \phi_2)$ which is orthogonal to ψ_1. We normalise $\tilde{\psi}_2$ to get $\psi_2 = \tilde{\psi}_2/\sqrt{(\tilde{\psi}_2, \tilde{\psi}_2)}$ and construct $\tilde{\psi}_3 = \phi_3 - \psi_2(\psi_2, \phi_3) - \psi_1(\psi_1, \phi_3)$ which is orthogonal to both ψ_1 and ψ_2 and which is then normalised to give $\psi_3 = \tilde{\psi}_3/\sqrt{\tilde{\psi}_3, \tilde{\psi}_3)}$ In this way we have constructed an orthonormal set of functions and we can see that for a general case we have

$$\tilde{\psi}_n = \phi_n - \sum_{i=1}^{n-1} \psi_i(\psi_i, \phi_n)$$

3.2 Symmetry Transformations

A symmetry transformation G with respect to a given function $f(x, y, z)$ is a real linear coordinate transformation that preserves the length (real unitary transformation)

$$\mathbf{r}' = G\mathbf{r} \rightarrow r_i' = \sum_j G_{ij} r_j, \quad r_i = x, y, z$$

such that the function calculated with the new variables r_i by the above substitution of coordinates is the same as the function calculated with the old variables: $f(x', y', z') = f'(x, y, z) = f(x, y, z) \rightarrow f(G\mathbf{r}) = f(\mathbf{r})$. In

other words, the function looks the same in the old and the new coordinate system. This also implies that

$$f(G\mathbf{r}) = f(\mathbf{r}) = f(G^{-1}\mathbf{r})$$

because $f(\mathbf{r}') = f(\mathbf{r}) = f(G^{-1}\mathbf{r}')$ and $\mathbf{r}'$ is just a dummy variable.

A symmetry operator $\hat{T}(G)$ associated with a symmetry transformation G is defined by

$$\hat{T}(G)f(\mathbf{r}) = f(G^{-1}\mathbf{r})$$

It is important to note that the operator acts upon the coordinates $\mathbf{r}$, and not upon the argument of f. Thus we mean that

$$\hat{T}(G)f(A\mathbf{r}) = f(AG^{-1}\mathbf{r}) \neq f(G^{-1}A\mathbf{r})$$

We also have G^{-1} instead of G in our definition. This is a natural choice because two successive operations $\hat{T}(G_1)$ and $\hat{T}(G_2)$ on a function $f(\mathbf{r})$ correspond to the same order of coordinate transformation:

$$\hat{T}(G_2)\hat{T}(G_1)f(\mathbf{r}) = \hat{T}(G_2)f(G_1^{-1}\mathbf{r}) = f(G_1^{-1}G_2^{-1}\mathbf{r}) = f([G_2G_1]^{-1}\mathbf{r})$$

Theorem 1:
If $\{G\}$ is a set of all symmetry transformations of a function, then the associated symmetry operators $\{\hat{T}(G)\}$ form a group.

Proof:
The set $\{G\}$ evidently form a group because if G is a symmetry transformation, then so is G^{-1} as discussed above. A succession of two symmetry transformations is itself a symmetry transformation and the identity transformation is obviously a symmetry transformation. From the definition, we have

$$\begin{aligned}
\hat{T}(G_1)\hat{T}(G_2)f(\mathbf{r}) &= \hat{T}(G_1)f(G_2^{-1}\mathbf{r}) \\
&= f(G_2^{-1}G_1^{-1}\mathbf{r}) \\
&= f([G_1G_2]^{-1}\mathbf{r}) \\
&= \hat{T}(G_1G_2)f(\mathbf{r})
\end{aligned}$$

Hence $\hat{T}(G_1)\hat{T}(G_2) = \hat{T}(G_1G_2)$ and the symmetry operators form a group.

3.3 Invariant Subspace and Its Generation

A set of functions or vectors $\{\phi_i\}$ is said to span an invariant subspace V_S under a given set of symmetry operators $\{\hat{T}(G)\}$ if $\hat{T}(G)\phi_i$ is also in V_S for all G and i.

An invariant subspace can be generated from an arbitrary function f and a set of symmetry operators $\{\hat{T}(G)\}$ by applying each of the operators on f. The set of functions $\{\hat{T}(G)f\}$ form an invariant subspace under $\{\hat{T}(G)\}$ because $\hat{T}(G')[\hat{T}(G)f] = \hat{T}(G'G)f$, which must lie in the subspace since $\hat{T}(G'G)$ is just another member of $\{\hat{T}(G)\}$. We note that the number of functions that span the subspace is not necessarily equal to the number of G. Some of the functions may be the same or can be expressed as linear combinations of the others. The largest number of linearly independent functions in V_S is called the dimension of the subspace.

It may happen that we can construct a function f' in V_S such that the invariant subspace $\{\hat{T}(G)f'\}$ has a smaller dimension than that of V_S. In this case the subspace V_S is said to be reducible. When such a function cannot be found than V_S is said to be irreducible.

3.4 Basis Functions for a Representation

Let $\{\phi_i\}$ be a set of orthonormal functions that span an invariant subspace V_S. Then $\hat{T}(G)\phi_i(\mathbf{r}) = \phi_i(G^{-1}\mathbf{r})$ is in V_S by definition and it can therefore be expanded as a linear combination of $\{\phi_i\}$:

$$\hat{T}(G)\phi_i = \sum_j \phi_j T_{ji}(G) \tag{3.1}$$

If the basis functions are orthonormal, then $T(G)$ is unitary because

$$\begin{aligned}(\hat{T}(G)\phi_i, \hat{T}(G)\phi_j) = \delta_{ij} &= (\sum_k \phi_k T_{ki}(G), \sum_l \phi_l T_{lj}(G)) \\ &= \sum_{kl} T^*_{ki}(G) T_{lj}(G)(\phi_k, \phi_l) \\ &= \sum_k T^\dagger_{ik}(G) T_{kj}(G)\end{aligned}$$

Theorem 2:
The matrices $\{T(G)\}$ form a representation for $\{\hat{T}(G)\}$

Proof:

$$\begin{aligned}
\hat{T}(G_1)\hat{T}(G_2)\phi_i &= \sum_j \hat{T}(G_1)\phi_j T_{ji}(G_2) \\
\hat{T}(G_1G_2)\phi_i &= \sum_{jk} \phi_k T_{kj}(G_1)T_{ji}(G_2) \\
\sum_k \phi_k T_{ki}(G_1G_2) &= \sum_k \phi_k T_{kj}(G_1)T_{ji}(G_2)
\end{aligned}$$

Thus $T(G_1)T(G_2) = T(G_1G_2)$. The functions $\{\phi_i\}$ are said to form a basis for a representation, which may be reducible. Evidently, if the subspace is irreducible under $\{\hat{T}(G)\}$, then the representation is also irreducible. This simply follows from the fact that one always generates the entire subspace starting from any function in the subspace. If the representation were reducible, then it would be possible to start from a function that does not generate the entire subspace, in which case the subspace is reducible. We now see the relevance of matrix representation theory studied in the previous chapter. Since the theorems were developed for arbitrary matrices, they are also applicable here.

Theorem 3:
A change of basis vectors $\psi_j = \sum_i \phi_i S_{ij}$ corresponds to a similarity transformation of the original representation, which is an equivalent representation. S is assumed to be unitary so that $(\psi_i, \psi_j) = \delta_{ij}$.

Proof:

$$\begin{aligned}
\hat{T}(G)\phi_i &= \sum_j \phi_j T_{ji}(G) \\
\hat{T}(G)\sum_j \psi_j S^{-1}_{ji} &= \sum_j \sum_k \psi_k S^{-1}_{kj} T_{ji}(G)
\end{aligned}$$

Multiplying both sides by S_{im} and summing over i yields

$$\hat{T}(G)\psi_m = \sum_k \psi_k T'_{km}(G)$$

where $T'_{km}(G) = \sum_{ji} S^{-1}_{kj} T_{ji}(G) S_{im}(G)$ or $T' = S^{-1}TS$ which is a similarity transformation. It is clear that the reverse is also true, i.e. a similarity transformation of the representation with a unitary matrix S corresponds to a unitary transformation of the basis vectors.

3.5 Projection Operators

It is possible to construct a projection operator $\hat{P}^\beta$ such that given an arbitrary function ψ, $\hat{P}^\beta\psi$ is a component of ψ in the irreducible subspace β, i.e. $\hat{P}^\beta\psi$ transforms according to the irreducible representation β. This is a very useful tool. In the following, we construct these projection operators.

Suppose $\{\psi_i^\alpha\}$ span an irreducible subspace transforming according to the irreducible representation α of $\{\hat{T}(G)\}$. That is

$$\hat{T}(G)\psi_i^\alpha = \sum_j \psi_j^\alpha T_{ji}^\alpha(G)$$

Multiplying by $T_{kl}^{\beta*}(G)$ and summing over G yields

$$\sum_G T_{kl}^{\beta*}(G)\hat{T}(G)\psi_i^\alpha = \sum_G \sum_j \psi_j^\alpha T_{ji}^\alpha(G) T_{kl}^{\beta*}(G)$$

Using the Orthogonality Theorem on the right side, we get

$$\begin{aligned} \sum_G T_{kl}^{\beta*}(G)\hat{T}(G)\psi_i^\alpha &= \sum_j \psi_j^\alpha (h/l_\beta)\delta_{jk}\delta_{il}\delta_{\alpha\beta} \\ &= (h/l_\beta)\delta_{il}\delta_{\alpha\beta}\psi_k^\alpha \end{aligned}$$

We define

$$\hat{P}_{kl}^\beta \equiv (l_\beta/h)\sum_G T^{\beta*}{}_{kl}(G)\hat{T}(G)$$

so that

$$\hat{P}_{kl}^\beta \psi_i^\alpha = \delta_{il}\delta_{\alpha\beta}\psi_k^\beta \rightarrow \hat{P}_{ki}^\alpha \psi_i^\alpha = \psi_k^\alpha \tag{3.2}$$

Starting from a given function that belongs to the ith row of a given irreducible representation α, the projection operator can be used to generate the other "partner functions" corresponding to the other rows. These functions form a basis for the irreducible representation α.

Moreover, we can also define

$$\begin{aligned} \hat{P}^{\beta} &\equiv \sum_i \hat{P}^{\beta}_{ii} \\ &\equiv (l_\beta/h) \sum_G \chi^{\beta *}(G) \hat{T}(G) \end{aligned}$$

so that

$$\hat{P}^{\beta} \psi^{\alpha}_i = \delta_{\beta\alpha} \psi^{\alpha}_i \tag{3.3}$$

The projection operators allow us to decompose the space, in which the symmetry operators are defined, into irreducible subspaces. Any function ψ can therefore be written as follows

$$\psi = \sum_\alpha \sum_i \psi^{\alpha}_i \tag{3.4}$$

where ψ^{α}_i belongs to the ith row of the irreducible representation α. We note also that if ϕ^{α}_i and ψ^{α}_i belong to the ith row of the irreducible representation α, so does any linear combination $a\phi^{\alpha}_i + b\psi^{\alpha}_i$.

Suppose that a given representation T is reducible. Then there is a unitary matrix S such that $T' = S^{-1}TS = \sum_\alpha \oplus m_\alpha T^\alpha$ has the block form and each block cannot be reduced any further. α labels the irreducible representation and m_α tells us how many times the irreducible representation α appears in the reduction. We note that when $m_\alpha > 1$ the irreducible representations T^α are assumed to be the same. This can always be done by means of similarity transformations in each subspace which transforms according to the same irreducible representation α. The new basis vectors according to Theorem 3 are given by $\psi_j = \sum_i \phi_i S_{ij}$ and they may be labelled according to the irreducible subspaces to which they belong. Any vector in V_S can therefore be expanded as follows:

$$\begin{aligned} v &= \sum_{\alpha,t,i} \psi^{\alpha t}_i c^{\alpha t}_i \\ &= \sum_{\alpha,i} v^{\alpha}_i \end{aligned} \tag{3.5}$$

where t labels the different possible subspaces transforming according to the same irreducible representation α, which is necessary when $m_\alpha > 1$, and i labels the basis functions in the subspace α, t. We have also defined $v_i^\alpha = \sum_t \psi_i^{\alpha t} c_i^{\alpha t}$. However, $\hat{T}(G) v_i^\alpha$ is not necessarily equal to $\sum_j v_j^\alpha T_{ji}(G)$ unless there is only one t.

3.6 Orthogonality of Basis Functions

Theorem 4:
Two vectors belonging to two inequivalent irreducible representations must be orthogonal. If they transform according to the same irreducible representation, they are still orthogonal if they belong to different rows.

Proof:
Let ϕ_i^α and ψ_j^β belong to the irreducible representations T^α and T^β respectively. Then

$$\hat{T}(G)\phi_i^\alpha = \sum_k \phi_k^\alpha T_{ki}^\alpha(G)$$

$$\hat{T}(G)\psi_j^\beta = \sum_l \psi_l^\beta T_{lj}^\beta(G)$$

Recalling that T is or may always be chosen to be unitary, we have

$$\begin{aligned}
(\phi_i^\alpha, \psi_j^\beta) &= (\hat{T}(G)\phi_i^\alpha, \hat{T}(G)\psi_j^\beta) \\
&= \sum_{kl} T_{ki}^{\alpha *}(G) T_{lj}^\beta(G) (\phi_k^\alpha, \psi_l^\beta) \\
&= (1/h) \sum_G \sum_{kl} T_{ki}^{\alpha *}(G) T_{lj}^\beta(G) (\phi_k^\alpha, \phi_l^\beta) \\
&= (1/l_\alpha) \delta_{\alpha\beta} \delta_{ij} \sum_k (\phi_k^\alpha, \psi_k^\beta)
\end{aligned}$$

3.7 Examples

As an example, we consider the group D_3 which is the group of permutations of three objects. The elements are e = unit element, c_1, c_2 = anticlockwise rotations about the $z-$axis by $2\pi/3$ and $4\pi/3$ respectively, and d_1, d_2, d_3 = rotations by π about axes lebelled $1, 2, 3$ in Figure 3.1.

The classes are $C_e = e$, $C_c = (c_1, c_2)$, and $C_d = (d_1, d_2, d_3)$. We choose a set of basis vectors or functions in order to form a representation for the group elements. The choice is arbitrary.

1. The first obvious choice is the three Cartesian unit vectors $\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z$ as shown in the figure. Let us see how they transform under the group operations.

	$\mathbf{e}_x$	$\mathbf{e}_y$	$\mathbf{e}_z$
$\hat{T}(e)$	$\mathbf{e}_x$	$\mathbf{e}_y$	$\mathbf{e}_z$
$\hat{T}(c_1)$	$-\frac{1}{2}\mathbf{e}_x + \frac{\sqrt{3}}{2}\mathbf{e}_y$	$-\frac{\sqrt{3}}{2}\mathbf{e}_x - \frac{1}{2}\mathbf{e}_y$	$\mathbf{e}_z$
$\hat{T}(c_2)$	$-\frac{1}{2}\mathbf{e}_x - \frac{\sqrt{3}}{2}\mathbf{e}_y$	$\frac{\sqrt{3}}{2}\mathbf{e}_x - \frac{1}{2}\mathbf{e}_y$	$\mathbf{e}_z$
$\hat{T}(d_1)$	$-\mathbf{e}_x$	$\mathbf{e}_y$	$-\mathbf{e}_z$
$\hat{T}(d_2)$	$\frac{1}{2}\mathbf{e}_x + \frac{\sqrt{3}}{2}\mathbf{e}_y$	$\frac{\sqrt{3}}{2}\mathbf{e}_x - \frac{1}{2}\mathbf{e}_y$	$-\mathbf{e}_z$
$\hat{T}(d_3)$	$\frac{1}{2}\mathbf{e}_x - \frac{\sqrt{3}}{2}\mathbf{e}_y$	$-\frac{\sqrt{3}}{2}\mathbf{e}_x - \frac{1}{2}\mathbf{e}_y$	$-\mathbf{e}_z$

We see that applying the group operations on $\mathbf{e}_x$ or $\mathbf{e}_y$ generate an invariant subspace $(\mathbf{e}_x, \mathbf{e}_y)$ whereas $\mathbf{e}_z$ forms an invariant subspace by itself. The set of Cartesian unit vectors $(\mathbf{e}_x, \mathbf{e}_y, \mathbf{e}_z)$ do form a basis for the representation of the group. The matrices can be calculated by using the definition $T_{ij}(G) = (\phi_i, \hat{T}(G)\phi_j)$:

$$T(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad T(c_1) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$T(c_2) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad T(d_1) = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$T(d_2) = \begin{pmatrix} \frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad T(d_3) = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

The characters are $\chi(C_e) = 3$, $\chi(C_c) = 0$, and $\chi(C_d) = -1$. As can be seen, the 3×3 representation is reducible into a 2×2 and a 1×1

representations. The 1×1 representation is obviously irreducible, but it may be possible to further reduce the 2×2 representation. We recall that the character of a given representation can be written as $\chi = \sum_\alpha m_\alpha \chi^\alpha$ and by using the first orthonormality relation between characters the coefficients m_α can be calculated as follows:

$$m_\alpha = \frac{1}{h} \sum_k N_k \chi^{\alpha *}(C_k) \chi(C_k)$$

For convenience, we reproduce the character table of the group D_3.

	C_e	$2C_c$	$3C_d$
T^1	1	1	1
T^2	1	1	-1
T^3	2	-1	0

Thus

$$\begin{aligned} m_1 &= \frac{1}{6}[1 \cdot 1 \cdot 3 + 2 \cdot 1 \cdot 0 + 3 \cdot 1 \cdot (-1)] = 0 \\ m_2 &= \frac{1}{6}[1 \cdot 1 \cdot 3 + 2 \cdot 1 \cdot 0 + 3 \cdot (-1) \cdot (-1) = 1 \\ m_3 &= \frac{1}{6}[1 \cdot 2 \cdot 3 + 2 \cdot (-1) \cdot 0 + 3 \cdot 0 \cdot (-1) = 1 \end{aligned}$$

Hence the representation breaks up into $T = T^2 \oplus T^3$ and therefore $(\mathbf{e}_x, \mathbf{e}_y)$ do form an irreducible subspace for the representation T^3. We could have arrived at this conclusion simply by calculating the characters of the 2×2 representation which are $\chi(C_e) = 2$, $\chi(C_c) = -1$, and $\chi(C_d) = 0$ and which agree with the characters of the T^3 representation.

2. As a second example, we consider the same group but we choose a basis which consists of functions rather than the Cartesian vectors. We can take an arbitrary function, say x^2, and generate an invariant subspace from it. We construct an orthonormal basis that spans this subspace and we form the representation for the group. We then use

the projection operator method to figure out which functions belong to a given irreducible subspace.

What we need to know is how x transforms under the group operations. We have defined $\hat{T}(G)f(\mathbf{r}) = f(G^{-1}\mathbf{r})$, i.e. $\hat{T}(G)x = \hat{T}(G)(\mathbf{e}_x \cdot \mathbf{r}) = (\mathbf{e}_x \cdot G^{-1}\mathbf{r}) = (G\mathbf{e}_x \cdot \mathbf{r})$. Thus x, y and z transform like the Cartesian vectors $\mathbf{e}_x$, $\mathbf{e}_y$, and $\mathbf{e}_z$ and we have

$$\begin{aligned}
\hat{T}(e)x^2 &= x^2 \\
\hat{T}(c_1)x^2 &= (-\frac{1}{2}x + \frac{\sqrt{3}}{2}y)^2 = \frac{1}{4}x^2 + \frac{3}{4}y^2 - \frac{\sqrt{3}}{2}xy \\
\hat{T}(c_2)x^2 &= (-\frac{1}{2}x - \frac{\sqrt{3}}{2}y)^2 = \frac{1}{4}x^2 + \frac{3}{4}y^2 + \frac{\sqrt{3}}{2}xy \\
\hat{T}(d_1)x^2 &= (-x)^2 = x^2 \\
\hat{T}(d_2)x^2 &= (\frac{1}{2}x + \frac{\sqrt{3}}{2}y)^2 = \frac{1}{4}x^2 + \frac{3}{4}y^2 + \frac{\sqrt{3}}{2}xy \\
\hat{T}(d_3)x^2 &= (\frac{1}{2}x - \frac{\sqrt{3}}{2}y)^2 = \frac{1}{4}x^2 + \frac{3}{4}y^2 - \frac{\sqrt{3}}{2}xy
\end{aligned}$$

These six functions form an invariant subspace for D_3 but all of them can be written as linear combinations of only three distinct functions $\chi_1 = x^2$, $\chi_2 = y^2$, and $\chi_3 = xy$. Evidently none of these three functions can be written as a linear combination of the other two so that they are linearly independent and form a basis for the invariant subspace, although they are neither orthogonal nor normalised.

We now use the Gramm-Schmidt orthogonalisation procedure to construct a set of orthonormal basis needed to construct a unitary representation for the group. We can start with any of the three functions or any linear combination of them. Let us start with $\chi_1 = x^2$ which we normalise inside a unit sphere so that

$$|A|^2(\chi_1, \chi_1) = \int_0^1 dr\ r^2 \int_0^\pi d\theta sin\ \theta \int_0^{2\pi} d\phi\ \chi_1^* \chi_1 = 1$$

which gives $A = \sqrt{35/4\pi}$. The normalised function is then

$$\phi_1 = Ax^2$$

The second function is constructed by using $\tilde{\phi}_2 = \chi_2 - \phi_1(\phi_1, \chi_2)$ which yields after normalisation

$$\phi_2 = A\frac{1}{2\sqrt{2}}(3y^2 - x^2)$$

The function xy is already orthogonal to both x^2 and y^2 due to antysymmetry so that the third orthonormalised function is

$$\phi_3 = A\sqrt{3}xy$$

To construct the representation matrices, we need to know how these basis functions transform into one another under the group operations.

	ϕ_1	ϕ_2	ϕ_3
$\hat{T}(e)$	ϕ_1	ϕ_2	ϕ_3
$\hat{T}(c_1)$	$\frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 - \frac{1}{2}\phi_3$	$\frac{1}{\sqrt{2}}(\phi_1 + \phi_3)$	$\frac{1}{2}\phi_1 - \frac{1}{\sqrt{2}}\phi_2 - \frac{1}{2}\phi_3$
$\hat{T}(c_2)$	$\frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 + \frac{1}{2}\phi_3$	$\frac{1}{\sqrt{2}}(\phi_1 - \phi_3)$	$-\frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 - \frac{1}{2}\phi_3$
$\hat{T}(d_1)$	ϕ_1	ϕ_2	$-\phi_3$
$\hat{T}(d_2)$	$\frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 + \frac{1}{2}\phi_3$	$\frac{1}{\sqrt{2}}(\phi_1 - \phi_3)$	$\frac{1}{2}\phi_1 - \frac{1}{\sqrt{2}}\phi_2 + \frac{1}{2}\phi_3$
$\hat{T}(d_3)$	$\frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 - \frac{1}{2}\phi_3$	$\frac{1}{\sqrt{2}}(\phi_1 + \phi_3)$	$-\frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 + \frac{1}{2}\phi_3$

The matrix representations can be easily obtained and these are

$$T(e) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad T(c_1) = \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ -\frac{1}{2} & \frac{1}{\sqrt{2}} & -\frac{1}{2} \end{pmatrix}$$

$$T(c_2) = \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & -\frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & -\frac{1}{2} \end{pmatrix} \quad T(d_1) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$T(d_2) = \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \\ \frac{1}{2} & -\frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix} \quad T(d_3) = \begin{pmatrix} \frac{1}{2} & \frac{1}{\sqrt{2}} & -\frac{1}{2} \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ -\frac{1}{2} & \frac{1}{\sqrt{2}} & \frac{1}{2} \end{pmatrix}$$

Unlike the previous example, these matrices are not in block form but we know that they are reducible because there is no three dimensional representation of D_3. Let us figure out which irreducible representations are contained in these matrices by using the same formula as in the previous example. The reducible characters are $\chi(C_e) = 3$, $\chi(C_c) = 0$, and $\chi(C_d) = 1$. We get

$$\begin{aligned} m_1 &= \frac{1}{6}[1 \cdot 1 \cdot 3 + 2 \cdot 1 \cdot 0 + 3 \cdot 1 \cdot 1] = 1 \\ m_2 &= \frac{1}{6}[1 \cdot 1 \cdot 3 + 2 \cdot 1 \cdot 0 + 3 \cdot (-1) \cdot 1] = 0 \\ m_3 &= \frac{1}{6}[1 \cdot 2 \cdot 3 + 2 \cdot (-1) \cdot 0 + 3 \cdot 0 \cdot 1] = 1 \end{aligned}$$

Hence the representation breaks up into $T = T^1 \oplus T^3$.

Since the representation contains an identity representation, it must be possible to construct a linear combination of ϕ_1, ϕ_2, and ϕ_3 such that it is invariant under the group operations. We do this in a systematic way using the projection operator method. The projection operator is given by

$$\hat{P}^\alpha = \frac{l_\alpha}{h} \sum_G \chi^{\alpha *}(G) \hat{T}(G)$$

which when applied to an arbitrary function gives the component of the function in the irreducible subspace α. Let us apply $\hat{P}^1$ to ϕ_1, ϕ_2, and ϕ_3:

$$\begin{aligned} \hat{P}^1\phi_1 &= \frac{1}{6}\Big[\phi_1 + (\frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 - \frac{1}{2}\phi_3) + (\frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 + \frac{1}{2}\phi_3) \\ &\qquad + \phi_1 + (\frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 + \frac{1}{2}\phi_3) + (\frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 - \frac{1}{2}\phi_3)\Big] \\ &= \frac{\sqrt{2}}{3}(\sqrt{2}\phi_1 + \phi_2) \\ \hat{P}^1\phi_2 &= \frac{1}{6}\Big[\phi_2 + (\frac{1}{\sqrt{2}}(\phi_1 + \phi_3)) + (\frac{1}{\sqrt{2}}(\phi_1 - \phi_3)) \\ &\qquad + \phi_2 + (\frac{1}{\sqrt{2}}(\phi_1 - \phi_3)) + (\frac{1}{\sqrt{2}}(\phi_1 + \phi_3))\Big] \end{aligned}$$

$$= \frac{1}{3}(\sqrt{2}\phi_1 + \phi_2)$$

$$\hat{P}^1\phi_3 = 0$$

The linear combination $(\sqrt{2}\phi_1+\phi_2)/\sqrt{3}$ transforms according to the identity representation. The component of ϕ_1 in the third irreducible subspace is given by

$$\begin{aligned}\hat{P}^3\phi_1 &= \frac{2}{6}\left[2\phi_1 - (\frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 - \frac{1}{2}\phi_3) - (\frac{1}{2}\phi_1 + \frac{1}{\sqrt{2}}\phi_2 + \frac{1}{2}\phi_3)\right] \\ &= \frac{1}{3}(\phi_1 - \sqrt{2}\phi_2)\end{aligned}$$

Thus we may choose a new basis

$$\begin{aligned}\psi_1 &= \frac{1}{\sqrt{3}}(\sqrt{2}\phi_1 + \phi_2) \\ \psi_2 &= \frac{1}{\sqrt{3}}(\phi_1 - \sqrt{2}\phi_2) \\ \psi_3 &= \phi_3\end{aligned}$$

which brings the representation into block form with ψ_1 transforming according to the identity representation T^1 and (ψ_2, ψ_3) transforming according to the irreducible representation T^3. The new basis may be written as $\psi_i = \sum_j \phi_j S_{ji}$ where S is the unitary matrix that reduces the representation into block form which is given by

$$S = \begin{pmatrix} \sqrt{\frac{2}{3}} & \sqrt{\frac{1}{3}} & 0 \\ \sqrt{\frac{1}{3}} & -\sqrt{\frac{2}{3}} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

3.8 Relationship to Quantum Mechanics

A basic problem in quantum mechanics is finding the eigenvectors and eigenvalues of a Hamiltonian $\hat{H}$. A general procedure is to calculate the Hamiltonian matrix in an arbitrary basis and diagonalise it, but in most cases, this procedure is too difficult to carry out. Instead one tries to find

a basis in which the off diagonal elements of H are small or zero so that they can be neglected or treated perturbatively. It is here that the study of the symmetry of the Hamiltonian is of great value because group theory can tell us which matrix elements are zero and how the matrix elements are related to one another. The results are exact and depend only on the symmetry of the systems and not on the particular form of interactions or potentials.

3.8.1 The Group of the Schrödinger Equation

If $\{G\}$ is a set of all symmetry transformations of a Hamiltonian, $\hat{H}$, then according to Theorem 1 the associated symmetry operators $\{\hat{T}(G)\}$ form a group which is called the group of the Schrödinger equation or in short the Schrödinger group.

Theorem 5:
Each element of the Schrödinger group commutes with the Hamiltonian. Moreover, if $\psi(\mathbf{r})$ is an eigenvector of $\hat{H}$, then $\hat{T}(G)\psi(\mathbf{r}) = \psi(G^{-1}\mathbf{r})$ is also an eigenvector of $\hat{H}$ with the same eigenvalue.

Proof:
By definition

$$\hat{T}(G)\hat{H}(\mathbf{r}) = \hat{H}(G^{-1}\mathbf{r}) = \hat{H}(\mathbf{r})$$

Let us investigate the consequences of this symmetry by considering the effect of $\hat{T}(G)$ on $\hat{H}\psi(\mathbf{r})$ where ψ is an arbitrary function .

$$\begin{aligned} \hat{T}(G)\hat{H}(\mathbf{r})\psi(\mathbf{r}) &= \hat{H}(G^{-1}\mathbf{r})\psi(G^{-1}\mathbf{r}) \\ &= \hat{H}(\mathbf{r})\hat{T}(G)\psi(\mathbf{r}) \\ \left[\hat{T}(G)\hat{H}(\mathbf{r}) - \hat{H}(\mathbf{r})\hat{T}(G)\right]\psi(\mathbf{r}) &= 0 \end{aligned}$$

Since $\psi(\mathbf{r})$ is arbitrary, $[\hat{T}, \hat{H}] = 0$. The second part of the theorem follows directly from this result:

$$\hat{H}(\mathbf{r})\hat{T}(G)\psi(\mathbf{r}) = \hat{T}(G)\hat{H}(\mathbf{r})\psi(\mathbf{r}) = \epsilon\hat{T}(G)\psi(\mathbf{r})$$

3.8.2 Degeneracy and Invariant Subspace

The implication of Theorem 5 is that a degenerate set of eigenfunctions of $\hat{H}$ form an invariant subspace under the symmetry operations of the Schrödinger group and therefore form a basis for a representation of the group. Let $\{\psi_i\}$ be a set of degenerate eigenfunctions with energy ϵ. Since $\hat{T}(G)\psi_i(\mathbf{r}) = \psi_i(G^{-1}\mathbf{r})$ is also an eigenfunction with the same energy ϵ, it must be possible to expand $\hat{T}(G)\psi_i(\mathbf{r})$ as a linear combination of $\{\psi_i\}$:

$$\hat{T}(G)\psi_i = \sum_j \psi_j T_{ji}(G)$$

The matrices $\{T(G)\}$ form a representation for the Schrödinger group.

The representation is normally irreducible but if it is reducible, then there are two possibilities:

1. There is an accidental degeneracy so that the subspace can be broken up into two or more irreducible subspaces. A vector in one irreducible subspace evidently cannot be brought into another irreducible subspace by the symmetry operators.

2. The group is a subgroup of a larger group.

In practice, accidental degeneracies my be lifted up by varying parameters in the Hamiltonian without changing the symmetry of it. If the subspace is irreducible, the degeneracy is termed "normal".

Assuming that there is no accidental degeneracy, each degenerate set of eigenfunctions of $\hat{H}$ form a basis for an irreducible representation of the Schrödinger group. We may label each eigenfunction by the row and the irreducible representation to which it belongs. In this sense, the row index and the irreducible representation provide "quantum numbers". The degeneracy is simply given by the dimensionality of the irreducible representation. Thus by knowing the symmetry of the Hamiltonian, we can tell the degrees of degeneracy possible in any problem. It follows that these degeneracies can only be broken by a perturbation if it has a lower symmetry than the unperturbed Hamiltonian. Moreover, by knowing the symmetry of the perturbation, we can also tell how the degeneracies are split.

3.8.3 Partial Diagonalisation of $\hat{H}$

Theorem 6:
The matrix element $(\phi_i^\alpha, \hat{H}\psi_j^\beta)$ is zero unless $\alpha = \beta$ and $i = j$.

Proof:

$$\begin{aligned}
(\phi_i^\alpha, \hat{H}\psi_j^\beta) &= (\hat{T}(G)\phi_i^\alpha, \hat{T}(G)\hat{H}\psi_j^\beta) \\
&= (\hat{T}(G)\phi_i^\alpha, \hat{H}\hat{T}(G)\psi_j^\beta) \\
&= \sum_{kl} T^{\alpha *}{}_{ki}(G) T^\beta_{lj}(G)(\phi_k^\alpha, \hat{H}\psi_l^\beta) \\
&= \frac{1}{h}\sum_G \sum_{kl} T^{\alpha *}{}_{ki}(G) T^\beta_{lj}(G)(\phi_k^\alpha, \hat{H}\psi_l^\beta) \\
&= \frac{1}{l_\alpha}\sum_{kl} \delta_{kl}\delta_{ij}\delta_{\alpha\beta}(\phi_k^\alpha, \hat{H}\psi_l^\beta) \\
&= \frac{1}{l_\alpha}\delta_{\alpha\beta}\delta_{ij}\sum_k (\phi_k^\alpha, \hat{H}\psi_k^\beta)
\end{aligned}$$

This result is very useful because by choosing basis functions with the appropriate symmetry, the Hamiltonian is partially diagonalised with very little effort. Also, $(\phi_i^\alpha, \hat{H}\psi_i^\beta)$ is independent of i. This is a special case of the so called Wigner-Eckart theorem discussed later.

3.9 Irreducible Sets of Operators

We have studied the concept of irreducible subspace formed by a set of functions which transform among themselves under the group operations. A similar concept may be extended to operators and we define an irreducible set of operators $\hat{O}_i^\alpha$ by the closure property

$$\hat{O}_i^{\alpha'} = \hat{T}(G)\hat{O}_i^\alpha \hat{T}^{-1}(G) = \sum_j \hat{O}_j^\alpha T^\alpha_{ji}(G) \tag{3.6}$$

Thus the irreducible set of operators $\hat{O}_i^\alpha$ transform among themselves under the irreducible representation T^α. The number of operators in such a set is equal to the dimension l_α of the irreducible representation. An example of an irreducible set of operators is given by the momentum operators p_x, p_y, and p_z under rotation.

3.10 Direct Product Representations of a Group

The direct product of an $n \times n$ matrix A and and $m \times m$ matrix B is defined by

$$(A \otimes B)_{ii',jj'} = A_{ij} B_{i'j'} \tag{3.7}$$

$(A \otimes B)$ is an $(mn \times mn)$ matrix and it is *not* the same as a matrix multiplication of A and B.

Theorem 7:
If T^α and T^β are two representations of a group, then $T^{\alpha\otimes\beta} = T^\alpha \otimes T^\beta$ is also a representation of the group.

Proof:

$$\begin{aligned}
[T^{\alpha\otimes\beta}(G_1)T^{\alpha\otimes\beta}(G_2)]ii', jj' &= \sum_{kk'} T^{\alpha\otimes\beta}_{ii',kk'}(G_1) T^{\alpha\otimes\beta}_{kk',jj'}(G_2) \\
&= \sum_{kk'} T^{\alpha}_{ik}(G_1) T^{\beta}_{i'k'}(G_1) T^{\alpha}_{kj}(G_2) T^{\beta}_{k'j'}(G_2) \\
&= T^{\alpha}_{ij}(G_1G_2) T^{\beta}_{i'j'}(G_1G_2) \\
&= T^{\alpha\otimes\beta}_{ii',jj'}(G_1G_2)
\end{aligned}$$

Theorem 8:
The character of a direct product representation $T^{\alpha\otimes\beta}$ is the product of the characters of T^α and T^β.

Proof:

$$\begin{aligned}
\chi^{\alpha\otimes\beta} &= \sum_{ii'} T^{\alpha\otimes\beta}_{ii',ii'} \\
&= \sum_{ii'} T^{\alpha}_{ii} T^{\beta}_{i'i'} \\
&= \chi^\alpha \chi^\beta
\end{aligned}$$

Theorem 9:
If $\{\psi_i^\alpha\}$ transform according to the representation T^α and $\{\psi_j^\beta\}$ transform according to the representation T^β, then $\{\psi_i^\alpha \psi_j^\beta\}$ transform according to the direct product representation $T^{\alpha\otimes\beta}$.

Proof:

$$\begin{aligned}\hat{T}(G)(\psi_i^\alpha \psi_j^\beta) &= \sum_k \sum_l \psi_k^\alpha T_{ki}^\alpha(G) \psi_l^\beta T_{lj}^\beta(G) \\ &= \sum_{kl} (\psi_k^\alpha \psi_l^\beta) T_{kl,ij}^{\alpha\otimes\beta}\end{aligned}$$

In general, the direct product representation is reducible even when the two constituent representations are irreducible. There is a unitary matrix U, independent of the group elements, which transforms $T^{\alpha\otimes\beta}$ into a block form:

$$\sum_{ij,i'j'} U_{\gamma mk,ij} T_{ij,i'j'}^{\alpha\otimes\beta} U_{ij,\gamma' m' k'}^\dagger = \delta_{\gamma\gamma'} \delta_{mm'} T_{kk'}^\gamma \tag{3.8}$$

The label m distinguishes blocks with the same irreducible representation. Thus, we may write

$$T^{\alpha\otimes\beta} = \sum_\gamma \oplus m_\gamma T^\gamma \tag{3.9}$$

γ labels the irreducible representations and the coefficients m_γ, which tells us the number of times the irreducible representation γ occurs in the decomposition, can be calculated using the first orthogonality relation of the characters

$$\begin{aligned}\chi^{\alpha\otimes\beta} &= \sum_\gamma m_\gamma \chi^\gamma \\ \chi^\alpha \chi^\beta &= \sum_\gamma m_\gamma \chi^\gamma \\ m_\gamma &= (1/h) \sum_k N_k \chi^\alpha(C_k) \chi^\beta(C_k) \chi^{\gamma *}(C_k)\end{aligned}$$

3.11 Clebsch-Gordan Coefficients

Since the set of product functions $\psi_i^\alpha \psi_j^\beta$ transform according to the product representation $T^{\alpha\otimes\beta}$ which is in general reducible, evidently the space formed by the product functions are also reducible and the product functions may then be projected into these irreducible subspaces:

$$\psi_i^\alpha \psi_j^\beta = \sum_{\gamma m} F_{ij}^\gamma(m)$$

where $F_{ij}^\gamma(m)$ belongs to the irreducible subspace γ. The label m distinguishes functions with the same γ which is necessary only when $m_\gamma > 1$ in the decomposition of the product representation. In other words, there may be more than one subspace which transform according to the same irreducible representation. $F_{ij}^\gamma(m)$ itself may be expanded in an orthogonal basis which spans the irreducible subspace γ:

$$F_{ij}^\gamma(m) = \sum_k f_k^\gamma(m) C_{k,ij}^\gamma(m)$$

and therefore

$$\psi_i^\alpha \psi_j^\beta = \sum_{\gamma m} \sum_k f_k^\gamma(m) C_{k,ij}^\gamma(m) \tag{3.10}$$

The coefficients C are called the Clebsch-Gordan coefficients and they depend on α and β.

Apart from a possible phase factor, the Clebsch-Gordan coefficients are actually identical to the unitary matrix U defined in the previous section. To see this, we consider how the state $\Psi_k^\gamma(m) = \sum_{ij} \psi_i^\alpha \psi_j^\beta U^\dagger_{ij,\gamma mk}$ transform under a group symmetry operation:

$$\begin{aligned}
\hat{T}(G)\Psi_k^\gamma(m) &= \sum_{ij,i'j'} \psi_{i'}^\alpha \psi_{j'}^\beta T^{\alpha\otimes\beta}_{i'j',ij} U^\dagger_{ij,\gamma mk} \\
&= \sum_{i'j'k'} \psi_{i'}^\alpha \psi_{j'}^\beta U^\dagger_{i'j',\gamma mk'} T^\gamma_{k'k} \\
&= \sum_{k'} \Psi_{k'}^\gamma(m) T^\gamma_{k'k}
\end{aligned}$$

We have used Eq. (3.8) in the second step. Thus the states $\Psi_k^\gamma(m)$ transform according to the irreducible representation γ. We may also write

$$\psi_i^\alpha \psi_j^\beta = \sum_{k\gamma m} \Psi_k^\gamma(m) U_{\gamma mk,ij} \tag{3.11}$$

which shows that the Clebsch-Gordan coefficients are identical to the unitary matrix U, apart from a phase factor. By convention, they are normalised as follows:

$$\sum_{ij} |C^{\gamma}_{ijk}(m)|^2 = 1 \tag{3.12}$$

Since C is unitary, it satisfies the following relations

$$\sum_{ij} C^{\gamma}_{k,ij}(m) C^{*\gamma'}_{k',ij}(m') = \delta_{\gamma\gamma'}\delta_{mm'}\delta_{kk'}$$

$$\sum_{\gamma km} C^{\gamma}_{k,ij}(m) C^{*\gamma}_{k,i'j'}(m) = \delta_{ii'}\delta_{jj'}$$

3.12 The Wigner-Eckart Theorem

In physics, we are often faced with a problem of calculating matrix elements of an operator $\hat{O}$ between two states ψ and ϕ: $(\psi, \hat{O}\phi)$. In practice, the calculation of matrix elements can be very complicated and we would like to study if group theory can help us in simplifying this problem.

First of all, from previous sections, we know that an arbitrary function belonging to a linear space L which transforms into itself under group operations can be projected into the different irreducible components of the group. Consequently, we need only consider matrix elements of the type:

$$(f^{\gamma}_k, \hat{O}^{\alpha}_i f^{\beta}_j)$$

We study the transformation of the function $\psi_{ij} = \hat{O}^{\alpha}_i f^{\beta}_j$ under a group symmetry operation:

$$\begin{aligned}
\hat{T}(G)\psi_{ij} &= \hat{T}(G)\hat{O}^{\alpha}_i f^{\beta}_j \\
&= [\hat{T}(G)\hat{O}^{\alpha}_i \hat{T}^{-1}(G)]\, \hat{T}(G) f^{\beta}_j \\
&= \sum_k \hat{O}^{\alpha}_k T^{\alpha}_{ki}(G) \sum_m f^{\beta}_m T^{\beta}_{mj}(G) \\
&= \sum_{km} \psi_{km} T^{\alpha\otimes\beta}_{km,ij}(G)
\end{aligned}$$

The new function ψ_{ij} may then be completely expanded into its irreducible components as in Eq. (3.11):

$$\psi_{ij} = \sum_{\gamma' k' m} \Psi^{\gamma'}_{k'}(m) C^{\gamma'}_{k',ij}(m)$$

The matrix element is then given by

$$\begin{aligned}(f_k^\gamma, \hat{O}_i^\alpha f_j^\beta) &= \sum_{\gamma' k' m} (f_k^\gamma, \Psi_{k'}^{\gamma'}(m)) C_{k',ij}^{\gamma'}(m) \\ &= \sum_m (f_k^\gamma, \Psi_k^\gamma(m)) C_{k,ij}^\gamma(m)\end{aligned}$$

The significance of the above result is that the Clebsch-Gordan coefficients $C_{k,ij}^\gamma(m)$ are obtained entirely from symmetry and they do not depend on the details of the potential of the system. Information about the details of the system is contained in the matrix elements $(f_k^\gamma, \Psi_k^\gamma(m))$ which do not depend on i and j. In fact, it does not depend on k as shown in section 3.6. These matrix elements are often referred to as reduced matrix elements and they are written as

$$(f_k^\gamma, \Psi_k^\gamma(m)) = \langle f^\gamma || \hat{O}^\alpha || f^\beta \rangle_m$$

emphasising the fact that the reduced matrix elements are independent of i, j, and k. Thus we have

$$(f_k^\gamma, \hat{O}_i^\alpha f_j^\beta) = \sum_m \langle f^\gamma || \hat{O}^\alpha || f^\beta \rangle_m C_{k,ij}^\gamma(m) \tag{3.13}$$

This is known as the Wigner-Eckart theorem which tells us that the matrix element $(f_k^\gamma, \hat{O}_i^\alpha f_j^\beta)$ is zero unless the product representation $T^{\alpha \otimes \beta}$ contains the irreducible representation γ. This is a general form of selection rules. The Clebsch-Gordan coefficients relate the matrix elements for a given α, β, and γ but with different i, j, and k to one another.

We can see that theorem 6 follows immediately from the Wigner-Eckart theorem because the Hamiltonian is an invariant under the group symmetry operations, i.e. $\hat{T}(G)\hat{H}\hat{T}^{-1}(G) = \hat{H}$, so that $\hat{H}$ transforms according to the identity representation.

3.13 Applications

We list a few of the common applications of group theory.

1. Selection rules: As an example we consider optical transitions in a molecule which has a D_3 symmetry. This could correspond to a

molecule with three identical atoms at the corners of a triangle. Actually, the full symmetry is higher than D_3 but as an illustration it is sufficient to consider the D_3 symmetry. Optical transitions are governed by dipole operators x, y, and z which transform like the three Cartesian unit vectors. The groundstate of the molecule may be assumed to be non-degenerate and symmetric so that it transforms according to the identity representation. From the previous example, the dipole operators transform according to the representation $T = T^2 \oplus T^3$ and therefore the final states can only be those which transform according to $(T^2 \oplus T^3) \otimes T^1 = T^2 \oplus T^3$.

2. Symmetry breaking: In the above example, we know from symmetry alone that the eigenfunctions can only be at most doubly degenerate. If we replace one of the atoms by a different atom so that the symmetry becomes C_2, then this degeneracy, if it exists, must split into two non-degenerate levels because C_2 is an Abelian group and the irreducible representations are one dimensional. The actual reduction can be figured out straightforwardly using the orthogonality relation between the characters. The ordering of the energy levels, however, cannot be determined by group theory alone.

3. Variational principle: We are often interested in finding the groundstate of a given Hamiltonian which usually cannot be solved analytically. One method of obtaining an approximate groundstate is based on variational principle. We start with some basis functions $\{\phi_i\}$ and approximate the true groundstate Ψ as a linear combination of these functions.

$$\Psi = \sum_i c_i \phi_i$$

From the variational principle, the energy expectation value $< E >= (\Psi, \hat{H}\Psi) \geq E_0$, where E_0 is the true groundstate energy. The coefficients $\{c_i\}$ are determined by minimising $< E >$ subject to the condition $(\Psi, \Psi) = 1$:

$$\begin{aligned} \frac{\partial}{\partial c_i^*}\left[< E > -\lambda(\Psi, \Psi)\right] &= \frac{\partial}{\partial c_i^*}\left[\sum_{jk} c_j^*(\phi_j, \hat{H}\phi_k)c_k - \lambda \sum_j c_j^* c_j\right] \\ &= \sum_k H_{ik}c_k - \lambda c_i = 0 \end{aligned}$$

which is just an eigenvalue problem.

From Theorem 6, it is clear that we should sort out the basis functions, using the projection operator method for example, according to the rows and irreducible representations $\{\phi_i^{\alpha m}\}$ where m labels different possible subspaces transforming according to the same irreducible representation α. It is only necessary to express the trial function as follows: $\psi = \sum_m c_i^{\alpha m}\phi_i^{\alpha m}$. When $m = 1$, the Hamiltonian is already diagonal and when $m > 1$, we need only diagonalise an $m \times m$ matrix instead of an $l \times l$ matrix where $l = \sum_{\alpha m i} 1$, which is usually much larger than m.

4. Degenerate perturbation theory: In many cases, the Hamiltonian may be broken up into two terms $\hat{H} = \hat{H}_0 + \hat{H}_1$ such that $\hat{H}_1$ may be treated as a small perturbation to $\hat{H}_0$. $\hat{H}_0$ usually has a higher symmetry than $\hat{H}_1$. A typical example of this is an atom placed in a crystal where the crystal field symmetry is lower than the rotational symmetry of the atom. If the eigenfunctions of $\hat{H}_0$ are degenerate, we may use the variational principle to calculate the energy shifts. The eigenfunction of $\hat{H}$ is approximated as a linear combination of the degenerate eigenfunctions of $\hat{H}_0$. This leads to an eigenvalue problem for $\hat{H}_1$ and the eigenvalues give the first order shifts. As before, we should sort out the degenerate eigenfunctions of $\hat{H}_0$ according to the rows and irreducible representations of the symmetry group of $\hat{H}_1$ in order to minimise the size of the matrix to be diagonalised.

3.14 Examples

1. Bloch Theorem: A lattice is a parallelepiped formed by three linearly independent vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$. A set of vectors $\mathbf{t} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$ for all possible integers n_1, n_2, n_3 generate lattice points which together with the associated lattices form a crystal. The set $t = \{\mathbf{t}\}$ clearly form a group under vector addition and the group is Abelian. In fact, it is a direct product of three groups

$$t = t_1 \otimes t_2 \otimes t_3$$

where $t_1 = \{n_1\mathbf{a}_1\}$, $t_2 = \{n_2\mathbf{a}_2\}$, and $t_3 = \{n_3\mathbf{a}_3\}$. It is customary to have a periodic boundary condition such that

$$\hat{T}(N_1\mathbf{a}_1)\psi(\mathbf{r}) = \psi(\mathbf{r} + N_1\mathbf{a}_1) = \psi(\mathbf{r}) \rightarrow \hat{T}(N_1\mathbf{a}_1) = \hat{T}(0) = 1$$

Similarly for the other two groups. N_1 is taken to be infinite at the end. The groups t_1, t_2, and t_3 become cyclic and the irreducible representations are given by $e^{i2\pi k_1/N_1}$, $k_1 = 1, 2, \ldots, N_1$, and their powers. It is useful at this stage to introduce the concept of reciprocal space defined by

$$\begin{aligned}
\mathbf{g}_1 &= 2\pi\frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} \\
\mathbf{g}_2 &= 2\pi\frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3} \\
\mathbf{g}_3 &= 2\pi\frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot \mathbf{a}_2 \times \mathbf{a}_3}
\end{aligned}$$

so that

$$\mathbf{g}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$$

With this definition, the direct product representations can be written

$$T^{\mathbf{k}}(\mathbf{t}) = e^{i\mathbf{k}\cdot\mathbf{t}}$$

where $\mathbf{k} = (k_1/N_1)\mathbf{g}_1 + (k_2/N_2)\mathbf{g}_2 + (k_3/N_3)\mathbf{g}_3$. It follows that the eigenfunctions of a Hamiltonian with translational lattice symmetry form basis functions for the irreducible representations of the group of translations and they may be labelled by the irreducible representations $\mathbf{k}$. This means

$$\hat{T}(\mathbf{t})\psi_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}(\mathbf{r} + \mathbf{t}) = \psi_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{t}}$$

which is the Bloch theorem.

2. Normal modes (chapter 6 of Elliot and Dawber): When the atoms in a molecule are displaced from their equilibrium positions, the potential energy will increase. If the atoms are let free, there will be an interchange between potential and kinetic energies resulting in vibrations. These vibrations may be thought of as being composed

of eigen modes or normal modes, each with a well defined frequency, in the same way that a wavefunction can be decomposed into a sum of eigenstates with well defined energies. The eigen modes may be classified according to the irreducible representations of the symmetry group of the molecule, just like the the eigenstates of the Hamiltonian.

The potential energy for arbitrary displacements of N atoms in a molecule is given by

$$V = V_0 + \sum_i \frac{\partial V}{\partial q_i} q_i + \sum_{ij} \frac{\partial^2 V}{\partial q_i \partial q_j} q_i q_j$$

The sums run from 1 to $3N$. At equilibrium, $\partial V/\partial q_i = 0$ so that the Hamiltonian for molecular vibrations is given by

$$H = \sum_i \frac{1}{2} M_i \dot{q}_i^2 + \sum_{ij} \frac{1}{2} B_{ij} q_i q_j$$

where $B_{ij} = \partial^2 V/\partial q_i \partial q_j$. It is conventional to absorb the masses into the displacement coordinates by defining

$$\alpha_i = \sqrt{M_i} q_i, \quad D_{ij} = B_{ij}/\sqrt{M_i M_j}$$

The Hamiltonian becomes

$$H = \sum_i \frac{1}{2} \dot{\alpha}_i^2 + \sum_{ij} \frac{1}{2} D_{ij} \alpha_i \alpha_j$$

The matrix D is known as the dynamical matrix.

We can now introduce a $3N$ dimensional abstract space with orthonormal basis vectors $\{\mathbf{e}_i\}$. The $3N$ displacements of atoms in real space may be mapped into a vector in the $3N$ dimensional abstract space:

$$(q_1, q_2, \ldots, q_{3N}) \rightarrow \mathbf{q} = \sum_i \mathbf{e}_i \alpha_i$$

The unit vector $\mathbf{e}_i$ corresponds to a displacement $q_i = 1/\sqrt{M_i}$ in real space but we note that $\mathbf{e}_i$ itself is not a displacement in real space

but rather a displacement in the abstract space. We may define an operator $\hat{D}$ in the abstract space so that

$$\begin{aligned} V(\mathbf{q}) &= \frac{1}{2}(\mathbf{q}, \hat{D}\mathbf{q}) \\ &= \frac{1}{2}\sum_{ij}\alpha_i\alpha_j(\mathbf{e}_i, \hat{D}\mathbf{e}_j) \end{aligned}$$

which implies

$$D_{ij} = (\mathbf{e}_i, \hat{D}\mathbf{e}_j) \rightarrow \hat{D}\mathbf{e}_j = \sum_i \mathbf{e}_i D_{ij}$$

We would like to transform the Hamiltonian into the form $H = \sum_i h_i$ so that the eigenvenctors of H can be written as a product of the eigenvectors of h. This can be done by a unitary transformation

$$\mathbf{u}_k = \sum_i \mathbf{e}_i a_{ik}$$

An arbitrary vector $\mathbf{q}$ may be written as

$$\mathbf{q} = \sum_i \mathbf{e}_i\alpha_i = \sum_k \mathbf{u}_k Q_k = \sum_{ki} \mathbf{e}_i a_{ik} Q_k \rightarrow \alpha_i = \sum_k a_{ik}Q_k$$

By choosing $\mathbf{u}_k$ to be an eigenvector of $\hat{D}$, i.e. $\hat{D}\mathbf{u}_k = \omega_k\mathbf{u}_k$ or $\sum_j D_{ij}a_{jk} = \omega_k a_{ik}$, the Hamiltonian becomes

$$H = \sum_k \left[\frac{1}{2}\dot{Q}_k^2 + \frac{1}{2}\omega_k Q_k^2\right]$$

which is the desired form. Quantum mechanically, we replace $\dot{Q}_k^2$ with $-\partial^2/\partial Q_k^2$ and the solutions to $h = -\partial^2/\partial Q_k^2 + \frac{1}{2}\omega_k Q_k^2$ are

$$\begin{aligned} \psi_{n(k)} &= AH_{n(k)}(\sqrt{\omega_k}Q_k)exp(-\omega_k Q_k/2) \\ \epsilon_{n(k)} &= (n(k) + \frac{1}{2})\omega_k \end{aligned}$$

We have set the Planck constant $h/2\pi = 1$.

So far we have not made any use of group theory and in principle we can calculate the dynamical matrix D and diagonalise it to obtain

the normal modes and the corresponding eigen frequencies. The diagonalisation of D is greatly simplified by using group theory. The eigen frequencies, however, cannot be obtained from group theory alone because they depend on the strength of the potential. By definition, we have

$$[\hat{T}(G), \hat{D}] = 0$$

for all G and it immediately follows from Theorem 5 that the degenerate eigenvectors of $\hat{D}$ (normal modes) form basis vectors for the irreducible representations of the group.

The $3N$ dimensional space forms a $3N \times 3N$ representation which is in general reducible:

$$\chi^{3N} = \sum_{\gamma} m_\gamma \chi^\gamma$$

To calculate χ^{3N}, we first write the basis vector as $\mathbf{e}_i(R)$, $i = x, y, z$, $R = 1, 2, \ldots, N$, which corresponds to a displacement of atom R along the i-axis. The effect of the symmetry operation on the basis vector is given by

$$\hat{T}(G)\mathbf{e}_i(R) = \sum_{R'j} \mathbf{e}_j(R') T_{ji}^{R'R}(G)$$

The character is given by

$$\chi^{3N} = \sum_{Ri} T_{ii}^{RR} = N_R \chi^V$$

where N_R is the number of atoms unmoved by the symmetry operation $\hat{T}(G)$ and χ^V is the character of the three dimensional vector representation. This result can be understood by observing that when $\hat{T}(G)$ moves atom R to atom R', $\sum_i T_{ii}^{RR} = 0$. When atom R is not moved, then $\sum_i T_{ii}^{RR} = \chi^V$.

As an example, we consider a molecule with D_3 symmetry (three atoms at the corners of an equilateral triangle). We have already worked out the characters for the vector representation χ^V and they are given by $\chi^V(C_e) = 3$, $\chi^V(C_c) = 0$, and $\chi^V(C_d) = -1$. Thus $\chi^{3N}(C_e) = 3 \cdot 3 = 9$, $\chi^{3N}(C_c) = 0$, and $\chi^{3N}(C_d) = 1 \cdot (-1) =$

-1. It is then straightforward to decompose χ^{3N} into the different irreducible components using the character table of D_3. We get

$$\begin{aligned} m_1 &= \frac{1}{6}(1 \cdot 1 \cdot 9 + 2 \cdot 1 \cdot 0 + 3 \cdot 1 \cdot (-1)) = 1 \\ m_2 &= \frac{1}{6}(1 \cdot 1 \cdot 9 + 2 \cdot 1 \cdot 0 + 3 \cdot (-1) \cdot (-1)) = 2 \\ m_3 &= \frac{1}{6}(1 \cdot 2 \cdot 9 + 2 \cdot (-1) \cdot 0 + 3 \cdot 0 \cdot (-1)) = 3 \end{aligned}$$

There are three non-degenerate modes and three doubly degenerate modes. Actually, six of them correspond to rigid motions, i.e. there is no relative motion between the atoms. The significance of classifying the vibrations into normal modes is that when calculating absorption or emission spectra it is possible to figure out which modes are allowed in the absorption process. The simplest absorption processes are caused by electric dipole transitions from the groundstate to some vibrational excited states. The groundstate usually tranforms according to the identity representation and the dipole operators transform according to the vector representation. Thus the modes allowed are given by those corresponding to the irreducible representations occuring in the decomposition of the vector representation. In more complicated absorption processes, there are intermediate states involved. In this case the dominant operators are of the form xy, yz, zx, x^2, y^2, and z^2 (Raman spectra). These are in fact products of x, y, and z, i.e. they transform according to the product of the vector representations which can be decomposed into the irreducible components. Care, however, has to be taken due to the fact that the product functions are not linearly independent. See chapter 6 of Elliot and Dawber for more examples and details.

Chapter 4

Lie Groups

4.1 Definitions

So far we have considered groups with a finite number of elements. In this Chapter, we will study the so called continuous groups in which the elements G are defined uniquely by a set of n *independent* continuous real parameters $\mathbf{a} = (a_1, a_2, \ldots, a_n)$ so that $G(\mathbf{a}) \neq G(\mathbf{b})$ unless $\mathbf{a} = \mathbf{b}$. The number n is called the dimension of the group. Such groups have an infinite number of elements. The elements of a continuous group satisfy the multiplication law:

$$G(\mathbf{a})G(\mathbf{b}) = G(\mathbf{c}) \tag{4.1}$$

This means that operating a group element $G(\mathbf{b})$ followed by $G(\mathbf{a})$ has the same effect as operating a group element $G(\mathbf{c})$ represented by a set of parameters $\mathbf{c}$. $\mathbf{c}$ must be a function of the paramaters $\mathbf{a}$ and $\mathbf{b}$:

$$\mathbf{c} = \mathbf{F}(\mathbf{a}, \mathbf{b}) \tag{4.2}$$

and we may write the multiplication law as:

$$G(\mathbf{a})G(\mathbf{b}) = G(\mathbf{F}(\mathbf{a}, \mathbf{b})) \tag{4.3}$$

As a convention, $\mathbf{a} = \mathbf{0}$ is chosen to represent the unit element:

$$G(\mathbf{0}) = 1 \tag{4.4}$$

With this definition, it follows from Eqs. (4.1) and (4.2) that

$$\mathbf{F}(\mathbf{a}, \mathbf{0}) = \mathbf{a}\ ;\ \mathbf{F}(\mathbf{0}, \mathbf{b}) = \mathbf{b}\ ;\ \mathbf{F}(\mathbf{0}, \mathbf{0}) = \mathbf{0} \tag{4.5}$$

$$\frac{\partial \mathbf{F}(\mathbf{0},\mathbf{0})}{\partial \mathbf{a}} = \frac{\partial \mathbf{F}(\mathbf{0},\mathbf{0})}{\partial \mathbf{b}} = 1 \tag{4.6}$$

In addition, every element must have an inverse i.e. for a given set of parameters $\mathbf{a}$, there is a set of parameters $\mathbf{q}$ such that

$$G(\mathbf{a})G(\mathbf{q}) = G(\mathbf{q})G(\mathbf{a}) = G(\mathbf{0}) = 1 \tag{4.7}$$

The functions $\mathbf{F(a,b)}$ are assumed to be analytic functions of the parameters $\mathbf{a}$ and $\mathbf{b}$, and this kind of group is called a Lie-group.

4.2 Infinitesimal Operators

An important concept in continuous groups is the concept of infinitesimal operators which are obtained by considering group elements near the unit element i.e. elements with small $\mathbf{a}$:

$$G(\mathbf{a}) = 1 + \mathbf{X}\cdot\mathbf{a} + \ldots \tag{4.8}$$

$$X_i = \left[\frac{\partial G}{\partial a_i}\right]_{\mathbf{a}=\mathbf{0}} \tag{4.9}$$

The set of operators $\mathbf{X} = (X_1, X_2, \ldots, X_n)$ are called the infinitesimal operators, or generators, which are *independent* of the parameters $\mathbf{a}$. It will be shown below that every group element may be expressed in terms of the infinitesimal operators so that the study of continuous groups may be restricted in most cases to the study of these infinitesimal operators.

For small $\mathbf{a}$ and $\mathbf{b}$ we have

$$\begin{aligned}\mathbf{F}(\mathbf{a},\mathbf{b}) &= \mathbf{F}(\mathbf{a},\mathbf{0}) + \frac{\partial \mathbf{F}(\mathbf{0},\mathbf{0})}{\partial \mathbf{b}}\cdot\mathbf{b} \\ &= \mathbf{a}+\mathbf{b}\end{aligned}$$

using Eq. (4.6). As a convention, a dot denotes a dot product or a summation over the lower and upper vectors. This implies that

$$G(\mathbf{a})G(\mathbf{b}) = G(\mathbf{F}(\mathbf{a},\mathbf{b})) = G(\mathbf{a}+\mathbf{b})$$

$$G(\mathbf{b})G(\mathbf{a}) = G(\mathbf{F}(\mathbf{b},\mathbf{a})) = G(\mathbf{b}+\mathbf{a})$$

i.e. the group elements are commutative in the vicinity of the unit element.

To relate the group elements and the infinitesimal operators, we study the product $G(\mathbf{a})G(\mathbf{b})$ for an arbitrary $\mathbf{a}$ but small $\mathbf{b}$. To simplify the writing, we define a matrix

$$\mathbf{M}(\mathbf{a}) \equiv \frac{\partial \mathbf{F}(\mathbf{a},\mathbf{0})}{\partial \mathbf{b}} \rightarrow \mathbf{M}_{ij}(\mathbf{a}) \equiv \frac{\partial F_i(\mathbf{a},\mathbf{0})}{\partial b_j} \tag{4.10}$$

and a convention that a dot on the left of $\mathbf{M}$ means a summation over the rows whereas a dot on the right means a summation over the columns.

$$\begin{aligned} G(\mathbf{a})G(\mathbf{b}) &= G(\mathbf{F}(\mathbf{a},\mathbf{b})) \\ &= G(\mathbf{F}(\mathbf{a},\mathbf{0}) + \mathbf{M}(\mathbf{a})\cdot\mathbf{b}) \\ &= G(\mathbf{a} + \mathbf{M}(\mathbf{a})\cdot\mathbf{b}) \\ &= G(\mathbf{a}) + \frac{\partial G(\mathbf{a})}{\partial \mathbf{a}}\cdot\mathbf{M}(\mathbf{a})\cdot\mathbf{b} \end{aligned}$$

On the other hand

$$G(\mathbf{a})G(\mathbf{b}) = G(\mathbf{a})[1 + \mathbf{X}\cdot\mathbf{b}]$$

so that

$$G(\mathbf{a})\mathbf{X}\cdot\mathbf{b} = \frac{\partial G(\mathbf{a})}{\partial \mathbf{a}}\cdot\mathbf{M}(\mathbf{a})\cdot\mathbf{b}$$

Since $\mathbf{b}$ are arbitrary and independent parameters, it must be that

$$G(\mathbf{a})\mathbf{X} = \frac{\partial G(\mathbf{a})}{\partial \mathbf{a}}\cdot\mathbf{M}(\mathbf{a}) \tag{4.11}$$

This equation relates the group element and its derivative at $\mathbf{a}$ to the infinitesimal operators $\mathbf{X}$.

We now try to find an explicit expression relating $G(\mathbf{a})$ to $\mathbf{X}$. Let $\mathbf{u} = (u_1, u_2, \ldots, u_n)$ be a unit vector $(\mathbf{u}\cdot\mathbf{u} = 1)$ in the parameter space and let us project Eq. (4.11) along this unit vector:

$$G(\mathbf{a})\mathbf{X}\cdot\mathbf{u} = \frac{\partial G(\mathbf{a})}{\partial \mathbf{a}}\cdot\mathbf{M}(\mathbf{a})\cdot\mathbf{u} \tag{4.12}$$

We define a curve in the parameter space by the following equation

$$\frac{d\mathbf{a}(t)}{dt} = \mathbf{M}(\mathbf{a})\cdot\mathbf{u} \tag{4.13}$$

with boundary condition $\mathbf{a}(0) = \mathbf{0}$. The direction of this curve at $t = 0$ is along the unit vector $\mathbf{u}$ because $\mathbf{M}(\mathbf{0}) = \frac{\partial \mathbf{F}(\mathbf{0},\mathbf{0})}{\partial \mathbf{b}} = 1$. Using Eq. (4.13) in (4.12) yields

$$\begin{aligned} G(\mathbf{a})\mathbf{X}\cdot\mathbf{u} &= \frac{\partial G(\mathbf{a})}{\partial \mathbf{a}}\cdot\frac{d\mathbf{a}}{dt} \\ &= \frac{dG(\mathbf{a})}{dt} \end{aligned}$$

which can be formally solved to give

$$G(\mathbf{a}(t)) = e^{t\mathbf{X}\cdot\mathbf{u}} \tag{4.14}$$

Thus, the group elements at finite parameters $\mathbf{a}$ can be obtained from the infinitesimal operators $\mathbf{X}$. The global properties of Lie groups are determined by the infinitesimal operators $\mathbf{X}$ which are independent of the parameters $\mathbf{a}$. We have made an assumption, however, that every point $\mathbf{a}$ in the parameter space can be reached by the curve defined in Eq. (4.13), by starting along an appropriate direction $\mathbf{u}$ from the origin.

4.3 Lie Algebra

The infinitesimal operators satisfy commutation relations and to find these relations, we differentiate Eq. (4.11) with respect to a parameter a_i for each component j:

$$\frac{\partial G(\mathbf{a})}{\partial a_i}X_j = \sum_k \left[\frac{\partial^2 G(\mathbf{a})}{\partial a_i \partial a_k}\frac{\partial F_k(\mathbf{a},\mathbf{0})}{\partial b_j} + \frac{\partial G(\mathbf{a})}{\partial a_k}\frac{\partial^2 F_k(\mathbf{a},\mathbf{0})}{\partial a_i \partial b_j}\right]$$

Evaluating this expression for $\mathbf{a} = \mathbf{0}$, we get

$$X_i X_j = \frac{\partial^2 G(\mathbf{0})}{\partial a_i \partial a_j} + \sum_k X_k \frac{\partial^2 F_k(\mathbf{0},\mathbf{0})}{\partial a_i \partial b_j}$$

Interchanging $i \leftrightarrow j$ and taking the difference, we get

$$[X_i, X_j] = \sum_k X_k c_{ij}^k \tag{4.15}$$

where

$$c_{ij}^{k} = \frac{\partial^2 F_k(\mathbf{0},\mathbf{0})}{\partial a_i \partial b_j} - \frac{\partial^2 F_k(\mathbf{0},\mathbf{0})}{\partial a_j \partial b_i} \tag{4.16}$$

We see that the infinitesimal operators possess a closure property under commutation. Operators possessing this property are said to form an algebra and for Lie groups it is called Lie algebra. For every Lie group there is a corresponding Lie algebra.

The coefficients c_{ij}^{k} are called the structure constants and they are purely determined by the functions $\mathbf{F(a,b)}$ which means that they are *independent of any particular representation of the group.*

The structure constants are antisymmetric in the lower indices:

$$c_{ij}^{k} = -c_{ji}^{k} \tag{4.17}$$

We can construct symmetric and anti-symmetric quantities from the structure constants. By summing over products of two structure constants, we obtain symmetric matrices

$$g_{ij} = \sum_{kl} c_{il}^{k} c_{jk}^{l} = g_{ji} \tag{4.18}$$

Summing over products of these matrices and the structure constants yields

$$a_{ijk} = \sum_{m} g_{im} c_{jk}^{m} \tag{4.19}$$

which are anti-symmetric with respect to an interchange of two indices. This is because we have the following relation

$$\sum_{l} \left[c_{ij}^{l} c_{lk}^{m} + c_{jk}^{l} c_{li}^{m} + c_{ki}^{l} c_{lj}^{m} \right] = 0 \tag{4.20}$$

which follows from the Jacobi identity

$$[[A,B],C] + [[B,C],A] + [[C,A],B] = 0$$

In this way, we can continue forming symmetric and antisymmetric quantities from the structure constants.

4.4 Casimir Operators

To construct the irreducible representations of a continuous group, it will be useful to have some operators which commute with all of the infinitesimal operators. The degenerate eigenfunctions of these operators may then be used as basis functions for the irreducible representations because they transform among themselves under group operations. We recall from Chapter 3 that when $[\hat{T}(G), \hat{H}] = 0$, the sets of degenerate eigenfunctions of $\hat{H}$ form basis sets for the irreducible representations of the group (assuming we have the full group, not a subgroup of a larger group).

The simplest operator that commute with the infinitesimal operators $\mathbf{X}$ must be at least of second order in these operators because a linear combination of X_i clearly will not in general commute with $\mathbf{X}$ due to Eq. (4.15). Thus we form the most general linear combination of second order operators

$$C = \sum_{ij} g^{ij} X_i X_j \tag{4.21}$$

The matrix g^{ij} must be symmetric since every matrix can be written as a sum of symmetric and anti-symmetric matrices and from Eq. (4.15) the anti-symmetric part reduces to a linear combination of X_i. We evaluate the commutation of this operator with an arbitrary X_k:

$$\begin{aligned}
[C, X_k] &= \sum_{ij} g^{ij} [X_i X_j, X_k] \\
&= \sum_{ij} g^{ij} \{X_i [X_j, X_k] + [X_i, X_k] X_j\} \\
&= \sum_{ij} g^{ij} \sum_{l} \left\{ X_i X_l c^l_{jk} + X_l c^l_{ik} X_j \right\} \\
&= \sum_{ijl} g^{ij} c^l_{jk} \{X_i X_l + X_l X_i\}
\end{aligned}$$

The last step makes use of the fact that g^{ij} is symmetric. If we can find g^{ij} such that $\sum_j g^{ij} c^l_{jk}$ is anti-symmetric with respect to the interchange $i \leftrightarrow l$ then C is the required operator. We have in Eq. (4.19) an anti-symmetric quantity with three indices but it involves no upper indices in the structure constant. We may, however, write

$$c^l_{jk} = \sum_{ml'} g^{lm} g_{ml'} c^{l'}_{jk}$$

$$= \sum_m g^{lm} a_{mjk}$$

where we have defined the inverse of g^{ij}

$$\sum_m g^{lm} g_{ml'} = \delta_{ll'}$$

and

$$a_{mjk} = \sum_{l'} g_{ml'} c^{l'}_{jk}$$

as in Eq. (4.19) Continuing the evaluation of $[C, X_k]$ we get

$$\begin{aligned}
[C, X_k] &= \sum_{ijl} g^{ij} \sum_m g^{lm} a_{mjk} \{X_i X_l + X_l X_i\} \\
&= \frac{1}{2} \sum_{ijlm} [g^{ij} g^{lm} + g^{lj} g^{im}] a_{mjk} \{X_i X_l + X_l X_i\} \\
&= \frac{1}{4} \sum_{ijlm} [g^{ij} g^{lm} + g^{lj} g^{im}][a_{mjk} + a_{jmk}] \{X_i X_l + X_l X_i\}
\end{aligned}$$

Since $a_{mjk} = -a_{jmk}$ we obtain $[C, X_k] = 0$.

In general, it may be possible to form higher order Casimir operators, which also commute with all of the infinitesimal operators. The irreducible representations of the group may be labelled by the eigenvalues of these Casimir operators. In the rotation group discussed later, we need only one Casimir operator to label the irreducible representations.

4.5 Ladder Operators and Multiplets

For a given Lie group, some of the infinitesimal operators may commute among themselves. The largest number of mutually commuting infinitesimal operators is called the rank of the group. Let $\{\hat{H}_i\}$ be such a set and $\{\hat{E}_\alpha\}$ be the rest of the infinitesimal operators. Let also $\{\hat{C}_i\}$ be a set of Casimir operators. Since $\{\hat{C}_i\}$ commute with $\{\hat{H}_i\}$ it is possible to construct simultaneous eigenstates of $\{\hat{C}_i\}$ and $\{\hat{H}_i\}$ with eigenvalues $\{C_i\}$ and $\{H_i\}$:

$$\begin{aligned}
\hat{C}_i |C_i,\ H_i\rangle &= C_i |C_i,\ H_i\rangle \\
\hat{H}_i |C_i,\ H_i\rangle &= H_i |C_i,\ H_i\rangle
\end{aligned}$$

The remaining set of operators $\{\hat{E}_\alpha\}$ can be expressed as ladder operators:

$$[\hat{H}_i, \hat{E}_\alpha] = \epsilon_{i\alpha}\hat{E}_\alpha \tag{4.22}$$

This can be done by forming a linear combination $\hat{E}_\alpha = \sum_i \hat{X}_i a_{i\alpha}$ and requiring that

$$\begin{aligned} [\hat{H}_i, \sum_j \hat{X}_j a_{j\alpha}] &= \epsilon_{i\alpha}\sum_j \hat{X}_j a_{j\alpha} \\ \sum_{jk} \hat{X}_k c_{ij}^k a_{j\alpha} &= \epsilon_{i\alpha}\sum_j \hat{X}_j a_{j\alpha} \\ \sum_k \hat{X}_k \sum_j [c_{ij}^k - \epsilon_{i\alpha}\delta_{jk}]a_{j\alpha} = 0 &\rightarrow \sum_j c_{ij}^k a_{j\alpha} = \epsilon_{i\alpha}a_{k\alpha} \end{aligned}$$

The coefficients $a_{i\alpha}$ are the eigenvectors of the structure constants and $\epsilon_{i\alpha}$ are called the root vectors. Eq. (4.22) implies that

$$\begin{aligned} [\hat{H}_i, \hat{E}_\alpha]|C_i,\ H_i\rangle &= \epsilon_{i\alpha}\hat{E}_\alpha|C_i,\ H_i\rangle \\ (\hat{H}_i - H_i)\hat{E}_\alpha|C_i,\ H_i\rangle &= \epsilon_{i\alpha}\hat{E}_\alpha|C_i,\ H_i\rangle \\ \hat{H}_i(\hat{E}_\alpha|C_i,\ H_i\rangle) &= (H_i + \epsilon_{i\alpha})(\hat{E}_\alpha|C_i,\ H_i\rangle) \end{aligned}$$

i.e. $\hat{E}_\alpha|C_i,\ H_i\rangle$ is also an eigenstate of $\hat{H}_i$ but with an eigenvalue $(H_i+\epsilon_{i\alpha})$. This means

$$\hat{E}_\alpha|C_i,\ H_i\rangle = A_\alpha(C_i, H_i)|C_i,\ H_i + \epsilon_{i\alpha}\rangle \tag{4.23}$$

The constants A_α can be determined from the Lie algebra. The states generated by the ladder operators are the degenerate eigenstates of the Casimir operators. This is because the Casimir operators commute with all the infinitesimal operators and therefore the degenerate eigenstates of the Casimir operators form an invariant subspace under the infinitesimal operators. Acting $\hat{X}_i$ on $|C_i,\ H_i\rangle$ results in a linear combination of states with the same eigenvalues $\{C_i\}$. Such a set of degenerate states are called a multiplet and they form an invariant subspace under the group operations.

Assuming that the multiplet spans a finite space, there must be a state $|\psi_+\rangle$ and $|\psi_-\rangle$ with the largest and smallest values of $\{H_i\}$ such that

$$\hat{E}_\alpha|\psi_+\rangle = 0, \quad \hat{E}_\beta|\psi_-\rangle = 0$$

if $\hat{E}_\alpha$ and $\hat{E}_\beta$ increases and decreases the eigenvalues.

We also have

$$\left[\hat{H}_i,[\hat{E}_\alpha,\hat{E}_\beta]\right]=\left[[\hat{H}_i,\hat{E}_\alpha],\hat{E}_\beta\right]+\left[\hat{E}_\alpha,[\hat{H}_i,\hat{E}_\beta]\right]=(\epsilon_{i\alpha}+\epsilon_{i\beta})[\hat{E}_\alpha,\hat{E}_\beta]$$

so that the commutator $[\hat{E}_\alpha,\hat{E}_\beta]$ is itself a ladder operator with a root $(\epsilon_{i\alpha}+\epsilon_{i\beta})$. If $\epsilon_{i\alpha}+\epsilon_{i\beta}=0$, then $[\hat{E}_\alpha,\hat{E}_\beta]$ is a linear combination of $\{\hat{H}_i\}$.

It is clear from the above discussion that the number of Casimir operators needed to specify a multiplet is equal to the rank of the Lie group.

4.6 Summation over group elements

Many of the theorems that we have encountered involve summation over group elements. In this section, we will study how to perform this summation for continuous groups. We have to replace the summation by an integral over the parameters in the following way:

$$\sum_G f(G)\rightarrow\int d\mathbf{a}\;w(\mathbf{a})f(G(\mathbf{a})) \tag{4.24}$$

$w(\mathbf{a})$ is a weight function describing the "density" of elements in the parameter space.

In proving some theorems for finite groups, we make use of the rearrangement theorem. For these theorems to remain valid in the case of continuous groups, we must require

$$\int d\mathbf{a}\;w(\mathbf{a})f(G(\mathbf{a})G(\mathbf{b}))=\int d\mathbf{a}\;w(\mathbf{a})f(G(\mathbf{c}))=\int d\mathbf{c}\;w(\mathbf{c})f(G(\mathbf{c})) \tag{4.25}$$

From Eq. (4.3), $G(\mathbf{a})G(\mathbf{b})=G(\mathbf{c})=G(\mathbf{F}(\mathbf{a},\mathbf{b}))$, and for a fixed $\mathbf{b}$, $\mathbf{c}$ is a function of $\mathbf{a}$.

$$\begin{aligned}\int d\mathbf{a}\;w(\mathbf{a})f(G(\mathbf{a})) &= \int d\mathbf{c}\;w(\mathbf{c})f(G(\mathbf{c}))\\ &= \int d\mathbf{a}\;\frac{\partial\mathbf{c}}{\partial\mathbf{a}}w(\mathbf{c})f(G(\mathbf{c}))\end{aligned}$$

Comparison with Eq. (4.25) gives

$$\frac{\partial\mathbf{c}}{\partial\mathbf{a}}w(\mathbf{c})=w(\mathbf{a}) \tag{4.26}$$

where $\partial\mathbf{c}/\partial\mathbf{a}$ is the Jacobian.

To relate $\mathbf{a}$ to $\mathbf{c}$ we consider a small $\mathbf{b}$:

$$\begin{aligned}\mathbf{c} &= \mathbf{F}(\mathbf{a},\mathbf{b}) \\ &= \mathbf{F}(\mathbf{a},\mathbf{0}) + \frac{\partial \mathbf{F}(\mathbf{a},\mathbf{0})}{\partial \mathbf{b}} \cdot \mathbf{b} \\ &= \mathbf{a} + \mathbf{M}(\mathbf{a}) \cdot \mathbf{b}\end{aligned}$$

where the matrix $\mathbf{M}$ is defined as in Eq. (4.10). To first order in $\mathbf{b}$, the Jacobian is given by

$$\frac{\partial \mathbf{c}}{\partial \mathbf{a}} = 1 + \frac{\partial}{\partial \mathbf{a}} \cdot \mathbf{M}(\mathbf{a}) \cdot \mathbf{b}$$

Expanding $w(\mathbf{c})$ about $\mathbf{a}$ to first order in $\mathbf{b}$ yields

$$\begin{aligned}w(\mathbf{c}) &= w\left(\mathbf{a} + \mathbf{M}(\mathbf{a}) \cdot \mathbf{b}\right) \\ &= w(\mathbf{a}) + \frac{\partial w(\mathbf{a})}{\partial \mathbf{a}} \cdot \mathbf{M}(\mathbf{a}) \cdot \mathbf{b}\end{aligned}$$

Substituting the above expressions into Eq. (4.26) gives

$$\left[1 + \frac{\partial}{\partial \mathbf{a}} \cdot \mathbf{M}(\mathbf{a}) \cdot \mathbf{b}\right]\left[w(\mathbf{a}) + \frac{\partial w(\mathbf{a})}{\partial \mathbf{a}} \cdot \mathbf{M}(\mathbf{a}) \cdot \mathbf{b}\right] = w(\mathbf{a})$$

Since $\mathbf{b}$ is arbitrary, we thus have

$$\frac{1}{w(\mathbf{a})}\frac{\partial w(\mathbf{a})}{\partial \mathbf{a}} \cdot \mathbf{M}(\mathbf{a}) = -\frac{\partial}{\partial \mathbf{a}} \cdot \mathbf{M}(\mathbf{a})$$

or

$$\frac{\partial\, ln\, w(\mathbf{a})}{\partial \mathbf{a}} = -\frac{\partial}{\partial \mathbf{a}} \cdot \mathbf{M}(\mathbf{a}) \cdot \mathbf{M}^{-1}(\mathbf{a}) \tag{4.27}$$

4.7 Rotation Group R_3

As an example, we consider the rotation group in three dimensions, R_3, which often appears in many applications in physics, in particular in the theory of angular momentum. The technique used in constructing the irreducible representations of the rotation group is actually quite common in Lie groups.

4.7.1 Infinitesimal operators

A rotation in three dimensions may be denoted by $R(\alpha\mathbf{a})$ where $\mathbf{a}$ is the axis of rotation and α is the angle of anti-clockwise rotation. It is easy to show that

$$R(\alpha\mathbf{a})\mathbf{r} = cos\ \alpha\ \mathbf{r} + (1 - cos\ \alpha)(\mathbf{r}\cdot\mathbf{a})\mathbf{a} + sin\ \alpha\ (\mathbf{a}\times\mathbf{r}) \tag{4.28}$$

For small α we have to first order

$$\begin{aligned} R(\mathbf{a},\alpha)\mathbf{r} &= (1 + \alpha\ \mathbf{a}\times)\mathbf{r} \\ &= (1 + \alpha\ \sum_i a_i\mathbf{e}_i\times)\mathbf{r} \\ &= (1 + \sum_i \alpha_i\mathbf{e}_i\times)\mathbf{r} \end{aligned} \tag{4.29}$$

We identify

$$X_x = \mathbf{e}_x\times,\quad X_y = \mathbf{e}_y\times,\quad X_z = \mathbf{e}_z\times,$$

as the infinitesimal operators of the rotation group associated with the parameters $\alpha_x = \alpha a_x$, $\alpha_y = \alpha a_y$ and $\alpha_z = \alpha a_z$ corresponding to rotations about $x-$, $y-$ and $z-$ axes respectively. In other words, when α is small, the rotation can be regarded as a vector sum of rotations about $x-$, $y-$ and $z-$ axes.

In the Cartesian basis, we have explicitly

$$X_x = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$X_y = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}$$

$$X_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

4.7.2 Commutation Relations

In Cartesian coordinates, the commutation relations for the infinitesimal operators are

$$[X_x, X_y] = X_z, \quad [X_y, X_z] = X_x, \quad [X_z, X_x] = X_y \tag{4.30}$$

The infinitesimal operators are $skew\ Hermitian$ (this is true in general if the representation is unitary) but it is possible to define equivalent infinitesimal operators $J_k = iX_k$ which are Hermitian. The commutation relations become

$$[J_x, J_y] = iJ_z, \quad [J_y, J_z] = iJ_x, \quad [J_z, J_x] = iJ_y \tag{4.31}$$

We will show below that the commutation relations also follow from the general results derived in the previous sections.

We consider a rotation $R(\beta\mathbf{b})$ followed by $R(\alpha\mathbf{a})$ which may be affected by a rotation $R(\gamma\mathbf{c})$:

$$R(\gamma\mathbf{c}) = R(\alpha\mathbf{a})R(\beta\mathbf{b})$$

The main quantities to calculate are the three functions $\mathbf{F}(\alpha\mathbf{a}, \beta\mathbf{b}) = \gamma\mathbf{c}$. What we have to calculate are the structure constants defined in Eq. (4.16). Since the derivatives of $\mathbf{F}(\alpha\mathbf{a}, \beta\mathbf{b})$ are taken at $\alpha\mathbf{a} = \mathbf{0}$ and $\beta\mathbf{b} = \mathbf{0}$, it is sufficient to consider small α and β. For small α, $R(\alpha\mathbf{a})$ takes the form:

$$R(\alpha\mathbf{a}) = \begin{pmatrix} 1 & -\alpha_z & \alpha_y \\ \alpha_z & 1 & -\alpha_x \\ -\alpha_y & \alpha_x & 1 \end{pmatrix}$$

and similarly for $R(\beta\mathbf{b})$. Thus we have
$R(\gamma\mathbf{c}) = R(\alpha\mathbf{a})R(\beta\mathbf{b}) =$

$$\begin{pmatrix} 1 - \alpha_y\beta_y - \alpha_z\beta_z & -(\alpha_z + \beta_z - \alpha_y\beta_x) & \alpha_y + \beta_y + \alpha_z\beta_x \\ \alpha_z + \beta_z + \alpha_x\beta_y & 1 - \alpha_x\beta_x - \alpha_z\beta_z & -(\alpha_x + \beta_x - \alpha_z\beta_y) \\ -(\alpha_y + \beta_y + \alpha_x\beta_z) & \alpha_x + \beta_x - \alpha_y\beta_z & 1 - \alpha_x\beta_x - \alpha_y\beta_y \end{pmatrix}$$

The trace of $R(\gamma\mathbf{c})$ is $(1 + 2cos\ \gamma)$, independent of the basis. Equating this with the trace of $R(\alpha\mathbf{a})R(\beta\mathbf{b})$ gives

$$\begin{aligned} 1 + 2cos\ \gamma &= 3 - 2(\alpha_x\beta_x + \alpha_y\beta_y + \alpha_z\beta_z) \\ 1 + 2(1 - \gamma^2/2) &= 3 - 2(\alpha_x\beta_x + \alpha_y\beta_y + \alpha_z\beta_z) \\ \gamma^2 &= 2(\alpha_x\beta_x + \alpha_y\beta_y + \alpha_z\beta_z) \end{aligned}$$

We also know that $R(\gamma\mathbf{c})$ is unitary and it does not alter $\gamma\mathbf{c}$ so that $R(\gamma\mathbf{c})\gamma\mathbf{c} = R^\dagger(\gamma\mathbf{c})\gamma\mathbf{c} = \gamma\mathbf{c}$ or

$$[R(\gamma\mathbf{c}) - R^\dagger(\gamma\mathbf{c})]\gamma\mathbf{c} = 0$$

This gives us the following equations:

$$\begin{aligned} -C\gamma_y + B\gamma_z &= 0 \\ C\gamma_x - A\gamma_z &= 0 \\ -B\gamma_x + A\gamma_y &= 0 \end{aligned}$$

$$\begin{aligned} A &= 2(\alpha_x + \beta_x) + \alpha_y\beta_z - \alpha_z\beta_y \\ B &= 2(\alpha_y + \beta_y) + \alpha_z\beta_x - \alpha_x\beta_z \\ C &= 2(\alpha_z + \beta_z) + \alpha_x\beta_y - \alpha_y\beta_x \end{aligned}$$

With $\gamma^2 = \gamma_x^2 + \gamma_y^2 + \gamma_z^2$, the solution to the above equations is

$$\gamma_x = pA, \;\; \gamma_y = pB, \;\; \gamma_z = pC$$

where

$$p = \left[\frac{2(\alpha_x\beta_x + \alpha_y\beta_y + \alpha_z\beta_z)}{A^2 + B^2 + C^2}\right]^{1/2}$$

A straightforward algebra shows that $p = 1/2$ to linear order in α and β. The non-zero structure constants are then

$$c_{xy}^z = c_{zx}^y = c_{yz}^x = 1 \tag{4.32}$$

which gives the commutation relations in Eq. (4.30).

4.7.3 Casimir Operator

The Casimir operator can also be obtained directly from the results of the previous section. We calculate the matrix g_{ij} defined in Eq. (4.18):

$$\begin{aligned} g_{xx} &= \sum_{kl} c_{xl}^k c_{xk}^l \\ &= c_{xy}^z c_{xz}^y + c_{xz}^y c_{xy}^z \\ &= -2 \end{aligned}$$

The same results are obtained for g_{yy} and g_{zz} whereas the other matrix elements are zero. Thus we get

$$g_{ij} = -2\delta_{ij}, \;\; g^{ij} = -\frac{1}{2}\delta_{ij}$$

and the Casimir operator is therefore

$$\begin{aligned} C &= \sum_{ij} g^{ij} X_i X_j \\ &= -\frac{1}{2}(X_x^2 + X_y^2 + X_z^2) \\ &= -\frac{1}{2}X^2 = \frac{1}{2}J^2 \end{aligned} \tag{4.33}$$

4.8 Irreducible Representations of R_3

The method of constructing the irreducible representations for the rotation group R_3 is quite general since it is based on the commutation relations in Eqn. (4.30) alone. The method may therefore be applied to other continuous groups. Since every rotation can be built up from the infinitesimal operators, an irreducible subspace under these infinitesimal operators is also an irreducible subspace under the rotation group. The steps for constructing the irreducible representations are as follows:

1. The sets of degenerate eigenvectors of the Casimir operator $\hat{J}^2$ form irreducible subspaces under the infinitesimal operators $\hat{J}_x$, $\hat{J}_y$, and $\hat{J}_z$. The rank of R_3 is one because there are no two mutually commuting operators. Since $\hat{J}^2$ commutes with the infinitesimal operators, the eigenvectors of $\hat{J}^2$ may be chosen simultaneously to be eigenvectors of one of the infinitesimal operators. As a convention, we choose $\hat{J}_z$.

   We construct the following ladder operators

   $$\hat{J}_\pm = \hat{J}_x \pm i\hat{J}_y \tag{4.34}$$

   which may be obtained by solving the eigenvectors and eigenvalues of c^i_{zj}. Clearly, the set of operators $\hat{J}_\pm, \; \hat{J}_z$ are equivalent to the set

of operators $\hat{J}_x,\ \hat{J}_y,\ \hat{J}_z$. We may therefore work with the former set. The commutation relations of these operators are

$$[\hat{J}_z, \hat{J}_\pm] = \pm\hat{J}_\pm, \quad [\hat{J}_+, \hat{J}_-] = 2\hat{J}_z \tag{4.35}$$

The usefulness of these operators may be seen by applying $\hat{J}_z$ to $\hat{J}_\pm\psi_m$ where ψ_m is an eigenfunction of $\hat{J}_z$ with an eigenvalue m.

$$\begin{aligned} \hat{J}_z(\hat{J}_\pm\psi_m) &= (\hat{J}_\pm\hat{J}_z \pm \hat{J}_\pm)\psi_m \\ &= \hat{J}_\pm(\hat{J}_z \pm 1)\psi_m \\ &= \hat{J}_\pm(m \pm 1)\psi_m \\ &= (m \pm 1)(\hat{J}_\pm\psi_m) \end{aligned}$$

Thus, $\hat{J}_\pm\psi_m$ must be proportional to $\psi_{m\pm1}$.

2. We assume that the irreducible representations of R_3 have a finite dimension. We choose basis functions which are eigenfunctions of $\hat{J}_z$. Let j be the largest eigenvalue of $\hat{J}_z$ in this basis. Then

$$\hat{J}_+\psi_j = 0 \tag{4.36}$$

There may be more than one function with the largest eigenvalue. We take one of these and operate $\hat{J}_-$ repeatedly on this function:

$$\begin{aligned} \hat{J}_-\psi_j &= c_{j-1}\psi_{j-1} \\ \hat{J}_-\psi_{j-1} &= c_{j-2}\psi_{j-2} \ \ etc. \end{aligned}$$

The c's are normalisation constants. Since we have assumed that the dimension of the irreducible representations is finite, it must be that for some integer n we have

$$\hat{J}_-\psi_{j-n} = 0$$

The problem is to figure out what n is.

3. We show that ψ_m is an eigenfunction of $\hat{J}^2$ irrespective of the value of m. This is to be expected because a set of degenerate eigenvectors

of $\hat{J}^2$ form a basis for an irreducible representation.

$$\begin{aligned}\hat{J}^2 &= \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2 \\ &= \frac{1}{2}(\hat{J}_+\hat{J}_- + \hat{J}_-\hat{J}_+) + \hat{J}_z^2 \\ &= \hat{J}_+\hat{J}_- + \hat{J}_z^2 - \hat{J}_z \\ &= \hat{J}_-\hat{J}_+ + \hat{J}_z^2 + \hat{J}_z\end{aligned}$$

The last two relations have been obtained by using the the second commutation relation in Eq. (4.35). Operating $\hat{J}^2$ on ψ_j we get

$$\begin{aligned}\hat{J}^2\psi_j &= (\hat{J}_-\hat{J}_+ + \hat{J}_z^2 + \hat{J}_z)\psi_j \\ &= j(j+1)\psi_j\end{aligned}$$

Operating $\hat{J}^2\hat{J}_-$ on ψ_j yields

$$\begin{aligned}\hat{J}^2\hat{J}_-\psi_j &= \hat{J}_-\hat{J}^2\psi_j \\ &= j(j+1)\hat{J}_-\psi_{j-1}\end{aligned}$$

Thus ψ_{j-1} is also an eigenfunction of $\hat{J}^2$ with eigenvalue $j(j+1)$. We can continue the same procedure starting from ψ_{j-1} so that it follows that $\psi_m,\ m = j, j-1, \ldots, j-n$ is an eigenfunction of$\hat{J}^2$ with eigenvalue $j(j+1)$. We now operate $\hat{J}^2$ on ψ_{j-n}:

$$\begin{aligned}\hat{J}^2\hat{\psi}_{j-n} &= (\hat{J}_+\hat{J}_- + \hat{J}_z^2 - \hat{J}_z)\psi_{j-n} \\ &= [(j-n)^2 - (j-n)]\psi_{j-n} \\ &= (j-n)(j-n-1)\psi_{j-n}\end{aligned}$$

It follows that $(j-n)(j-n-1) = j(j+1)$, which implies that $n = 2j$ and therefore j can be an integer or a half-integer.

4. Finally we show that the $2j+1$ functions $\psi_j,\ \psi_{j-1},\ \ldots, \psi_{-j}$ form an irreducible subspace (transform among themselves or invariant) under the operators $\hat{J}_+,\ \hat{J}_-,\ \hat{J}_z$. It is clear that the functions transform among themselves under $\hat{J}_-$ and $\hat{J}_z$. We show that they also transform among themselves under $\hat{J}_+$:

$$\hat{J}_+c_m\psi_m = \hat{J}_+\hat{J}_-\psi_{m+1}$$

$$\begin{aligned} &= (\hat{J}^2 - \hat{J}_z^2 + \hat{J}_z)\psi_{m+1} \\ &= [j(j+1) - (m+1)^2 + (m+1)]\psi_{m+1} \\ &= (j+m+1)(j-m)\psi_{m+1} \end{aligned}$$

To calculate the normalisation constants c_m we take the dot product $c_m(\psi_{m+1}, \hat{J}_+\psi_m) = (j+m+1)(j-m)$. Using the fact that $J_- = J_+^\dagger$, we have

$$\begin{aligned} (\psi_{m+1}, \hat{J}_+\psi_m) &= (J_+^\dagger\psi_{m+1}, \psi_m) \\ &= (J_-\psi_{m+1}, \psi_m) \\ &= (c_m\psi_m, \psi_m) = c_m^* \end{aligned}$$

Thus $|c_m|^2 = (j+m+1)(j-m)$. There is an arbitrary phase factor in c_m and the usual convention due to Condon and Shortley is to choose c_m to be real and positive so that

$$c_m = \sqrt{(j+m+1)(j-m)} \tag{4.37}$$

$$\hat{J}_+\psi_m = \sqrt{(j+m+1)(j-m)}\psi_{m+1} \tag{4.38}$$

$$\hat{J}_-\psi_m = \sqrt{(j+m)(j-m+1)}\psi_{m-1} \tag{4.39}$$

To summarise, the irreducible representations of R_3 are labelled by R^j, with $j = 0,\ \pm 1/2,\ \pm 1,\ \pm 3/2,\ \pm 2\ldots$, which transform the $(2j+1)$ functions $\psi_j,\ \psi_{j-1},\ \ldots, \psi_{-j}$ among themselves.

4.9 Characters of R_3

Rotations by the same angle, $\hat{R}(\mathbf{a}, \phi)$ and $\hat{R}(\mathbf{b}, \phi)$, belong to the same class irrespective of the axes $\mathbf{a}$ and $\mathbf{b}$. This must be true because there is always a rotation $\hat{R}(\mathbf{c}, \phi')$ that brings the axis $\mathbf{a}$ to $\mathbf{b}$ or vice versa, i.e.

$$\hat{R}(\mathbf{a}, \phi) = \hat{R}^{-1}(\mathbf{c}, \phi')\hat{R}(\mathbf{b}, \phi)\hat{R}(\mathbf{c}, \phi')$$

Geometrically, $\hat{R}(\mathbf{c}, \phi')$ rotates $\mathbf{a}$ to $\mathbf{b}$, $\hat{R}(\mathbf{b}, \phi)$ does a rotation by ϕ about $\mathbf{b}$ and finally $\hat{R}^{-1}(\mathbf{c}, \phi')$ rotates $\mathbf{b}$ back to $\mathbf{a}$ and the net result is the same as a rotation by ϕ about $\mathbf{a}$.

Since the characters of representations belonging to the same class are the same, it is sufficient to consider the characters of R_z. We consider the subgroup R_z consisting of rotations about the z-axis. This subgroup is Abelian and the irreducible representations are therefore one dimensional. We require $R(z,\phi)R(z,\delta\phi) = R(z,\phi+\delta\phi)$. Expanding both sides in $\delta\phi$ we get

$$\begin{aligned} R(z,\phi)(1+\delta\phi R'(z,0)) &= R(z,\phi)+\delta\phi R'(z,\phi) \\ R'(z,0)R(z,\phi) &= R'(z,\phi) \end{aligned}$$

The solution is $R(z,\phi) = c\ exp(R'(z,0)\phi)$. For a unitary representation, we may choose $c=1$ and from the boundary condition $R(z,\phi) = R(z,\phi+2\pi)$, we deduce that $R'(z,0) = -im$ where m is a positive or negative integer. Thus the irreducible representations of R_z are

$$R_z^m(\phi) = exp(-im\phi) \tag{4.40}$$

labelled by $m = 0, \pm1, \pm2, \ldots$ and the angle ϕ. These are also the eigenfunctions of the infinitesimal operator $\hat{J}_z$ with eigenvalues m, as may be easily verified.

It is clear that representation $R^j(\mathbf{a},\phi)$ is reducible under the group R_z and by choosing the z-axis along $\mathbf{a}$, it may be decomposed as

$$\begin{aligned} R^j(\mathbf{a},\phi) &= R_z^{-j}(\phi)\oplus R_z^{-j+1}(\phi)\oplus\ldots\oplus R_z^j(\phi) \\ &= \sum_{m=-j}^{m=j}\oplus R_z^m(\phi) \end{aligned}$$

Thus the character is given by

$$\begin{aligned} \chi^j(\phi) &= \sum_{m=-j}^{m=j} exp(-im\phi) \\ &= \frac{sin\ (j+1/2)\phi}{sin\ \phi/2} \end{aligned} \tag{4.41}$$

which is easily obtained from the geometric series formula $S_n = \sum_{k=0}^{k=n-1} ar^k = a(1-r^n)/(1-r)$ with $n = (2j+1)$, $a = exp(ij\phi)$, and $r = exp(i\phi)$.

4.10 The Vector-Coupling Theorem

The direct product of two irreducible representations of R_3 referring to the same rotation ϕ about a given axis $\mathbf{a}$ is given by

$$R^{j_1}(\mathbf{a},\phi) \otimes R^{j_2}(\mathbf{a},\phi) = \sum_j \oplus c_j R^j(\mathbf{a},\phi) \tag{4.42}$$

To figure out the coefficient c_j we use the fact that the character of a direct product representation is the product of the characters of the individual representations:

$$\chi^{j_1}(\mathbf{a},\phi)\chi^{j_2}(\mathbf{a},\phi) \;=\; \sum_j \oplus c_j \chi^j(\mathbf{a},\phi)$$

The left hand side is given by

$$\begin{aligned}
\chi^{j_1}\chi^{j_2} &= \sum_{m_1=-j_1}^{j_1} \sum_{m_2=-j_2}^{j_2} e^{-im_1\phi} e^{-im_2\phi} \\
&= [e^{i(j_1+j_2)\phi} + e^{i(j_1+j_2-1)\phi} + \ldots + e^{-i(j_1+j_2)\phi}] \\
&+ [e^{i(j_1+j_2-1)\phi} + e^{i(j_1+j_2-2)\phi} + \ldots + e^{-i(j_1+j_2-1)\phi}] \\
&+ \ldots \\
&+ [e^{i(j_1-j_2)\phi} + e^{i(j_1-j_2-1)\phi} + \ldots + e^{-i(j_1-j_2)\phi}] \\
&= \chi^{j_1+j_2} + \chi^{j_1+j_2-1} + \ldots + \chi^{j_1-j_2}
\end{aligned}$$

assuming that $j_1 \geq j_2$ without loss of generality. Therefore $j_1 - j_2$ becomes $|j_1 - j_2|$ in the general case. Comparison with the previous equation shows that $c_j = 1$ for $j = j_1 + j_2,\ j_1 + j_2 - 1,\ \ldots\ + |j_1 - j_2|$ which yields the vector-coupling theorem:

$$R^{j_1}(\mathbf{a},\phi) \otimes R^{j_2}(\mathbf{a},\phi) = \sum_{j=|j_1-j_2|}^{j_1+j_2} \oplus R^j(\mathbf{a},\phi) \tag{4.43}$$

The rotation group is called simply reducible because $m_\gamma = 1$.

4.11 Clebsch-Gordan Coefficients

As discussed in section 3.11, a product of two states $\psi^{j_1}_{m_1}\psi^{j_2}_{m_2}$ transforming according to the product representation $R^{j_1\otimes j_2}$ of the rotation group may be expanded as follows:

$$\psi(m_1,m_2)=\psi^{j_1}_{m_1}\psi^{j_2}_{m_2}=\sum_{JM}\Psi^J_M C^{J*}_M(m_1,m_2)$$

where the C's are the Clebsch-Gordan coefficients which form a matrix that brings the product representation $R^{j_1\otimes j_2}$ into the block diagonal form (section 3.4, Theorem 3):

$$\begin{aligned}&R^{j_1}_{m_1'm_1}R^{j_2}_{m_2'm_2}\\&\quad=\sum_{J=|j_1-j_2|}^{j_1+j_2}\sum_{MM'}C^J_{M'}(m_1',m_2')R^J_{M'M}C^{J*}_M(m_1,m_2)\end{aligned}\tag{4.44}$$

This expansion is known as the Clebsch-Gordan series. No additional label is needed in C because the rotation group is simply reducible. We have dropped the dependence on j_1 and j_2 for clarity. We may also write, using the unitarity of C

$$\Psi^J_M=\sum_{m_1,m_2}C^J_M(m_1,m_2)\psi(m_1,m_2)\tag{4.45}$$

Thus

$$C^J_M(m_1,m_2)=(\psi(m_1,m_2),\Psi^J_M)\tag{4.46}$$

Since the new functions Ψ^J_M are orthonormal, we have

$$\sum_{m_1m_2}|C^J_M(m_1,m_2)|^2=1\tag{4.47}$$

By applying $\hat{J}_z$ to both sides of Eq. (4.45), it follows that $C^J_M(m_1,m_2)=0$ unless $m=m_1+m_2$ and from the vector-coupling theorem we also have $|j_1-j_2|\le J\le j_1+j_2$:

$$C^J_M(m_1,m_2)=0\ \ unless\ \begin{cases}M=m_1+m_2\ \ or\\ |j_1-j_2|\le J\le j_1+j_2\end{cases}\tag{4.48}$$

With the Condon and Shortley phase convention

$$\begin{aligned}\hat{J}_+\psi^j_m &= A_{j,+m}\psi^j_{m+1}\\ \hat{J}_-\psi^j_m &= A_{j,-m}\psi^j_{m-1}\end{aligned}$$

where

$$A_{j,m} = \sqrt{(j-m)(j+m+1)}, \quad A_{j,j} = A_{j,|m|>j} = 0 \tag{4.49}$$

the Clebsch-Gordan coefficients become real.

The Clebsch-Gordan coefficients for fixed j_1 and j_2 and a chosen j can be calculated from recursion relations obtained by applying $\hat{J}_-$ and $\hat{J}_+$ to both sides of Eq. (4.45):

$$\begin{aligned}&A_{J,-M}\Psi^J_{M-1}\\ &= \sum_{n_1 n_2} C^J_M(n_1,n_2)\,[\,A_{j_1,-n_1}\psi(n_1-1,n_2) + A_{j_2,-n_2}\psi(n_1,n_2-1)\,]\end{aligned}$$

$$\begin{aligned}&A_{J,+M}\Psi^J_{M+1}\\ &= \sum_{n_1 n_2} C^J_M(n_1,n_2)\,[\,A_{j_1,+n_1}\psi(n_1+1,n_2) + A_{j_2,+n_2}\psi(n_1,n_2+1)\,]\end{aligned}$$

Taking the dot product with $\psi(m_1,m_2)$ and setting $M \to M+1$ and $M \to M-1$ in the first and second equation above we get the recursion relations:

$$\begin{aligned}A_{J,+M}C_M(m_1,m_2) &= A_{j_1,+m_1}C_{M+1}(m_1+1,m_2)\\ &+ A_{j_2,+m_2}C_{M+1}(m_1,m_2+1) \qquad (4.50)\\ A_{J,-M}C_M(m_1,m_2) &= A_{j_1,-m_1}C_{M-1}(m_1-1,m_2)\\ &+ A_{j_2,-m_2}C_{M-1}(m_1,m_2-1) \qquad (4.51)\end{aligned}$$

To simplify the notation, we have dropped the superscript J since it is fixed. There is an ambiguity in the sign and this is fixed by choosing the convention that

$$C_J(j_1, J-j_1) > 0 \tag{4.52}$$

As an example we evaluate the Clebsch-Gordan coefficients for a given $j_2 = 1/2$ which gives possible values of $J = j_1 - 1/2,\ j_1 + 1/2$. To simplify the notation further, we drop the second argument in C since it can be obtained by substracting the first argument from the subscript. We consider the case $J = j_1 - 1/2$. With $m_2 = \pm 1/2$ we get from the recursion relations

$$\begin{aligned} A_{J,M}C_M(M-1/2) &= A_{j_1,M-1/2}C_{M+1}(M+1/2) \\ A_{J,-M-1}C_{M+1}(M+1/2) &= A_{j_1,-M-1/2}C_M(M-1/2) \\ &+ A_{j_2,-1/2}C_{M+1}(M+1/2) \\ A_{J,M-1}C_{M-1}(M-1/2) &= A_{j_1,M-1/2}C_M(M+1/2) \\ &+ A_{j_2,-1/2}C_M(M-1/2) \\ A_{J,-M}C_M(M+1/2) &= A_{j_1,-M-1/2}C_{M-1}(M-1/2) \end{aligned}$$

These are four linear equations with four unknowns but since the equations are homogeneous, the solutions can only be expressed as ratios. However, the additional condition in Eq. (4.47) determines the absolute magnitudes and condition 4.52 fixes the sign. Similarly we can generate the recursion relations for $J = j_2 + 1/2$. The solutions in complete notation are

$$\begin{aligned} C_M^{j_1\pm 1/2}(M-1/2,1/2) &= \pm\sqrt{\frac{j_1 \pm M + 1/2}{2j_1+1}} \\ C_M^{j_1\pm 1/2}(M+1/2,-1/2) &= \sqrt{\frac{j_1 \mp M + 1/2}{2j_1+1}} \end{aligned}$$

The Clebsch-Gordan coefficients can be also calculated by using the projection operator:

$$\hat{P}^J = \prod_{K\neq J} \hat{P}_K^J = \prod_{K\neq J}\left[\frac{\hat{J}^2 - K(K+1)}{J(J+1) - K(K+1)}\right] \tag{4.53}$$

which when applied to ψ_{m_1,m_2} will annihilate all components except $C_M^J(m_1,m_2)\Psi_M^J$ where $M = m_1 + m_2$:

$$\begin{aligned} \hat{P}^J\psi_{m_1,m_2} &= C_M^J(m_1,m_2)\Psi_M^J \\ \Rightarrow\ C_M^J(m_1',m_2')\ C_M^J(m_1,m_2) &= (\psi_{m_1',m_2'}, \hat{P}^J\psi_{m_1,m_2}) \end{aligned}$$

We evaluate $\hat{P}^J_K \psi_{m_1,m_2}$, using the identity $\hat{J}^2 = \hat{J}_- \hat{J}_+ + \hat{J}_z(\hat{J}_z + 1)$:

$$\begin{aligned}
\hat{P}^J_K \psi_{m_1,m_2} &= [J(J+1) - K(K+1)]^{-1} \\
&\times [\ \{\ A_{j_1,m_1} A_{j_1,-m_1-1} + A_{j_2,m_2} A_{j_2,-m_2-1} \\
&\quad + M(M+1) - K(K+1)\ \}\ \psi(m_1,m_2) \\
&\quad + A_{j_1,m_1} A_{j_2,-m_2} \psi(m_1+1, m_2-1) \\
&\quad + A_{j_2,m_2} A_{j_1,-m_1} \psi(m_1-1, m_2+1)\ ] \\
\\
&= [J(J+1) - K(K+1)]^{-1} \\
&\times [\ \{\ (j_1 - m_1)(j_1 + m_1 + 1) + (j_2 - m_2)(j_2 + m_2 + 1) \\
&\quad + M(M+1) - K(K+1)\ \}\ \psi(m_1,m_2) \\
&\quad + \sqrt{(j_1 - m_1)(j_1 + m_1 + 1)(j_2 + m_2)(j_2 - m_2 + 1)} \\
&\quad \times \psi(m_1+1, m_2-1) \\
&\quad + \sqrt{(j_2 - m_2)(j_2 + m_2 + 1)(j_1 + m_1)(j_1 - m_1 + 1)} \\
&\quad \times \psi(m_1-1, m_2+1)\ ]
\end{aligned}$$

We evaluate the previous example using the projection operator method. Consider the case $J = j_1 - 1/2$, $m_2 = -1/2 \Rightarrow m_1 = M + 1/2$. We have $\hat{P}^J = \hat{P}^J_{j_1+1/2}$ since there are only two possible values of $K = j_1 \pm 1/2$. Thus,

$$\begin{aligned}
&|C^{j_1-1/2}_M(M+1/2, -1/2)|^2 \\
&= (\psi(M+1/2,-1/2), \hat{P}^{j_1-1/2}_{j_1+1/2} \psi(M+1/2,-1/2)) \\
&= \frac{j_1 + M + 1/2}{2j_1 + 1}
\end{aligned}$$

Using the sign convention in (4.52) we get

$$C^{j_1-1/2}_M(M+1/2,-1/2) = \sqrt{\frac{j_1 + M + 1/2}{2j_1 + 1}}$$

because it must be positive when $M = j_1 - 1/2$. We also have

$$\begin{aligned}
&C^{j_1-1/2}_M(M-1/2, 1/2)\ C^{j_1-1/2}_M(M+1/2,-1/2) \\
&= \frac{\sqrt{(j_1 + M + 1/2)(j_1 - M + 1/2)}}{-(2j_1+1)}
\end{aligned}$$

so that

$$C_M^{j_1-1/2}(M-1/2,1/2 \;=\; -\sqrt{\frac{j_1-M+1/2}{2j_1+1}}$$

in agreement with the previous results.

The general formula for the Clebsch-Gordan coefficients has been evaluated by Wigner (Gruppentheorie, Vieweg-Verlag, Brunswick, 1931 or in the translated version, Group Theory, Academic Press, New York, 1959). Wigner's closed expression is

$$\begin{aligned} C_M^J(m_1,m_2) &= \delta_{M,m_1+m_2}\sqrt{2J+1} \\ &\times \sqrt{\frac{(J+j_1-j_2)!(J-j_1+j_2)!(j_1+j_2-J)!(J+M)!(J-M)!}{(j_1+j_2+J+1)!(j_1-m_1)!(j_1+m_1)!(j_2-m_2)!(j_2+m_2)!}} \\ &\times \sum_\nu \frac{(-1)^{\nu+j_2+m_2}}{\nu!}\frac{(j_2+J+m_1-\nu)!(j_1-m_1+\nu)!}{(J-j_1+j_2-\nu)!(J+M-\nu)!(\nu+j_1-j_2-M)!} \end{aligned} \tag{4.54}$$

Racah (G. Racah, *Phys. Rev.* **62**, 438 (1942)) derived a more symmetrical form:

$$\begin{aligned} C_M^J(m_1,m_2) &= \delta_{M,m_1+m_2}\sqrt{2J+1} \\ &\times \sqrt{\frac{(j_1+j_2-J)!(J+j_1-j_2)!(J+j_2-j_1)!}{(j_1+j_2+J+1)!}} \\ &\times \sqrt{(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!(J+M)!(J-M)!} \\ &\times \sum_\nu \frac{(-1)^\nu}{\nu!}\left\{\frac{1}{(j_1+j_2-J-\nu)!(j_1-m_1-\nu)!(j_2+m_2-\nu)!}\right. \\ &\qquad \left.\times\frac{1}{(J-j_2+m_1+\nu)!(J-j_1-m_2+\nu)!}\right\} \end{aligned} \tag{4.55}$$

The most frequently used Clebsch-Gordan coefficients are tabulated in many books on atomic physics.

4.12 Spherical Harmonics

We wish to find explicit basis functions for the irreducible representations of the rotation group. To do this, we need to know the form of the infinitesimal operators in function space. We form an operator representation of the group elements, $R \to \hat{T}(R)$, and study its effect on an arbitrary function $\psi(x, y, z)$. First we consider a small rotation about the z-axis:

$$\begin{aligned}\hat{T}(R(\gamma\mathbf{z}))\psi(x,y,z) &= \psi(R^{-1}(\gamma\mathbf{z})(x,y,z)) \\ &= \psi(x+\gamma y, y-\gamma x, z) \\ &= \left[1+\gamma\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right)\right]\psi(x,y,z)\end{aligned}$$

The same procedure can be applied to the x- and y-axes. The infinitesimal operators in function space are therefore

$$\hat{J}_z = i\left(y\frac{\partial}{\partial x}-x\frac{\partial}{\partial y}\right) \tag{4.56}$$

$$\hat{J}_y = i\left(x\frac{\partial}{\partial z}-z\frac{\partial}{\partial x}\right) \tag{4.57}$$

$$\hat{J}_x = i\left(z\frac{\partial}{\partial y}-y\frac{\partial}{\partial z}\right) \tag{4.58}$$

These are identical to the angular momentum operators in quantum mechanics.

The procedure for constructing the irreducible representations of R_3 tells us that we should start with an eigenfunction of $\hat{J}_z$ and $\hat{J}^2$ and then we apply the ladder operators repeatedly in order to span the irreducible subspace corresponding to a set of degenerate eigenvectors of $\hat{J}^2$. The simplest function, other than a constant, that one can think of is $x - iy$ which is an eigenfunction of $\hat{J}_z$ with eigenvalue -1 and it is also an eigenfunction of $\hat{J}^2$. Furthermore,

$$\hat{J}_- = (\hat{J}_x - iJ_y)(x - iy) = 0$$

which implies that $(x - iy)$ has the smallest value of m among the degenerate eigenfunctions of $\hat{J}^2$. To generate the irreducible subspace, we apply

the operator $\hat{J}_+$ repeatedly on $(x - iy)$ until it vanishes:

$$\begin{aligned} \hat{J}_+(x - iy) &= 2z \\ \hat{J}_+ z &= -(x + iy) \\ \hat{J}_+(x + iy) &= 0 \end{aligned}$$

$(x-iy)$, z, and $-(x+iy)$ thus form an irreducible subspace with eigenvalues of $\hat{J}_z$ equal to $m = -1, 0, 1$ respectively. We immediately recognise that this set corresponds to the $j = 1$ representation with eigenvalue of $\hat{J}^2$ equal to $j(j+1) = 2$, as may be easily verified. These functions are proportional to the spherical harmonics for $l = 1$. Since $r^2 = x^2 + y^2 + z^2$ is invariant under rotation, we may choose $r = 1$. In polar coordinates, we then have $z = cos\ \theta$, $y = sin\ \theta\ sin\ \phi$, and $x = sin\ \theta\ cos\ \phi$, so that

$$\begin{aligned} Y_1^1 &= -\sqrt{\tfrac{3}{8\pi}}\,(x + iy) &&= -\sqrt{\tfrac{3}{8\pi}}\ sin\ \theta\ e^{i\phi} \\ Y_0^1 &= \sqrt{\tfrac{3}{4\pi}}\ z &&= \sqrt{\tfrac{3}{4\pi}}\ cos\ \theta \\ Y_{-1}^1 &= \sqrt{\tfrac{3}{8\pi}}\,(x - iy) &&= \sqrt{\tfrac{3}{8\pi}}\ sin\ \theta\ e^{-i\phi} \end{aligned}$$

which are the spherical harmonics Y_m^l for $l = 1$. The normalisation constants are determined by integrating the square of each function over the solid angle and requiring the integral to be unity. Higher l spherical harmonics may be generated in the same fashion by applying the operator $\hat{J}_+$ on $(x - iy)^l$ repeatedly and normalising the resulting functions as just mentioned above. There is an ambiguity in the sign. As a convention, the spherical harmonics are defined such that

$$Y_{-l}^l = \frac{\sqrt{(2l)!}}{2^l l!}\sqrt{\frac{2l+1}{4\pi}}(x - iy)^l \tag{4.59}$$

which fixes the sign.

The spherical harmonics for each l form an irreducible subspace under rotation and therefore provide an irreducible representation of the rotation group R_3. Under rotation, the spherical harmonics transform among themselves with the same l. Two spherical harmonics with different l values will never transform to each other under rotation because they belong to two

distinct irreducibe subspaces of the rotation group. This means that we can decompose an arbitrary function $f(r,\theta,\phi)$ into the irreducible subspaces formed by the spherical harmonics as follows:

$$f(r,\theta,\phi) = \sum_{lm} f_{lm}(r) Y_m^l(\theta,\phi)$$

From the definition of the spherical harmonics it is easy to show that:

$$Y_m^l(0,\phi) = \sqrt{\frac{2l+1}{4\pi}}\delta_{m,0} \tag{4.60}$$

$$Y_0^l(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}} P_l(cos\ \theta) \tag{4.61}$$

The last equation may be thought of as the definition of the Legendre polynomials.

We can now derive some useful identities but first we write down the transformation of spherical harmonics under an arbitrary rotation R in the following way:

$$\hat{T}(R) Y_m^l(\theta,\phi) = Y_m^l(\theta',\phi') = \sum_{m'} Y_{m'}^l(\theta,\phi) R_{m'm}^l \tag{4.62}$$

or

$$Y_m^l(\theta,\phi) = \sum_{m'=-l}^{l} R_{mm'}^{l*} Y_{m'}^l(\theta',\phi') \tag{4.63}$$

where $R_{m'm}^l$ is the irreducible representation of a rotation R in the spherical harmonics basis. We take the point of view that (θ,ϕ) and (θ',ϕ') correspond to the same physical point, i.e. it is the coordinate system which is rotated. Considering a point $(\theta,\phi) = (\theta_z,\phi_z)$ on the rotated z axis corresponding to $\theta' = 0$ we get

$$R_{m0}^l = \sqrt{\frac{4\pi}{2l+1}} Y_m^{l*}(\theta_z,\phi_z) \tag{4.64}$$

It follows immediately by substituting this into Eq. (4.62) for $m = 0$ that

$$Y_0^l(\theta',\phi') = \sqrt{\frac{4\pi}{2l+1}} \sum_{m=-l}^{l} Y_m^l(\theta,\phi) Y_m^{l*}(\theta_z,\phi_z) \tag{4.65}$$

By Eq. (4.61) we get the addition theorem

$$P_l(cos\ \theta') = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_m^{l*}(\theta_z, \phi_z) Y_m^l(\theta, \phi) \tag{4.66}$$

For the special case of $\theta = \theta_z$ and $\phi = \phi_z$ we have $\theta' = 0$ so that

$$\sum_{m=-l}^{l} Y_m^{l*}(\theta, \phi) Y_m^l(\theta, \phi) = \frac{2l+1}{4\pi}$$

Thus the quantity on the left hand side is invariant under rotation since the (θ, ϕ) is arbitrary.

A product of two spherical harmonics transforms according to the direct product representation which is in general reducible. Using Eq. (4.64) in Eq. (4.44) we obtain

$$\begin{aligned} Y_{m_1}^{l_1}(\theta, \phi) Y_{m_2}^{l_2}(\theta, \phi) &= \sum_{L=|l_1-l_2|}^{l_1+l_2} \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2L+1)}} \\ &\quad \times C_0^L(0,0) C_M^L(m_1, m_2) Y_M^L((\theta, \phi) \end{aligned} \tag{4.67}$$

where $M = m_1 + m_2$. From this we can evaluate the frequently encountered integral of three spherical harmonics:

$$\int d\Omega\ Y_M^{L*} Y_{m_1}^{l_1} Y_{m_2}^{l_2} = \sqrt{\frac{(2l_1+1)(2l_2+1)}{4\pi(2L+1)}} C_0^L(0,0) C_M^L(m_1, m_2) \tag{4.68}$$

Chapter 5

Atomic Physics

The Hamiltonian $\hat{H}$ of an atom in the absence of external fields is given by

$$\hat{H} = \sum_i [t_i - Z/r_i] + 1/2 \sum_{i \neq j} 1/r_{ij} + \sum_i \xi(r_i) \mathbf{l}_i \cdot \mathbf{s}_i \tag{5.1}$$

It is useful to break up $\hat{H}$ as follows:

$$\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_2 \tag{5.2}$$

where

$$\hat{H}_0 = \sum_i \hat{h}_0(\mathbf{r}_i) = \sum_i [t_i - Z/r_i + V_{eff}(r_i)] \tag{5.3}$$

$$\hat{H}_1 = 1/2 \sum_{i \neq j} 1/r_{ij} - \sum_i V_{eff}(r_i) \tag{5.4}$$

$$\hat{H}_2 = \sum_i \xi(r_i) \mathbf{l}_i \cdot \mathbf{s}_i \tag{5.5}$$

V_{eff} is a spherically symmetric single-particle potential. The reason for the above division of $\hat{H}$ is that $\hat{H}_0$ is a single-particle operator which can be solved easily. By choosing V_{eff} appropriately, $\hat{H}_1$ may be made small so that it can be treated as a perturbation. $\hat{H}_2$ is usually small and can also be treated as a perturbation and we assume that $\hat{H}_2 << \hat{H}_1$.

The objective of the present chapter is to set up the Hamiltonian matrix and exploit the symmetry properties of the Hamiltonian by means of group theory in order to simplify our task. We consider the terms in the Hamiltonian one by one starting with $\hat{H}_0$.

5.1 $\hat{H}_0$

$\hat{H}_0$ has two kinds of symmetry. It is invariant under permutations of the electron coordinates (indistinguishability) and under separate rotations of the electron coordinates. The eigenfunctions of $\hat{H}_0$ must therefore form basis functions for the irreducible representations of the permutation and rotation groups. For a permutation group of N elements, there is always a one-dimensional irreducible representation whose basis functions are totally anti-symmetric, meaning that the functions change sign whenever two coordinates are interchanged. It does not follow from group theory that the eigenfunctions of the Hamiltonian should be totally anti-symmetric but for fermions, these are the only ones found in nature (Pauli principle). These anti-symmetric functions can be written most conveniently as Slater determinants which are linear combinations of $\prod_i \psi_i(\mathbf{r}_i)$, where $\hat{h}_0\psi_i = \epsilon_i\psi_i$, with the coordinates permuted:

$$\Psi(1,2,\ldots,Z) = \frac{1}{\sqrt{Z}} \begin{vmatrix} \psi_1(1) & \psi_2(1) & \ldots & \psi_Z(1) \\ \psi_1(2) & \psi_2(2) & \ldots & \psi_Z(2) \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots \\ \psi_1(Z) & \psi_2(Z) & \ldots & \psi_Z(Z) \end{vmatrix} \tag{5.6}$$

We have labeled the coordinates $\mathbf{r}_i$ by i for simplicity. Take for example the simplest non-trivial case of two electrons. The Slater determinant is

$$\Psi_{12}(1,2) = \frac{1}{\sqrt{2}}\left[\psi_1(1)\psi_2(2) - \psi_1(2)\psi_2(1)\right]$$

which changes sign when the coordinates or the quantum labels 1 and 2 are interchanged Moreover, it becomes zero when the coordinates or the quantum labels $1 = 2$, which is a general property of a determinant that it is zero whenever two rows or columns are the same. This is simply the Pauli exclusion principle. Since $\hat{H}_0$ is a sum of single-particle operators, its solution is just a single Slater determinant. From now on we assume that basis functions needed to set up the secular equation for $\hat{H}$ must be Slater determinants.

We now consider the rotational symmetry which implies that

$$[\hat{T}(R), \hat{h}_0] = 0$$

It follows that

$$[\hat{h}_0, \hat{L}_x] = [\hat{h}_0, \hat{L}_y] = [\hat{h}_0, \hat{L}_z] = [\hat{h}_0, \hat{L}^2] = 0$$

and the eigenstates of $\hat{h}_0$ may be chosen to be simultaneous eigenstates of $\hat{L}^2$ and $\hat{L}_z$. Each energy level of $\hat{h}_0$ is $(2l+1)$ degenerate since the irreducible representations of R_3 are labelled by R^l with dimensions $(2l+1)$. Neglecting spin, the eigenstates must have the following form:

$$\psi_{nlm}(\mathbf{r}) = u_{nl}(r) Y_m^l(\theta, \phi)$$

where Y_m^l is an eigenfunction of $\hat{L}_z$ and $\hat{L}^2$. Operating $\hat{h}_0$ on ψ_{nlm} shows that $u_{nl}(r)$ must be a solution to the radial Schrödinger equation corresponding to $\hat{h}_0$, which is a familiar result.

We now take into account spin and label the spin states by $\chi_{m_s}(\sigma)$ where the spin coordinate σ can only take two discrete values $\sigma = \pm 1$:

$$\chi_+(1) = 1, \;\; \chi_+(-1) = 0, \;\; \chi_-(1) = 0, \;\; \chi_-(-1) = 1,$$

Physical observation shows that the spin behaves like angular momentum so that

$$\hat{T}(R)\chi_{m_s}(\sigma) = \sum_{m_s'} \chi_{m_s'}(\sigma) T^{1/2}_{m_s' m_s}(R)$$

The spin states form a basis for the two dimensional irreducible representation of R_3 corresponding to $j = 1/2$. The eigenstate of $\hat{h}_0$ including spin is

$$\psi_{nlmm_s}(\mathbf{r}, \sigma) = u_{nl}(r) Y_m^l(\theta, \phi) \chi_{m_s}(\sigma)$$

To summarise, the eigenfunctions of $\hat{H}_0$ are simply single Slater determinants with the orbitals given by the eigenfunctions of $\hat{h}_0$. In determining the eigenstates of $(\hat{H}_0 + \hat{H}_1)$ we will use these eigenfunctions as basis functions.

5.2 $\hat{H}_0 + \hat{H}_1$

We now consider $(\hat{H}_0 + \hat{H}_1)$ which is invariant under *simultaneous* rotations of the position coordinates of the electrons. It is also implicitly invariant under *simultaneous* rotations in the spin coordinates. Although $(\hat{H}_0 +$

$\hat{H}_1)$ has no explicit spin dependence, it is assumed that each electron carries a spin and the spin dependence enters implicitly through the Pauli principle. The degenerate eigenfunctions of $(\hat{H}_0 + \hat{H}_1)$ must therefore form an invariant subspace under simultaneous rotations of the space or spin coordinates.

The infinitesimal operators for the simultaneous rotations in space or spin coordinates are given by the sum of the infinitesimal operators corresponding to each electron coordinate. Thus

$$\hat{L}_x = \sum_i \hat{L}_x(i), \quad \hat{L}_y = \sum_i \hat{L}_y(i), \quad \hat{L}_z = \sum_i \hat{L}_z(i)$$

where $\hat{L}_z(i)$ acts on the coordinate $\mathbf{r}_i$. Similarly for the infinitesimal operators in the spin space $\hat{S}_x$, $\hat{S}_y$, and $\hat{S}_z$. These six infinitesimal operators correspond to a direct product $R_3^L \otimes R_3^S$ since the orbital and spin operators commute. $(\hat{H}_0 + \hat{H}_1)$ commutes with $\hat{L}_x$, $\hat{L}_y$, $\hat{L}_z$, and $\hat{L}^2$ and with the spin counterpart. As before we may choose the eigenfunctions of $(\hat{H}_0 + \hat{H}_1)$ to be simultaneous eigenfunctions of $\hat{L}_z$ and $\hat{L}^2$ and of $\hat{S}_z$ and $\hat{S}^2$. $(\hat{H}_0 + \hat{H}_1)$ no longer commutes with the angular momentum or spin operators of each electron. The eigenfunctions of $\hat{H}_0$ are still eigenfunctions of $\hat{L}_z$ and $\hat{S}_z$ but not of $\hat{L}^2$ or $\hat{S}^2$.

5.2.1 Configuration and Term

In atoms, we need only consider the valence electrons because the electrons forming a closed shell act effectively like a spherically symmetric potential which can be combined with V_{eff}. We define a configuration by a symbol such as s^1p^1 meaning that there is one electron in an s-shell and one electron in a p-shell. Thus the superscript indicates the number of electrons. We use the spectroscopic notations $s, p, d, f, \ldots$ corresponding to $l = 0, 1, 2, 3, \ldots$ respectively.

When there are more than one electron, the representation for simultaneous rotations of the electron coordinates is given by a direct product of each rotation. According to the vector-coupling theorem, the direct product representation is in general reducible. Since $(\hat{H}_0 + \hat{H}_1)$ commute with rotation operators in space and spin coordinates separately, the energy levels of $(\hat{H}_0 + \hat{H}_1)$ can be labelled with L and S and each energy level is $(2L + 1)(2S + 1)$ degenerate. The corresponding states

are conventionally written as ${}^{2S+1}L$ and they are called "term" (multiplet). To illustrate the concept of term, consider two p electrons. According to the vector-coupling theorem, the irreducible representations for simultaneous rotations of the two electron space coordinates correspond to $L = l_1+l_2, l_1+l_2-1, \ldots, |l_1-l_2| = 2, 1, 0$ since $l_1 = l_2 = 1$. Similarly, the irreducible representations for simultaneous rotations of the two electron spin coordinates correspond to $S = 1, 0$ since $s_1 = s_2 = 1/2$. The possible terms are then given by ${}^3D,\ {}^3P,\ {}^3S,\ {}^1D,\ {}^1P,\ {}^1S$. Some of these terms may not be allowed by the Pauli exclusion principle when the two electrons are equivalent as we shall see below.

5.2.2 Ladder Operator Method

As just discussed above, the eigenfunctions of $\hat{H}_0$ are still eigenfunctions of $\hat{L}_z$ and $\hat{S}_z$ but not of $\hat{L}^2$ or $\hat{S}^2$. However, we know that we can always generate an invariant subspace by applying the symmetry operators repeatedly on an arbitrary function in that subspace. If we know one of the eigenfunctions of $\hat{L}^2$ and $\hat{S}^2$ then we can construct the other degenerate eigenfunctions by using the ladder operators. Let us illustrate this method by considering a specific example since the generalisation to an arbitrary case is quite clear.

Consider a configuration p^2 and let us use the notation $|+1^+\rangle|-1^-\rangle$ to represent a Slater determinant where one electron has $m_l = +1$ and $m_s = +1/2$ and the other electron has $m_l = -1$ and $m_s = -1/2$. m_l and m_s are respectively the eigenvalues of $\hat{L}_z$ and $\hat{S}_z$ of the individual electrons. Let us list the possible Slater determinants corresponding to this configuration starting with the largest possible value of $M_L = \sum_i m_l(i)$. We note also that the two electrons are equivalent because they occupy the same p shell. There are $(2 \times 3)!/2!(2 \times 3 - 2)! = 15$ possible ways of placing two identical electrons in a p-shell:

	M_L	M_S
$\Psi_1 = \|1^+\rangle\|1^-\rangle$	2	0
$\Psi_2 = \|1^+\rangle\|0^+\rangle$	1	1
$\Psi_3 = \|1^+\rangle\|0^-\rangle$	1	0
$\Psi_4 = \|1^-\rangle\|0^+\rangle$	1	0
$\Psi_5 = \|1^-\rangle\|0^-\rangle$	1	-1
$\Psi_6 = \|1^+\rangle\|-1^+\rangle$	0	1
$\Psi_7 = \|1^+\rangle\|-1^-\rangle$	0	0
$\Psi_8 = \|1^-\rangle\|-1^+\rangle$	0	0
$\Psi_9 = \|1^-\rangle\|-1^-\rangle$	0	-1
$\Psi_{10} = \|0^+\rangle\|0^-\rangle$	0	0
$\Psi_{11} = \|0^+\rangle\|-1^+\rangle$	-1	1
$\Psi_{12} = \|0^+\rangle\|-1^-\rangle$	-1	0
$\Psi_{13} = \|0^-\rangle\|-1^+\rangle$	-1	0
$\Psi_{14} = \|0^-\rangle\|-1^-\rangle$	-1	-1
$\Psi_{15} = \|-1^+\rangle\|-1^-\rangle$	-2	0

We keep in mind that Ψ_i is a Slater determinant so that e.g. $|1^+\rangle|1^-\rangle = -|1^-\rangle|1^+\rangle$. It is natural when using the ladder operator method to start from a Slater determinant with the largest values of M_L and/or M_S since it is more likely that it is an eigenstate of $\hat{L}^2$ and/or $\hat{S}^2$. Ψ_1 has the largest value of M_L and it is the only one. Moreover, it has $M_S = 0$ and therefore it must be an eigenfunction belonging to singlet ^1D. We check that it is an eigenfunction of $\hat{L}^2$ and $\hat{S}^2$:

$$\begin{aligned}
\hat{L}_+\Psi_1 &= [\hat{L}_+(1) + \hat{L}_+(2)]|+1^+\rangle|+1^-\rangle = 0 \\
\hat{L}_z\Psi_1 &= (\hat{L}_z(1) + \hat{L}_z(2))|+1^+\rangle|+1^-\rangle \\
&= (1+1)|+1^+ + 1^-\rangle \\
&= 2\Psi_1 \\
\hat{L}_z^2\Psi_1 &= 4\Psi_1 \\
\hat{L}^2\Psi_1 &= 6\Psi_1
\end{aligned}$$

$$\begin{aligned}
\hat{S}_+\Psi_1 &= [\hat{S}_+(1) + \hat{S}_+(2)]|+1^+\rangle|+1^-\rangle = 0 \\
\hat{S}_z\Psi_1 &= [\hat{S}_z(1) + \hat{S}_z(2)]|+1^+\rangle|+1^-\rangle = 0 \\
\hat{S}^2\Psi_1 &= 0
\end{aligned}$$

We generate the invariant subspace formed by the degenerate eigenfunctions of $\hat{L}^2$ corresponding to the term ^1D:

$$\begin{aligned}\hat{L}_-\Psi_1 &= [\hat{L}_-(1)+\hat{L}_-(2)]|+1^+\rangle|+1^-\rangle \\ &= \sqrt{(1+1)(1-1+1)}|0^+\rangle|+1^-\rangle \\ &\quad +\sqrt{(1+1)(1-1+1)}|+1^+\rangle|0^-\rangle \\ &= \sqrt{2}(\Psi_3-\Psi_4)\end{aligned}$$

We continue applying the lowering operator:

$$\begin{aligned}\hat{L}_-(\Psi_3-\Psi_4) &= \sqrt{2}(2\Psi_{10}+\Psi_7-\Psi_8) \\ \hat{L}_-(2\Psi_{10}+\Psi_7-\Psi_8) &= 3\sqrt{2}(\Psi_{12}-\Psi_{13}) \\ \hat{L}_-(\Psi_{12}-\Psi_{13}) &= 2\sqrt{2}\Psi_{15} \\ \hat{L}_-\Psi_{15} &= 0\end{aligned}$$

The functions Ψ_1, $(\Psi_3-\Psi_4)$, $(\Psi_7-\Psi_8+2\Psi_{10})$, $(\Psi_{12}-\Psi_{13})$, and Ψ_{15} are degenerate eigenfunctions of $\hat{L}^2$ and $\hat{S}^2$ corresponding to the term ^1D.

Ψ_2 must be an eigenfunction belonging to ^3P because it is the only one with $M_L = 1$ and $M_S = 1$ and the term ^3D does not exist. We operate $\hat{S}_-$ on Ψ_2 to obtain the triplets with $M_L = 1$.

$$\begin{aligned}\hat{S}_-\Psi_2 &= \hat{S}_-|1^+\rangle|0^+\rangle \\ &= |1^-\rangle|0^+\rangle+|1^+\rangle|0^-\rangle \\ &= \Psi_4+\Psi_3 \\ \hat{S}_-(\Psi_4+\Psi_3) &= 2\Psi_5 \\ \hat{S}_-\Psi_5 &= 0\end{aligned}$$

Operating $\hat{L}_+$ on Ψ_2 yields a state $|+1^+\rangle|+1^+\rangle$ which is forbidden by the Pauli exclusion principle. This state would be allowed if the two electrons occupied different p shells. We operate $\hat{L}_-$ on Ψ_2 and then use $\hat{S}_-$ to generate the triplets with $M_L = 0$:

$$\begin{aligned}\hat{L}_-\Psi_2 &= \sqrt{2}\Psi_6 \\ \hat{S}_-\Psi_6 &= \Psi_8+\Psi_7 \\ \hat{S}_-(\Psi_8+\Psi_7) &= 2\Psi_9 \\ \hat{S}_-\Psi_9 &= 0\end{aligned}$$

Continuing along the same fashion we generate the triplets with $M_L = -1$

$$\begin{aligned} \hat{L}_- \Psi_6 &= \sqrt{2}\Psi_{11} \\ \hat{S}_- \Psi_{11} &= \Psi_{13} + \Psi_{12} \\ \hat{S}_- (\Psi_{13} + \Psi_{12}) &= 2\Psi_{14} \\ \hat{S}_- \Psi_{14} &= 0 \end{aligned}$$

We have generated 14 eigenfunctions. The only one left must belong to the term ^1S. There are three Slater determinants, $\Psi_7,\ \Psi_8,\ \Psi_{10}$, with $M_L = 0$ and $M_S = 0$. We have already found two eigenfunctions $\Psi_7 - \Psi_8 + 2\Psi_{10}$ and $\Psi_7 + \Psi_8$ belonging to ^1D and ^3P respectively. The eigenfunction belonging to ^1S must be $\Psi_7 - \Psi_8 - \Psi_{10}$ since it is orthogonal to the previous two eigenfunctions.

Below we summarise our results, where the eigenfunctions have been normalised:

Term	M_L	M_S	Eigenfunction
^1D	2	0	Ψ_1
	1	0	$(\Psi_3 - \Psi_4)/\sqrt{2}$
	0	0	$(\Psi_7 - \Psi_8 + 2\Psi_{10})/\sqrt{6}$
	-1	0	$(\Psi_{12} - \Psi_{13})/\sqrt{2}$
	-2	0	Ψ_{15}
^3P	1	1	Ψ_2
		0	$(\Psi_3 + \Psi_4)/\sqrt{2}$
		-1	Ψ_5
	0	1	Ψ_6
		0	$(\Psi_7 + \Psi_8)/\sqrt{2}$
		-1	Ψ_9
	-1	1	Ψ_{11}
		0	$(\Psi_{12} + \Psi_{13})/\sqrt{2}$
		-1	Ψ_{14}
^1S	0	0	$(\Psi_7 - \Psi_8 - \Psi_{10})/\sqrt{3}$

The method that we have used to construct the eigenfunctions of $\hat{L}^2$ and $\hat{S}^2$ and hence of $(\hat{H}_0 + \hat{H}_1)$ is systematic but it becomes tedious as

the number of Slater determinants increases. We discuss below a different method which is more suitable for the latter case.

5.2.3 Projection Operator Method

Let us illustrate the method by using the example we have just considered. Each of the Slater determinant Ψ_1, $\Psi_2, \ldots$ must be a linear combination of eigenfunctions belonging to ^1D, ^3P, and ^1S. It is best to start with a Slater determinant with $M_L = 0$ and $M_S = 0$ since it is contained in all the terms. Let us take Ψ_7 and suppose that we are interested in finding the component of ^1D. We first project out the component of ^3P out of Ψ_7 and then we project out the comoponent of ^1S:

$$\begin{aligned} \left[\hat{L}^2 - 1(1+1)\right]\Psi_7 &= 2\Psi_{10} \\ \left[\hat{L}^2 - 0(0+1)\right]\Psi_{10} &= 2\Psi_{10} + \Psi_7 - \Psi_8 \end{aligned}$$

This is proportional to the eigenfunction of ^1D with $M_L = 0$ and $M_S = 0$ which is in agreement with the result obtained by using the ladder operator method.

We can arrive at the same result if we first find the eigenfunction of $\hat{S}^2$ with $S = 0$ by projecting out the component with $S = 1$:

$$\begin{aligned} [\hat{S}^2 - 1(1+1)]\Psi_7 &= \Psi_7 + \Psi_8 - 2\Psi_7 \\ &= \Psi_8 - \Psi_7 \end{aligned}$$

Thus $(\Psi_8 - \Psi_7)$ is an eigenfunction of $\hat{S}^2$ corresponding to $S = 0$ (singlet). Now we project out the component of ^1S. It is not necessary to project out the component of ^3P because $(\Psi_8 - \Psi_7)$ is a singlet and therefore it cannot contain eigenfunctions of ^3P.

$$\begin{aligned} [\hat{L}^2 - 0(0+1)](\Psi_8 - \Psi_7) &= 2(-\Psi_{10} + \Psi_8) - 2(\Psi_{10} + \Psi_7) \\ &= -2(\Psi_7 - \Psi_8 + 2\Psi_{10}) \end{aligned}$$

which is proportional to the previous result.

From a given Slater determinant, the projection operator method allows us to arrive at a particular eigenfunction of a term by projecting out all the other terms one by one.

5.2.4 Term Energies

In this section we discuss the calculations of term energies. To calculate the term energies, we need matrix elements of the type

$$\langle \Psi_i | \hat{H}_0 + \hat{H}_1 | \Psi_j \rangle$$

It is convenient to calculate them in the occupation number representation in which $(\hat{H}_0 + \hat{H}_1)$ is given by

$$\hat{H}_0 + \hat{H}_1 = \sum_{ij} \hat{c}_i \langle i|\hat{h}_0|j\rangle \hat{a}_j + \frac{1}{2} \sum_{ijkl} \hat{c}_i \hat{c}_j \langle ij|\hat{v}|kl\rangle \hat{a}_l \hat{a}_k \qquad (5.7)$$

where

$$\begin{aligned} \langle i|\hat{h}_0|j\rangle &= \delta(s_i, s_j) \int d1 \; \psi_i^*(1) h_0(1) \psi_j(1), \;\; 1 \equiv \mathbf{r}_1 \\ \langle ij|\hat{v}|kl\rangle &= \delta(s_i, s_k)\delta(s_j, s_l) \int d1d2 \; \frac{\psi_i^*(1)\psi_j^*(2)\psi_k(1)\psi_l(2)}{|1-2|} \end{aligned}$$

$\hat{c}_i = \hat{a}_i^\dagger$ and $\hat{a}_i = \hat{c}_i^\dagger$ are creation and annihilation operators respectively which obey the commutation relations

$$[\hat{c}_i, \hat{c}_j]_+ = 0, \;\; [\hat{a}_i, \hat{a}_j]_+ = 0, \;\; [\hat{c}_i, \hat{a}_j]_+ = \delta_{ij} \qquad (5.8)$$

We write the Slater determinants Ψ_i in the occupation number representation and order the single-particle states ψ_i as follows

$$|1^+,\ 1^-,\ 0^+,\ 0^-,\ -1^+,\ -1^-\rangle = \hat{c}_{1^+}\ \hat{c}_{1^-}\ \hat{c}_{0^+}\ \hat{c}_{0^-}\ \hat{c}_{-1^+}\ \hat{c}_{-1^-}|0\rangle$$

where $|0\rangle$ is a state with no electrons in the p shell. We note that for fermions the ordering of the states is very important. Thus we have

$$\begin{aligned} \Psi_1 &= \hat{c}_{1^+}\ \hat{c}_{1^-}|0\rangle \\ \Psi_2 &= \hat{c}_{1^+}\ \hat{c}_{0^+}|0\rangle \\ &\vdots \\ \Psi_{15} &= \hat{c}_{-1^+}\ \hat{c}_{-1^-}|0\rangle \end{aligned}$$

The matrix elements of $\hat{H}_1$ between $\Psi = \hat{c}_p\hat{c}_q|0\rangle$ and $\Psi' = \hat{c}_r\hat{c}_s|0\rangle$ will be of the following form:

$$\begin{aligned}\langle\Psi|\hat{H}_1|\Psi'\rangle &= \frac{1}{2}\sum_{ijkl}\langle ij|\hat{v}|kl\rangle\langle 0|\hat{a}_q\hat{a}_p\hat{c}_i\hat{c}_j\hat{a}_l\hat{a}_k\hat{c}_r\hat{c}_s|0\rangle \\ &= \langle pq|\hat{v}|rs\rangle - \langle pq|\hat{v}|sr\rangle\end{aligned}$$

The first term is the direct term and the second term is the so called exchange term.

The matrix elements of $\hat{H}_0$ between $\Psi = \hat{c}_p\hat{c}_q|0\rangle$ and $\Psi' = \hat{c}_r\hat{c}_s|0\rangle$ are quite simple:

$$\begin{aligned}\langle\Psi|\hat{H}_0|\Psi'\rangle &= \sum_{ij}\langle i|\hat{h}_0|j\rangle\langle 0|\hat{a}_q\hat{a}_p\hat{c}_i\hat{a}_j\hat{c}_r\hat{c}_s|0\rangle \\ &= [\langle p|\hat{h}_0|p\rangle + \langle q|\hat{h}_0|q\rangle](\delta_{pr}\delta_{qs} - \delta_{ps}\delta_{qr})\end{aligned}$$

We have made use of the fact that ψ_i are eigenfunctions of $\hat{h}_0$ so that $\langle i|\hat{h}_0|j\rangle = \delta_{ij}$. $\hat{H}_0$ is diagonal because the Slater determinants are eigenfunctions of $\hat{H}_0$ and they are degenerate. Therefore $\hat{H}_0$ only contributes the same constant term to all the terms.

We must also evaluate the integral $\langle pq|\hat{v}|rs\rangle$ before we can calculate the term energies. To do this, we use the multipole expansion of the Coulomb potential:

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{lm}\frac{4\pi}{2l+1}\frac{r_<^l}{r_>^{l+1}}Y_m^{l*}(\Omega_1)Y_m^l(\Omega_2) \tag{5.9}$$

where $r_>$ and $r_<$ are the greater and the smaller of r_1 and r_2. We recall that $\psi_i = \phi_l(r)Y_m^l(\Omega)$ where $\phi_l(r)$ is the solution to the radial Schrödinger equation.

$$\begin{aligned}\langle\psi_1\psi_2|\hat{v}|\psi_3\psi_4\rangle &= \int d^3r_1\, d^3r_2 \sum_{lm}\frac{4\pi}{2l+1}\frac{r_<^l}{r_>^{l+1}}\phi_{l_1}(r_1)\phi_{l_2}(r_2)\phi_{l_3}(r_1)\phi_{l_4}(r_2) \\ &\times \int d\Omega_1 Y_m^{l*}(\Omega_1)Y_{m_1}^{l_1*}(\Omega_1)Y_{m_3}^{l_3}(\Omega_1) \\ &\times \int d\Omega_2 Y_m^l(\Omega_2)Y_{m_2}^{l_2*}(\Omega_2)Y_{m_4}^{l_4}(\Omega_2)\end{aligned}$$

The integrals over three spherical harmonics are given by Eq. (4.68) and the Clebsch-Gordan coefficients are tabulated extensively in many books on atomic physics.

Let us calculate the energy of the term ^1D. Since all the eigenfunctions of ^1D are degenerate we can take the state Ψ_1:

$$\begin{aligned}\langle\Psi_1|\hat{H}_1|\Psi_1\rangle &= \langle pq|\hat{v}|rs\rangle - \langle pq|\hat{v}|sr\rangle \\ &= \int d^3r_1\, d^3r_2 \sum_{lm} \frac{4\pi}{2l+1}\frac{r_<^l}{r_>^{l+1}}\phi_1^2(r_1)\phi_1^2(r_2) \\ &\times \int d\Omega_1 Y_m^{l*}(\Omega_1)Y_1^{1*}(\Omega_1)Y_1^1(\Omega_1) \\ &\times \int d\Omega_2 Y_m^{l}(\Omega_2)Y_1^{1*}(\Omega_2)Y_1^1(\Omega_2)\end{aligned}$$

The second term (exchange term) vanishes because of the orthogonality of the spin states.

5.3 $\hat{H} = \hat{H}_0 + \hat{H}_1 + \hat{H}_2$

Finally we include the spin-orbit term $\hat{H}_2$ which is invariant under simultaneous rotations in space and spin coordinates. This implies

$$[\hat{H}, \hat{J}_x] = [\hat{H}, \hat{J}_y] = [\hat{H}, \hat{J}_z] = [\hat{H}, \hat{J}^2] = 0$$

where

$$\hat{J}_x = \sum_i [\hat{L}_x(i) + \hat{S}_x(i)] \;\; etc.$$

$\hat{H}$ does not commute with $\hat{L}_i$ or $\hat{S}_i$ and the group is now reduced to R_3. This means that the $(2L+1)(2S+1)$ degeneracy of each term will be in general split and each energy level of $\hat{H}$ is now $(2J+1)$ degenerate with $J = L+S, L+S-1, \ldots, |L-S|$ which follows from the vector-coupling rule $R^L \otimes R^S = \sum_{J=|L-S|}^{L+S} R^J$. The J dependence of the splitting for given L, S may be evaluated by using the Wigner-Eckart theorem. We assume that $\hat{H}_2$ is small enough so that it causes no mixing between the different terms. Let ψ_{JM} be an eigenstate of $\hat{J}^2$ which is also an eigenstate of $\hat{L}^2$ and $\hat{S}^2$ since it is formed as a linear combination of the eigenstates of a given term. We have

$$\begin{aligned}\Delta_J &= (\psi_{JM}, \sum_i \xi(r_i)\mathbf{l}_i \cdot \mathbf{s}_i\, \psi_{JM}) \\ &= A(\psi_{JM}, \mathbf{L}\cdot\mathbf{S}\, \psi_{JM}) \\ &= \frac{1}{2}A[J(J+1) - L(L+1) - S(S+1)]\end{aligned}$$

The second step follows from the fact that $\mathbf{L} \cdot \mathbf{S} = 1/2(\hat{J}^2 - \hat{L}^2 - \hat{S}^2)$ transforms exactly like $\sum_i \xi(r_i)\mathbf{l}_i \cdot \mathbf{s}_i$ and the fact that R_3 is simply reducible i.e. $m = 1$ in the Wigner-Eckart theorem. The actual magnitude of the splitting depends on the details of the wavefunctions which are contained in A.

Chapter 6

The Group SU_2: Isospin

It is found experimentally that the strong nuclear force that binds nucleons (protons and neutrons) is the same within $1\ \%$ between proton-proton, proton-neutron and neutron-neutron. We may regard a proton and a neutron as two different states of a nucleon. The Hamiltonian describing the nucleus is invariant under the interchange of proton and neutron states. This symmetry is called isospin. The group corresponding to isospin is called SU_2, which is homomorphic with the rotation group R_3 and the mathematical description is identical to that of the spin 1/2. This means that the results we have derived for the group R_3 may be readily used here.

6.1 The Group SU_2

A 2×2 unitary matrix has four independent parameters and it may be written as

$$U = exp(i\theta) \begin{pmatrix} \alpha & \beta \\ \gamma & \delta \end{pmatrix}$$

Since $UU^\dagger = 1$, we have $mod(det\ U) = 1$ and we may choose $\alpha\delta - \beta\gamma = 1$. A little algebra shows that $\delta = \alpha^*$ and $\gamma = -\beta^*$ so that

$$U = exp(i\theta) \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix}$$

The set of matrices U with $\theta = 0$ and determinant $= 1$ form a subgroup of U_2, called SU_2 (special unitary). Thus, SU_2 is a group with elements

$$U = \begin{pmatrix} \alpha & \beta \\ -\beta^* & \alpha^* \end{pmatrix} \tag{6.1}$$

and the condition $|\alpha|^2 + |\beta|^2 = 1$. We should note that these matrices are themselves the elements of the group SU_2 and they may be regarded as representations of rotation operators in a two-dimensional Hilbert space.

Since U are unitary, the corresponding infinitesimal matrices must be skew Hermitian which can be made Hermitian by including the factor i:

$$1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Since the determinant of SU_2 is $+1$, its infinitesimal matrices must have zero trace and the unit matrix is therefore excluded. The remaining three matrices are just the Pauli spin matrices which are also the infinitesimal matrices of the rotation group R_3 corresponding to $j = 1/2$. However, the relationship between the two group elements of SU_2 and R_3 is not necessarily one-to-one (isomorphic).

Physically, we may generate the group SU_2 by considering two nucleon states,

$$|p\rangle = c_p^+|0\rangle, \quad |n\rangle = c_n^+|0\rangle$$

corresponding to proton and neutron. The bilinear products of the annihilation and creation operators that conserve particle number are

$$c_p^+ c_p, \quad c_n^+ c_n, \quad c_p^+ c_n, \quad c_n^+ c_p$$

We define a new set of operators

$$\begin{aligned} \hat{B} &= c_p^+ c_p + c_n^+ c_n \\ \hat{\tau}_+ &= c_p^+ c_n \\ \hat{\tau}_- &= c_n^+ c_p \\ \hat{\tau}_z &= \frac{1}{2}(c_p^+ c_p - c_n^+ c_n) = \hat{Q} - \frac{1}{2}\hat{B} \end{aligned}$$

which have the following Lie algebra

$$[\hat{B}, \hat{\tau}_+] = [\hat{B}, \hat{\tau}_-] = [\hat{B}, \hat{\tau}_z] = 0$$

$$[\hat{\tau}_z, \tau_+] = \tau_+, \;\; [\hat{\tau}_z, \tau_-] = \tau_-, \;\; [\hat{\tau}_+, \hat{\tau}_-] = 2\hat{\tau}_z$$

The operator $\hat{B}$ may be interpreted as the Baryon number operator and it is an invariant reflecting the conservation of Baryon number. The three operators $\hat{\tau}_+$, $\hat{\tau}_-$, and $\hat{\tau}_z$ form a Lie algebra by themselves and it is identical to the Lie algebra of the rotation group R_3. The two dimensional representations of these operators are obtained by evaluating matrix elements such as $(\tau_+)_{12} = \langle p|c_p^+ c_n|n\rangle = 1$ and this gives:

$$B = 1 \;\; \tau_+ = \frac{1}{2}(\sigma_x + i\sigma_y), \;\; \tau_- = \frac{1}{2}(\sigma_x - i\sigma_y), \;\; \tau_z = \frac{1}{2}\sigma_z$$

In physical applications, it is usually the Lie algebra which is important rather than the Lie group. Two different Lie groups may have the same Lie algebra. As we have seen, the rotation group R_3 is not the same as the group SU_2 although they have the same Lie algebra.

6.2 Relationship between SU_2 and R_3

To relate the elements of R_3 to those of SU_2 we consider explicitly the two-dimensional representation of R_3 corresponding to $j = 1/2$. A rotation about an axis $\mathbf{a}$ by an angle ϕ is represented by

$$D^{1/2}(\mathbf{a}, \phi) = exp(\phi \hat{\mathbf{a}} \cdot \mathbf{X}) \tag{6.2}$$

with $\mathbf{X} = -i\sigma/2$. The anti-commutation relations of the infinitesimal matrices $\mathbf{X}$ are given by

$$\{X_i, X_j\} = -\frac{1}{2}\delta_{ij} \tag{6.3}$$

which implies

$$(\mathbf{a} \cdot \mathbf{X})^2 = \sum_{ij} a_i a_j X_i X_j = -\frac{1}{4}\sum_i a_i^2 \; E = -\frac{1}{4}E$$

sine $\hat{\mathbf{a}}$ is a unit vector. We can now easily work out the representation matrix $D^{1/2}(\mathbf{a}, \phi)$

$D^{1/2}(\mathbf{a}, \phi) \;\; = \;\; exp(\phi \hat{\mathbf{a}} \cdot \mathbf{X})$

$$
\begin{aligned}
&= 1+\phi(\hat{\mathbf{a}}\cdot\mathbf{X})+\frac{1}{2}\phi^2(\hat{\mathbf{a}}\cdot\mathbf{X})^2+\frac{1}{6}\phi^3(\hat{\mathbf{a}}\cdot\mathbf{X})^3+\frac{1}{24}\phi^4(\hat{\mathbf{a}}\cdot\mathbf{X})^4+\ldots \\
&= 1+\frac{1}{2}\phi^2(\hat{\mathbf{a}}\cdot\mathbf{X})^2+\frac{1}{24}\phi^4(\hat{\mathbf{a}}\cdot\mathbf{X})^4+\ldots \\
&\quad +(\hat{\mathbf{a}}\cdot\mathbf{X})[\phi+\frac{1}{6}\phi^3(\hat{\mathbf{a}}\cdot\mathbf{X})^2+\ldots] \\
&= 1-\frac{1}{2}(\phi/2)^2+\frac{1}{4}(\phi/2)^4+\ldots \\
&\quad +2(\hat{\mathbf{a}}\cdot\mathbf{X})[\phi/2-\frac{1}{3}(\phi/2)^3+\ldots] \\
&= cos\ \phi/2+2(\hat{\mathbf{a}}\cdot\mathbf{X})sin\ \phi/2 \\
&= \begin{pmatrix} cos\ \phi/2-ia_z sin\ \phi/2 & -(a_y+ia_x)sin\ \phi/2 \\ (a_y-ia_x)sin\ \phi/2 & cos\ \phi/2+ia_z sin\ \phi/2 \end{pmatrix}
\end{aligned}
$$

These matrices are the matrices of SU_2 in Eq. (6.1) if we make the identification $\alpha = cos\ \phi/2 - ia_z sin\ \phi/2$ and $\beta = -(a_y+ia_x)sin\ \phi/2$ with $0 \leq \phi < 2\pi$ and $\hat{\mathbf{a}}$ pointing in all possible directions. The representation $D^{1/2}$ for the rotation group is however double-valued because there are two matrices corresponding to the same rotation. This can be seen by noting that, to produce all rotations, the angle ϕ need only cover either 0 to π, or π to 2π since

$$R(\mathbf{a},\phi) = R(-\mathbf{a},-\phi) = R(-\mathbf{a},2\pi-\phi)$$

The $D^{1/2}$ representations corresponding to this same physical rotation are different because

$$D^{1/2}(-\mathbf{a},2\pi-\phi) = -D^{1/2}(\mathbf{a},\phi)$$

The relationship between SU_2 and R_3 is thus homomorphic because there are two distinct SU_2 matrices corresponding to the same physical rotation. The representation $D^{1/2}$ for the rotation group can be made single-valued by extending the physical rotation angle artificially to 4π (similar to Riemannian sheets in complex plane). A rotation $R(\mathbf{a},2\pi+\phi)$ is regarded as a new rotation different from $R(\mathbf{a},\phi)$ whereas $R(\mathbf{a},4\pi+\phi) = R(\mathbf{a},\phi)$ since $D^{1/2}(\mathbf{a},4\pi+\phi) = D^{1/2}(\mathbf{a},\phi)$. A rotation such as $R(-\mathbf{a},2\pi-\phi)$ is to be regarded as equivalent to a rotation $R(\mathbf{a},2\pi+\phi)$ because $R(-\mathbf{a},2\pi-\phi) = R(\mathbf{a},-(2\pi-\phi)) = R(\mathbf{a},4\pi-(2\pi-\phi)) = R(\mathbf{a},2\pi+\phi)$.

6.3 SU_2 in Nuclei

As we have discussed in the previous section, the infinitesimal operators of the group SU_2 have the same commutation relations as those of the rotation group R_3. Since the irreducible representations of R_3 were deduced entirely from the commutation relations of the infinitesimal operators, it follows that we have the same irreducible representations in SU_2 which we may label with D^T, $T = 0, 1/2, 1, 3/2 \ldots$, as in R_3. T is called the isospin, similar to L for angular momentum in R_3.

We recall that when a Hamiltonian is invariant under R_3, the eigenfunctions transforming according to the irreducible representations D^L are degenerate labelled by the z components of angular momentum $M_L = L, L-1, \ldots, -L$. Similarly, when a Hamiltonian is invariant under SU_2, the degenerate eigenfunctions tranforming according to the irreducible representation D^T will have z-components of isospin $M_T = T, T-1, \ldots, -T$. These multiplets are interpreted as different possible states of nuclei. For example, the two-dimensional space of proton and neutron, $|p\rangle$ and $|n\rangle$, tranforms according to $D^{1/2}$ and consequently the eigenfunctions of a single nucleon will have $M_T = 1/2, -1/2$. Conventionally, $M_T = 1/2$ corresponds to $|p\rangle$ and $M_T = -1/2$ to $|n\rangle$.

Physically, the operator $\hat{Q} = \frac{1}{2}\hat{B} + \hat{T}_z$ is regarded as a charge operator. A given nucleus with a fixed neutron number N and proton number Z corresponds to a state with $M_T = (Z-N)/2$ since $\langle Q \rangle = Z$. This state may correspond to a state with $T = |Z-N|/2$ or higher. It is found experimentally that the ground state of a nucleus has the minimum value of the total isospin T whereas in an atom, the ground state has the maximum value of the total spin S (Hund's rule). This is because the forces between the nucleons are attractive whereas the forces between the electrons are repulsive. The physical interpretation of this result is that a nucleus with a fixed mass number $A = N + Z$ can exist in different nucleon states with z-components of isospin $M_T = (Z-N)/2$, where Z and N may take any values constrained by the mass number. For a given nucleus with fixed N and Z, states with $M_T = (Z-N)/2$ but $T > |Z-N|/2$ correspond to excited states.

For the general case of several nucleons, we consider simultaneous SU_2 transformation in every nucleon. To find the irreducible representations of two nucleons, we use the same vector-coupling theory as in the angular

momentum theory:

$$D^{T_1} \otimes D^{T_2} = \sum_{|T_1-T_2|}^{T_1+T_2} \oplus D^T$$

which may be extended to an arbitrary number of nucleons.

As a first example, we consider two nucleons. From the vector-coupling theory, we have states with $T = 1$ and $T = 0$. The ground state will correspond to a singlet with $T = 0$ and the excited states to a triplet with $T = 1$ with $M_T = 1, 0, -1$. To work out these states, let us write down explicitly the four vectors that form the space of two nucleons:

$$|1\rangle = |p_1 p_2\rangle \;\; |2\rangle = |p_1 n_2\rangle \;\; |3\rangle = |n_1 p_2\rangle \;\; |4\rangle = |n_1 n_2\rangle$$

The vectors $|1\rangle$ and $|4\rangle$ have $M_T = 1$ and -1 respectively and therefore belong to $T = 1$ states. To find the other states, we apply the lowering operator

$$\hat{T}_- = \hat{t}_-(1) + \hat{t}_-(2)$$

on the vector $|1\rangle$ which conserves the value of T but lowers the value of M_T by one:

$$\begin{aligned} \hat{T}_-|1\rangle &= |n_1 p_2\rangle + |p_1 n_2\rangle \\ &= |2\rangle + |3\rangle \end{aligned}$$

The resulting vector has $M_T = 0$ and we conclude that the $T = 1$ states must be

$$|1\rangle, \;\; 1/\sqrt{2}(|2\rangle + |3\rangle), \;\; |4\rangle$$

The remaining vector

$$1/\sqrt{2}(|2\rangle - |3\rangle)$$

must have $T = 0$ as may be checked by considering

$$\begin{aligned} \hat{T}^2(|2\rangle - |3\rangle) &= (\hat{T}_+\hat{T}_- + \hat{T}_z^2 - \hat{T}_z)(|n_1 p_2\rangle - |p_1 n_2\rangle) \\ &= 0 \end{aligned}$$

Another example of isospin labelling is provided by nuclei with $A = 13$. The lowest value of $T = 1/2$ must be given by the nuclei with $Z = 6, \; N = 7, \; M_T = -1/2$ (C^{13}) and $Z = 7, \; N = 6, \; M_T = 1/2$ (N^{13}). Since $A = 13$ is odd, it is not possible to have states with $T = 1$. The next higher

states must be formed by the nuclei with $Z = 5,\ N = 8,\ M_T = -3/2$ and $Z = 8,\ N = 5,\ M_T = 3/2$ corresponding to $T = 3/2$. The remaining two states with $M_T = \pm 1/2$ must correspond to excited states of C^{13} and N^{13}.

6.4 Tensor Operators

Tensor operators are irreducible sets of operators associated in particular with the rotation group R_3. The general definition of an irreducible set of operators $\{\hat{O}_i^\alpha\}$ is

$$\hat{T}(G)\hat{O}_i^\alpha\hat{T}^{-1}(G) = \sum_k O_k^\alpha T_{ki}^\alpha(G)$$

In Lie groups, $\hat{T}(\mathbf{a}) = 1 + \sum_q a_q\hat{X}_q$ for small $\mathbf{a}$ so that

$$\begin{aligned}\hat{T}(\mathbf{a})\hat{O}_i^\alpha\hat{T}^{-1}(\mathbf{a}) &= (1+\sum_q a_q\hat{X}_q)\hat{O}_i^\alpha(1-\sum_q a_q\hat{X}_q)\\ &= \hat{O}_i^\alpha + \sum_q a_q[\hat{X}_q,\hat{O}_i^\alpha]\end{aligned}$$

Since

$$\sum_k O_k^\alpha T_{ki}^\alpha(\mathbf{a}) = \sum_k O_k^\alpha\left[\delta_{ki} + \sum_q a_q(X_q^\alpha)_{ki}\right]$$

we have

$$[\hat{X}_q,\hat{O}_i^\alpha] = \sum_k O_k^\alpha(X_q^\alpha)_{ki} \tag{6.4}$$

which is the equivalent definition of irreducible set of operators in Lie groups.

The relations defining tensor operators associated with the rotation group are

$$[\hat{J}_z,\hat{O}_m^j] = \sum_{m'}\hat{O}_{m'}^j(\psi_{m'}^j,\hat{J}_z\psi_m^j) = m\hat{O}_m^j$$

$$[\hat{J}_\pm,\hat{O}_m^j] = \sum_{m'}\hat{O}_{m'}^j(\psi_{m'}^j,\hat{J}_\pm\psi_m^j) = \sqrt{(j\pm m+1)(j\mp m)}O_{m\pm1}^j$$

j is called the rank of the tensor and the number of operators in a set is $(2j+1)$ with $m = -j, -j+1, \ldots, j$. For example, the angular momentum operators themselves form a tensor operator of rank 1 (vector operator):

$$\hat{O}^1_1 = -\hat{J}_+\sqrt{2}, \;\; \hat{O}^1_0 = \hat{J}_z, \;\; \hat{O}^1_{-1} = \hat{J}_-\sqrt{2}$$

Chapter 7

The Point Groups

7.1 Crystal Symmetry

A lattice is defined by three linearly independent vectors $\mathbf{a}_1$, $\mathbf{a}_2$, and $\mathbf{a}_3$ and a crystal is a regular array of lattices such that it is invariant under translations $\mathbf{t} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$. Apart from translations, there are also symmetry operations which are performed with a point fixed (origin) and which form a point group. The fundamental covering operations of point groups are

1. Rotations about axes through the origin.

2. Inversion

The complete set of symmetry operations including translations is called the space group.

7.2 Schoenflies Notation

There are several notations used in describing point groups. We follow the notation due to Schoenflies.

$E =$ identity
$C_n =$ rotation through $2\pi/n$.
$\sigma =$ reflection in a plane.

σ_h = reflection in the plane through the origin and perpendicular to the axis of highest rotation symmetry.
σ_v = reflection in the plane through the axis of highest rotation symmetry.
σ_d = reflection in the plane through the axis of highest rotation symmetry and bisecting the angle between the two-fold axes perpendicular to the symmetry axis. This is a special kind of σ_v.
S_n = improper rotation through $2\pi/n$. An improper rotation is a rotation followed by a reflection in a plane perpendicular to the axis of rotation.
$i = S_2$ = inversion.

7.3 Commuting Operations

We list pairs of operations which commute. They are useful for working out group multiplication tables.

1. Two rotations about the same axis.

2. Two reflections in perpendicular planes

3. Two rotations by π about perpendicular axes.

4. A rotation and a reflection in a plane perpendicular to the axis of rotation

5. The inversion and any rotation or reflection

The following rules are useful in determining the complete symmetry of the problem.

1. The intersection of two reflection planes is a symmetry axis. The axis is $n-$fold if the angle between the planes is π/n. If a reflection plane contains an $n-$fold axis, there must be $n-1$ other reflection planes at angles of π/n.

2. If two $2-$fold axes make an angle π/n, then there must be a perpendicular $n-$fold axis. A two-fold axis and an $n-$fold axis implies the existence of $n-1$ additional two-fold axes separated by angles of π/n.

3. Any two of the following: an even-fold axis, a reflection plane perpendicular to it, and an inversion centre implies the existence of the other.

7.4 Enumeration of Point Groups

The point groups may be divided into two categories:

1. Simple rotation groups which have one symmetry axis of highest symmetry.

2. Higher symmetry groups which have no unique axis of highest symmetry, but which have more than one $n-$fold axis where $n > 2$.

It is convenient to visualise the point group operations by means of stereographic projections as shown in Figure 7.1. These are formed by projecting on to the XY plane a general point on a unit sphere which is subjected to the symmetry operations. The labels $+/\circ$ mean that the point is above/below the plane respectively. The n-fold rotation axes are indicated by the symbols at the centre of the circle. Solid radial lines indicate vertical reflection planes and dashed radial lines indicate rotation axes. Horizontal reflection planes are indicated by unit circles with solid lines rather than broken lines.

There are thirty two point groups and we list them in order of increasing complexity.

Simple rotation groups:

C_n • These are groups of rotations about $n-$fold axes. They are cyclic groups of order n. It can be shown that n can only be 1, 2, 3, 4, and 6. Other rotations are not consistent with translational symmetry. The groups are therefore C_1, C_2, C_3, C_4, and C_6.

Proof: If $\mathbf{t}$ is a translational vector and $\mathbf{t}' = R\mathbf{t}$, then the translational vector $\mathbf{t}' - \mathbf{t}$ must be perpendicular to the rotation axis. Let $\mathbf{s}$ be the shortest translational vector perpendicular to the axis of rotation. Apply-

ing C_n on $\mathbf{s}$ generates a new vector $\mathbf{s}'$ and we must have

$$|\mathbf{s}' - \mathbf{s}| = 2ssin\ \pi/n \geq s$$

since $\mathbf{s}$ is defined to be the smallest translational vector perpendicular to the axis of rotation. It follows immediately that $n \leq 6$ and geometrical consideration shows that $n = 5$ is not possible.

C_{nh} • These groups have a σ_h reflection plane in addition to the C_n axis. When n is even, the group includes the inversion element so that $C_{2nh} = C_{2n} \otimes I$. The groups are C_{1h}, $C_{2h} = C_2 \otimes I$, C_{3h}, $C_{4h} = C_4 \otimes I$, and $C_{6h} = C_6 \otimes I$.

C_{nv} • These groups have a σ_v reflection plane in addition to the C_n axis. According to rule 1 there must also be n reflection planes separated by an angle π/n around the C_n axis. C_{1v} is identical to C_{1h}. The groups are C_{2v}, C_{3v}, C_{4v}, and C_{6v}.

S_{2n} • These groups have an $2n$-fold axis for improper rotations and each has C_n as a subgroup. The groups are S_2, S_4, and $S_6 = C_3 \otimes I$.

D_n • These groups have n two-fold axes perpendicular to the C_n axis. The groups are D_2, D_3, D_4, D_6.

D_{nh} • Each of these groups has D_n as a subgroup and in addition it contains the horizontal reflection plane σ_h. Since σ_h commutes with rotations, $D_{nh} = D_n \otimes I$.

D_{nd} • Each of these groups has D_n as a subgroup and in addition it contains diagonal reflection planes σ_d bisecting the angles between the twofold axes perpendicular to the principal rotation axis. The groups are D_{2d} and D_{3d}.

Higher symmetry groups:

T • This group consists of 12 proper rotations that take a regular tetrahedron into itself. This is shown in Figure 7.2. The elements are E, 3 C_2's about the X, Y, and Z axes and 8 C_3's about the body diagonals which

consist of two classes, clockwise and anticlockwise rotations by $2\pi/3$.

T_d • This group has T as a subgroup and in addition it contains 6 diagonal reflection planes σ_d normal to a cube face and containing a tetrahedral edge such as ac or ab. The presence of 6 σ_d's implies the existence of 6 S_4's about the X, Y and Z axes. The total number of elements is 24.

T_h • This group has T as a subgroup and in addition it contains inversion so that $T_h = T \otimes I$.

O • This is one of the most important point groups, shown in Figures 7.3a and 7.3b. This group consists of 24 proper rotations that take an octahedron into itself. These are E, 8 C_3's about the body diagonals, 3 C_2's and 6 C_4's about the X, Y, and Z axes, and 6 C_2's about axes through thr origin parallel to face diagonals. All the C_3's are in the same class but the two kinds of C_2 operations form two distinct classes.

O_h • This group has O as a subgroup and in addition it contains inversion so that $O_h = O \otimes I$.

The following point groups are useful to know but they are not consistent with translational symmetry because they contain fivefold axes.

Y • This group consists of 60 proper rotations that take an icosahedron or a dodecahedron into itself. This is illustrated in Figures 7.4a and 7.4b.

Y_h • This group has Y as a subgroup and in addition it contains inversion so that $Y_h = Y \otimes I$.

We list also in Table 7.1 the classification of the 32 point groups according to the crystal systems to which they belong. The unit cell required for compatibility with the point-group symmtery is specified by three translations $\mathbf{a}$, $\mathbf{b}$, and $\mathbf{c}$ and three angles α, β, and γ as illustrated in Figure 7.5.

7.5 Improper Point Groups

The product of two improper elements is a proper element since an improper element has a determinant -1. It follows also that a product of a proper and an improper element is an improper element. Let G be an improper group. We may write

$$G = P + Q$$

wher P and Q contain proper and improper elements respectively. Let i be any improper element. Then from the rearrangement theorem we have

$$G = iP + iQ$$

and therefore $iP = Q$ and $iQ = P$ so that

$$G = P(1 + i)$$

If i commutes with all elements in the group, then

$$G = P \otimes I$$

where $I = (1, i)$. For example, i can be the inversion or horizontal reflection. If the inversion is not contained in the group, it is isomorphic with the proper group $G' = P + iQ$. This isomorphism can be seen by noting that iQ cannot overlap with P since i is not contained in G. Thus we associate the element iQ_k of G' with the element Q_k of G while P is common to both groups.

7.6 Double-Group Representations

We have seen that the half-integer representations of the rotation group R_3 are double-valued. Each rotation is represented by two distinct matrices. The half-integer representations arise for example when the basis functions are the spin functions $\chi_\sigma(m_s)$ which give the representation $D^{1/2}$.

Since point groups are subgroups of the rotations group, we also expect to have double-valued representations when the basis functions transform according to the half-integer representations, which are often the case in physical applications.

Consider a point group g consisiting of proper rotations and the corresponding group G of matrices taken from the representation $D^{1/2}$, say. G contains twice as many elements as g does and the group G is called the double group of g. The two groups G and g are homomorphic. To work out the character table of the double group, we can proceed as usual but the following rules simplify the procedure:

1. Let $T(R)$ and $T(\bar{R})$ be two matrices of G representing the same rotation R. $T(\bar{R}) = \bar{E}T(R)$ where $\bar{E}$ is minus a unit matrix representing a rotation by 2π and $\bar{E}^2 = E$ represents a rotation by 4π. Evidently, $\bar{E}$ commutes with all elements of the double group. The characters of $T(R)$ and $T(\bar{R})$ must therefore have opposite sign:

$$\chi(\bar{R}) = -\chi(R)$$

   except when R is a rotation by π, in which case $\chi(\bar{R}) = \chi(R) = 0$.

2. Neglecting for the moment the special case of rotation by π, it follows that if a set of rotations R form a class of g, then the matrices $T(R)$ and $T(\bar{R})$ form two classes of G, such that if $T(R)$ belongs to one than $T(\bar{R})$ belongs to the other.

3. If R is rotation by π, then $T(R)$ and $T(\bar{R})$ may or may not belong to the same class. They belong to the same class if and only if the axis of rotation is bilateral, i.e. there is an element that reverses the direction of the axis. This is because for bilateral axis, $R(\pm\theta)$ belong to the same class so that in the double group $R(\pi)$ and $R(-\pi) = R(3\pi)$, or $T(R)$ and $T(\bar{R})$, belong to the same class.

As an example, we consider the double group of D_3. The classes of D_3 are C_e, C_c, and C_d. The classes of the double group can be worked out by using the rules discussed above. $\bar{e}$ is in a class by itself because it commutes with all elements. There is no bilateral axis so that the character table is given by

	C_e	$\bar{C}_e$	$2C_c$	$2\bar{C}_c$	$3C_d$	$3\bar{C}_d$
T^1	1	1	1	1	1	1
T^2	1	1	1	1	-1	-1
T^3	2	2	-1	-1	0	0
T^4	1	-1	1	-1	i	$-i$
T^5	1	-1	1	-1	$-i$	i
T^6	2	-2	-1	1	0	0

The first three are the single-valued representations of D_3 and the last three are the new representations arising from the double group. The characters $\chi(\bar{C}_d)$ can be obtained by observing that $d_1^2 = \bar{e}$ so that $\chi^2(\bar{C}_d) = -1$ and therefore $\chi(\bar{C}_d) = \pm i$. The rest of the table can be filled in by using the orthogonality between the characters.

$\bar{E}$ commutes with all elements and $\bar{E}^2 = E$ so that $(E, \bar{E})$ form a subgroup. The double group, however, is not a direct product of this subgroup and the original group because from the point of view of the double group, the original group g is no longer a group.

As a simple example of physical applications of the double groups we consider an atom with three s-electrons. The product of three spin functions tranform according to the product representation $D^{1/2} \otimes D^{1/2} \otimes D^{1/2} = D^{3/2} \oplus 2D^{1/2}$. Let us suppose that we break the rotational symmetry by putting the atom in a potential with D_3 symmetry. The product functions transform according to the double group of D_3 and not according to the group D_3. The representations $D^{3/2}$ and $D^{1/2}$ may be reduced by using the usual formula $\chi = \sum_\gamma m_\gamma \chi^\gamma$ where γ labels the irreducible representations of the double group.

7.7 Space Group

The space group, which is the full symmetry of a crystal, contains translational-symmetry operators, rotational-symmetry operators from the point group, and the combinations of the two. The elements of the space group are conventionally represented by $\{R|\mathbf{t}\}$ meaning

$$\{R|\mathbf{t}\}\mathbf{r} = R\mathbf{r} + \mathbf{t} \tag{7.1}$$

The multiplication rule for the elements of the space group is

$$\begin{aligned}\{R|\mathbf{t}\}\{R'|\mathbf{t}'\}\mathbf{r} &= \{R|\mathbf{t}\}(R'\mathbf{r}+\mathbf{t}') \\ &= R(R'\mathbf{r}+\mathbf{t}')+\mathbf{t} \\ &= \{RR'|R\mathbf{t}'+\mathbf{t}\}\mathbf{r} \end{aligned} \tag{7.2}$$

If $\{R'|\mathbf{t}'\} = \{R|\mathbf{t}\}^{-1}$ then $\{RR'|R\mathbf{t}'+\mathbf{t}\} = \{E|\mathbf{0}\}$ so that

$$R' = R^{-1}, \quad \mathbf{t}' = -R^{-1}\mathbf{t} \tag{7.3}$$

Thus the inverse element is

$$\{R|\mathbf{t}\}^{-1} = \{R^{-1}|-R^{-1}\mathbf{t}\} \tag{7.4}$$

We have already shown in example 1 (3.14) that the eigenfunctions of a Hamiltonian with a lattice translational symmetry must obey Bloch theorem:

$$\psi_{\mathbf{k}}(\mathbf{r}+\mathbf{t}) = e^{i\mathbf{k}\cdot\mathbf{t}}\psi_{\mathbf{k}}(\mathbf{r}) \tag{7.5}$$

Functions having this property are called Bloch functions. This means that we can write

$$\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \tag{7.6}$$

where $u_{\mathbf{k}}$ is periodic, i.e.

$$u_{\mathbf{k}}(\mathbf{r}+\mathbf{t}) = u_{\mathbf{k}}(\mathbf{r})$$

We consider here only simple space groups (symmorphic). By this we mean that all the point group elements are members of the space group or in other words, the point group is a subgroup of the space group. This is not true in general.

The form of the Bloch functions explicitly takes into account the lattice translational symmetry. Now we consider the effects of the point group operations on these functions.

$$\begin{aligned}\hat{T}(R)\psi_{\mathbf{k}}(\mathbf{r}) &= \hat{T}(R)u_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \\ &= u_{\mathbf{k}}(R^{-1}\mathbf{r})e^{i\mathbf{k}\cdot R^{-1}\mathbf{r}} \\ &= u_{\mathbf{k}}(R^{-1}\mathbf{r})e^{iR\mathbf{k}\cdot\mathbf{r}} \end{aligned} \tag{7.7}$$

The function $u_{\mathbf{k}}(R^{-1}\mathbf{r})$ is also periodic because

$$u_{\mathbf{k}}(R^{-1}(\mathbf{r}+\mathbf{t})) = u_{\mathbf{k}}(R^{-1}\mathbf{r}+\mathbf{t}') = u_{\mathbf{k}}(R^{-1}\mathbf{r})$$

where $\mathbf{t}' = R^{-1}\mathbf{t}$ is just another translational vector.

If we apply all the point-group operations on a wave vector $\mathbf{k}$ we obtain what is called the star of $\mathbf{k}$. If $\mathbf{k}$ lies on a symmetry point, some of the operations will take $\mathbf{k}$ into itself. These operations that take $\mathbf{k}$ into itself clearly form a subgroup because $R_1R_2\mathbf{k} = R_3\mathbf{k} = \mathbf{k}$ where $R_1R_2 = R_3$. This subgroup is called the group of the wave vector. Under the operations of this group, we have

$$\hat{T}(R)\psi_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(R^{-1}\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}} \tag{7.8}$$

Thus we see that $\{u_{\mathbf{k}}(R^{-1}\mathbf{r})$ transform among themselves under the group of $\mathbf{k}$ according to an irreducible representation of the group which is called the small representation.

The eigenfunctions of the Hamiltonian of a crystal are then specified by two quantities: the $\mathbf{k}$ vector (Bloch theorem) and the irreducible representation of the group of $\mathbf{k}$.

Formally, we have (in atomic units $\hbar = m = e = 1$)

$$\left[-\frac{1}{2}\nabla^2 + V(\mathbf{r})\right]\Psi_{\mathbf{k}} = E_{\mathbf{k}}\Psi_{\mathbf{k}} \tag{7.9}$$

Using the Bloch form, we get

$$-\frac{1}{2}\left[\nabla^2 + 2i\mathbf{k}\cdot\nabla - k^2\right]u_{\mathbf{k}} = E_{\mathbf{k}}u_{\mathbf{k}} \tag{7.10}$$

which may be rewritten

$$\left[-\frac{1}{2}\nabla^2 + V(\mathbf{r}) + \mathbf{k}\cdot\mathbf{p}\right]u_{\mathbf{k}} = E'_{\mathbf{k}}u_{\mathbf{k}} \tag{7.11}$$

where $E' = E - k^2/2$. This equation shows the significance of the group of $\mathbf{k}$. We can think of the last term as a perturbation which breaks the symmetry of the lattice potential $V(\mathbf{r})$.

Consider first the case of $\mathbf{k} = 0$. Then $u_{\mathbf{k}}$ will transform according to an irreducible representation of the full point group. The degeneracy at this

point is given by the dimension of the irreducible representation as usual. Let us now consider the case $\mathbf{k} \neq 0$ with the corresponding $\mathbf{k}$ vector group which is a subgroup of the full point group. In this case, the degenerate states at $\mathbf{k} = 0$ still form an invariant subspace for the subgroup but they are in general reducible. We expect that the degeneracy will be split. In this way we can figure out the degeneracies at any $\mathbf{k}$ point. As a simple example, consider a two dimensional crystal with a square primitive lattice. The reciprocal space is also a square. Let us assume that the point group is D_4. If we take a point along the x-axis, then the $\mathbf{k}$ vector group is (e, a_x) (using the same notation as in the exercise). This is an Abelian group and the irreducible representations are one dimensional. Thus the states at this point cannot be degenerate. If we consider the point $\mathbf{k} = 0$, we might have states which are doubly degenerate because there is a two dimensional irreducible representation of D_4. Along the x-axis, these degenerate states will in general be split.

Chapter 8

The Group SU_3

8.1 Infinitesimal Operators and Lie Algebra

The group SU_3 is an extension of the group SU_2. We derive the Lie algebra from a physical point of view by considering three states which may be associated with the proton, neutron and lambda particle states:

$$|p\rangle = c_p^+|0\rangle, \quad |n\rangle = c_n^+|0\rangle, \quad |\Lambda\rangle = c_\Lambda^+|0\rangle$$

The bilinear products of annihilation and creation operators that conserve particle number are:

$$\begin{array}{lll} c_p^+c_p, & c_n^+c_n, & c_\Lambda^+c_\Lambda, \\ c_p^+c_n, & c_n^+c_\Lambda, & c_\Lambda^+c_p, \\ c_p^+c_\Lambda, & c_n^+c_p, & c_\Lambda^+c_n \end{array}$$

These operators form a Lie algebra. We define a new set of infinitesimal operators as follows:

$$\begin{aligned} \hat{B} &= c_p^+c_p + c_n^+c_n + c_\Lambda^+c_\Lambda, \\ \hat{T}_z &= \frac{1}{2}(c_p^+c_p - c_n^+c_n), \\ \hat{Y} &= \frac{1}{3}(c_p^+c_p + c_n^+c_n - 2c_\Lambda^+c_\Lambda), \end{aligned}$$

$$\hat{T}_+ = c_p^+ c_n, \quad \hat{U}_+ = c_n^+ c_\Lambda, \quad \hat{V}_+ = c_\Lambda^+ c_p,$$
$$\hat{T}_- = c_n^+ c_p, \quad \hat{U}_- = c_\Lambda^+ c_n, \quad \hat{V}_- = c_p^+ c_\Lambda$$

We could have chosen

$$\hat{U}_z = \frac{1}{2}(c_n^+ c_n - c_\Lambda^+ c_\Lambda) = \frac{3}{4}\hat{Y} - \frac{1}{2}\hat{T}_z \tag{8.1}$$

or

$$\hat{V}_z = \frac{1}{2}(c_\Lambda^+ c_\Lambda - c_p^+ c_p) = -\frac{3}{4}\hat{Y} - \frac{1}{2}\hat{T}_z \tag{8.2}$$

instead of $\hat{T}_z$. The operator $\hat{B}$ commutes with all other operators and it may be interpreted as the (baryon) number operator. The rest of the operators form a Lie algebra by themselves and there are at most two operators that mutually commute, $\hat{T}_z$ and $\hat{Y}$, so that the corresponding Lie group is of rank 2. The other operators $\hat{T}_\pm$, $\hat{U}_\pm$, and $\hat{V}_\pm$ are the ladder operators, as the notation already suggests. Thus the desired Lie algebra is

$$\left[\hat{T}_z, \hat{Y}\right] = 0 \tag{8.3}$$
$$\left[\hat{T}_z, \hat{J}_\pm\right] = \pm\frac{1}{2}(3\delta_{JT} - 1)\hat{J}_\pm \tag{8.4}$$
$$\left[\hat{Y}, \hat{J}_\pm\right] = \pm(\delta_{JU} - \delta_{JV})\hat{J}_\pm \tag{8.5}$$

where $J = T, U, V$. The Lie algebras for U and V can be obtained from Eqs. (8.1), (8.2), (8.3), (8.4) and (8.5). In additions, we have commutation relations among the ladder operators which are useful for generating the multiplets:

$$\left[\hat{J}_\pm, \hat{J}'_\mp\right] = 2\delta_{JJ'}\hat{J}_z \tag{8.6}$$
$$\left[\hat{T}_\pm, \hat{U}_\pm\right] = \pm\hat{V}_\mp \quad \textit{and cyclic permutations} \tag{8.7}$$

We observe also that

$$[\hat{J}_z, \hat{J}_\pm] = \pm\hat{J}_\pm, \quad [\hat{J}_+, \hat{J}_-] = 2\hat{J}_z \tag{8.8}$$

which is the Lie algebra of SU_2.

The representation of the infinitesimal operators in the three dimensional space of $|p\rangle$, $|n\rangle$, and $|\Lambda\rangle$ is given by

$$T_z = \begin{pmatrix} \frac{1}{2} & 0 & 0 \\ 0 & -\frac{1}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad Y = \begin{pmatrix} \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & 0 \\ 0 & 0 & -\frac{2}{3} \end{pmatrix}$$

$$T_+ = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad T_- = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$U_+ = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \quad U_- = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

$$V_+ = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \quad V_- = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

These are in fact the generators of the group SU_3.

8.2 Subgroups

Knowledge of the subgroups is useful for working out the multiplet structure. Eq. (8.8) shows that there are three SU_2 subgroups. $\hat{Y}$ is a generator of an Abelian group as indicated by the diagonal form of Y, just like $\hat{T}_z$ is a generator of an Abelian group R_2. The generators $(\hat{Y}, \hat{T}_z, \hat{T}_\pm)$ form a direct product group $SU_2 \otimes U_1$ since $\hat{Y}$ commutes with $\hat{T}_z$ and $\hat{T}_\pm$. The Abelian group U_1 can be shown to be isomorphic with the group R_2. There are other subgroups but they are not important for the purpose of working out the multiplet structure.

8.3 Multiplet Structure

There are two mutually commuting operators, $\hat{T}_z$ and $\hat{Y}$, so that a multiplet may be labelled by two numbers related to the eigenvalues of two Casimir operators. Each state in a multiplet may be labelled by the eigenvalues of $\hat{T}_z$ and $\hat{Y}$. However, due to the presence of SU_2 subgroups, the states

may be degenerate and additional labels are required to distinguish these degenerate states. Thus the states in a given multiplet can be written as

$$\psi(M_T, Y, \alpha)$$

where M_T and Y are the eigenvalues of $\hat{T}_z$ and $\hat{Y}$ respectively and α is a set of additional labels required to distinguish states with the same M_T and Y. Since $\hat{Y}$ corresponds to an Abelian group, its representation is one dimensional and uniquely labelled by Y. The label M_T on the other hand may arise from several different values of T. To label each state uniquely, we may then choose $\alpha = T$.

From Eq. (8.8), the operators $(\hat{T}_z, \hat{T}_+, \hat{T}_-)$ are the infinitesimal operators of the group SU_2 and therefore M_T takes the values $M_T = 0, \pm 1/2, \pm 1, \ldots$. Similarly for $(\hat{U}_z, \hat{U}_+, \hat{U}_-)$ and $(\hat{V}_z, \hat{V}_+, \hat{V}_-)$. It follows from Eq. (8.1) or (8.2) that the eigenvalues of $\hat{Y}$ are $Y = 0, \pm 1/3, \pm 2/3, \pm 1, \ldots$. Each state in a given multiplet may then be represented by a point in (M_T, Y)-plane as illustrated in Fig. (8.1), keeping in mind that each point may represent more than one state. Each state is not only an eigenstate of $\hat{T}_z$ and $\hat{Y}$ but it is also an eigenstate of $\hat{U}_z$ and $\hat{V}_z$ as follows from Eqs. (8.1) and (8.2) but $\hat{T}_z$, $\hat{U}_z$, and $\hat{V}_z$ are interrelated so that one of them determines the other two.

The ladder operators may be conveniently represented by arrows as shown in Fig. (8.2). For example, Eqs. (8.4) and (8.5) tell us that

$$\hat{V}_- \; \psi(M_T, Y, T) = \sum_{T'} c(T') \; \psi(M_T + \frac{1}{2}, Y + 1, T')$$

To generate a multiplet, we use the same procedure as in the case of the rotation group. We start from a state ψ with the highest value of Y and for this Y the highest value of M_T. Or alternatively, we could start from the highest value of M_T and for this M_T the highest value of Y. The first alternative implies:

$$\hat{T}_+ \psi = \hat{U}_+ \psi = \hat{V}_- \psi = 0$$

Although $\hat{U}_-$ increases M_T, $\hat{U}_- \psi$ is not necessarily zero because $\hat{U}_-$ lowers the value of Y. The above equations imply that ψ is an eigenfunction of $\hat{T}^2$, $\hat{U}^2$, and $\hat{V}^2$ which may be verified by operating $\hat{T}^2 = \hat{T}_- \hat{T}_+ + \hat{T}_z^2 + \hat{T}_z$

on ψ, and similarly for $\hat{U}^2$ and $\hat{V}^2$. In other words it has definite T, U, and V. Conventionally, ψ is labelled by two numbers $\lambda = 2T$ and $\mu = 2U$, which implies from Eqs. (8.1) and (8.2) that $\lambda + \mu = 2V$. Or

$$T = \frac{1}{2}\lambda, \quad U = \frac{1}{2}\mu, \quad V = \frac{1}{2}(\lambda + \mu) \tag{8.9}$$

The two numbers λ and μ may also be used to label the multiplet: $D^{\lambda\mu}$. The state ψ has the following values of M_T and Y:

$$M_T = \frac{1}{2}\lambda, \quad Y = \frac{1}{3}(\lambda + 2\mu)$$

and let us denote the state by the point $A = [\frac{1}{2}\lambda, \frac{1}{3}(\lambda + 2\mu)]$ as shown in the Fig. (8.3). The steps to generate the multiplet is as follows:

1. We apply $\hat{T}_-$ repeatedly on $\psi(A)$ until we reach point F at which $\hat{T}_-\psi(F) = 0$. The coordinate of point F is $F = [-\frac{1}{2}\lambda, \frac{1}{3}(\lambda + 2\mu)]$

2. We apply $\hat{U}_-$ repeatedly on $\psi(A)$ until we reach point B at which $\hat{U}_-\psi(B) = 0$. To figure out the coordinate of point B, we observe that $\hat{U}_-$ increases M_T by $1/2$ and decreases Y by 1 and $\hat{U}_-$ has been applied μ times from A to B. Thus $B = [\frac{1}{2}(\lambda+\mu), \frac{1}{3}(\lambda-\mu)]$. There cannot be states to the right of AB because from Eq. (8.6) we have $\hat{T}_+\hat{U}_-^n\psi = \hat{V}_-\hat{U}_-^n\psi = 0$ Thus the states along AB still have definite but different values of T and V and the same value of U.

3. The states along BC can be obtained by applying $\hat{V}_+$ repeatedly on $\psi(B)$ or we can argue from symmetry that the states must be symmetrical about the diagonal bisecting AB. The rest of the hexagon can be obtained by symmetry about the diagonal bisecting BC. We have shown that the states in a given multiplet must lie on or inside a hexagon. In general, it can also be a triangle which is the case when $\lambda = 0$ or $\mu = 0$. States on the outermost hexagon are unique and they have definite T, U, and V.

4. We can now generate states inside the hexagon and there may be more than one independent state at each point. Consider the state

labelled by point G. There are three basic ways of reaching point G from A which generate the states:

$$\phi_1 = \hat{T}_-\hat{U}_-\psi \quad \phi_2 = \hat{U}_-\hat{T}_-\psi \quad \phi_3 = \hat{V}_+\psi,$$

The states ϕ_1 and ϕ_2 are linearly independent since $\hat{T}_-$ and $\hat{U}_-$ do not commute but ϕ_3 is not independent of the other two because

$$[\hat{T}_-, \hat{U}_-]\psi = -\hat{V}_+\psi \rightarrow \phi_1 - \phi_2 = -\phi_3$$

The state ϕ_1 has a definite $T = \frac{1}{2}(\lambda + 1)$ and it is possible to form a linear combination of ϕ_2 and ϕ_3 so that it has a definite T:

$$\begin{aligned} \hat{T}_+(\phi_2 + c\phi_3) &= \hat{T}_+\hat{U}_-\hat{T}_-\psi + c\hat{T}_+\hat{V}_+\psi \\ &= \hat{U}_-\hat{T}_+\hat{T}_-\psi + c(\hat{V}_+\hat{T}_+ - \hat{U}_-)\psi \\ &= \hat{U}_-(\hat{T}_-\hat{T}_+ + 2\hat{T}_z)\psi - c\hat{U}_-\psi \\ &= (\lambda - c)\hat{U}_-\psi \end{aligned}$$

using the fact that $\hat{T}_+\psi = 0$. By choosing $c = \lambda$ the linear combination $\tilde{\phi}_2 = \phi_2 + \lambda\phi_3$ has a definite $T = \frac{1}{2}(\lambda - 1)$ since $\hat{T}_+\tilde{\phi}_2 = 0$ and $\hat{T}_z\tilde{\phi}_2 = \frac{1}{2}(\lambda - 1)\tilde{\phi}_2$. It is of course possible to choose the states to have definite U or V. Applying $\hat{T}_-$ on $\psi(G)$ generate two sets of states parallel to AF. Continuing along the same fashion, it is not difficult to show that the next line parallel to AF consists of three sets of states with $T = \frac{1}{2}(\lambda - 2),\ \frac{1}{2}\lambda,\ \frac{1}{2}(\lambda + 2)$. For example, the state $\hat{U}_-^2\psi$ has $T = \frac{1}{2}(\lambda + 2)$ while the state $\hat{U}_-\tilde{\phi}_2$ has $T = \frac{1}{2}\lambda$ since $\hat{T}_+\hat{U}_-\tilde{\phi}_2 = \hat{U}_-\hat{T}_+\tilde{\phi}_2 = 0$. The third state may be formed by a similar linear combination as the one described above.

The multiplet structure consists of hexagons of decreasing size with the degeneracy increased by one as we move inside. Eventually we may arrive at a triangle instead of a hexagon at which stage the degeneracy remains constant as we move further. The reason is that with a triangle we cannot generate an new state such as $\tilde{\phi}_2$. This implies that when $\lambda = 0$ or $\mu = 0$ each point corresponds to one state because we start with a triangle and no extra states are generated as we move inside. This is illustrated by the representation D^{30} in

Fig. (8.4) where the point O can be reached from A by $\hat{V}_+\hat{T}_-\psi(A)$ or $\hat{T}_-\hat{V}_+\psi(A)$ but $[\hat{V}_+, \hat{T}_-] = 0$ so that the two paths are equivalent.

The multiplet structure also allows us to work out the dimension of the irreducible representation. Thus the outermost hexagon contributes $3(\lambda + \mu)$ states and the next one inside contributes $2 \times 3(\lambda + \mu - 2)$ states and so on taking care of the special case of a triangle. The general formula is given by

$$d(\lambda, \mu) = \frac{1}{2}(\lambda + 1)(\mu + 1)(\lambda + \mu + 2) \tag{8.10}$$

which is symmteric with respect to interchange of λ and μ. Given a representation $D^{\lambda\mu}$ it is straightforward to map the states in the $(M_T, Y)-$plane. Starting from the point $A = [\frac{1}{2}\lambda, \frac{1}{3}(\lambda + 2\mu)]$, we form the line AF by moving λ steps along $\hat{T}_-$ and μ steps along $\hat{U}_-$. The rest of the hexagon and the inner hexagons can be formed from the rules discussed above.

8.4 Example

As an example, let us construct explicitly the multiplet D^{21} as shown in Fig. (8.5). We start with the state

$$\psi(A) = \psi(1, \frac{4}{3}, 1)$$

which has definite values of $T = 1$, $U = \frac{1}{2}$, and $V = \frac{3}{2}$. Applying $\hat{T}_-$ twice generates

$$\psi(0, \frac{4}{3}, 1), \quad \psi(-1, \frac{4}{3}, 1)$$

Applying $\hat{U}_-$ on $\psi(A)$ gives

$$\psi(B) = \psi(\frac{3}{2}, \frac{1}{3}, \frac{3}{2})$$

The $T = \frac{3}{2}$ multiplet is generated by repeated applications of $\hat{T}_-$ on $\psi(B)$. The $T = \frac{1}{2}$ multiplet is generated from the linear combination

$$\psi(\frac{1}{2}, \frac{1}{3}, \frac{1}{2}) = c(\hat{U}_-\hat{T}_- + 2\hat{V}_+)\psi(A)$$

The normalisation constant is obtained by requiring

$$|c|^2 \left((\hat{U}_-\hat{T}_- + 2\hat{V}_+)\psi(A),\ (\hat{U}_-\hat{T}_- + 2\hat{V}_+)\psi(A)\right) = 1$$

We have

$$\begin{aligned}
(\hat{U}_-\hat{T}_-\psi(A),\ \hat{U}_-\hat{T}_-\psi(A)) &= (\psi(A),\ \hat{T}_+\hat{U}_+\hat{U}_-\hat{T}_-\psi(A)) \\
&= (\psi(A),\ \hat{T}_+(\hat{U}_-\hat{U}_+ + 2\hat{U}_z)\hat{T}_-\psi(A)) \\
&= 2(\psi(A),\ \hat{T}_+(\hat{T}_-\hat{U}_z + \frac{1}{2}\hat{T}_-\psi(A)) \\
&= 2(\psi(A),\ \hat{T}_+\hat{T}_-\psi(A)) \\
&= 4
\end{aligned}$$

$$\begin{aligned}
(\hat{U}_-\hat{T}_-\psi(A),\ \hat{V}_+\psi(A)) &= (\psi(A),\ \hat{T}_+\hat{U}_+\hat{V}_+\psi(A)) \\
&= (\psi(A),\ \hat{T}_+(\hat{V}_+\hat{U}_+ + \hat{T}_-\psi(A)) \\
&= 2
\end{aligned}$$

$$(\hat{V}_+\psi(A),\ \hat{V}_+\psi(A)) = 3$$

Thus the normalisation constant is given by $c = 1/\sqrt{24}$. The states at C are given by

$$\psi(0, -\frac{2}{3}, 1) = c_1\hat{T}_-\hat{V}_+\psi(B), \quad \psi(0, -\frac{2}{3}, 0) = c_2\hat{U}_-\psi(\frac{1}{2}, \frac{1}{3}, \frac{1}{2})$$

The normalisation constants can be calculated in the same way as above.

8.5 Product Representations

In physical applications such as analysing the possible final states in a collision between two particles, we have to decompose product representations:

$$D^{\lambda_1\mu_1} \otimes D^{\lambda_2\mu_2} = \sum_{\lambda\mu} \oplus\, m_{\lambda\mu} D^{\lambda\mu} \tag{8.11}$$

The general formula for the coefficients $m_{\lambda\mu}$ is complicated but it possible to obtain them directly by the method of reduction. We illustrate this

method by considering the product $D^{11} \otimes D^{11}$. First we list all possible T and Y multiplets contained in D^{11} and label them by (T, Y):

$$D^{11} = (\frac{1}{2}, 1) \oplus (1, 0) \oplus (0, 0) \oplus (\frac{1}{2}, -1)$$

We form products of (T, Y)

$$(T_1, Y_1) \otimes (T_2, Y_2) = \sum_{T=|T_1-T_2|}^{T_1+T_2} \oplus (T, Y_1 + Y_2)$$

To determine T we have used the usual vector coupling theorem and to determine Y we note that it represents an Abelian group so that the representation is of the form $exp(icY)$ and therefore the product of two representations Y_1 and Y_2 is $exp[ic(Y_1 + Y_2)]$. Forming all products and substracting all possible representations contained in the product representation we have:

	$Y =$	2	1	0	-1	-2
$D^{11} \otimes D^{11}$	$T =$	$1, 0$	$2(\frac{3}{2}), 4(\frac{1}{2})$	$2, 5(1), 4(0)$	$2(\frac{3}{2}), 4(\frac{1}{2})$	$1, 0$
D^{22}	$T =$	1	$\frac{3}{2}, \frac{1}{2}$	$2, 1, 0$	$\frac{3}{2}, \frac{1}{2}$	1
	$T =$	0	$\frac{3}{2}, 3(\frac{1}{2})$	$4(1), 3(0)$	$\frac{3}{2}, 3(\frac{1}{2})$	0
D^{03}	$T =$	0	$\frac{1}{2}$	1	$\frac{3}{2}$	
	$T =$		$\frac{3}{2}, 2(\frac{1}{2})$	$3(1), 3(0)$	$3(\frac{1}{2})$	0
D^{30}	$T =$		$\frac{3}{2}$	1	$\frac{1}{2}$	0
	$T =$		$2(\frac{1}{2})$	$2(1), 3(0)$	$2(\frac{1}{2})$	
$2D^{11}$	$T =$		$2(\frac{1}{2})$	$2(1), 2(0)$	$2(\frac{1}{2})$	
	$T =$			0		
D^{00}	$T =$			0		

The first row is a list of all possible Y that arise from the product representation. The second row is a list of all possible T and the number preceeding each bracket is the number of times the T multiplets arise for a given Y. The product $D^{11} \otimes D^{11}$ must contain a representation with $T = 1, Y = 2$ which is the representation D^{22}. We substract the T values of D^{22} listed in the third row from the product representation which yields the fourth row. Following the same argument, there must be a representation with $T = 0, Y = 2$ which is the representation D^{03}. We substract

the T values of D^{03} from the remaining T's and continue along the same fashion. Thus we conclude finally

$$D^{11} \otimes D^{11} = D^{22} \oplus D^{03} \oplus D^{30} \oplus 2D^{11} \oplus D^{00}$$

8.6 SU_3 Multiplets and Hadrons

Hadrons are strongly interacting particles with decay time $< 10^{-8}$ sec, except proton and neutron. By strong we mean that the energy involved in a reaction is of the order of MeV or greater. Apart from, mass, spin, charge, and parity, hadrons may be assigned the following intrinsic quantities:

1. Isospin T: Among an isospin multiplet, hadrons have (almost) the same masses. For example, proton and neutrons which correspond to $T = 1/2$ or the three π-particles which correspond to $T = 1$. Strong interactions are found to be invariant under isospin tranformation, i.e. states in a given isospin multiplets transform among themselves under isospin transformation such as transformation among (p, n) or (π^+, π^-, π^0) (c.f. angular momentum states).

2. Hypercharge Y: The quantity Y in the group SU_3 is related to the charge and the z-component of isospin by

   $$Y = 2(Q - M_T)$$

   This relation is a physical interpretation which does not follow from group theory. It is known experimentally that the hypercharge is conserved in strong interaction. Hadrons can be divided into baryons with half-integer spins and mesons with integer spins, the former are heavier than the latter.

3. Baryon number B: It is conserved in all reactions, including weak ones. The assignment of baryon number if as follows: $B = +1$ for baryons, $B = -1$ for anti-baryons, and $B = 0$ for mesons.

With the above assignments of intrinsic quantities, hadrons can be beautifully classified according to SU_3 multiplets. Fig. (8.6) (figure 11.8 of Elliot and Dawber) shows some of these classifications. The corresponding

particles are listed in Table (8.1) (from table 11.1 of Elliot and Dawber). The representation D^{11} and D^{30} consist of baryons with spin $1/2$ and $3/2$ respectively while the other D^{11} representation corresponds to the mesons. Particles with short life-time, which arise as resonances in collisions, may often be regarded as excited states of the more stable ones.

It has been suggested that baryons are composed of three more fundamental spin $1/2$ particles known as quarks which are labelled by u, d, and s. These three quarks are supposed to correspond to the representation D^{10} so that

$$\begin{aligned} u &\rightarrow T = \frac{1}{2}, \quad M_T = +\frac{1}{2}, \quad Y = +\frac{1}{3}, \quad Q = +\frac{2}{3} \\ d &\rightarrow T = \frac{1}{2}, \quad M_T = -\frac{1}{2}, \quad Y = +\frac{1}{3}, \quad Q = -\frac{1}{3} \\ s &\rightarrow T = 0, \quad M_T = \ 0, \quad\ Y = -\frac{2}{3}, \quad Q = -\frac{1}{3} \end{aligned}$$

Since the largest spin is $S = 3/2$, it is then proposed that the baryons can be constructed from the triple product

$$D^{10} \otimes D^{10} \otimes D^{10} = D^{30} \oplus 2D^{11} \oplus D^{00}$$

A more complicated model involving nine quarks has also been proposed which introduces, apart from spin, additional intrinsic properties known as colours.

8.7 Casimir Operators

We have not made any explicit use of the Casimir operators in working out the structure of the multiplets. To construct the second order Casimir operator, it is possible to use the general formula derived before and a similar formula for higher order Casimir operators can also be derived although they become more complicated. For the group SU_3 there is a simple way of working out the Casimir operators which is based on the observation that the infinitesimal operators may be written in terms of the matrices defined by:

$$(A_i^j)_{kl} = \delta_{ik}\delta_{jl} - \frac{1}{3}\delta_{ij}\delta_{kl} \tag{8.12}$$

We have

$$T_z = (A_1^1 - A_2^2)/2, \quad Y = -A_3^3, \quad T_+ = A_1^2, \quad T_- = A_2^1$$

$$U_+ = A_2^3, \quad U_- = A_3^2, \quad V_+ = A_3^1, \quad V_- = A_1^3$$

The commutation relations for the A_i^j are

$$[A_i^j, A_k^l] = \delta_{jk} A_i^l - \delta_{il} A_k^j$$

It is then easy to show that the operators

$$C_2 = \sum_{ij} A_i^j A_j^i, \qquad C_3 = \sum_{ijk} A_j^k A_i^j A_k^i$$

commute with all of the infinitesimal operators. Instead of C_3 it is more convenient to define

$$C_3' = C_3 + \frac{3}{2} C_2$$

so that

$$\begin{aligned} \hat{C}_2 \psi &= \left[\frac{2}{3}(\lambda^2 + \mu^2 + \lambda\mu) + 2(\lambda + \mu) \right] \psi \\ \hat{C}_3' \psi &= \frac{1}{9}(\lambda - \mu)(2\lambda + \mu + 3)(2\mu + \lambda + 3)\, \psi \end{aligned}$$

which may be easily verified by using the Lie algebra.