Group Theory in Solid State Physics I

Preface

This lecture introduces group theoretical concepts and methods with the aim of showing how to use them for solving problems in atomic, molecular and solid state physics. Both finite and continuos groups will be discussed in this lectures. Finite groups are important because the symmetry elements in molecular and solid state physics consist of discrete rotations and translations. Continuos groups are crucial in problems containing the spin. The relevant literature for the topics presented in this lectures is:
L.D. Landau, E.M. Lifshitz, Lehrbuch der Theor. Pyhsik, Band III, "Quantenmechanik", Akademie-Verlag Berlin, 1979, Kap. XII and Band V, "Statistische Physik", Teil 1, Akademie-Verlag 1987, Kap. XIII.

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Contents

Chapter 1

Groups

A set G of elements $g_1, g_2...$ is said to form a group if

1. a law of composition (or multiplication) $\circ$ of two elements g_1 and g_2 is defined, so that $g_1 \circ g_2 \in G$
2. a identity element e exists such that $e \circ g = g \circ e = g$
3. the associative law is fullfiled, i.e. $g_1 \circ (g_2 \circ g_3) = (g_1 \circ g_2) \circ g_3$
4. there exists an inverse element g^{-1}such that $g \circ g^{-1} = g^{-1} \circ g = e$

In general, changing the order of multiplication produces a different result. A group for which $g_1 \circ g_2 = g_2 \circ g_1$ is said to be a commutative or Abelian group. The number of elements in a group might be finite, in which case it is denoted by h and called the order of the group. It might also be infinite, in which case the group is called an infinite group. A special class of groups are transformation groups. We consider a set M containing, as elements, objects $x, y, ..$ such as e.g. vectors and numbers. A **transformation** g is a one-to one map from M to M, i.e

$$g : x \longrightarrow a(x) \in M, \forall x \in M$$

Of particular importance in physics are a such transformations which transform a physical body into itself: such a transformation is called **symmetry transformations**.
Theorem: The set G of all symmetry transformations form a group. The group is called the symmetry group of the system.
Proof.
First, we define a composition law $\circ$ consisting of performing two symmetry transformations of the system successively: by convention, $b \circ a$ means that

a is performed first, followed by b. The result of performing two symmetry transformations successively is to transform the system into itself: i.e.

- a and b are symmetry operations, $b \circ a$ is also a symmetry operation

This means that the set G is closed under the law of successive transformations. We can also define an identity transformation e which leaves the system invariant:

- e belongs obviously to G

Given a symmetry transformation a we see that there exists an inverse transformation a^{-1} which transform back the system into itself:

- a^{-1} also belongs to G

Finally, successive symmetry transformations of the system obeys the associative laws, i.e

- $a \circ (b \circ c) = (a \circ b) \circ c$

QED

Exercise. Show that the following sets are groups

- the set consisting of $(1, -1)$
- the set complex numbers $(1, i, -1, -i)$
- the set of all integers $\mathcal{Z} = (..., -2, -1, 0, 1, 2, ...)$ with the addition as law of composition and the set of rational numbers $\mathcal{Q}$ under ordinary multiplication (but not $\mathcal{N} = 1, 2, 3, ...$)
- the set of real numbers $\mathcal{R}$ under addition or under multiplication (if zero is excluded)
- the set of all matrices of order $m \times n$ under addition

Symmetry transformations can be divided into three types:

1. Rotations by a certain angle about some axis and reflections at a certain plane
2. translations by some vector and
3. combination of the type 1. and type 2. transformations.

Type 2 and 3 exist only in an infinite body: a physical system with finite dimensions (a molecule, for instance) can only have symmetry transformations which leave at least one point of the body undisplaced in position. Type 1. transformations are symmetry transformations of a finite body provided they all have a point of intersection: rotating one body around two non-intersecting axes or reflecting at two non-intersecting planes leads to a translation of the finite body, which is not transformed into itself. When a group of transformations of a certain system consists of operations which leaves one point of the system undisplaced, it is called a **point group**. Symmetry groups containing translations are **space groups**. In the following, we use the Schönflies notation to label the symmetry transformations. When a body is transformed into itself by a rotation about a given axis by an angle $\frac{2\pi}{n}$ $(n = 1, 2, 3, ...)$, the axis is an n-fold rotation axis. The value $n = 1$ corresponds to a rotation by 2π (or equivalently, 0): the corresponding operation is the identity transformation and is usually denoted by e. The rotation with $n \neq 0$ are denoted by C_n. Its integral power will be denoted by C_n^k: this operation represents k successive operations of C_n on the system or a rotation by $\frac{2\pi k}{n}$. Evidently, $C_n^k = C_{n/k}$, if n is a multiple of k and $C_n^n = E$.
When a body transforms into itself by reflection at a plane, the plane is said to be a symmetry plane. Reflections are denoted by σ. An important property is that $\sigma^2 = e$. A reflection at a plane perpendicular to a certain rotational axis will be denoted by σ_h (the subscript h means horizontal). Reflections at planes containing the rotational axis are indicated by σ_v (v stands for 'vertical'). A body may transform into itself by the combination of a rotation and a reflection: this operation is a so called improper rotation and is denoted by S_n. S_n fulfills the equation $S_n = C_n\sigma_h = \sigma_h C_n$. The special case S_2,

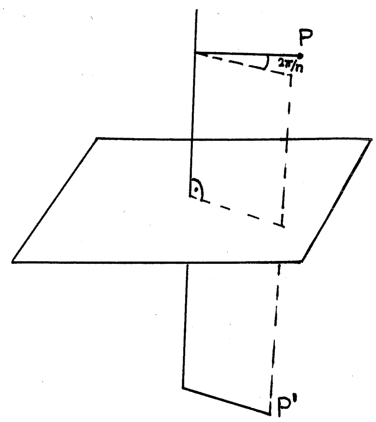

Figure 1.1:

corresponding to a rotation by π and a reflection to a plane perpendicular to the rotation axis, is an inversion, denoted by I: each point P is mapped into a point P_t (the index t means 'transformed') lying on the straight line passing through P and O (O being the intersection of the rotation axis with the symmetry plane). The distance PO is the same as the distance P_tO. If a body is symmetric with respect to $S_2 = C_2\sigma_h = I$, we speak of O as its inversion center. A rotation followed by a reflection or the inversion is called an improper rotation, to be compared with a proper rotation, which does not contain reflections.
Example 1: the symmetry group of a square. Suppose to have identical atoms arranged on the corners of a square, label each atom with a number $1, 2, 3, 4$ and think of all possible symmetry operation of the square, i.e. such operation which move the atoms from one corner to another without changing the position of the corners (and of the boundaries). It can be readily

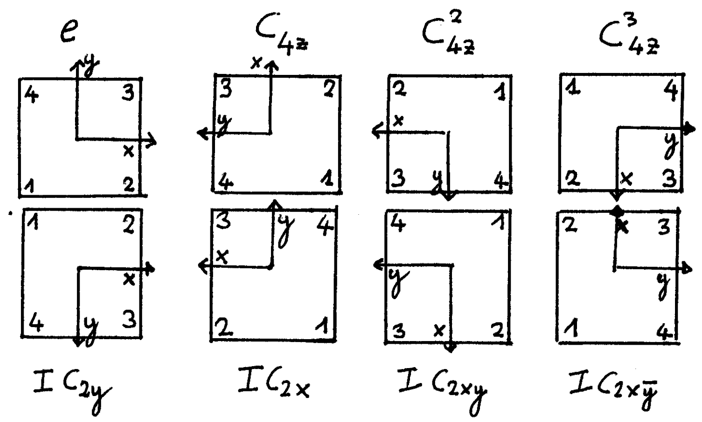

Figure 1.2:

verified that the set of eight transformations listed in the figure is a group and that it is the complete group of symmetry of a square. This symmetry group of order 8 is denoted by C_{4v} and is one of the point groups. We might also describe the symmetry operations by listing the result of the map of the basis vector $\vec{e}_x$, $\vec{e}_y$ under the transformation operation x, y, see figure. In the table, we list all operations and their result on x, y.
Exercise Find the symmetry group of a planar equilateral triangle and write down the table with the transformation of the coordinates (x, y).
Example 2: The symmetry group of a cube. This group is called the cubic group O_h and is a very important example in solid state physics. With the aid of the figure, we can illustrate all 48 symmetry elements of O_h.

Type	Operation	Coordinate
e	e	xyz
C_4	C_{4z}	y$\bar{x}$z
C_4^2	C_{4z}^2	$\bar{x}\bar{y}$z
C_4^3	C_{4z}^3	$\bar{y}$xz
$2\sigma_v$	$IC_{2y}(m_x)$	x$\bar{y}$z
	$IC_{2x}(m_y)$	$\bar{x}$yz
$2\sigma_v'$	$IC_{2xy}(\sigma_u)$	$\bar{y}\bar{x}$z
	$IC_{2x\bar{y}}(\sigma_v)$	yxz

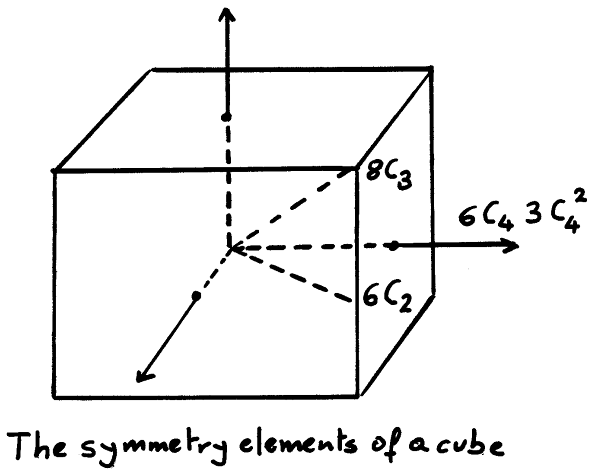

Figure 1.3:

- the identity e
- 3 rotations by π about the axes x, y, z $(3C_4^2)$
- 6 rotations by $\pm\pi/2$ about the axes x, y, z $(6C_4)$
- 6 rotations by π about the bisectrices in the planes xy, yz, xz $(6C_2)$
- 8 rotations by $\pm 2\pi/3$ about the diagonals of the cube $(8C_3)$
- the combination of the inversion I with the listed 24 proper rotations

For finite groups, the products of the group elements can be ordered into a Table, known as the group multiplication table. This Table is given for the group C_{4v}. Note that in establishing the result of the product ba, the operation a is performed first, followed by the operation b. In the multiplication

Type	Operation	Coordinate	Type	Operation	Coordinate
C_1	C_1	xyz	I	I	$\bar{x}\bar{y}\bar{z}$
C_4^2	C_{2z}	$\bar{x}\bar{y}z$	IC_4^2	IC_{2z}	$xy\bar{z}$
	C_{2x}	$x\bar{y}\bar{z}$		IC_{2x}	$\bar{x}yz$
	C_{2y}	$\bar{x}y\bar{z}$		IC_{2y}	$x\bar{y}z$
C_4	C_{4z}^{-1}	$\bar{y}xz$	IC_4	IC_{4z}^{-1}	$y\bar{x}\bar{z}$
	C_{4z}	$y\bar{x}z$		IC_{4z}	$\bar{y}x\bar{z}$
	C_{4x}^{-1}	$x\bar{z}y$		IC_{4x}^{-1}	$\bar{x}z\bar{y}$
	C_{4x}	$xz\bar{y}$		IC_{4x}	$\bar{x}\bar{z}y$
	C_{4y}^{-1}	$zy\bar{x}$		IC_{4y}^{-1}	$\bar{z}\bar{y}x$
	C_{4y}	$\bar{z}yx$		IC_{4y}	$z\bar{y}\bar{x}$
C_2	C_{2xy}	$yx\bar{z}$	IC_2	IC_{2xy}	$\bar{y}\bar{x}z$
	C_{2xz}	$z\bar{y}x$		IC_{2xz}	$\bar{z}y\bar{x}$
	C_{2yz}	$\bar{x}zy$		IC_{2yz}	$x\bar{z}\bar{y}$
	$C_{2x\bar{y}}$	$\bar{y}\bar{x}\bar{z}$		$IC_{2x\bar{y}}$	yxz
	$C_{2\bar{x}z}$	$\bar{z}\bar{y}\bar{x}$		$IC_{2\bar{x}z}$	zyx
	$C_{2y\bar{z}}$	$\bar{x}\bar{z}\bar{y}$		$IC_{2y\bar{z}}$	xzy
C_3	C_{3xyz}^{-1}	zxy	IC_3	IC_{3xyz}	$\bar{z}\bar{x}\bar{y}$
	C_{3xyz}	yzx		IC_{3xyz}	$\bar{z}\bar{x}\bar{y}$
	$C_{3x\bar{y}z}^{-1}$	$z\bar{x}\bar{y}$		$IC_{3x\bar{y}z}^{-1}$	$\bar{z}xy$
	$C_{3x\bar{y}z}$	$\bar{y}\bar{z}x$		$IC_{3x\bar{y}z}$	$yz\bar{x}$
	$C_{3x\bar{y}\bar{z}}^{-1}$	$\bar{z}\bar{x}y$		$IC_{3x\bar{y}\bar{z}}^{-1}$	$zx\bar{y}$
	$C_{3x\bar{y}\bar{z}}$	$\bar{y}z\bar{x}$		$IC_{3x\bar{y}\bar{z}}$	$y\bar{z}x$
	$C_{3xy\bar{z}}^{-1}$	$\bar{z}x\bar{y}$		$IC_{3xy\bar{z}}$	$z\bar{x}y$
	$C_{3xy\bar{z}}$	$y\bar{z}\bar{x}$		$IC_{3xy\bar{z}}$	$\bar{y}zx$

Table 1.1: Coordinate transformations under the action of the elements of the group O_h

	e	C_4	C_4^2	C_4^3	m_y	m_x	σ_v	σ_u
e	e	C_4	C_4^2	C_4^3	m_y	m_x	σ_v	σ_u
C_4^3	C_4^3	e	C_4	C_4^2	σ_u	σ_v	m_y	m_x
C_4^2	C_4^2	C_4^3	e	C_4	m_x	m_y	σ_u	σ_v
C_4	C_4	C_4^2	C_4^3	e	σ_v	σ_u	m_x	m_y
m_y	m_y	σ_u	m_x	σ_v	e	C_4^2	C_4^3	C_4
m_x	m_x	σ_v	m_y	σ_u	C_4^2	e	C_4	C_4^3
σ_v	σ_v	m_y	σ_u	m_x	C_4	C_4^3	e	C_4^2
σ_u	σ_u	m_x	σ_v	m_y	C_4^3	C_4	C_4^2	e

Table 1.2: Multiplication Table for C_{4v}

table, the operation performed first is found in the top row, the operation performed successively is found in the first column. The bulk of the table gives the results. The ordering of the rows and the column is immaterial: the one chosen in the figure in such that along the principal diagonal one finds the operation e.
Exercise: Check the result of the operation $\sigma_u C_4$.
Exercise: Prove that each element of the group occurs once and only once in each column or in each row. **Exercise**: prove that a cyclic group (cyclic means that all the group elements may be formed by taking powers of a single element) are Abelian.

An isomorphism between two groups $G = g_1, g_2, ..$ and $F = f_1, f_2, ...$ is a one-to-one map between the elements of G and F. If two groups are isomorphic, then they have the same multiplication table, i.e. they are essentially the same, although the concrete significance of their elements may be different. **Exercise**: show that between two groups (E, C_4, C_4^2, C_4^3) and $(1, i, -1, -i)$ there is an isomorphism.
An homomorphism is a map $\phi : g_i \rightarrow \phi(g_i)$ that associates to each element g_i one and only one element $\phi(g_i)$ such that $\phi(g_l g_k) = \phi(g_l)\phi(g_k)$. The element $\phi(g_i)$ is called the image or map of the element g_i under the homomorphism. Although each element has only one image, several elements of G may be mapped onto the same image. Thus it might happen that $\phi(g_i) = \phi(g_j)$ although $g_i \neq g_j$. Two elements a and b of a group G are **conjugate elements** if there exists a group element x such that $a = xbx^{-1}$ (or equivalently, $a = x^{-1}bx$). Applying the conjugation operation to one element a using every possible element x of the group produces classes of mutually conjugate elements. All element of one class are conjugated to each other but no two

element belonging to different classes are conjugate to each other (this is because if a is conjugate to b and to c, then b and c are also conjugate: for from $a = x^{-1}bx$ and $a = y^{-1}cy$ follows $b = (yx^{-1})^{-1}c(yx^{-1})$. The identity element e constitutes a class by itself. Each class is therefore completely determined by giving one single element of the class, which might be taken as the representative of the class. Each element of the group can only belong to one single class.
Exercise: construct the classes of C_{4v} using the multiplication table.
Exercise: Show that if the group is Abelian, each element is a class on its own. There are simple rules that establish commuting transformation operations:

- Two consecutive rotations about the same axis
- Two reflections at orthogonal planes (they are equivalent to a rotation by π at the axis forming the intersection of the two planes)
- two rotations by π about two orthogonal axis (they are equivalent to a rotation by the same angle about a third axis, orthogonal to both
- A rotation and a reflection at a plane orthogonal to the rotation axis
- a rotation (or a reflection) and an inversion at a point lying on the rotation axis (reflection plane)

In the case we are dealing with groups of transformations consisting of rotations, reflections and inversion of a physical system, there are some simple rules which allow the determination of the classes of a non-Abelian group without having to perform explicit calculations for all elements:

- Rotations through angles of different magnitudes must belong to different classes. Thus, e.g. C_4 and C_4^2 belong to different classes.
- Rotations by $\pm$ the same angle about an axis belong to the same class only if there is an element in the group that change the handiness of the coordinate system. Thus, C_4 and C_4^3 belong to the same class because of the existence of a vertical reflection plane
- Rotations through the same angle about different axes or reflections with respect two different planes belong to the same class only if the two different axis of the two different planes can be brought into each other by an element of the group. Thus, m_x and m_y belong to the same class as they can be brought into each other by C_4.

Some physical systems have continuos symmetry groups of transformation, i.e. are tranformed into themselves by a set of transformations which can be labeled by one or more **continuous** parameters. Continuos groups are an example of infinite groups. The elements of a continuous group G can be characterized by a set of real parameters $a_1, a_2, ..., a_r$, of which at least one varies continuously over a certain interval. (r is called the order of the continuos group).

Example. C_∞ consists of all rotations by an angle $\varphi \in [0, 2\pi]$ around a fixed axis in three dimensional Euclidean space (the two-dimensional or axial rotation group). The transformation operations of this continuous group can be regarded as mapping one point residing on a circle into another point residing on the same circle. The most natural way of describing this transformation group is to establish two mutual orthogonal vectors $\vec{e}_i$ in a plane and write down the transformation of these two vectors under a rotation aroung a third vector pointing perpendicular to the plane, using an orthogonal matrix with determinant 1:

$$\begin{pmatrix} e_1^t & e_2^t \end{pmatrix} = \begin{pmatrix} e_1 & e_2 \end{pmatrix} \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}$$

This establishes a matrix group which is isomorphic to the axial rotation group C_∞ and is called the two-dimensional special orthogonal group $SO(2)$. This matrix group does not have a finite number of elements but there are a non-denumerable infinite number of them.

Exercise: prove that the set of such matrices forms indeed a group with respect to matrix multiplication.

In order to deal with continuos groups (and to prove some theorem about them), we require them to have some special properties. We consider first only groups whose elements x can be put in one to one correspondence with the points of a subset of an r-dimensional space S_r, which we assume to be a vector space with scalar product. We shall refer to this subset as the parameter space. For instance, the parameter space of $SO(2)$ can be identified with the points residing on a circle in a plane with radius 1. Second, we require continuous groups to be *connected* (in german: zusammenhängend). This means that given two elements x_1 and x_2 of the group G with images $P(x_1), P(x_2)$ in S_r, it is possible to connect $P(x_1)$ with $P(x_2)$ by one or more paths lying entirely within the parameter space.

Exercise: Why is $SO(2)$ a connected group?

Third, we require connected groups to be compact, i.e. their parameter space is a compact space (closed and bounded).

Exerxise: explain why $SO(2)$ is compact. Show that O_2 (= the group containing all rotations about one axis and their composition with the inversion)

is not connected.
Fourth, after choosing the continuous parameters of a connected compact group such that the image of the identity element e is the origin of the parameter space, i.e. $e = x(0, 0, ...0)$, we require that any element near the identity may be written as

$$x(0, 0, ..., \epsilon_j, 0, ...0) \approx x(0, 0, ...0) + i \cdot \epsilon_j I_j(0, 0, ...0)$$

to first order in ϵ_j. If this is possible in the neighbouroud of any element, than the group is a **Lie group**. There are r such operators I_j and they are given by

$$I_j \doteq \frac{1}{i} \frac{\partial x(a_1, ..., a_r)}{\partial a_j} |_{a_j=0}$$

Notice that knowing these operators near to the identity operator, we can construct all elements of a Lie group at any finite distance from the identity element. Suppose to wish to generate the element $x(0, 0, ..., a_j, 0, ...0)$. Let us write $a_j = N \cdot \epsilon_j$, where N is a large positive integer so that ϵ_j is a small quantity. Then allowing N to tend to infinity and using the algebraic identity

$$lim_{N \to \infty}(1 + x/N)^N = exp(x)$$

we obtain

$$\begin{aligned} x(0, 0, ..., a_j, 0, ...0) &= [x(0, 0, ..., \epsilon_j, ...0)]^N \\ &= [e + i \cdot \epsilon_j I_j]^N \\ &= [e + i(a_j/N)I_j]^N \\ &= exp(ia_j I_j) \end{aligned}$$

which is an exact result. The exponential function on the right hand side is to be understood as being equivalent to its expansion in the powers of the operator I_j. For a general element of the group we can easily extend the above result to the general formula

$$x(a_1, a_2, ...a_r) = exp[\sum_{j=1}^{r} ia_j I_j]$$

All the elements of the Lie group belonging to the subset containing the identity can be generated using the operators I_j and giving variuous values to the parameters a_j within the respective prescribed intervals. The operators I_j are therefore called the **generators** (german: infinitesimale Erzeugende) of the Lie group. A Lie group with r continuous parameters has r generators.
Example: the generators of $SO(2)$.

As $SO(2)$ is a one-parameter group, it has only one generator. As the unit matrix is given by $\varphi = 0$, according to our definition

$$I = \frac{1}{i} \frac{d \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}}{d\varphi} |_{\varphi=0} = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}$$

which is just $-\sigma_y$, i.e. one of the Pauli matrices. Accordingly, any $2x2$ orthogonal matrix with determinant 1 can be written as follows:

$$\begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} = exp[-i \cdot \sigma_y \varphi]$$

Exercise: prove this last statement by directly summing the Taylor expansion of the exponential function.

In compact Lie Groups one can define an **average** over the group elements. Let $f(x)$ be a complex function defined on G. If for a wide class of such functions the average

$$M_{x \in G} f(x)$$

exists and has the properties

1. linearity:

$$M_{x \in G}[\alpha f(x) + \beta g(x)] = \alpha M_{x \in G} f(x) + \beta M_{x \in G} g(x)$$

2. positiv: if $f(x) \geq 0$ and real, then $M_{x \in G} \geq 0$, being 0 only if $f(x) \equiv 0$

3. normalized: if $f(x) = 1$, then $M_{x \in G} f(x) = 1$

4. invariant with respect to group operations: $\forall y$

$$M_{x \in G} f(yx) = M_{x \in G} f(xy) = M_{x \in G} f(x)$$

then the group is said to be a group with average (in german: eine Gruppe mit Mittelwert).
Exercise: Show that for a finite group

$$M_{a \in G} f(a) \doteq \frac{1}{h} \sum_a f(a)$$

ist an average (h: order of the group).
For compact Lie groups the average takes the form of an integral over an

appropriate element $d\tau_G$, $d\tau_G$ being determined bei some differential form within the parameter space. According to the previous definition of average, one chooses $d\tau_g$ such that the "group volume" $\int d\tau_g$ assumes the value of 1.
Example. A possible average for $SO(2)$ is

$$\frac{1}{2\pi}\int_0^{2\pi} f(\varphi)d\varphi$$

where $f(\varphi)$ is a periodic function of φ with period 2π and $d\varphi$ is the length of the differential element on the unit circle in the plane.
Exercise: show that this integral is indeed an average according to our general definition.

1.1 Exercises

1. Show that the following sets are groups
   - the set consisting of $(1, -1)$
   - the set complex numbers $(1, i, -1, -i)$
   - the set of all integers $\mathcal{Z} = (..., -2, -1, 0, 1, 2, ...)$ with the addition as law of composition and the set of rational numbers $\mathcal{Q}$ under ordinary multiplication (but not $\mathcal{N} = 1, 2, 3, ...$)
   - the set of real numbers $\mathcal{R}$ under addition or under multiplication (if zero is excluded)
   - the set of all matrices of order $m \times n$ under addition
2. Find the symmetry group of a planar equilateral triangle and write down the table with the transformation of the coordinates (x, y).
3. Prove that each element of the group occurs once and only once in each column or in each row.
4. Prove that a cyclic group (cyclic means that all the group elements may be formed by taking powers of a single element) are Abelian.
5. Show that between two groups (E, C_4, C_4^2, C_4^3) and $(1, i, -1, -i)$ there is an isomorphism.
6. Construct the classes of C_{4v} and C_{3v}

7. Show that if the group is Abelian, each element is a class on its own.

8. Prove that the set of $SO(2)$ matrices forms a group with respect to matrix multiplication

9. Show by summung the Taylor expansion that

$$\begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix} = exp[-i \cdot \sigma_y \varphi]$$

10. Show that for a finite group

$$M_{a \in G} f(a) \doteq \frac{1}{h} \sum_a f(a)$$

ist an average (h: order of the group)

11. Show that

$$\frac{1}{2\pi} \int_0^{2\pi} f(\varphi) d\varphi$$

where $f(\varphi)$ is a periodic function of φ with period 2π and $d\varphi$ is the length of the differential element on the unit circle in the plane is an average

Chapter 2

Group Representations

2.1 Unitary Representations

For groups with average there exists a precise representation theory due to H. Weyl. Let $G = e, a, b...$ be a group with average, and L an Hilbert space.
Definition: A representation of the group G is an homomorphism associating to every element a of the group a linear operator $T(a)$ acting on L. L is the representation space of G. If the dimension of L is n, the representation is n dimensional. In practice, one usually define a linear operator on L by its matrix with respect to some VONS $e_1, ..., e_n$. Hence we construct a matrix representation of G within the space L by means of the equation

$$T(a)e_i = \sum_j T_{ji}(a)e_j$$

The matrix $T = [T_{ij}(a)]$ is the matrix representing the operator $T(a)$ and the set of matrices $T_{ij}(a) = (e_i, T(a)e_j)$ generate a matrix representation of G in L.
Proof:

$$T(a)T(b)e_i = \sum_k T_{ki}(ab)e_k = T(a)\sum_k T_{ki}(b)e_k =$$
$$\sum_{kl} T_{lk}(a)T_{ki}(b)e_l = \sum_k(\sum_l T_{kl}(a)T_{li}(b))e_k$$

By comparison we deduce that

$$T_{ki}(ab) = \sum_l T_{kl}(a)T_{li}(b)$$

or

$$T(ab) = T(a)T(b)$$

which is just the requirement for a matrix representation where the law of composition between matrices is the matrix multiplication. It is evident that the vector space L which is used to generate a representation of the group G has the following property: for every element a of G and every vector $\phi \in L_n$ $T(a)\phi$ also belong to L: We say that the space L is closed under the transformations of G or simply closed under G.
Exercise: show that $T(e)$ is the unit matrix and $T(a^{-1}) = T^{-1}(a)$.
As the correspondence is merely an homomorphism, several elements of G may be represented by the same matrix. In the special case of an isomorphism, the representation is said to be 'faithful'. The simplest representation of a group is obtained when we associate the number '1' with every element of the group. Thus, in our example of C_{4v}, we would have the correspondence

E	C_4	C_4^2	C_4^3	m_x	m_y	σ_u	σ_v
1	1	1	1	1	1	1	1

The set of numbers 1 does indeed form a representation of any group, in general. This representation is known as the identity or $'1'$-representation. The identity representation is clearly an unfaithful representation of the group.
Theorem. Suppose we have a representation $T_1(a)$ of dimension l. Then the set of matrices $T_2(a) \equiv S^{-1}T_1(a)S$ also form a representation of dimension l with S being any non-singular matrix.
Proof:

$$T_2(a)T_2(b) = S^{-1}T_1(a)SS^{-1}T_1(b)S = S^{-1}T_1(ab)S = T_2(ab)$$

The two representations T_2 and T_1 are said to be equivalent and the transformation between the two is similarity transformation. Clearly, by similarity transformation, one can produce an infinite number of equivalent representations.
Exercise. Prove that a similarity transformation is produced by a transformation of the basis functions according to $(e_1^t, e_2^t, ...) = (e_1, e_2, ...)S$, taking into account that under this transformation the coordinates of the various vectors transform according to $\vec{x} = \mathbf{S}\vec{x}^t$.
Maschke's Theorem. Any representation of a group with average is equivalent to a unitary representation, i.e. a representation for which all matrices are unitary (their inverse coincides with the complex conjugate transpose).
Proof: having a representation $T(a)$, we must find a matrix S such that $(ST(a)S^{-1})^\dagger = (ST(a)S^{-1})^{-1}$. We now show that the matrix S for which $S^2 = M_b T^\dagger(b)T(b)$ is the sought for matrix. The first step is to write

$$T^\dagger(a)S^2T(a) \quad = \quad M_b T^\dagger(a)T^\dagger(b)T(b)T(a)$$

$$\begin{aligned} &= M_b T^\dagger(ba) T(ba) \\ &= M_c T^\dagger(c) T(c) \\ &= S^2 \end{aligned}$$

Since S is hermitic, postmultiplying both sides by $T^{-1}(a)S^{-1}$ and pre-multiplying by S^{-1} we obtain the required unitarity condition. Owing to this theorem, we need to consider representations by unitary matrices only. This will produce a great simplification: for instance, the scalar product in L remains invariant if two vectors are transformed by $T(a)$. Notice that unitary representations are not unique, for if T_1 is a unitary representation and S is a unitary matrix, then T_2 is also an equivalent unitary representation.
Exercise: prove this.
Theorem. The basis set carrying unitary representations is an orthonormal set.
Proof The following equation

$$(e_i, e_j) = (T(a)e_i, T(a)e_j) = (\sum_l T_{li}(a)e_l, \sum_m T_{mj}(a)e_m) = \\ \sum_{l,m} T^*_{li}(a)T_{mj}(a)(e_l, e_m) = \sum_{l,m} T^{-1}_{il}(a)T_{mj}(a)(e_l, e_m)$$

has the solution $(e_i, e_j) = \delta_{ij}$.

Examples of representation

Exercise: Find two and four dimensional representations of the 8 operations of C_{4v}.
Exercise: find two and four dimensional representations for the symmtry group of an equilateral triangle.
Example. C_∞ is a Lie group with average and consists of all rotations by an angle $\varphi \in [0, 2\pi]$ around a fixed axis in three dimensional Euclidean space (the two-dimensional or axial rotation group). The transformation operations of this continuous group can be regarded as mapping one point residing on a circle into another point residing on the same circle. The most natural way of representing this transformation group is to establish two mutual orthogonal vectors $\vec{e}_i$ in a plane and write down the transformation of these two vectors under a rotation aroung a third vector pointing perpendicular to the plane, using an orthogonal matrix with determinant 1:

$$\begin{pmatrix} e_1^t & e_2^t \end{pmatrix} = \begin{pmatrix} e_1 & e_2 \end{pmatrix} \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}$$

Exercise: prove that the such matrices (called the set $SO(2)$) generate a representation of C_∞.

Example: The previous examples of representations were constructed within familiar vector spaces. We now show how a representation can be constructed within a function space. This is a most important step when considering quantum mechanical problems. We consider a map associating to every vector $\vec{r}$ a transformed vector $\vec{r}_t = T\vec{r}$. Examples of T are rotations, translations and combination of both. Any scalar function function ϕ at $\vec{r}$ will have a different value ϕ_t. $\phi(\vec{r})$ and $\phi_t(\vec{r})$ are related by the equation

$$\phi_t(\vec{r}) = \phi(T^{-1}\vec{r})$$

which is a practical way to find the expression for the transformed wave function. By defining $\phi_t(\vec{r}) \doteq O_T\phi(\vec{r})$, we obtain

$$O_T\phi(\vec{r}) = \phi(T^{-1}\vec{r})$$

If the elements T form a group, then $O_S O_R = O_{SR}$, where the convention is used, that the operator O_R is applied first and the operator O_S acts on the whole expression placed right to it. In other words: the operators O_T form a representation of the group G within a function space. In fact

$$O_S O_R\phi(\vec{r}) = O_S\phi(R^{-1}\vec{r}) = \phi(R^{-1}S^{-1}\vec{r}) = \phi((SR)^{-1}\vec{r}) = O_{SR}\phi(\vec{r})$$

the identity operator corresponds to the identity transformation and $(O_R)^{-1} = O_{R^{-1}}$.

Other properties of O_T:

1. O_T is a linear operator

$$O_T(af(\vec{r}) + bg(\vec{r})) = af(T^{-1}\vec{r}) + bg(T^{-1}\vec{r}) = aO_T(\vec{r}) + bO_Tg(\vec{r})$$

2. O_T is a unitary operator

$$(O_Tf, O_Tg) = \int\int\int dV f^*(T^{-1}\vec{r})g(T^{-1}\vec{r}) = (f, g)$$

as the integral is over all space and after a variable substitution $R^{-1}\vec{r} = \vec{y}$.

The matrix representation of O_T is achieved (for a given VONS ψ_i) by the equation

$$O_T\psi_j(\vec{r}) = \sum_i O_{ij}(T)\psi_i(\vec{r})$$

Exercise. Show that a possible representation of C_∞ in the Hilbert space of square integrable functions over R^2 is defined by the equation

$$O(\varphi)\psi(x, y) = \psi(x\cos\varphi + y\sin\varphi, -x\sin\varphi + y\cos\varphi)$$

2.2 Reducible and irreducible representations

Suppose that T_1 and T_2 are two matrix representations of a group of dimensions l_1 and l_2 respectively, and define for each element of the group a $(l_1 + l_2)$-dimensional matrix T by the direct sum

$$T(a) = \begin{pmatrix} T_1(a) & 0 \\ 0 & T_2(a) \end{pmatrix}$$

The direct sum of two or more Hilbert spaces. Consider a vector space L_n with a coordinate system $e_1, ..., e_n$ and a vector space L_m with basis vectors $i_1, ..., i_m$. Provided that the two spaces have no common vector except the null vector, the direct sum space $L_t \equiv L_n \oplus L_m$ is the vector space defined by the $t = n+m$ basis vectors $(e_1, ..., e_n, i_1, ...i_m)$. If L_n and L_m are complete spaces, so is L_t, i.e. any vector in L_t can be expanded as a linear combination of the basis vectors. As a simple example we consider a plane with basis vectors e_x, e_y and a line with basis vector e_z which does not lie in the x, y plane. The direct sum of the two spaces is the three dimensional vector space with basis vectors e_x, e_y, e_z. In conjunction with the direct sum of spaces one can introduce the direct sum of two square matrices $[A_{ij}]$ of the order n and $[B_{ij}]$ of the order m. The resulting matrix C is of the order $n + m$ and is defined as

$$C = A \oplus B = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix} = \begin{pmatrix} A_{11} & ... & A_{1n} & 0 & ... & 0 \\ A_{21} & ... & A_{2n} & 0 & ... & 0 \\ ... & ... & ... & 0 & ... & 0 \\ A_{n1} & ... & A_{nn} & 0 & ... & 0 \\ 0 & ... & 0 & B_{11} & ... & B_{1m} \\ 0 & ... & 0 & B_{21} & ... & B_{2m} \\ 0 & ... & 0 & ... & ... & ... \\ 0 & ... & 0 & B_{m1} & ... & B_{mm} \end{pmatrix}$$

The direct sum of matrices can be easily extended to more than two matrices. Such a matrix, which has non-vanishing elements in square blocks along the main diagonal and zeros elsewhere, is said to be in a block-diagonalized form. It has the important properties that $detC = detA \cdot detB$ and $trC = trA + trB$ (det = determinant and tr = trace). Also if A_1 and A_2 are matrices with the same order n and B_1 and B_2 are matrices with the same order m, then

$$(A_1 \oplus B_1)(A_2 \oplus B_2) = (A_1 A_2) \oplus (B_1 B_2)$$

$T(a)$ is a partitioned matrix in which the elements of the top-right-hand block and bottom left-hand block are all zero, i.e. $T(a) = T_1(a) \oplus T_2(a)$. As

$$T(a)T(b) = \begin{pmatrix} T_1(a)T_1(b) & 0 \\ 0 & T_2(a)T_2(b) \end{pmatrix} = \begin{pmatrix} T_1(ab) & 0 \\ 0 & T_2(ab) \end{pmatrix} = T(ab)$$

T is also a representation of the group. The representation T constructed by direct sum of representations are said to be reducible, as they can be partitioned in block form. The representation T_1 and T_2 are said to appear in the 'reduction' of T. Notice that a similarity transformation could obscure the block form by making the zero matrix elements disappear, but the representation would be still considered to be reducible, that is a representation is said to be reducible if it can be put into block form by an appropriate similarity transformation.

It might be possible that the representations T_1 and T_2 are further reducible, i.e. that a similarity transformation exists, which transforms all matrices $T_1(a)$ and $T_2(a)$ into block forms themselves. Clearly, this process of reduction can be carried out until we can find no unitary transformation which reduces all matrices of the representation further. Thus, the final form of the matrices of a representation T may look like

$$T(a) = \begin{pmatrix} T_1(a) & 0 & ... & 0 \\ 0 & T_2(a) & ... & 0 \\ ... & ... & ... & ... \\ 0 & 0 & .... & T_s(a) \end{pmatrix}$$

with all matrices of T having the same reduced structure. When such a complete reduction of a representation is achieved, the component representations T_1, T_2,... are called **irreducible** representations of the group and the representation T is said to be fully reduced. Clearly, the irreducible representations are the 'basic' representations from which all others can be constructed. Notice that an irreducible representation may occur more than once in the reduction of a reducible representation: in general

$$T = \oplus_i n_i T_i$$

Notice that when the representation T is reduced according to this direct sum, a number of subspaces are produced which are invariant with respect to all operations of G, i.e. the operations of G do not bring outside the subspace. The invariant subspaces are pairwise orthogonal, i.e. L_n is the orthogonal sum of a number of invariant subspaces, each sustaining an irreducible representation:

$$L_n = \oplus_m n_m L_m$$

It is the main aim of group theory

- to construct all irreducible representations
- to test any representation for its irreducibility and
- to construct the invariant subspaces.

To this aim the key theorem is the the orthogonality theorem for the matrix elements of irreducible representation.

Orthogonality Theorem

Suppose that T_α and T_β are two unitary irreducible representations of a group, and that they are not equivalent if $\alpha \neq \beta$ and identical if $\alpha = \beta$. then

$$\mathcal{M}_a T^{(\alpha)*}_{ik}(a) T^{\beta}_{lm}(a) = \frac{1}{l_\alpha} \cdot \delta_{\alpha\beta}\delta_{il}\delta_{km}$$

where l_α the dimension of T^α. Thus, knowing the matrix elements of the representations allows, in principle, to find out whether the representation is irreducible without having to search for the similarity transformation that puts the representation in block form. The proof of the orthogonality theorem involves two theorems of fundamental importance which go by the name of Schur's lemmas and which are extremely useful for the study of the irreducible representation of a group.
Schur's Lemma 1: If T^α is an irreducible representation of a group G and a matrix A commutes with all matrices of T^α, then $A = \lambda \cdot E$.
Schur's Lemma 2: If T^α and T^β are two irreducible representations of dimensions l_α and l_β of a group G and A is a matrix of order $l_\alpha \times l_\beta$ satisfying the relation

$$T^\alpha(a)A = AT^\beta(a), \forall a$$

then $A = 0$ (the null matrix) or the two representations are equivalent. The proof of both Lemmas can be found in the numerous standard books of group theory. Here we give the proof of the key orthogonality theorem involving matrix elements of irreducible representations. Let X be a non-singular $l_\alpha \times l_\beta$ matrix. We first show that the matrix defined by

$$\mathcal{M}_b T^\alpha(b) X T^\beta(b^{-1})$$

has the property of the A matrix in Schur's lemmas. In fact,

$$\begin{aligned}
T^\alpha(a)A &= \mathcal{M}_b T^\alpha(a) T^\alpha(b) X T^\beta(b^{-1}) \\
&= \mathcal{M}_b T^\alpha(ab) X T^\beta(b^{-1}) T^\beta(a^{-1})(T^\beta(a) \\
&= \mathcal{M}_b T^\alpha(ab) X T^\beta((ab)^{-1} T^\beta(a) \\
&= AT^\beta(a)
\end{aligned}$$

by virtue of the definition of M. If $T^\alpha = T^\beta$ then $A = \lambda E$, otherwise is $A = 0$, i.e. the matrix $A = \lambda \cdot \delta_{\alpha\beta} \cdot E$. The matrix equation worked out above writes

$$\lambda\delta_{\alpha\beta} \cdot \delta_{ij} = \mathcal{M}_a \sum_{k,m} T^\alpha(a)_{ik} X_{km} T^\beta(a^{-1})_{mj}$$

in which the rectangular matrix is quite arbitrary but λ will be determined by the choice of X. We make use of this freedom to simplify this last equation by taking for X a matrix with zero elements everywhere except for the element in the row k and columns m which is taken to be 1. In this special case we have

$$\lambda\delta_{\alpha\beta}\cdot\delta_{ij} = \mathcal{M}_a T^{\alpha}(a)_{ik} T^{\beta}(a^{-1})_{mj}$$

We determine λ by setting $\alpha = \beta$ and $i = j$ and summing over i, in which case the right hand side of theis last equation becomes $\lambda \cdot l_{\alpha}$ and the left hand side is just δ_{km}. Setting this value of λ into the equations leads to the sought for orthogonality relation, taking into account that $T^{\beta}(a^{-1})_{mj} = T^{*\beta}(a)_{jm}$ for unitary representations.

2.3 Characters of a representation and theorems involving them

Because representation related by a similarity transformation are equivalent, there is a considerable degree of arbitrariness in the actual form of the matrices. However, there are quantities which do not change under similarity transformations, and which therefore provides a unique way of characterizing a representation. These quantities are appropriately called the characters of a representation.

Definition. Let T be a representation (reducible or irreducible) of a group G. Then

$$\chi(a) \doteq \sum_k T_{kk}(a)$$

is defined as the **character** of the group element a in this representation (that is the character is the sum of the diagonal elements). The set of characters corresponding to a representation is called the character system of the representation. If the representations are one dimensional, their character is the same as the representation.

Theorem: The character is invariant under similarity transformation.

Proof:

$$\begin{aligned}
(T(a)T(b))_{ik} &= \sum_j T(a)_{ij}T(b)_{jk} \\
tr(T(a)T(b)) &= \sum_{i,j} T(a)_{ij}T(b)_{ji} \\
&= \sum_{ij} T(b)_{ji}T(a)_{ij} \\
&= \sum_{ij} T(b)_{ij}T(a)_{ji} \\
&= trT(b)T(a)
\end{aligned}$$

$$\Longrightarrow$$
$$tr(S^{-1}T(a)S) \quad = \quad tr(T(a)SS^{-1}) = trT(a)$$

Thus, equivalent representations have the same characters. The dimension of a representation is the character of the matrix representing the identity element of the group.
Conjugate elements have the same character, i.e. the character is identical within the same class of conjugate elements (in other words: the character is a map associating to every **class** a complex number, i.e. it is a class function). Each class is therefore completely determined – as far as its character is concerned – by giving one single element of the class, which might be taken as the representative of the class. Each element of the group can only belong to one single class.
There is a number of important theorems involving characters, which can be used to give very useful results from the knowledge of the characters alone, without requiring the explicit knowledge of the matrices.

Theorem 1: orthogonality theorems for characters

We can immediately transform the orthogonality relation

$$\mathcal{M}_a T_{ik}^{(\alpha)*}(a) T_{lm}^{\beta}(a) = (1/l_\alpha) \cdot \delta_{\alpha\beta}\delta_{il}\delta_{km}$$

into an orthogonality relation for the characters of a group. In fact, setting $i = k$ and $l = m$ and summing both sides over the indices i and l we obtain

$$\mathcal{M}_a \chi^{\alpha*}(a)\chi^{\beta}(a) = \delta_{\alpha\beta}$$

This theorem allows for an immediate test for irreducibility because **the average of the square of the absolute value of the characters of an irreducible representation of a Lie group with average is just one**:

$$\mathcal{M}_a \mid \chi^{\alpha}(a) \mid^2 = 1$$

if T^α is irreducible. As each group admits the 1-representation, a further consequence oif this orthogonality theorem is the equation

$$\mathcal{M}_a \chi(a)^{\alpha} = 0$$

provided T^α is not the 1-representation.

Theorem 2: reduction formula

It very often happens that we have a representation of the group which is a reducible one. Such a representation T may be written as the direct sum of various irreducible representations, according to

$$T = \oplus_\alpha n_\alpha T^\alpha$$

where T^α are irreducible representations of the group. n_α is the number of times the irreducible representation T_α is contained in the direct sum. To find n_α, we take the traces of both sides in the expression for the direct sum. If $\chi(a)$ is the trace of the representation T and $\chi^{(\alpha)}(a)$ is the character of the element a in the irreducible representation T^α, then

$$\chi(a) = \sum_\alpha n_\alpha \chi^\alpha(a)$$

for all $a \in G$. Multiplying both sides by $\chi^{\gamma*}(a)$ and averaging over a we obtain

$$\begin{aligned} \mathcal{M}_a \chi^{\gamma*}(a)\chi(a) &= n_\gamma \Longleftrightarrow \\ n_\gamma &= \mathcal{M}_a \chi^{\gamma*}(a)\chi(a) \end{aligned}$$

This last equation gives a method for obtaining the coefficients n_γ solely knowing the characters of the representation to be reduced and those of the irreducible component, without needing explicitly the matrix elements.

Theorem 3: the number of irreducible representations of a group

For continuos Lie groups with average there is an important theorem proved by by F. Peter and H. Weyl: The number of irreducible representations of a continuos Lie group with measure is denumerably infinite, i.e. **the irreducible representations build a discrete set**. For finite groups there is an equally important theorem, which allows to obtain the number of irreducible representations: the number of irreducible representations of a group is exactly equal to the number of conjugacy classes.
Thus, the characters of the irreducible representations of a finite group are conveniently displayed in the form of **character tables**. The classes of the group are usually listed along the top row of the table, and the irreducible representations down the left-hand side. As a consequence of this theorem, this table is always square and the corresponding rows are normalized to the order of the finite group and orthogonal to each other. As the matrix is a square one, its columns are orthogonal to each other (see linear algebra).

A formula for finite groups

For finite groups, there is an important formula which is very helpful in constructing the character table of finite groups. This formula states that the sum of the squares of the dimensions of the inequivalent irreducible representations is equal to the order of the group. To prove this formula, we introduce the regular representation T_r of a finite group. As a first step, one associates by a one-to-one map to every element of the group a basis vector in a space R^h. In a second step, one associates to each element a – taken as the top entry in the multiplication table – a $h \times h$ matrix whose columns consist of the basis vectors of the elements in the corresponding column of the multiplication table. This representation has some important properties. As each element appears only once in a column of the representation table, (when multiplied by e), all diagonal elements are 0, except for the identity operation, which has exactly '1' on the diagonal. In other words: the regular representation of e is the unit matrix in R^h and has character $\chi_r(e) = h$. The character for the representation of all other elements is zero, as their matrices have all zero on the diagonal. We shall now find the coefficients n_i in

$$T_r = \oplus n_i T_i$$

Using the suitable formula we obtain

$$n_i = \frac{1}{h}\sum_a \chi^{i*}(a)\chi_r(a) = \frac{1}{h}\chi^{i*}(e)\cdot h = l_i$$

with l_i being the dimension of the $i-th$ irreducible representation. We thus have the equation

$$T_r = \oplus_i l_i T_i.$$

Taking the traces on both side of this equation for the matrix represenating e leads to

$$\sum_i l_i^2 = h$$

which is the important formula we have anticipated. A consequence of this theorem is that all irreducible representations of Abelian groups are one-dimensional.

We summarize now some rules for constructing the character table of a finite group.

1. It is convenient to display in table form the characters of the irreducible representations. Such a table gives less information than a complete set of matrices, but it is sufficient for classifying the electronic states

2. The number of irreducible representations is equal to the number of classes in the group

3. The sum of the squares of the dimensions l_α of the irreducible representations is equal to the number of elements of the group

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

4. The characters of the irreducible representation must be mutually orthogonal and normalized to the order of the group:

$$\sum_a \chi^\alpha(a)^* \chi^\beta(a) = h \cdot \delta_{\alpha\beta}$$

5. Every group admits the one-dimensional identical representation in which each element of the group is represented by the number 1. The orthogonality relation between characters then shows that for any irreducible representation other than the identity representation

$$\sum_a \chi(a) = 0$$

2.4 Exercises

1. Prove that a similarity transformation is produced by a transformation of the basis functions according to $(e_1^t, e_2^t, ...) = (e_1, e_2, ...)S$, taking into account that under this transformation the coordinates of the various vectors transform according to $\vec{x} = \mathbf{S}\vec{x}^t$

2. Find two and four dimensional representations of the 8 operations of C_{4v} and the two and three dimensional representations for C_{3v}.

3. Show that the $SO(2)$ matrices generate a representation of C_∞

4. Show that a possible representation of C_∞ in the Hilbert space of square integrable functions over R^2 is defined by the equation

$$O(\varphi)\psi(x, y) = \psi(x\cos\varphi + y\sin\varphi, -x\sin\varphi + y\cos\varphi)$$

5. Table 1.1. gives a three-dimensional representation of the group of the Γ point in cubic lattices O_h. Show that it is irreducible and find it within the character table of this group, shown here.

Irr.Rep.	E	$6C_4$	$3C_4^2$	$6C_2$	$8C_3$	I	$I6C_4$	$I3C_4^2$	$I6C_2$	$I8C_3$
Γ_1	1	1	1	1	1	1	1	1	1	1
Γ_2	1	-1	1	-1	1	1	-1	1	-1	1
Γ_{12}	2	0	2	0	-1	2	0	2	0	-1
$\Gamma_{15'}$	3	1	-1	-1	0	3	1	-1	-1	0
$\Gamma_{25'}$	3	-1	-1	1	0	3	-1	-1	1	0
$\Gamma_{1'}$	1	1	1	1	1	-1	-1	-1	-1	-1
$\Gamma_{2'}$	1	-1	1	-1	1	-1	1	-1	1	-1
$\Gamma_{12'}$	2	0	2	0	-1	-2	0	-2	0	1
Γ_{15}	3	1	-1	-1	0	-3	-1	1	1	0
Γ_{25}	3	-1	-1	1	0	-3	1	1	-1	0

6. Find the characters of the 2 and 4 dimensional representations of C_{4v} constructed in Serie 1 and test for irreducibility.

7. Find the characters of the two and three dimensional representations of C_{3v} contructed in Serie 1 and test for irreducibility

8. Construct the character table of C_{3v}

9. Construct the character table of C_4 and C_{2v}.

10. Let G be a trasformation group consisting of rotations and reflections, and let the inversion I be an element of the group. Find all possible irreducible matrix representations of I.

11. Show: if $T = \bigoplus_r n_r T_r^{irred.}$ and $n_T = \sum_r n_r^2$, then $\sum_a \chi_T^*(a)\chi_T(a) = n_T g$, g being the order of the group.

Chapter 3

Group theory and Quantum Mechanics

The fundamental problem of quantum physics is to determine the eigenvalues and eigenfunctions of the Schrödinger equation

$$H\psi_n = E_n\psi_n$$

where H is a linear hermitian operator suited to the physical problem and ψ_n and E_n are the eigenfunctions and eingenvectors of the operator. The operator H may correspond to any physical observable such as position, momentum, angular momentum (spin or orbital) energy and so on. The spectrum of H can be finite or infinite. It is an axiom of quantum mechanics that the set of all eigenfunctions of an hermitian operator is a complete set and that these eigenfunctions define an Hilbert space on which operator act.
In general, it is very difficult to find the exact eigenfunctions and eigenvalues of an operator, except in some simple 'exactly solvable' cases. However, group theory helps in (a) simplifying the eigenvalues problem and (b) classifying the various eigenfunctions of an operator by the irreducible representations of the **symmetry group** of the H-operator.

3.1 The symmetry group of the Schrödinger equation

The key operator is the Hamilton operator. H is in general a function of various parameters of the system such as the position vector, time, derivatives, angular momentum, etc. Its most familiar form is, e.g.,

$$H = \frac{-\hbar^2 \cdot \vec{\nabla} \cdot \vec{\nabla})}{2m} + V(\vec{r})$$

We write $H = H(\vec{r}, \vec{p})$. Relevant for the classification of the various eigenvalues and for applying group theoretical methods are the transformation properties of the Hamiltonian. For the Hamiltonian reported above we consider the general map

$$(R \mid \vec{t}) \doteq T : \vec{r} \rightarrow \vec{r}_t = R\vec{r} + \vec{t}$$

with $\vec{t}$ being some translation and R a rotation.
Exercise: show that the kinetic energy is invariant with respect to T.
The transformation behaviour of H under the map is thus governed by the transformation properties of the function V. Under any transformation T, $H(\vec{r})$ transforms to $H_t(\vec{r}) = H(T\vec{r})$. In general, the expression for H_t as a function of $\vec{r}$, constructed by inserting $T\vec{r}$ into H, differs from the expression of H as a function of $\vec{r}$. However, when the system is transformed into itself – i.e. when T is a symmetry transformation – H is invariant under the transformation: $H(T\vec{r}) = H(\vec{r})$. This means that, after substituting all vectors $\vec{r}$ in H with $T\vec{r}$, one obtain an expression for H in the coordinates $\vec{r}$ which look exactly the same as the original expression for the Hamiltonian. For instance, the symmetry group of the Hamiltonian describing an electron moving in the field of a nucleous consists of all rotations around axes passing through the nucleous.Thes rotations transfroms the nucleous into itself, so that the potential energy must be invariant under the whole rotation group. If V refers to an electron in a crystal, V would then be invariant under some set of translations which transform the crystal into itself. The symmetry group G of a system becomes, in this way, the (symmetry) group of the Schrödinger equation or the symmetry group of H.

The significance of G for solving problems in quantum mechanics is contained in an important theorem.
Consider a l-fold degenerate energy eigenvalue E_l of H and let $\phi_n(\vec{r})$, $n = 1, 2, ..., l$ the set of linearly independent eigenfunctions corresponding to this eigenvalue, so that

$$H(\vec{r})\phi_n(\vec{r}) = E_l\phi_n(\vec{r}), \forall n$$

Suppose to have a set G of transformations T which leave the Hamiltonian invariant, and that G forms a group. Consider the function $O_T\phi(\vec{r})$, where O_T is defined by the equation $O_T\phi(\vec{r}) = \phi(T^{-1}\vec{r})$.
Lemma: $[O_T, H] = 0$.
Proof:

$$O_T(H\phi)(\vec{r}) = H(T^{-1}\vec{r})\phi(T^{-1}\vec{r}) = H(\vec{r})\phi(T^{-1}\vec{r}) = HO_T\phi(\vec{r})$$

As O_T commute with $H(\vec{r})$,

$$H(\vec{r})O_T\phi_n(\vec{r}) = O_T H(\vec{r})\phi_n(\vec{r}) = O_T E_l \phi_n(\vec{r}) = E_l O_T \phi_n(\vec{r})$$

so that $O_T\phi_n(\vec{r})$ **is also an eigenfunctions of** $H(\vec{r})$ **with the same eigenvalue** E_l. As E_l was assumed to have only l linear independent eigenfunctions, $O_T\phi_n$ must be some linear combination of the eigenfunctions ϕ_n. Thus, $O_T\phi_n$ may be written as

$$O_T\phi_n(\vec{r}) = \sum_{mn} D(T)_{mn}\phi_m(\vec{r})$$

Repeating this procedure for each of the l functions establishes an array of l^2 numbers D_{mn} for each transformation O_T of the symmetry group.
Theorem: this set of matrices form a l-dimensional matrix representation of the symmetry group of the Hamiltonian.
Proof: From

$$\begin{aligned}
O_S\phi_n &= \sum_m D(S)_{mn}\phi_m \\
O_R\phi_q &= \sum_p D(R)_{pq}\phi_p \\
O_S O_R\phi_n &= O_S(\sum_p D(R)_{pn}\phi_p) \\
&= \sum_p D(R)_{pn}\sum_m D(S)_{mp}\phi_m \\
&= \sum_m(\sum_p D(S)_{mp}D(R)_{pn})\phi_m
\end{aligned}$$

and

$$O_{SR}\phi_n = \sum_m D_{mn}(SR)\phi_m$$

we obtain, because of $O_{SR} = O_S O_R$

$$D_{mn}(SR) = \sum_p D_{mp}(S)D_{pn}(R)$$

which can be written as the matrix product $D(RS) = D(S)D(R)$.
We have therefore demonstrated that a set of energy eigenfunctions corresponding to an l-fold degenerate eigenvalue form a basis for a l dimensional representation of the symmetry group. These functions form a basis for the representation D, the function $\phi_n(\vec{r})$ being said to transform according to the n-the column of this representation (or to belong to the n-th column of the representation D). This means that the coefficients of the linear combination

determining the transformed n-the basis function are to be read out from the n-the column of the matrix. Every energy level therefore corresponds to some representation of the group of the Schrödinger equation. Notice that the representation could be reducible of irreducible. Quite generally, we expect that the representation behind an energy level be an irreducible one, but we cannot exclude that some energy levels sustain reducible representations. An energy eigenvalue corresponding to a reducible representation is then considered an 'accidental' degeneracy between energy levels corresponding to its constituent irreducible representations. Accidental degeneracy is not demanded by the symmetry of the system, in contrast to essential degeneracy, which is demanded by the dimension of some irreducible representations being larger than one. Notice that we might be overlooking some symmetries of the system, and this might produce extra degeneracy, which is also accidental – because of our ignorance in capturing all symmetries of the system. If other symmetry elements are present, they might render a representation, which is reducible under a more restricted number of elements, irreducible under the enlarged set of symmetry operations.

3.2 Construction of Basis functions and matrix representations

We have just proved that the eigenspaces of the Hamilton operator carry representations of the symmetry group of the Hamiltonian. Group theoretical methods work the other way around: one tries to construct – using symmetry arguments alone, without solving explicitely any eigenvalue equation – subspaces which are invariant with respect to a given irreducible representation of the symmetry group. These symmetry constructed functions might immediately diagonalize H, i.e. some of the eigenvalues of H can be immediately derived by applying H onto each representative wave function in each subspace. The way to construct such invariant subspaces is described by the following theorem: **Theorem**: Consider any vector ϕ within the Hilbert space L acted upon by the operator H and let G the symmetry group of H. The wave function

$$P_n^{(p)}\phi \doteq l_p \cdot \mathcal{M}_T D_{nn}^{*(p)}(T) O_T \phi \doteq \psi_n^{(p)}$$

transforms according to the n-th row of the irreducible representation D^p of the group G. The so defined operator $P_n^{(p)}$ projects out of any wave function those parts transforming according to the various rows of an irreducible representation. The set of functions generated by repeated application of the projection operator for all indices n are so called "symmetry adapted" wave

functions, i.e. they represent an invariant subspace L^p of L carrying the irreducible representation D^p.
Proof: We think on the expansion psi as a linear combination of wave functions of the type psi^q_m, where some m and q will appear with some coefficient (which can be zero). Let us apply P^p_n onto each single $\phi^{(q)}_m$. Then

$$\begin{aligned}
P^p_n \phi^q_m &= l_p \mathcal{M}_T D^{*(p)}_{nn} O_T \phi^q_m \\
&= l_p \mathcal{M}_T D^{*(p)}_{nn}(T) \sum_k D^{(q)}_{km}(T) \phi^q_k \\
&= \delta_{pq} \cdot \sum_k \delta_{nm} \delta_{nk} \phi^{(q)}_k \\
&= \delta_{pq} \cdot \delta_{nm} \phi^q_n
\end{aligned}$$

This equation states that applying the projector P^p_n onto the functions ψ^q_m forthcoming in the expansion of psi gives either zero if $p \neq q$ and $m \neq n$ or else the function itself. Thus, using the projector, one can project out symmetry adapted wave functions out of any function. Of course, it might be that the sought for symmetry adapted wave functions are not contained in ψ, so that the result of applying the projector is zero. In that case, in order to generate symmetry adapted wave functions, one must repeat the the procedure with another "trial" wave function ψ. This projector technique is a direct procedure for constructing basis functions of any Hamiltonian using symmetry arguments alone, without solving explicitly the eigenvalue problem. It requires an explicit knowledge of the matrix element of the various representations, and not merely a knowledge of the characters alone, which is the usual information given in the published literature. For one-dimensional representations the characters are the matrix elements them selves, so that this projector technique provide the complete answer for the basis functions of one-dimensional representations. For representations with larger dimension, the procedure to obtain n-partners of a basis set for an irreducible representation from the characters is based on the projector

$$P^{(p)} \doteq \sum_n P^{(p)}_n = l_p \mathcal{M}_T \chi^{*(p)}(T) O_T$$

which projects out of any normalizable wave function the sum of all basis functions transforming according to the columns of the p-th irreducible representation. This last projector reuqires only the knowledge of the characters of the irreducible represenation of which one would like to construct symmetry adapted wave functions. Of course, the projector dos not produce all partners within the irreducible subspace. However, having determined $\phi^{(p)}$, we can then apply to $\phi^{(p)}$ the operations of the symmetry group to obtain exactly l_p-linear independent functions which can be made orthonormal and thus can be used as a basis set for the irreducible representation D^p (remember taht application of the operations of the group to a function belonging to an invariant subspace carrying the irreducible representation D^p does not bring us outside this subspace). Notice that, after having generated the basis functions transforming according to the irreducible representation D^p, it is possible to construct the matrix representation of D^p (in practice, this is the procedure most adopted to construct matrix representations of the irreducible representations), using

$$O_T \phi_n^{(p)} = \sum_m D^p_{nm}(T)\phi^p_m$$

This procedure requires only the initial knowledge of the characters.

3.3 Applications to quantum mechanical problems

We have now produced a set of symmetry adapted basis functions and our intuitive knowledge of group theory tells us that they can be used produce eigenvalues of H without explicitely solving any eigenvalue problem. What can we do exactly with these functions? Their application to quantum mechanics rests on the following Lemma.

Lemma: Let G be a group with average and $\phi(k, m_k, r)$ be a basis function transforming according to the m_k-th column of the unitary irreducible representation D^k of the group G.

The index r must be introduced because functions having the same symmetry under the operations of G might differ on aspects other then their symmetry. In the case of $SO(3)$, for example, functions which have a certain symmetry under rotations might have a different radial dependence (i.e. they might have a different quantum number n).

Let also $\phi(l, m_l, s)$ be a basis function transforming according to the m_l-th column of the irreducible representation D^l. Then

$$\Big(\phi(k, m_k, r), \phi(l, m_l, s)\Big) = \delta_{kl}\delta_{m_k m_l} \cdot C(r, s, k)$$

i.e. the scalar product of two basis functions is vanishing if the basis functions belong to different irreducible representations or to different columns of the same irreducible representation. Else is the scalar product a constant which does not depend on m_k but only on k, r, s.

Proof: Since the scalar product of two functions is invariant under unitary transformations, for any operation $T \in G$

$$\begin{aligned}
\Big(\phi(k,m_k,r),\phi(l,m_l,s)\Big) &= \Big(O_T\phi(k,m_k,r),O_T\phi(l,m_l,s)\Big) \Longrightarrow \\
\Big(\phi(k,m_k,r),\phi(l,m_l,s)\Big) &= (\sum_{m_p}^{l_k} D^k_{m_p m_k}(T)\phi(k,m_p,r),\sum_{m_q}^{l_l} D^l_{m_q m_l}(T)\phi(l,m_q,s)) \\
&= \sum_{m_p,m_q} D^{*k}_{m_p m_k}(T)D^l_{m_q m_l}(T)(\phi(k,m_p,r),\phi(l,m_q,s))
\end{aligned}$$

Taking the average over both sides we obtain

$$\begin{aligned}
\Big(\phi(k,m_k,r),\phi(l,m_l,s)\Big) &= \sum_{m_p,m_q}(\phi(k,m_p,r),\phi(l,m_q,s))\cdot\Big(M_{T\in G}D^{*k}_{m_p m_k}(T)D^l_{m_q m_l}(T)\Big) \\
&= \frac{1}{l_k}\delta_{kl}\delta_{m_k m_l}\sum_{m_p m_q}\delta_{m_p m_q}(\phi(k,m_p,r),\phi(l,m_q,s)) \\
&= \delta_{kl}\delta_{m_k m_l}\frac{1}{l_k}\sum_{m_p}(\phi(k,m_p,r),\phi(l,m_p,s))
\end{aligned}$$

This proves the orthogonality of the basis functions. As the right hand side is independent of m_k and m_l, provided m_k and m_l are equal, the scalar product does not depend on the column index but only on k, r and s. The remaining constant i.e. $\frac{1}{l_k}\cdot\sum_{m_p}(\phi(k,m_p,r),\phi(l,m_p,s))$ must, in general, be explicitly computed, as symmetry arguments no longer help.

Example 1: The Hamiltonian matrix

A simple application of this Lemma involves the Hamilton operator. It can be shown, using the same proof introduced for the Lemma, that

$$\Big(\phi(k,m_k,r),H\phi(l,m_l,s)\Big) = \delta_{kl}\delta_{m_k m_l}\cdot H(r,s,k)$$

This formula tells us that symmetry adapted basis funtions can be used to block diagonalize the Hamilton operator. In fact, suppose to group together all basis functions belonging to the same irreducible representation k and with different index r and take, for each group r, only one basis function $\phi(k,m_k,r)$. Then the Hamiltonian matrix takes a block-diagonalized form, the dimension of each block being equal to the number of times an irreducible representation occurs in the level scheme. The problem is then considerably simplified because it has essentially been reduced to determining the eigenvalues of the blocks separately.

$$\begin{pmatrix} H(1,1) & 0 & 0 & 0 & ... & 0 & 0 & ... \\ 0 & H(1,2) & 0 & ... & 0 & 0 & 0 & ... \\ 0 & 0 & H(3) & 0 & ... & 0 & 0 & ... \\ ... & ... & ... & ... & ... & ... & ... & ... \\ 0 & 0 & 0 & ... & 0 & H(k,m) & 0 & ... \\ ... & ... & ... & ... & ... & ... & ... & ... \end{pmatrix}$$

with

$$H(k,m)_{r,s} = \Big(\phi(k,m_k,r), H\phi(k,m_k,s)\Big)$$

Depending on how many time the irreducible representation can occur in the energy level scheme, this block can still be quite large, but a sizeable reduction has been achieved, without loosing accuracy. Should we decide, in the spirit of perturbation theory, that only matrix elements with $r = s$ are sizeable, then the Hamilton matrix is immediately diagonalized (although we have lost accuracy). Should we truncate the number of different levels r considered to a small one, e.g. only considering those r's which are 'close' in energy, then we loose again accuracy, but, having used symmetrized wave functions, we hope that the loss of accuracy is minimized.

Example 2: Symmetry-breaking perturbations

A further application of group theory is the problem of static perturbation of a well know Hamiltonian. Consider a system with a Hamiltonian H_0, and suppose that a static perturbation V is applied giving a new Hamiltonian $H = H_0 + V$. Let G_0 and G_V be the respective groups of the Schrödinger equation. In general, not every transformation of G_0 will leave V invariant, although every transformation of G_V will leave H invariant, so that in general, we can assume that G_V is a subgroup of G_0. By assumption, the eigenfunctions of H_0 are known. As discussed, they can be grouped into invariant subsets (according to their degeneracy) where each subset forms a basis of an irreducible representation of G_0. Let us denote the eigenvalues of H_0 by E^0_α, which is l_α-fold degenerate so that there are l_α independent eigenfunctions $\phi_1, ..., \phi_{l_\alpha}$, all having the same eigenvalue. These eigenfunctions form a basis for an irreducible representation D^α of G_0. If we now imagine that the perturbation V is switched on, the group of symmetry will be reduced to G_V. Since G_V is a subgroup of G_0, the same functions ϕ_i will still generate an l_α-dimensional representation of G. However, whne restricted to the elements of G_V, this representation is, in general, a reducible one. Suppose that,

$$D^\alpha = \oplus_i n_i D^i$$

Γ_1	Γ_2	Γ_{12}	Γ'_{25}	Γ'_{15}
Δ_1	Δ_2	$\Delta_1 + \Delta_2$	$\Delta'_2 + \Delta_5$	$\Delta'_1 + \Delta_5$
Γ'_1	Γ'_2	Γ'_{12}	Γ_{25}	Γ_{15}
Δ'_1	Δ'_2	$\Delta'_1 + \Delta'_2$	$\Delta_2 + \Delta_5$	$\Delta_1 + \Delta_5$

where D^i are irreducible representation of G_V. This means that we get new subsets from the set of original functions ϕ_i such that a function in a subset mixes only with the functions of the same subset under the operations of the restricted group G_V. These subsets must all belong to different eigenvalues (except in the case of accidental degeneracy) and hence the original energy level E^0_α splits into a number of energy levels due to the lowering of symmetry. Using e.g. the projector operator technique, we are able to project out from the original invariant subspace all the subspaces which are invariant under the restricted number of symmetry operatoion. These are symmetry adapted wave functions that (block) diagonalize $H_0 + V$. If D^α is an irreducible representation of G, then the level will not split, although its value may be changed.

Example 3: Compatibility relations

Let us consider a group G and a subgroup S. Given a representation of G, let us choose from these matrices only those matrices corresponding to the elements of the subgroup S. We obtain, in this way, a set of matrices representing S. The representation obtained for S is in general reducible, even when the original representation of the full group is irreducible. It may be decomposed using the standard procedure into a number of irreducible representations of the subgroup that are said to be **compatible** with the given irreducible representation of G. Consider for instance the group O_h and the subgroup C_{4v}. The decomposition of the irreducible representations Γ_i of the group O_h into the irreducible representations Δ_i of the group C_{4v} is given in the table.
Exercise: Find the $\Gamma - \Lambda$ the $L - \Lambda$ and the $X - \Delta$ compatibility tables.

3.4 Exercises

1. Find the invariant subspaces in the three dimensional space carrying the three dimensional representation of C_{3v}. For which value of x in R^x we will find invariant subspaces belonging to all irreducible representations of C_{3v}?

2. Find the symmetry adapted vectors belonging to $\Delta_1, \Delta_2, \Delta_{2'}, \Delta_5$ in the four dimensional representation of C_{4v}.

3. Hückel theorie of molecular binding. Within a single electron model for the binding energy of molecules, the one electron levels are first calculated. The various levels are then filled taking the Pauli principle into account, and the total energy of the molecule is found by summing the energy of the electrons which has found place in the levels. Our understanding of the H_2^+ molecule tells us that the one-electron Hamilton operator consists of two parts: a diagonal one describing the energy of the electron residing close to each atom, and a non-diagonal one which describes the interaction of the electron with the neighbouring atoms. The non-vanishing matrix elements of this interaction Hamiltonian are between the basis function describing the electron residing at one atom and the basis functions describing the electrons residing on the neighbouring atoms. If the corners of the molecule are loaded with numbers, the interaction operator can be seen as a map associating to each corner the sum of the numbers residing of the neighbours corners.
i) Construct the interaction Hamiltonian for molecules arranged on a regular planar polyeder with N corners and show that it is invariant with respect to the symmetry operations of the system.
ii) find (without solving explicitely the determinantal equation) eigenvalues and eigenvectors for one electron moving in the field of atoms centered at the corners of a planar equilateral tringle and of a square.

4. Find the symmetry adapted polynomials transforming according to $\Delta_1, \Delta_2, \Delta_{2'}, \Delta_5$ within the Hilbertspace $f(|\vec{r}|)\cdot$ polynomial with degree ≤ 2 in the variables x, y, z. Discuss the splitting of the corresponding atomic levels when the electrons are immersed in a potential with C_{4v} symmetry.

5. Find the irreducible representations of O_h according to which the spherical harmonics $Y_{l,m}$ with $m = -l, ..+l$ and $l = 0, 1, 2$ transforms. Discuss the splitting of s, p, d atomic levels when the electrons are immersed in a potential with O_h symmetry.

6. Plot a possible bandstructure due to s, p, d-electrons at the Γ-point and along Δ for Na,Si,Ge,and Cu.

In the following, you will find some tables and figizers that will help in solving the exercises.

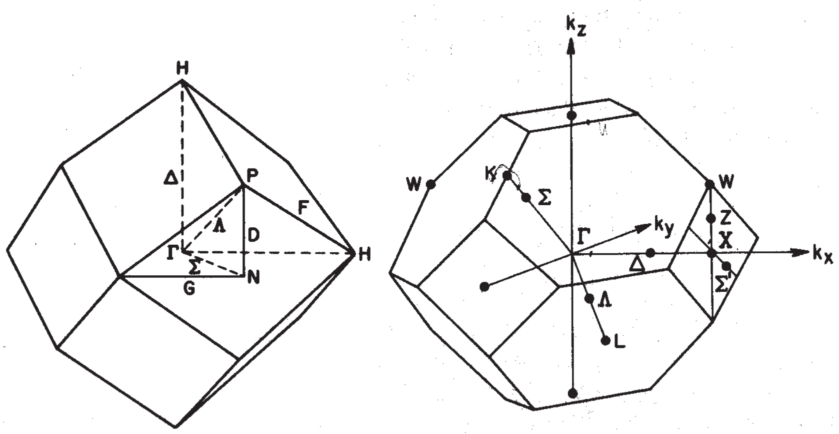

Figure 3.1: Brillouin zone for the bcc-lattice (left) and for the fcc lattice (right), showing the symmetry points and lines.

Character Table for the Cubic Group

Representation	Basis	E	$3C_4^2$	$6C_4$	$6C_2$	$8C_3$	J	$3JC_4^2$	$6JC_4$	$6JC_2$	$8JC_3$
Γ_1	1	1	1	1	1	1	1	1	1	1	1
Γ_2	$x^4(y^2 - z^2) + y^4(z^2 - x^2) + z^4(x^2 - y^2)$	1	1	−1	−1	1	1	1	−1	−1	1
Γ_{12}	$x^2 - y^2$, $2z^2 - x^2 - y^2$	2	2	0	0	−1	2	2	0	0	−1
Γ_{15}	x, y, z	3	−1	1	−1	0	−3	1	−1	1	0
Γ_{25}	$z(x^2 - y^2)$	3	−1	−1	1	0	−3	1	1	−1	0
Γ_1'	$xyz[x^4(y^2 - z^2) + y^4(z^2 - x^2) + z^4(x^2 - y^2)]$	1	1	1	1	1	−1	−1	−1	−1	−1
Γ_2'	xyz	1	1	−1	−1	1	−1	−1	1	1	−1
Γ_{12}'	$xyz(x^2 - y^2)$, $x \cdot y \cdot z(z^2 - 1/2(x^2+y^2))$	2	2	0	0	−1	−2	−2	0	0	1
Γ_{15}'	$xy(x^2 - y^2)$	3	−1	1	−1	0	3	−1	1	−1	0
Γ_{25}'	xy, yz, zx	3	−1	−1	1	0	3	−1	−1	1	0

Character Table: Group of Δ

Representation	Basis	E	C_4^2	C_4	JC_4^2	JC_2
Δ_1	$1, x, 2x^2 - y^2 - z^2$	1	1	1	1	1
Δ_2	$y^2 - z^2$	1	1	−1	1	−1
Δ_2'	yz	1	1	−1	−1	1
Δ_1'	$yz(y^2 - z^2)$	1	1	1	−1	−1
Δ_5	$y, z; xy, xz$	2	−2	0	0	0

Figure 3.2:

CHARACTER TABLE, GROUP OF $P = (2\pi/a)\ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

Representation	Basis	E	$3C_4^2$	$8C_3$	$6JC_4$	$6JC_2$
P_1	$1, xyz$	1	1	1	1	1
P_2	$x^4(y^2 - z^2) + y^4(z^2 - x^2) + z^4(x^2 - y^2)$	1	1	1	-1	-1
P_3	$x^2 - y^2, xyz(x^2 - y^2)$	2	2	-1	0	0
P_4	$x, y, z; xy; yz; zx$	3	-1	0	-1	1
P_5	$z(x^2 - y^2)$	3	-1	0	1	-1

TABLE VI

CHARACTER TABLE, GROUP OF $N = (2\pi/a)\ (\frac{1}{2}, \frac{1}{2}, 0)$

Representation	Basis	E	C_4^2	$C_2\Vert$	$C_2\perp$	J	JC_4^2	$JC_2\perp$	$JC_2\Vert$
N_1	$1, xy, 3z^2 - r^2$	1	1	1	1	1	1	1	1
N_2	$z(x - y)$	1	-1	1	-1	1	-1	-1	1
N_3	$z(x + y)$	1	-1	-1	1	1	-1	1	-1
N_4	$x^2 - y^2$	1	1	-1	-1	1	1	-1	-1
N_1'	$x + y$	1	-1	1	-1	-1	1	1	-1
N_2'	$z(x^2 - y^2)$	1	1	1	1	-1	-1	-1	-1
N_3'	z	1	1	-1	-1	-1	-1	1	1
N_4'	$x - y$	1	-1	-1	1	-1	1	-1	1

TABLE VII

CHARACTER TABLE, GROUP OF Λ, F^a

Representation	Basis	E	$2C_3$	$3JC_2$
Λ_1	$1, x + y + z$	1	1	1
Λ_2	$x(y^2 - z^2) + y(z^2 - x^2) + z(x^2 - y^2)$	1	1	-1
Λ_3	$2x - y - z, y - z$	2	-1	0

[a] $F = (2\pi/a)(\frac{1}{2} + x, \frac{1}{2} - x, \frac{1}{2} - x); \quad 0 \leqslant x \leqslant \frac{1}{2}$

Figure 3.3:

CHARACTER TABLE, GROUP OF $\Sigma = (2\pi/a)\ (x, x, 0)$

Representation	Basis	E	C_2	$JC_4{}^2$	JC_2
Σ_1	$1, x + y$	1	1	1	1
Σ_2	$z(x - y);\quad z(x^2 - y^2)$	1	1	-1	-1
Σ_3	$z;\quad z(x + y)$	1	-1	-1	1
Σ_4	$x - y;\quad x^2 - y^2$	1	-1	1	-1

TABLE XII

CHARACTER TABLES OF G, K, U, D, Z, S

	Z	E	$C_4{}^2$	$JC_4{}^2$	$JC_4{}^2 \perp$
Representation	G, K, U, S	E	C_2	$JC_4{}^2$	JC_2
	D	E	$C_4{}^2$	JC_2	$JC_2 \perp$
K_1	$1, x + y$	1	1	1	1
K_2	$z(x - y),\quad z(x^2 - y^2)$	1	1	-1	-1
K_3	$z,\quad z(x + y)$	1	-1	-1	1
K_4	$x - y;\quad x^2 - y^2$	1	-1	1	-1

$$G = \frac{2\pi}{a}\left(\tfrac{1}{2} + x, \tfrac{1}{2} - x, 0\right) \quad \text{(bcc)}; \qquad K = \frac{2\pi}{a}\left(\tfrac{3}{4}, \tfrac{3}{4}, 0\right) \quad \text{(fcc)}$$

$$U = \frac{2\pi}{a}\left(1, \tfrac{1}{4}, \tfrac{1}{4}\right) \quad \text{(fcc)}; \qquad D = \frac{2\pi}{a}\left(\tfrac{1}{2}, \tfrac{1}{2}, x\right) \quad \text{(bcc)}$$

$$Z = \frac{2\pi}{a}(1, x, 0) \quad \text{(fcc)}; \qquad S = \frac{2\pi}{a}(1, x, x) \quad \text{(fcc)}$$

Figure 3.4:

CHARACTER TABLE, GROUP OF $X = (2\pi/a)\ (1, 0, 0)$

Representation	Basis	E	$2C_4^2\perp$	$C_4^2\parallel$	$2C_4\parallel$	$2C_2$	J	$2JC_4^2\perp$	$JC_4^2\parallel$	$2JC_4\parallel$	$2JC_2$
X_1	$1, 2x^2 - y^2 - z^2$	1	1	1	1	1	1	1	1	1	1
X_2	$y^2 - z^2$	1	1	1	−1	−1	1	1	1	−1	−1
X_3	yz	1	−1	1	−1	1	1	−1	1	−1	1
X_4	$yz(y^2 - z^2)$	1	−1	1	1	−1	1	−1	1	1	−1
X_5	xy, xz	2	0	−2	0	0	2	0	−2	0	0
X_1'	$xyz(y^2 - z^2)$	1	1	1	1	1	−1	−1	−1	−1	−1
X_2'	xyz	1	1	1	−1	−1	−1	−1	−1	1	1
X_3'	$x(y^2 - z^2)$	1	−1	1	−1	1	−1	1	−1	1	−1
X_4'	x	1	−1	1	1	−1	−1	1	−1	−1	1
X_5'	y, z	2	0	−2	0	0	−2	0	2	0	0

CHARACTER TABLE, GROUP OF $L = (2\pi/a)\ (\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$

Representation	Basis	E	$2C_3$	$3C_2$	J	$2JC_3$	$3JC_2$
L_1	$1, xy + yz + xz$	1	1	1	1	1	1
L_2	$yz(y^2 - z^2) + xy(x^2 - y^2) + xz(z^2 - x^2)$	1	1	−1	1	1	−1
L_3	$2x^2 - y^2 - z^2;\ \ y^2 - z^2$	2	−1	0	2	−1	0
L_1'	$x(y^2 - z^2) + y(z^2 - x^2) + z(x^2 - y^2)$	1	1	1	−1	−1	−1
L_2'	$x + y + z$	1	1	−1	−1	−1	1
L_3'	$y - z;\ \ 2x - y - z$	2	−1	0	−2	1	0

TABLE X

CHARACTER TABLE, GROUP OF $W_1 = (2\pi/a)\ (1, \frac{1}{2}, 0)$

Representation	Basis	E	C_4^2	$2C_2$	$2JC_4$	$2JC_4^2$
W_1	$1, 2y^2 - x^2 - z^2$	1	1	1	1	1
W_1'	xz	1	1	1	−1	−1
W_2	xyz	1	1	−1	1	−1
W_2'	$y, z^2 - x^2$	1	1	−1	−1	1
W_3	$xy, yz; x, z$	2	−2	0	0	0

Figure 3.5:

Linear combination of spherical harmonics up to $l = 3$ that are partner functions for the irreducible representations of point group O_h. The expression of spherical harmonics in cartesian coordinates is given on the left side of the table. The phase convention is that of Condon and Shortley after C. J. Ballhausen, *Ligand Field Theory* (McGraw-Hill, 1962)

s state	$Y_{00} = \frac{1}{\sqrt{4\pi}}$	Γ_1	$s = \frac{1}{\sqrt{4\pi}} = Y_{00}$
p state	$Y_{11} = -\sqrt{\left(\frac{3}{8\pi}\right)}\frac{x+iy}{r}$	Γ_{15}	$p_x = \sqrt{\left(\frac{3}{4\pi}\right)}\frac{x}{r} = \frac{1}{\sqrt{2}}(-Y_{11}+Y_{1-1})$
	$Y_{10} = \sqrt{\left(\frac{3}{4\pi}\right)}\frac{z}{r}$		$p_y = \sqrt{\left(\frac{3}{4\pi}\right)}\frac{y}{r} = \frac{i}{\sqrt{2}}(Y_{11}+Y_{1-1})$
	$Y_{1-1} = \sqrt{\left(\frac{3}{8\pi}\right)}\frac{x-iy}{r}$		$p_z = \sqrt{\left(\frac{3}{4\pi}\right)}\frac{z}{r} = Y_{10}$
d state	$Y_{22} = \sqrt{\left(\frac{15}{32\pi}\right)}\frac{(x+iy)^2}{r^2}$	Γ'_{25}	$d_{xz} = \sqrt{\left(\frac{15}{4\pi}\right)}\frac{xz}{r^2} = \frac{1}{\sqrt{2}}(-Y_{21}+Y_{2-1})$
	$Y_{21} = -\sqrt{\left(\frac{15}{8\pi}\right)}\frac{(x+iy)z}{r^2}$		$d_{xy} = \sqrt{\left(\frac{15}{4\pi}\right)}\frac{xy}{r^2} = \frac{-i}{\sqrt{2}}(Y_{22}-Y_{2-2})$
	$Y_{20} = \sqrt{\left(\frac{5}{16\pi}\right)}\frac{3z^2-r^2}{r^2}$		$d_{yz} = \sqrt{\left(\frac{15}{4\pi}\right)}\frac{yz}{r^2} = \frac{i}{\sqrt{2}}(Y_{21}+Y_{2-1})$
	$Y_{2-1} = \sqrt{\left(\frac{15}{8\pi}\right)}\frac{(x-iy)z}{r^2}$	Γ_{12}	$d_{3z^2-r^2} = \sqrt{\left(\frac{5}{16\pi}\right)}\frac{3z^2-r^2}{r^2} = Y_{20}$
	$Y_{2-2} = \left(\sqrt{\frac{15}{32\pi}}\right)\frac{(x-iy)^2}{r^2}$		$d_{x^2-y^2} = \sqrt{\left(\frac{15}{16\pi}\right)}\frac{x^2-y^2}{r^2} = \frac{1}{\sqrt{2}}(Y_{22}+Y_{2-2})$
f state	$Y_{33} = -\sqrt{\frac{7}{4}}\sqrt{\left(\frac{5}{16\pi}\right)}\frac{(x+iy)^3}{r^3}$	Γ_{15}	$f_{(5x^2-3r^2)x} = \sqrt{\frac{7}{4}}\sqrt{\left(\frac{1}{4\pi}\right)}\frac{(5x^2-3r^2)x}{r^3} = \sqrt{\left(\frac{3}{16}\right)}(Y_{31}-Y_{3-1}) - \sqrt{\left(\frac{5}{16}\right)}(Y_{33}-Y_{3-3})$
	$Y_{32} = \sqrt{\frac{7}{4}}\sqrt{\left(\frac{15}{8\pi}\right)}\frac{(x+iy)^2 z}{r^3}$		$f_{(5y^2-3r^2)y} = \sqrt{\frac{7}{4}}\sqrt{\left(\frac{1}{4\pi}\right)}\frac{(5y^2-3r^2)y}{r^3} = -i\sqrt{\left(\frac{3}{16}\right)}(Y_{31}+Y_{3-1}) - i\sqrt{\left(\frac{5}{16}\right)}(Y_{33}+Y_{3-3})$
	$Y_{31} = -\sqrt{\frac{7}{4}}\sqrt{\left(\frac{3}{16\pi}\right)}\frac{(x+iy)(5z^2-r^2)}{r^3}$		$f_{(5z^2-3r^2)z} = \sqrt{\frac{7}{4}}\sqrt{\left(\frac{1}{4\pi}\right)}\frac{(5z^2-3r^2)z}{r^3} = Y_{30}$
	$Y_{30} = \sqrt{\frac{7}{4}}\sqrt{\left(\frac{1}{4\pi}\right)}\frac{(5z^2-3r^2)z}{r^3}$	Γ_{25}	$f_{(x^2-z^2)y} = \sqrt{\frac{7}{4}}\sqrt{\left(\frac{15}{4\pi}\right)}\frac{(x^2-z^2)y}{r^3} = -i\sqrt{\left(\frac{5}{16}\right)}(Y_{31}+Y_{3-1}) + i\sqrt{\left(\frac{3}{16}\right)}(Y_{33}+Y_{3-3})$
	$Y_{3-1} = \sqrt{\frac{7}{4}}\sqrt{\left(\frac{3}{16\pi}\right)}\frac{(x-iy)(5z^2-r^2)}{r^3}$		$f_{(x^2-y^2)z} = \sqrt{\frac{7}{4}}\sqrt{\left(\frac{15}{4\pi}\right)}\frac{(x^2-y^2)z}{r^3} = \frac{1}{\sqrt{2}}(Y_{32}+Y_{3-2})$
	$Y_{3-2} = \sqrt{\frac{7}{4}}\sqrt{\left(\frac{15}{8\pi}\right)}\frac{(x-iy)^2 z}{r^3}$		$f_{(y^2-z^2)x} = \sqrt{\frac{7}{4}}\sqrt{\left(\frac{15}{4\pi}\right)}\frac{(y^2-z^2)x}{r^3} = \sqrt{\left(\frac{5}{16}\right)}(Y_{31}-Y_{3-1}) + \sqrt{\left(\frac{3}{16}\right)}(Y_{33}-Y_{3-3})$
	$Y_{3-3} = \sqrt{\frac{7}{4}}\sqrt{\left(\frac{5}{16\pi}\right)}\frac{(x-iy)^3}{r^3}$	Γ'_2	$f_{xyz} = \sqrt{\frac{7}{4}}\sqrt{\left(\frac{15}{\pi}\right)}\frac{xyz}{r^3} = -\frac{i}{\sqrt{2}}(Y_{32}-Y_{3-2})$

Figure 3.6:

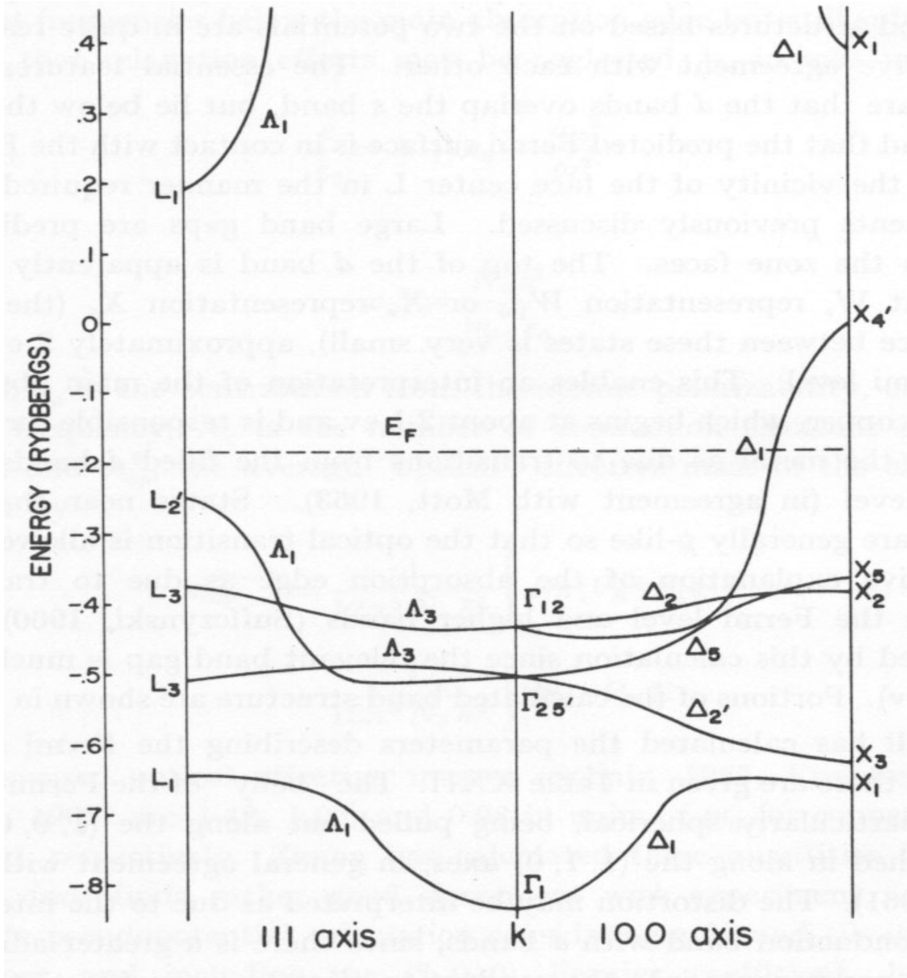
ENERGY (RYDBERGS)
.4
.3
.2
.1
0
-.1
-.2
-.3
-.4
-.5
-.6
-.7
-.8
E_F
L_1
L_2'
L_3
L_3
L_1
Λ_1
Λ_1
Λ_3
Λ_3
Λ_1
Γ_{12}
$\Gamma_{25'}$
Γ_1
Δ_1
Δ_1
Δ_2
Δ_5
$\Delta_{2'}$
Δ_1
X_1
$X_{4'}$
X_5
X_2
X_3
X_1
111 axis
K
100 axis

Figure 3.7:

Chapter 4

$SO(3)$ and $SU(2)$

The simplest example of quantum mechanical problem, the Hydrogen atom, has a symmetry group consisting of all rotations. We discuss now this important group and its representations.

4.1 Lie Algebra

The equation

$$x(a_1, a_2, ...a_r) = exp[\sum_{j=1}^{r} i a_j I_j]$$

defines a set of operators I_j, $j = 1, .., r$ which can be used to generate the entire Lie group by means of an exponential mapping.
Theorem: The r generators of a Lie group are the basis for an r-dimensional vector space.
Proof. We must prove that if I_l and I_k are infinitesimal generators of the group then any linear conbination of them is also a generator. Let

$$x_l = x(0, 0, ..., \epsilon_l, 0, ...0) = e + i\epsilon I_l$$
$$x_k = x(0, 0, ..., \epsilon_k, 0, ...0) = e + i\epsilon I_k$$

Then the following equation holds true:

$$x(0, 0, ..., \epsilon_l \cdot \alpha, 0.., 0)x(0, 0, ..., \epsilon_k \cdot \beta, 0...0) = e + i\epsilon(\alpha I_l + \beta I_k)$$

(QED).
In order to use the exponential expression of the group elements in terms of infinitesimal generators to perform the group operation between any two or more elements of the group, we need to be able to calculate expression such as $exp(A_1) \cdot exp(A_2)$, A_1 and A_2 being, in general, matrices. This is performed by

means of the Baxter-Campell-Haussdorf (BCH) formula, $exp(A_1) \cdot exp(A_2) = exp(A)$ with

$$A = A_1 + A_2 + \frac{1}{2}[A_1, A_2] + \frac{1}{12}\Big(\big[[A_1, A_2], A_2\big] + \big[[A_2, A_1], A_1\big]\Big) + ...$$

where $[A, B] \doteq AB - BA$ is the commutator of the two operators A, B. This formula implies that the product of two elements of the group involves commutators between any I_l and I_k. This establishes a further law of composition within the vector space of the generators, which becomes a **Lie algebra**. Quite generally, a Lie-Algebra is a r dimensional vector space L_G with elements $A, B, ...$ endowed with a law of composition for any two elements of L_G denoted by $[A, B]$ such that

1. $[A, B] \in L$
2. $[A, B] = -[A, B]$
3. (Jacobi identity) $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$

for all elements in L. The law of composition [....] is known as the commutator of A, B. A set of r-linear independent vectors of L_G is called a basis of the Lie algebra in analogy with the basis of a vector space. Because the Lie algebra is closed with respect to the commutator operation, we are able to calculate all possible commutators once the so called structure relations between the vectors of the basis are known:

$$[I_l, I_k] = \sum_{J=1}^{r} c_{lk}^{j} I_j,$$

$1 \leq l, k \leq r$, where c_{lk}^{j} are certain coefficients. The commutators of pairs of generators of a Lie group determine the structure of the Lie group completely, in analogy with the multiplication table for a finite group. Therefore, the coefficients c_{lk}^{j} appearing in the structure relations are known as **structure constants** of the Lie algebra and of the Lie group. They are a characteristic property of the Lie group and do not depend on any particular representation of the generators. However, they are not unique, since the generators of a Lie group are themselves not unique.
Theorem: provided the representation of the Lie group is chosen to be unitary, the generators are hermitic operators and the structure constants are purely imaginary numbers.
Proof: We require from any element $exp(iI_ja_j)$ that $exp(-ia_jI_j^\dagger)exp(ia_jI_j) =$

$exp(0)$, which is only possible if $I_j^\dagger = I_j$, i.e. the generators are hermitic (here we have used the fact that $(A^n)^t = (A^t)^n$). Furthermore, from

$$\sum_{j=1}^{r}(-c_{lk}^j)I_j = -[I_l, I_k] = [I_l, I_k]^\dagger = \sum_{j=1}^{r}\bar{c}_{lk}^j I_j^\dagger = \sum_{j=1}^{r}\bar{c}_{lk}^j I_j$$

we obtain $-c_{lk}^j = \bar{c}_{lk}^j$, i.e. the structure constants are purely imaginary numbers, with $c_{lk}^j = -c_{kl}^j$.
Exercise: Find and characterize the Lie algebra of $SO(2)$. In particular, find the structure constants.
Exercise: Show that the set of matrices

$$\begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix}$$

with a real parameter t forms a group. Find its Lie Algebra and the structure constants.

The importance of the Lie algebra lies in the fact that we may generate a matrix representation of the Lie group by considering a matrix representation of the Lie algebra: if we are able to find a set of r square matrices all of order p, such that they satisfy the structure relations with the given structure constants, then we would be able to generate a p-dimensional representation of the associated Lie group by using the exponential expansion. Those representations of the Lie algebra which are irreducible will provide irreducible representation of the Lie group, so that we might restrict ourselves to studying the representation theroy of the Lie algebra, which is often less cumbersome from the algebraic point of view than the representations of the Lie group. We recall, at this point, that the matrices of the Lie algebra are themselves matrix representations of those elements of the Lie group which are "close" to the identity element of the Lie group ("close" within the spirit of the Lie linearization procedure).

4.2 The group $SO(3)$

Consider the set of all orthogonal transformations in a three dimensional real vector space (i.e. a space defined over the field of real numbers). It is a group which we shall debote by $O(3)$. This set can be defined alternatively as the set of all 3×3 orthogonal matrices. The two sets are isomorphic to each other. An orthogonal matrix satisfies the relation $R^tR = RR^t = E$. Taking the determinant at both sides and noting that $detR^t = detR$, we have

$detR = \pm 1$. Thus, the orthogonal matrices are divided into two distinct sets – one containing the matrices with determinant 1 and the other containing the matrices with determinant -1. It can be easily checked that each set forms a group: with $SO(3)$ we denote the group of all real orthgogonal matrices of order 3 with determinant $+1$. $SO(3)$ describe pure (or proper) rotations by a finite angle around any axis $\vec{n}$, while $ISO(3)$ describes improper rotations ($ISO(3)$ contains all the orthogonal matrices with determinant -1). We shall now construct all the irreducible representations of $SO(3)$ by working out the representations of its Lie algebra.

To contruct the Lie algebra of $SO(3)$ we consider a rotation about the axis $\vec{n}$ by an infinitesimally small angle $\delta\varphi$. This rotation produces a map

$$\vec{r} \longrightarrow \vec{r}_t = \vec{r} + (\vec{n} \times \vec{r}) \cdot \delta\varphi$$

and the $\vec{r}$-dependent wave functions transform according to

$$\begin{aligned} O_{\vec{n},\delta\varphi}\phi(\vec{r}) &= \phi\Big(\vec{r} - (\vec{n} \times \vec{r}) \cdot \delta\varphi\Big) \\ &= (1 - \vec{n} \cdot \delta\varphi \cdot [\vec{r} \times \vec{\nabla}])\phi(\vec{r}) \\ &= \Big(1 - \frac{i}{\hbar}(\vec{n}\vec{L})\delta\varphi\Big)\phi(\vec{r}) \end{aligned}$$

Thus,

$$O_{\vec{n},\delta\varphi} = E - \frac{i}{\hbar}(\vec{n}\vec{L})\delta\varphi$$

Any rotation of a finite angle about the $\vec{n}$ axis can be written as

$$\begin{aligned} O_{\vec{n},\varphi} &= lim_{l \to \infty}(E - \frac{i}{\hbar}(\vec{n}\vec{L})\frac{\varphi}{l})^l \\ &= exp^{-\frac{i}{\hbar}(\vec{L}\vec{n})\varphi} \end{aligned}$$

This equation shows explicitely that the rotation group is a three parameter continuos group ($\vec{n} = (n_x, n_y, \sqrt{1 - n_x^2 - n_y^2})$ and φ). It has therefore three

linear independent infinitesimal generators. As a basis set for the Lie Algebra we can use $I_j = L_j/\hbar$, L_j being the three components of the quantum mechanical angular momentum vector in carstesian coordinates. The commutators of the various components can be explicitey evaluated and leads to the the structure relations

$$[I_i, I_j] = i \sum_{i,j,k} \epsilon_{ijk} I_k$$

A useful set of parameters for $SO(3)$ are the three Euler angles. Alternatively, one can express $\vec{n}$ with its direction cosines l, m, n, $l^2 + m^2 + n^2 = 1$, and use the angle φ as rotation angle. Finally, we introduce spherical coordinates in $\mathcal{R}^4$ according to

$$x_0 = \cos\phi, x_1 = \sin\phi\cos\vartheta, x_2 = \sin\phi\cos\vartheta\cos\psi, x_3 = \sin\phi\sin\vartheta\sin\psi$$

so that the parameter space is represented by the surface of the unit sphere S^3 in $\mathcal{R}^4$. From this representation of the parameter space it is clear that $SO(3)$ is a compact group.

It is our aim to construct all finite irreducible representations D_j of $SO(3)$. To this purpose we have to work out all possible irreducible representations of its Lie Algebra, the basis set of which must fullfill the structure relations

$$[I_i, I_j] = i\sum_{i,j,k} \epsilon_{ijk} I_k, (i,j,k) = 1,2,3$$

It is convenient to define the (non-hermitic) operators $I_\pm \doteq I_1 \pm iI_2$ as a basis of the Lie algebra, which obey the structure relations

$$[I_3, I_\pm] = \pm I_\pm, [I_+, I_-] = 2I_3$$

As I_3 is an hermitic operator, we can assume it to be a diagonal matrix, i.e

$$I_3\psi = z \cdot \psi$$

z being a real number.
Lemma: $z \pm 1$ is also an Eigenvalue of I_3, provided $I_\pm\psi \neq 0$.
Proof:

$$I_3(I_\pm\psi) = I_\pm I_3\psi \pm [I_3, I_\pm]\psi = (z \pm 1) \cdot I_\pm\psi$$

As we require the dimension of the irreducible vector space to be finite, there must be an eigenvalue j with the eigenfucntion ψ_j so that

$$I_3\psi_j = j\psi_j, I_+\psi_j = 0$$

Applying successively the operator I_- to ψ_j we produce an eigenfunction ψ_{j-1} of I_3 with the eigenvalue $j-1$. This procedure can be repeated so that

$$\begin{aligned} I_-\psi_p &= \psi_{p-1} \\ I_3\psi_p &= p\psi_p, p = j, j-1, ... \\ I_3\psi_{j-k} &= (j-k)\psi_{j-k} \\ I_-\psi_{j-k} &= 0 \end{aligned}$$

i.e. there is an integer number k that terminates the eigenvalue sequence. What is left to do, in order to specify completey a matrix representation of the Lie algebra, is to find the numbers j and k. For this purpose we introduce an operator which commutes with all generators of the Lie group: such an operator is known as **Casimir** operator. According to a theorem by Racah, the number of independent Casimir operators of a Lie group is equal to the minimum nunber of commuting operators (the so called *rank* of a Lie Group). In the case of $SO(3)$, the mimimum number of commuting operators is 1, because no two of its generators commute with each others. The one and only Casimir operator of $SO(3)$ is $\vec{I}^2 \doteq I_1^2 + I_2^2 + I_3^2$.
Exercise: prove this by explicitely calculating the commutation relations of $\vec{I}^2$ with the generators.
Exercise: prove the following equations:

$$\vec{I}^2 = I_+ I_- + I_z^2 - I_z = I_- I_+ + I_z^2 + I_z$$

To find j and k we have to prove following Lemmas:

1. $\vec{I}^2 \psi_j = j(j+1)\psi_j$. This is because $\vec{I}^2 \psi_j = (0 + j^2 + j)\psi_j$.
2. $\vec{I}^2 \psi_p = j(j+1)\psi_p$. By induction: we assume that $\vec{I}^2 \psi_{p+1} = j(j+1)\psi_{p+1}$ This leads, using the equations proved in the Exercise above, to $I_+ \psi_p = \mu_p \psi_{p+1}$, $\mu_p = j(j+1) - (p+1)^2 + (p+1)$. Then,

$$\vec{I}^2 \psi_p = I_- \mu_p \psi_{p+1} + (p^2 + p)\psi_p = j(j+1)\psi_p$$

3. j and k are related by $j = k/2$ $k \in \mathcal{N}$: this is because

$$\vec{I}^2 \psi_{j-k} = j(j+1)\psi_{j-k} = \Big((j-k)^2 - (j-k)\Big)\psi_{j-k}$$

This last equation establishes that a representation – called D_j– of the Lie algebra is associated to each half integer number $j = 0, \frac{1}{2}, 1, \frac{3}{2}, ...$ The representation has dimension $2j+1$ and the non-vanishing matrix elements of the generators are given by $(m = j, j-1, ... - j)$ (Condon-Shortley convention)

$$\begin{aligned}
(\psi_{j,m}, I_z \psi_{j.m}) &= m \\
(\psi_{j,m\pm 1}, I_x \psi_{j,m}) &= \frac{1}{2}\sqrt{(j \mp m)(j \pm m + 1)} \\
(\psi_{j,m\pm 1}, I_y \psi_{j,m}) &= \mp \frac{i}{2}\sqrt{(j \mp m)(j \pm m + 1)}
\end{aligned}$$

Theorem: The representation D_j is irreducible.
First proof: We assume that the representation is reducible. Then, there is

a true subset of the vector space $[\psi_j, ..., \psi_{-j}]$ which is invariant under the application of both I_+ and I_-. Let this subspace be determined by some of the vectors ψ_m. Applying $I_\pm$ onto these vectors will inevitably lead to $2j+1$ linearly independent vectors, thus contradicting the hypothesis that a true subset exists.

We can provide an alternative proof of the theorem above and prove that D_j, with j half integer, constitute *all* irreducible representations of $SO(3)$ by introducing the characters of D_j and an average within the group. Let us first consider the class structure of the group $SO(3)$. Consider the two operations $R_{\vec{u}}(\varphi)$ and $R_{\vec{v}}(\varphi)$, which denote rotations through the same angle φ about two distinct axes $\vec{u}$ and $\vec{v}$, both passing thorugh the origin. Since there exists in $SO(3)$ an operation which can bring the axis $\vec{u}$ into the axis $\vec{v}$, we see that rotations by the same angle about different axis must belong to the same class.

In any representation, therefore, the characters of the elements of $SO(3)$ depend only on the angle of rotation and not on the axis of rotation. It is thus not necessary to know the complicated transformation matrices under all rotations to obtain the characters of an element within a given representation: we only need to know the matrix representing a rotation about the z axis. For instance, the generator of these rotations is, in the D_j representations, a diagonal matrix, and the matrix representing the actual rotation by an angle φ is given by

$$\begin{pmatrix} e^{-ij\varphi} & 0 & . & . & 0 & 0 \\ 0 & e^{-i(j-1)\varphi} & . & . & 0 & 0 \\ 0 & 0 & . & . & 0 & 0 \\ 0 & 0 & . & . & 0 & 0 \\ 0 & 0 & . & . & e^{-i(-j+1)\varphi} & 0 \\ 0 & 0 & . & . & 0 & e^{-i(-j)\varphi} \end{pmatrix}$$

The character of this representation, and *thus of all the elements in the same class* is

$$\begin{aligned} \chi_j(\varphi) &= \sum_{k=-j}^{k=j} e^{ik\varphi} \\ &= e^{-ik\varphi}(1 + e^{i\varphi} + e^{2i\varphi} + ... \\ &= \frac{\sin(j+1/2)\varphi}{\sin\varphi/2} \\ &= \frac{\sin(2j+1)\phi}{\sin\phi} \end{aligned}$$

with the angle $\varphi \in [0, 2\pi]$. As only $\varphi/2$ enters the characters, we might use a new variable $\phi \doteq \varphi/2 \in [0, \pi]$. We define an average within the Lie group by noting that the elements of a class can be seen as occupying a circle with radius $\sin\phi$ on a unit sphere in a 4-dimensional space specified by the three direction cosines and the angle ϕ so that $d\tau_{SO(3)} = \frac{1}{2\pi^2}\sin^2\phi d\phi do$, with do being the differential angle for the direction of the rotation axis. Thus,

$$M_{S^3} f(\phi, \vec{n}) = \frac{1}{2\pi^2}\int f(\phi, \vec{n}) \sin^2\phi d\phi \cdot do$$

where $f(\phi, \vec{n})$ is a continuos function defined on S^3.
We are now in the position of proving that
Theorem
i) the representation D_j are irreducible and that *ii*) they constitute all possible irreducible representations.
i). We have to prove that $M_{S^3}\chi_j^*(\phi)\chi_j(\phi) = 1$. In fact

$$\frac{4\pi}{2\pi^2}\int \sin^2\phi d\phi do \frac{\sin^2(2j+1)\phi}{\sin^2\phi} = 1$$

ii). Let D be an irreducible representation besides D_j. For all $n \in \mathcal{N}$ the characters χ of D must obey the equation

$$\frac{1}{2\pi^2}\int (\sin\phi \cdot \chi^*(\phi)) \cdot \sin n\phi d\phi = 0$$

As the functions $\sin\phi, \sin 2\phi, ...$ build a complete orthonormal basis set on the intervall $[0, \pi]$ for all continuos functions on this intervall, $\sin\phi \cdot \chi(\phi)$ must be zero, i.e. $\chi(\phi) \equiv 0$. As the norm of this representation is not 1, it cannot be irreducible, contrary to the assumption.

4.3 The $j = 1/2$ irreducible representation: $SU(2)$.

The D_0 representation associates to every element of the group $SO(3)$ the number 1 and it is thus the identity representation. The subspace supporting D_0 is a one-dimensional vector space whose vectors are invariant with respect to all rotations of $SO(3)$. The next non-trivial irreducible representation $D_{1/2}$ is of fundamental importance in Physics. The generators of the representation are $1/2(\sigma_x, \sigma_y, \sigma_z)$, where the $\sigma's$ are **Pauli Matrices**

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

Using $\vec{n} = (l, m, n)$ and the rotation angle $\varphi \in [0, 2\pi]$ we can write the rotation matrix as

$$O_{l,m,n}(\varphi) = e^{-i\frac{\varphi}{2}\begin{pmatrix} n & l - i\cdot m \\ l + i\cdot m & -n \end{pmatrix}}$$

As $l^2 + n^2 + m^2 = 1$, we have

$$\begin{pmatrix} n & l - i\cdot m \\ l + i\cdot m & -n \end{pmatrix}^2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

so that

$$\begin{aligned} O_{l,m,n}(\varphi) &= \sum_{k_{even}} \frac{(-i\varphi/2)^k}{k!} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \\ &+ \sum_{k_{odd}} \frac{(-i\varphi/2)^k}{k!} \begin{pmatrix} n & l - i\cdot m \\ l + i\cdot m & -n \end{pmatrix} \\ &= \begin{pmatrix} \cos\frac{\varphi}{2} - i\cdot n \sin\frac{\varphi}{2} & (-i\cdot l - m)\sin\frac{\varphi}{2} \\ (-i\cdot l + m)\sin\frac{\varphi}{2} & \cos\frac{\varphi}{2} + i\cdot n\sin\frac{\varphi}{2} \end{pmatrix} \end{aligned}$$

An alternative way to construct the representation $D_{1/2}$ is to parametrize rotations by the Euler angles α, β, γ These angles determine the set of consecutive rotations which are necessary to drive the orthogonal vector system $K = (x, y, z)$ onto the system $K_t = (x_t, y_t, z_t)$. Three rotations are required:
a) a rotation by $\alpha (0 \le \alpha \le 2\pi)$ about the z axis drives K into K_1. We call this rotation $R(\alpha, z)$.
b) a rotation by $\beta (0 \le \beta \le \pi)$ about the next axis x_1 transforms K_1 into K_2 – this operation we call $R(\beta, x_1)$.
c) the last rotation is by $\gamma (0 \le \gamma \le 2\pi)$ about the z_2 axis – operation $R(\gamma, z_t)$.
The composition of the three operations is

$$e^{\frac{-i}{2}\sigma_z \alpha} \cdot e^{\frac{-i}{2}\sigma_x \beta} \cdot e^{\frac{-i}{2}\sigma_z \gamma}$$

The evaluation of the exponential functions by summing the corresponding series gives

$$\begin{aligned} e^{\frac{-i}{2}\sigma_z \varphi} &= \sum_n \frac{\left(-i \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{\varphi}{2}\right)^n}{n!} \\ &= \begin{pmatrix} e^{-i\frac{\varphi}{2}} & 0 \\ 0 & e^{i\frac{\varphi}{2}} \end{pmatrix} \end{aligned}$$

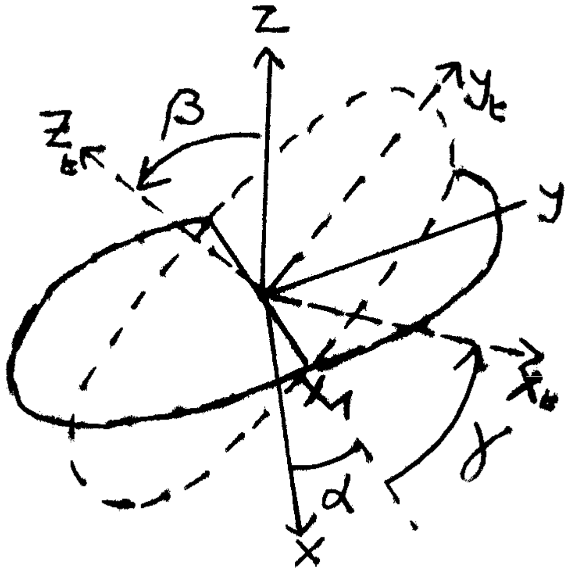

Figure 4.1:

and

$$\begin{aligned}\sum_n \frac{(\frac{-i}{2}\sigma_x\beta)^n}{n!} &= \sum_n (\frac{(-i)^n(\sigma_x\frac{\beta}{2})^n}{n!} \\ &= \sigma_0 \cdot \cos(\frac{\beta}{2}) - i \cdot \sigma_x \cdot \sin(\frac{\beta}{2}) \\ &= \begin{pmatrix} \cos\frac{\beta}{2} & -i\sin\frac{\beta}{2} \\ -i\sin\frac{\beta}{2} & \cos\frac{\beta}{2} \end{pmatrix}\end{aligned}$$

Building the product of the three matrices corresponding to the three rotations we obtain

$$O_{\alpha\beta\gamma} = \begin{pmatrix} \cos\frac{\beta}{2}e^{-i\frac{\alpha+\gamma}{2}} & -i\sin\frac{\beta}{2}e^{i\frac{\gamma-\alpha}{2}} \\ -i\sin\frac{\beta}{2}e^{i\frac{\alpha-\gamma}{2}} & \cos\frac{\beta}{2}e^{i\frac{\alpha+\gamma}{2}} \end{pmatrix}$$

The matrices of $D_{1/2}$, independent of their parametrization, all have an important property: they are unitary matrices with determinant 1, and the set of them obtained by running over the parameter space build the group $SU(2)$. This group is known as the special unitary group. It is a 3 parameters continuos Lie group with average. By construction, each matrix of $D_{1/2}$ corresponds to a unique rotation of $SO(3)$. However, notice that

$$D_{1/2}(\vec{n}, \varphi + 2\pi) = \bar{E} \cdot D_{1/2}(\vec{n}, \varphi)$$

with

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

Thus, an element of $SO(3)$ corresponds to two distinct unitary matrices of $SU(2)$, one of which is the negative of the other. One refer in general to half-integer representations of $SO(3)$ as the *doubled valued* representations of $SO(3)$. In Physics, these double valued representations are relevant when particles with half-integer spins are considered, such as the electron. Our result shows that the spinor describing the electron does not return to its original value after a rotation by 2π but becomes the negative of its original value, returning to its original value only after a rotation by 4π. Thus, the symmetry group governing the behaviour of a spinor with half integer spin is not $SO(3)$. Following H.A. Bethe (1929), we introduce a new symmetry group, where a rotation by 2π about any axis is not identical to the identity element but only a rotation through 4π is. This new group is obtained by adding to $SO(3)$ the new element $\bar{E}$ to mean the rotation by 2π about, say, the z-axis and the product of $\bar{E}$ with all other elements of $SO(3)$. The double-valued irreducible representations of $SO(3)$ becomes single valued representations of this new group. The new group is said to be the **double group** of $SO(3)$ and is often denoted by $SO'(3)$. It is isomorpohic to $SU(2)$: this is why one speak of $SU(2)$ as the the symmetry group of an electron, and not $SO(3)$.
Exercise : show that $SO(3)$ is not a subgroup of $SO'(3)$.

4.4 Double finite groups

Finite groups such as C_{3v} and C_{4v} must also be expanded to a double group when double valued representations are considered. A new element $\bar{E}$ is introduced, which is again the rotation by 2π around any axis, for which $\bar{E}\cdot\bar{E} = E$. Accordingly, we have the equations

$$C_n^n = \bar{E}, C^{2n} = E$$

The inversion I commute with each rotation and must give E by two-fold application. But the two-fold application of a reflection at a plane will be equal $\bar{E}$ rather than E:

$$\sigma^2 = \bar{E}, \sigma^4 = E$$

This is because a reflection can be written as IC_2. The result of the group expansion is a symmetry group that contains twice the number of symmetry elements as the original group. Again, the double valued representations

E	$\bar{E}$
1	1
1	-1

Table 4.1: The character Table of C_1^D

of the original *single* group are singled valued representations of the generated double group. Thus, we can use standard theorems to search for the irreducible double group representations. At this point we have to issue a warning: a double group will have, in general, a larger number of irreducible representations, but not necessarily twice as much. This is because the number of classes does not necessarily double. $\bar{E}$ commutes with all other elements and will always form a class on its own. But C_2 and $\bar{E}C_2$, for instance, belong to the same class, in virtue of $C_2C_2 = \bar{E}$.

4.4.1 The group C_1^D

The simple group C_1 contains the identity E. The double group contains E and $\bar{E}$. They form two distinct classes and there are two one-dimensional irreducible representations. The $D^{1/2}$-representation of E and $\bar{E}$ is

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}$$

It is clearly reducible into the sum of two identical one dimensional representations with $E = 1, \bar{E} = -1$ Clearly, the only physical irreducible representation is the extra representation contained in the second line of the table.

4.4.2 The group C_i^D

The single group C_i contains the identity and the inversion I. The double group C_i^D contains the four elements $E, \bar{E}, I, \bar{I}$. Because all these elements commute, there are four classes and four one-dimensional irreducible representations given in the table. Notice that, again, the two-dimensional representation $D^{1/2}$ is clearly reducible: it is the direct sum of two identical one-dimensional representations with $1, -1, 1, -1$.

E	$\bar{E}$	I	$\bar{I}$
1	1	1	1
1	1	-1	-1
1	-1	-1	1
1	-1	-1	1

4.4.3 The double group C_{3v}^D

The single group C_{3v} contains six elements:
$E, C_{3xyz}, C_{3xyz}^{-1}, IC_{2x\bar{y}}, IC_{2\bar{x}z}, IC_{2y\bar{z}}$, all transforming the $\vec{k}$-vector along the Λ-direction into itself ($\vec{k}_\Lambda = \pi/a(\lambda, \lambda, \lambda)$ with $0 < \lambda < 1$). The symbols C_{3xyz} and C_{3xyz}^{-1}, for instance, means rotations by an angle $2\pi/3$ around an axis with director cosines on the ratio $1 : 1 : 1$, see the table and figure for O_h. There are three classes: the identity element, the two there-fold rotations and the three reflections. We can easily construt the character table of the single point group C_{3v}. The double group C_{3v}^D has twice the number of elements and twice the number of classes as C_{3v}. The matrices representing the $2C_3$ group elements in the $D^{1/2}$ representation can be constructed by using $l = m = n = \sqrt{\frac{1}{3}}$ and a rotation angle $\pm\varphi = \frac{2\pi}{3}$:

$$C_{3xyz} = \begin{pmatrix} \frac{1-i}{2} & -\frac{1+i}{2} \\ \frac{1-i}{2} & +\frac{1+i}{2} \end{pmatrix}$$

Similarly, one can obtain the matrices $IC_{2x\bar{y}}, IC_{2\bar{x}z}, IC_{2y\bar{z}}$ by considering that the inversion is followed by the rotation of $2\pi/2$ around an axis with director cosines in the ration $1 : \bar{1} : 0$, i.e. $\varphi = \pi$ and $l = /\sqrt{2}$, $m = -1/\sqrt{2}$ $n = 0$. Thus, for instance,

$$IC_{2x\bar{y}} = I \cdot \begin{pmatrix} 0 & \frac{1-i}{\sqrt{2}} \\ -\frac{1+i}{\sqrt{2}} & 0 \end{pmatrix}$$

The remaining matrices can be constructed in a similar way.

$$E = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad ; \quad \bar{E} = \begin{pmatrix} \bar{1} & 0 \\ 0 & \bar{1} \end{pmatrix}$$

$$C_{3xyz} = 1/2 \begin{pmatrix} 1-i & -1-i \\ 1-i & 1+i \end{pmatrix} \quad ; \quad \bar{C}_{3xyz} = 1/2 \begin{pmatrix} -1+i & 1+i \\ -1+i & -1-i \end{pmatrix}$$

$$C_{3xyz}^{-1} = 1/2 \begin{pmatrix} 1+i & 1+i \\ -1+i & 1-i \end{pmatrix} \quad ; \quad \bar{C}_{3xyz}^{-1} = 1/2 \begin{pmatrix} -1-i & -1-i \\ 1-i & -1+i \end{pmatrix}$$

$$IC_{2x\bar{y}} = \sqrt{1/2}I \begin{pmatrix} 0 & 1-i \\ -1-i & 0 \end{pmatrix} \quad ; \quad I\bar{C}_{2x\bar{y}} = \sqrt{1/2}I \begin{pmatrix} 0 & -1+i \\ 1+i & 0 \end{pmatrix}$$

Irr.Rep.	E	$2C_3^2$	$3\sigma_v$
Λ_1	1	1	1
Λ_2	1	1	-1
Λ_3	2	-1	0

Irr.Rep.	E	$\bar{E}$	$2C_3^2$	$2\bar{C}_3^2$	$3\sigma_v$	$3\bar{\sigma}_v$
Λ_1	1	1	1	1	1	1
Λ_2	1	1	1	1	-1	-1
Λ_3	2	2	-1	-1	0	0
Λ_4	1	-1	-1	1	i	-i
Λ_5	1	-1	-1	1	-i	i
Λ_6	2	-2	1	-1	0	0

$$IC_{2\bar{x}z} = \sqrt{1/2}I\begin{pmatrix} -i & i \\ i & i \end{pmatrix} \quad ; \quad I\bar{C}_{2\bar{x}z} = \sqrt{1/2}I\begin{pmatrix} i & -i \\ -i & -i \end{pmatrix}$$
$$IC_{2y\bar{z}} = \sqrt{1/2}I\begin{pmatrix} i & -1 \\ 1 & -i \end{pmatrix} \quad ; \quad I\bar{C}_{2y\bar{z}} = \sqrt{1/2}I\begin{pmatrix} -i & 1 \\ -1 & i \end{pmatrix}$$

The 12 elements are thus divided into 6 classes, and the equation $\sum_\alpha (l_\alpha)^2 = 12$ has the solution $1^2 + 1^2 + 2^2 + 1^2 + 1^2 + 2^2 = 12$. Thus, there are a total of four one dimensional representations and two two-dimensional representations. The three irreducible representations of C_{3v} can be extended as irreducible representations of C_{3v}^D by representing $\bar{E}$ with E and the $\bar{C}$ elements as the non-$\bar{C}$ elements. There are three extra additional irreducible representations to be found. We notice that the two dimensional $D^{1/2}$ representation is irreducible: in fact with the characters

$$\chi(E) = 2, \chi(\bar{E}) = -2, \chi(C_3) = 1, \chi\bar{E}C_3 = -1, \chi(\sigma_v) = 0$$

we have $\sum_A \chi(A)^2 = 12$, which is a necessary and sufficient condition for an irreducible representation. The remaining two-extra one dimensional representations are found by applying the unitarity conditions. Λ_6 is the name of $D^{1/2}$ when restricted to this point group.

4.5 Exercises

1. Show that the set of matrices

$$\begin{pmatrix} 1 & t \\ 0 & 1 \end{pmatrix} \begin{pmatrix} t>0 & 0 \\ 0 & 1 \end{pmatrix}$$

with a real parameter t form groups (why is zero excluded in the second set of matrices?). Find the generator for both groups and integrate it to obtain the group elements.

2. Show that the set of transfromations $x' = a \cdot x$ and $y' = b \cdot y$ forms a group, find the generators and the structure relations.

3. Find the generator of $A(t) \cdot B(t)$ where A and B are matrices, t is a real parameter and the generators of $A(t)$ and $B(t)$ are known.

4. Show that $\chi_j(\varphi) = \sum_{k=-j}^{k=j} e^{ik\varphi} = \frac{\sin(j+1/2)\varphi}{\sin\varphi/2}$

5. Construct the 1-parameter continuos group generated by

$$I = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$$

Tip: construct a suitable differential equation fullfilled by I.

6. Let the commutator relations within a Lie Algebra be given by $[e_1, e_2] = e_3$, $[e_2, e_3] = 2e_2$, $[e_3, e_1] = 2e_1$. Find e_3 if

$$e_1 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; e_2 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

and find the generated continuos group.

7. Let S be a non-singular matrix. Show that all matrices A with $A^t SA = S$ build a group. What is the characteristic of the generators of this group? Show that they form a Lie Algebra.

8. The D_1 representation of $SO(3)$. A famous expression for a three dimensional representation of $SO(3)$ is the Euler rotation formula. The starting point is the definition of new generators J_k as $J_k = -i \cdot I_k$. Find the stucture relations for these new generators and show that the matrices

$$J_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \bar{1} \\ 0 & 1 & 0 \end{pmatrix}; J_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ \bar{1} & 0 & 0 \end{pmatrix}; J_3 = \begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix};$$

obey the structure relations. These generators can be used to constuct the exponential mapping of a rotation by an angle φ around an axis $\vec{n}$ specified by (l, m, n) with $l^2 + m^2 + n^2 = 1$, according to $D_1(\vec{n}, \varphi) = exp(U \cdot \varphi)$. Find U, which is the most general form of a skew-symmetric matrix. Use the Cayley-Hamilton theorem to show that $U^3 = -U$ (the theorem states that each square matrix fulfil its characteristic equation) and show, by summing the serie arising from the exponential map, that

$$D_1(\vec{n}, \varphi) = E + U \sin\varphi + U^2(1 - \cos\varphi)$$

(Euler rotation formula). Show that this formula is equivalent to

$$D_1(\vec{n}, \varphi)\vec{r} = \vec{r} + \vec{n} \times \vec{r} \sin\varphi + \vec{n} \times (\vec{n} \times \vec{r})(1 - \cos\varphi)$$

where $\times$ vector product.

9. Find the character table for the double group of C_{4v}. Pay notice to the class separation of the double group.