Symmetries and Groups in Quantum Mechanics

From Concrete to abstract!

M.V.N. Murthy

Institute of Mathematical Sciences, CIT Campus, Chennai 600113 (Retd.)

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Contents

Chapter 1

Brief review of some basic concepts

These notes are based on the lectures delivered at the IMSc Foundation series for undergraduate students. The notes begins with some concrete examples starting from unitary transformations in quantum mechanics, a discussion of symmetry transformations, groups of such transformations. The focus is mainly on the rotation group and its representations in the theory of angular momentum which plays a central role in the quantum mechanical systems the we study in any introductory course.

State Space: We represent a physical system in quantum mechanics(QM) by a ket $|\alpha\rangle$. This notation was introduced by Dirac and denotes the state of the system. In principle this state has the complete information about the state of the physical system. The set of all such states is a vector space, also known as Hilbert space. It can be finite as in the case of spin systems but may also be infinite. Two kets may be superposed resulting in another ket,

$$|\alpha\rangle + |\beta\rangle = |\gamma\rangle \tag{1.1}$$

or multiplied by a complex number

$$c|\alpha\rangle = |\alpha\rangle c \tag{1.2}$$

in any order. In quantum mechanics when $c \neq 0$, both $|\alpha\rangle$ and $c|\alpha\rangle$ represent the same state. Without loss of generality we use normalized kets. This is some times called the ray space instead of the vector space.

Corresponding to every ket vector $|\alpha\rangle$, there is a bra vector denoted by $\langle\alpha|$. It is some times called the dual vector. Therefore, corresponding to every ket space, there

is a dual bra space in one-to-one correspondence such that

$$|c\alpha\rangle = c|\alpha\rangle; \quad \langle c\alpha| = c^*\langle\alpha|, \tag{1.3}$$

where c is a complex number. The inner product between any two such states is defined by the (bra)c(ket)

$$\langle\beta|\alpha\rangle \geq 0 \tag{1.4}$$

which is a complex number in general. The inner product is similar to the scalar product between two vectors[1] The states are said to be "orthogonal" when the equality is satisfied. This also means the "length" of the vector

$$\langle\alpha|\alpha\rangle \geq 0 \tag{1.5}$$

is positive definite. It is zero only when it is a null vector (like the origin of a coordinate system).

Operators: An observable is represented by an operator $\hat{O}$ which acts on the system

$$\hat{O}|\alpha\rangle \tag{1.6}$$

which is also a ket. In QM, we are interested in Hermitian operators

$$\hat{O}^\dagger = \hat{O}.$$

The eigenvalues of a Hermitian operator are real. Familiar observables are the momentum, angular momentum, energy etc. We will discuss these separately later on. Often the operators acting on a state may change the state. There are a special class of vectors or kets which are unchanged under the action of an operator-

$$\hat{A}|\alpha\rangle = a|\alpha\rangle, \tag{1.7}$$

then a is called the eigenvalue and $|\alpha\rangle$ is called the eigenvector. In the case of Hermitian operators the eigenvalues are always real. This is the main reason why the observables are represented by Hermitian operators.

The set of all eigenvectors of a Hermitian operator form a complete set- that is eigenvectors belonging different eigenvalues are orthogonal. Therefore any arbitrary state may be expanded in terms of the complete set of vectors belonging to a Hermitian operator acting on the system:

$$|\psi\rangle = \sum_{i=1}^{N} a_n|\alpha_i\rangle; \quad a_n = \langle\alpha_n|\psi\rangle; \quad \langle\alpha_i|\alpha_j\rangle = \delta_{ij}. \tag{1.8}$$

We have assumed that the space of states is finite, but that is not necessary since it depends on the system. Here a_n are a set of complex coefficients.

[1]Much of the discussion here may be understood using the analogy of usual vectors in R^3 keeping in mind the space is real where as in general the inner product is a complex number.

Position space representation: The position basis is defined by the kets $|x\rangle$ where x is a real number which represents position of the system- it would be a vector with components in higher dimensions. Here we restrict our discussion to one dimension only. States corresponding to different position are orthogonal, that is

$$\langle x|y\rangle = \delta(x-y) \tag{1.9}$$

and the completeness relation is

$$I = \int dx|x\rangle\langle x|\,. \tag{1.10}$$

Position operator is defined as

$$\hat{x}|x\rangle = x|x\rangle.$$

State vector in position space is a projection given by

$$\psi(x) = \langle\psi|x\rangle; \quad \langle\phi|\psi\rangle = \int dx\ \langle\phi|x\rangle\langle x|\psi\rangle = \int dx\ \phi^*(x)\psi(x). \tag{1.11}$$

Expectation value of an operator is given by

$$\langle\phi|\hat{A}|\psi\rangle = \int dx\ \langle\phi|x\rangle\langle x|\hat{A}|y\rangle\langle y|\psi\rangle = \int dx\ dy\ \phi^*(x)\langle x|\hat{A}|y\rangle\psi(y). \tag{1.12}$$

If suppose the operator is a combination of x and derivatives with respect to x, $\hat{A} = A(x, \partial/\partial x)$, then

$$\langle\phi|\hat{A}|\psi\rangle = \int dx\phi^*(x)A(x,\partial/\partial x)\langle x|y\rangle\langle y|\psi\rangle = \int dx\ \phi^*(x)A(x,\partial/\partial x)\psi(x). \tag{1.13}$$

Momentum in position basis is

$$\langle x|p\rangle = \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}} \tag{1.14}$$

which is properly normalised such that

$$\langle p'|p\rangle = \delta(p'-p). \tag{1.15}$$

By definition therefore

$$-i\hbar\frac{d}{dx}\langle x|p\rangle = p\langle x|p\rangle. \tag{1.16}$$

This defines the hermitian operator whose eigenvalues are given by the momentum. Furthermore

$$\langle x|\hat{p}|\psi\rangle = \int dp\ \langle x|p\rangle\langle p|\hat{p}|\psi\rangle = \int dp\ p\langle x|p\rangle\langle p|\psi\rangle \tag{1.17}$$

which may be simplified as

$$\langle x|\hat{p}|\psi\rangle = -i\hbar\frac{d}{dx}\int dp\ \langle x|p\rangle\langle p|\psi\rangle = -i\hbar\frac{d}{dx}\int dp\ \frac{e^{ipx/\hbar}}{\sqrt{2\pi\hbar}}\langle p|\psi\rangle. \tag{1.18}$$

Using the property of Fourier transform we have

$$\langle x|\hat{p}|\psi\rangle = -i\hbar\frac{d}{dx}\psi(x) \tag{1.19}$$

Time evolution: How does the state of a system evolve in QM? A very fundamental principle in QM is that the time evolution must preserve the relation between any two vectors (Information about the system is not lost during its time evolution). Consider a dynamical transformation of a state from $t = 0$ to a time t. Let

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle$$
$$|\phi(t)\rangle = U(t)|\phi(0)\rangle.$$

The time variation is continuous. We require the inner product between the states to remain the same as time evolves. That is

$$\langle\phi(t)|\psi(t)\rangle = \langle\phi(0)|U^\dagger(t)U(t)|\psi(0)\rangle = \langle\phi(0)|\psi(0)\rangle. \tag{1.20}$$

Therefore we get the condition that the transformation U should be a unitary operator with the property

$$U^\dagger U = I. \tag{1.21}$$

Thus, in QM all states evolve unitarily. Since the inner product is preserved, states which are orthogonal to begin with will remain orthogonal for all times.

Let us now look at the "generator" of such transformations. Since it is a continuous transformation, we may take the time elapsed as small as possible. For an infinitesimal transformation let

$$U = I + \epsilon G + O(\epsilon^2), \tag{1.22}$$

where ϵ is infinitesimal and we stop at the first order. The unitarity condition then implies

$$U^\dagger U = I + \epsilon(G + G^\dagger) \Longrightarrow G = -G^\dagger. \tag{1.23}$$

Here G is called the generator of the transformation and is anti-hermitian. We may instead use a hermitian generator by substituting $G = -iH$. We then have for infinitesimal unitary transformations

$$U = I - i\epsilon H + O(\epsilon^2); \quad i = \sqrt{-1}. \tag{1.24}$$

Note that ϵH must be dimensionless. We call H the **Hamiltonian operator** or simply Hamiltonian which is the generator of time translations of the system. By classical analogue, the Hamiltonian has the dimensions of energy, hence ϵ has the dimensions of inverse energy. We may keep track of dimensions by noting that $E = \hbar\omega$. We can make ϵ as small as we like and take n steps, where n is an integer such that

$$U = [I - i\epsilon H]^n \tag{1.25}$$

and define $t = n\epsilon\hbar$ so that t has the dimensions of time and is finite in the limit of $n \to \infty$ and $\epsilon \to 0$. Thus

$$U(t) = \lim_{n\to\infty}[I - i\frac{t}{n\hbar}H]^n = \exp[-\frac{i}{\hbar}Ht] \tag{1.26}$$

which is a familiar relation. Of course since we have not specified the system, the Hamiltonian is not specified either. But given a state vector at some time t, there exists a Hamiltonian that determines the state for all times, that is

$$|\psi(t)\rangle = \exp[-\frac{i}{\hbar}Ht]|\psi(0)\rangle. \tag{1.27}$$

Consider the time evolution of a state for an infinitesimal interval in time Δt. We may write

$$|\psi(t+\Delta t)\rangle = [I - \frac{i}{\hbar}H\Delta t]|\psi(t)\rangle \tag{1.28}$$

or

$$|\psi(t+\Delta t)\rangle - |\psi(t)\rangle = -\frac{i}{\hbar}H\Delta t\psi(t)\rangle. \tag{1.29}$$

In the limit of very small times we take the limit

$$i\hbar \lim_{\Delta t\to 0}\frac{|\psi(t+\Delta t)\rangle - |\psi(t)\rangle}{\Delta t} = H|\psi(t)\rangle. \tag{1.30}$$

and therefore we get the well known Time Dependent Schroedinger Equation:

$$i\hbar\frac{\partial|\psi(t)\rangle}{\partial t} = H|\psi(t)\rangle. \tag{1.31}$$

If in particular the state of the system is an eigenstate of the Hamiltonian operator then we have the time independent Schroedinger equation

$$H|\psi(t)\rangle = E|\psi\rangle, \tag{1.32}$$

where E is the eigenvalue of the Hamiltonian operator which we call as "Energy".

Next consider the expectation value of an operator denoted by

$$\langle\hat{O}\rangle = \langle\psi|\hat{O}|\psi\rangle. \tag{1.33}$$

We are interested in its time evolution given by

$$\frac{d}{dt}\langle\hat{O}\rangle = \partial_t(\langle\psi|)\hat{O}|\psi\rangle + \langle\psi|\partial_t\hat{O}|\psi\rangle + \langle\psi|\hat{O}(\partial_t|\psi\rangle). \tag{1.34}$$

Using the time-dependent Schroedinger equation we get

$$\frac{d}{dt}\langle\hat{O}\rangle = \frac{i}{\hbar}[\langle\psi|H\hat{O} - \hat{O}H\psi\rangle] + \langle\psi|\partial_t\hat{O}|\psi\rangle = \frac{i}{\hbar}[\langle\psi|[H,\hat{O}]\rangle\psi > + \langle\psi|\partial_t\hat{O}|\psi\rangle. \tag{1.35}$$

This an important result since now one can make connection with classical equations of motion. If in particular the operator is not explicitly dependent on time then the equation becomes simpler

$$\frac{d}{dt}\langle\hat{O}\rangle = \frac{i}{\hbar}[\langle\psi|H\hat{O} - \hat{O}H\psi\rangle] + \langle\psi|\partial_t\hat{O}|\psi\rangle = \frac{i}{\hbar}[\langle\psi|[H,\hat{O}]\rangle\psi > . \tag{1.36}$$

Furthermore if the operator commutes with the Hamiltonian of the system, then we have

$$\frac{d}{dt}\langle\hat{O}\rangle = 0, \tag{1.37}$$

the expectation value of the operator is conserved. That is any operation that commutes with the Hamiltonian is a symmetry operation. What it means is that under the symmetry transformation, the properties of the system are unaltered. All observables retain the same value. Symmetry is a very powerful concept in physics in general. Examples of such transformations are translation, rotation etc which are familiar. Fundamental symmetries operate across various sub-fields and are fundamental in understanding any physical system.

We shall end this very brief review with some comments; As we have seen the dynamics of a quantum system is determined by the Hamiltonian of the system. This has to be specified for every system. In classical dynamics the time evolution of a system is traced through the points in the (2n)-dimensional phase space which yield a phase curve. The evolution of the point in phase is deterministic. In quantum mechanics the Hamiltonian evolution of the state vector is also deterministic given by the linear Schroedinger equation. However calculation of observables through the state vectors involves probabilistic interpretation. This makes QM very different from classical dynamics. However, we must always remember that all physical phenomena are ultimately described by Quantum Mechanics. Any other description can only be an approximation for ease of application.

Chapter 2

Symmetries and Conservation Laws

Symmetry considerations are a powerful tool to explore and understand the behaviour of physical systems. They provide the backbone of our theoretical formulations. Even when some of the apparent symmetries are not exact they provide a basis for classification of states assuming exact symmetry and allow us to look at possible sources and pattern of symmetry breaking. Broadly, a symmetry transformation is one in which the laws of physics are unchanged.

Symmetries may be classified into two broad categories: Continuous and discrete. We shall briefly discuss them here.

2.1 Continuous symmetries

We are familiar with continuous symmetries from Classical Mechanics. If the classical Lagrangian of a system is invariant under a set of continuous transformations, there exists a conservation law. This is essentially the content of Noether's[1] theorem. For example:

- Invariance of the Lagrangian under time translation results in the conservation of energy.

- Invariance of the Lagrangian under spatial translation results in the conservation of linear momentum.

[1]Emmy Noether was one of the leading mathematicians of her time, she developed theories of rings, fields, and algebras. Noether's theorem explains the connection between symmetry and conservation laws.

- Invariance of the Lagrangian under rotations results in the conservation of angular momentum.

provided the system obeys the Lagrangian equations of motion.

Any continuous transformation, like rotation or translation, say G may be generated, as seen earlier, from transformations which differ infinitesimally from the identity transformation

$$G = 1 - i\epsilon g,$$

where g is the Hermitian generator of the "Unitary" symmetry transformation G in question. For example for rotations about z-axis, it is the z-component of the angular momentum (to be shown later).

Suppose the Hamiltonian is invariant under G, that is G is symmetry, then we have

$$G^\dagger H G = H$$

or equivalently

$$[G, H] = 0.$$

In terms of the infinitesimal transformation, this may also be written in terms of the generator.

$$[g, H] = 0.$$

It is more meaningful to write the operator relation in terms of their expectation values given by

$$i\hbar \frac{d\langle g \rangle}{dt} = \langle [g, H] \rangle = 0$$

and hence g, or more precisely its quantum expectation value, is a constant of motion. For example if H is invariant under rotations then the generator of rotations, namely angular momentum about the axis of rotation, is a constant of motion.

Furthermore, when two operators commute, they can be simultaneously diagonalised. The set of eigenfunctions will be labelled by the eigenvalues, quantum numbers, of both operators. If the Hamiltonian for a transition is invariant under the transformation, then the quantum numbers labelling the initial state will also be conserved. This is a very powerful result which results in selection rules for reactions to occur.

Suppose we have two operator

$$[A, H] = 0, \quad [B, H] = 0$$

and if

$$iC = [A, B]$$

then

$$[C, H] = -i[H, [A, B]] = 0$$

using Jacobi identity

$$[H, [A, B]] + [A, [B, H]] + [B, [H, A]] = 0.$$

Thus C is also a symmetry of the system. It is possible that C may be a null operator or a linear combination of A, B. In that case no new symmetry results. However, if C is neither null nor a linear combination of A, B, then it is a new symmetry of the system. By examining the commutators of C with A or B, we may come across of another new symmetry. This way it is possible to discover a whole tower of symmetries of the system. Obviously, the tower of symmetries can not be too large as we know from experience.

In the next chapter, we shall discuss the example of rotation symmetry in detail leading to the "Quantum Theory of Angular Momentum".

2.2 Discrete symmetries

All symmetry operations in quantum mechanics are not necessarily continuous. The Hamiltonian may also be invariant under discrete transformations, for example space-time inversion. We consider three important symmetries here, namely, Parity, and Time Reversal. In contrast in a classical system, even when such discrete symmetries are apparent, they may not be consequential.

Permutation Symmetry A state of a system of identical, indistinguishable particles must be either symmetric or anti-symmetric under the exchange of any two particles within the system. It is an observed fact that all particles in the free state are either bosons are fermions depending on their behaviour with respect to another particle of the same kind. The state of a system of identical bosons is symmetric under permutations whereas a system of identical fermions is anti-symmetric under permutations. While one may be able to define systems with mixed symmetry (symmetric under some exchanges and antisymmetric under others) they are not realised in nature.

Note that the permutation symmetry or exchange symmetry is a discrete symmetry but is always operates in relation between particles.

Parity We first consider parity or space inversion. Classically under a parity transformation (in 3 dimensions) $\vec{r} \to -\vec{r}$ and $\vec{p} \to -\vec{p}$. That is a right-handed coordinate

system is changed to a left-handed coordinate system. This can not be achieved by rotation which is a continuous transformation in three-space dimensions. Hence it is a discrete symmetry. In fact it is easy to verify (we will do this in the next chapter) that the determinant of the transformation matrix is positive for rotation matrices where as for Parity it is negative.

If $|\alpha\rangle$ is a quantum mechanical state then we require under space inversion,

$$\langle\alpha|P^\dagger\vec{r}P|\alpha\rangle = -\langle\alpha|\vec{r}|\alpha\rangle$$

We accomplish by stating that under parity transformation,

$$P^\dagger\vec{r}P = -\vec{r}$$

or

$$\vec{r}P = -P\vec{r}$$

where we have used the fact that P is unitary. Thus the position and parity anticommute. Further, since two inversions cancel the effect of each other, we have,

$$P^2 = 1$$

or equivalently,

$$P^{-1} = P^\dagger = P$$

The Parity operator is not only unitary but also hermitian with eigenvalues +1 or -1.

By definition the angular momentum is $\vec{L} = \vec{r} \times \vec{p}$. Clearly,

$$P^\dagger\vec{L}P = \vec{L}; \quad \text{therefore } [\vec{L}, P] = 0.$$

Since $\vec{L}$ is the generator of rotations, parity commutes with rotations,

$$[R, P] = 0$$

.

If the Hamiltonian is invariant under parity transformation, then the states are definite eigenstates of the parity. Consider for example, a one dimensional system under the action of a potential such that $V(x) = V(-x)$. The Schroedinger equation for the system is

$$[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + v(x)]\psi(x) = E\psi(x). \tag{2.1}$$

Changing $x \to -x$ we get

$$[\frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + v(x)]\psi(-x) = E\psi(-x). \tag{2.2}$$

Obviously both $\psi(x)$ and $\psi(-x)$ are solutions of the equation with the same energy eigenvalue; they can only differ by a constant. That is

$$\psi(-x) = P\psi(x); \quad \psi(x) = P\psi(-x) = P^2\psi(x).$$

Therefore

$$P^2 = 1; \quad P = \pm.1$$

$$\psi(-x) = \psi(x) \Rightarrow Even\ paritystate$$

$$\psi(-x) = -\psi(x) \Rightarrow Odd\ paritystate$$

The solutions of Schroedinger equation for a parity invariant system have definite parity- even or odd. We see this in the solutions of one dimensional oscillator where the ground state has even parity where as the first excited state is an odd parity state.

For a rotationally invariant system in three dimensions, the eigenstates of the Hamiltonian are also eigenstates of parity. They are denoted by

$$\psi_{nlm} = R_{nl}(r)Y_{lm}(\theta, \phi).$$

Here n is the radial quantum number, while l, denote the eigenvalues of total angular momentum and its third component. Under parity transformation we have, $r \rightarrow r, \theta \rightarrow \pi - \theta, \phi \rightarrow \pi + \phi$ in spherical coordinates. Thus

$$P\psi_{nlm} = (-1)^l\psi_{nlm}$$

using the property of the spherical harmonics. We will discuss this in detail later.

Time-reversal The discussion of time reversal symmetry is some what more complicated. Classically both Newton's equations and Maxwell's equations are invariant under time reversal. We briefly discuss the situation in quantum mechanics where at the outset it appears not to be so since the Schroedinger equation is first order in time.

Suppose $\psi(x, t)$ is a solution of the Schroedinger equation,

$$i\hbar\frac{\partial\psi}{\partial t}(x, t) = (-\frac{\hbar^2}{2m}\nabla^2 + V)\psi(x, t)$$

then it is easy to see that the time reversed state $\psi(x, -t)$ is not a solution because of the first order time derivative. However, it is easy to check that $\psi^*(x, -t)$ is a solution by complex conjugation:

$$i\hbar\frac{\partial\psi^*}{\partial t}(x, -t) = (-\frac{\hbar^2}{2m}\nabla^2 + V)\psi^*(x, -t)$$

Thus we can conjecture that the time reversal has some thing to do with complex conjugation. Another way of looking at this is to preserve the probability invariant under time reversal. Following Wigner we may then require

$$\langle\psi|\psi\rangle = \langle T\psi|T\psi\rangle$$

There are two ways of achieving this which is obvious if we look at two different quantum states. We may have

$$\langle\phi|\psi\rangle = \langle T\phi|T\psi\rangle$$

as in ordinary transformations or

$$\langle\phi|\psi\rangle^* = \langle T\phi|T\psi\rangle$$

Since the first choice leads to the trouble mentioned above with respect to the dynamical equation, we may choose,

$$T\psi(x,t) = \psi^*(x,-t)$$

Therefore for any Hermitian operator O,

$$\langle\psi|O|\phi\rangle = \langle T\phi|TOT^{-1}|T\psi\rangle$$

Taking the absolute square gets rid of the complex conjugate problem and the probability remains invariant.

CPT theorem Apart from Parity and Time-reversal, another discrete symmetry is C- charge conjugation which transforms a particle state to anti-particle state and vice versa. We have not discussed this here; it is a fundamental symmetry of elementary particles. While the discrete symmetries C,P and T appear to violated, the combined operation CPT is an exact symmetry. Any theory that is invariant under Lorentz transformations must have CPT symmetry- CPT theorem. There is no known violation of the CPT symmetry and is consistent with all known experimental observations. The theorem has many consequences:

1. Spin-Statistics theorem: The connection between the spin of the particle and its statistics- for example the spin half particles obey Fermi statistics where as the integer spin particles obey Bose-Einstein statistics.

2. Particles and anti-particles have identical masses and life times.

3. All internal quantum numbers, charges, of anti-particles are opposite to those of the particles.

Summary To summarise, symmetry considerations are a powerful tool to explore and understand the behaviour of physical systems. They provide the backbone of our theoretical formulations. Even when some of the apparent symmetries are not exact they provide a basis for classification of states assuming exact symmetry and allow us to look at possible sources and pattern of symmetry breaking as in particle physics. Broadly, a symmetry transformation is one in which the laws of physics are unchanged.

Following Wigner, it was realised that invariance is an important principle for understanding key concepts. Wherever the application of the concept of symmetry is applied, it involves recognising a set of symmetry transformations under which the properties of the system under consideration remain unaltered. In all such cases the set of symmetry transformations form a *group*. The theory of groups deals with mathematical properties of a set of such transformations.

There are many examples in physics- for example: In geometry the distance between any two points, called metric, does not change under rotations. Invariance of the metric leads to the rotation group. In special theory of relativity the metric involves space-time and its invariance is characterised by a set of transformations which form the well known Lorentz group.

In the case of a crystal, the set of transformations that leave the the crystal structure invariant form a group which involves finite rotations and reflections. This is a powerful tool in the field of Crystallography.

In Quantum Mechanics we are interested in state space of a system characterised by a set of quantum numbers. The set of transformations on the state space of interest form a group. Next we consider the most important and commonly used group of transformations- namely the Rotation Group.

Chapter 3

Group of transformations

Formally a group is defined as follows:

Definition : Consider a set G defined by elements

$$G = g_1, g_2, g_3, \cdots \tag{3.1}$$

We say the elements $g \in G$ from a **Group** provided the set of elements satisfy the following properties:

1. If $g_i, g_j \in G$, then $g_i \star g_j \in G$, for all i, j where $\star$ denotes the group operation– for example multiplication, addition etc.

2. The set contains an identity element, $g_i \star I = I \star g_i = g_i$.

3. For all $g \in G$, there exists an inverse $g^{-1} \in G$ such that $g \star g^{-1} = g^{-1} \star g = I$

4. The group operation is associative: $g_i \star (g_j \star g_k) = (g_i \star g_j) \star g_k$.

If in particular the group elements commute, that is

$$g_i * g_j = g_j * g_i$$

for all i, j, the group is called an **Abelian Group**.

Here the set of elements g_i may represent a transformation or operation, which may be continuous or discrete, stated in abstract. The group operation may represent addition, multiplication (matrix multiplication), etc depending on the nature of transformation.

As an example consider the set of transformations on an equilateral triangle:

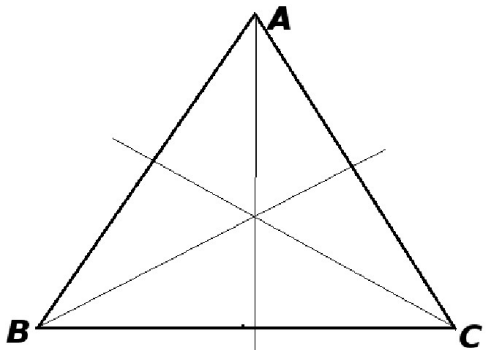


Figure 3.1:

We may treat the letters denoting the vertices (ABC) as a word. We may define many transformations which interchange the vertices leaving the triangle intact in the same orientation. For example consider the rotation of the triangle by 120^o and 240^o and 360^o or reflections about the three axes leaving one of the vertices unchanged. We may express these transformations in the form

$$g_i(word) = (word)'$$

where $(word)$ and $(word)'$ are some arrangements of the letters (A,B,C) and g_i effects some permutations of the letters in the words leaving the triangle intact. We may express the operation of g_i on the words explicitly as

$$(123)[ABC] = [ABC]; \quad (231)[ABC] = [BCA]; \quad (312)[ABC] = [CAB],$$

where each operation corresponds to a rotation of the triangle by 120^o. We also have the following set of operations

$$(132)[ABC] = [ACB]; \quad (321)[ABC] = [CBA]; \quad (213)[ABC] = [BAC],$$

where each operation corresponds to a reflection leaving a vertex intact.

Thus the set of transformations

$$g_1 = (123) = I,\ g_2 = (231),\ g_3 = (312),\ g_4 = (132),\ g_5 = (321),\ g_6 = (213)$$

leave the triangle invariant and the first operation is an identity. It is now easy to check that the set of $g_i, i = 1, 6$ form a group satisfying the properties of the group as defined above. This is the permutation group of 3-objects and is called **Permutation Group** S_3. One can extend this to the permutation of $n-$ objects (or vertices) corresponding to the invariance of regular geometric objects to define the Permutation group S_n.

In general the Theory of Groups deals with the properties of these transformations, their representations etc. In these lectures we try to understand the properties the key mathematical concepts regarding groups through some concrete examples, starting from the rotation group in two dimensions which is the simplest of all rotation groups.

3.1 Rotational Transformations

Let us begin with the simplest of rotational transformations- namely in two dimensions. Using this as template we consider the three dimensional rotations later.

3.1.1 Rotations in two-dimensions

Normally we represent a vector on a two dimensional plane by

$$\vec{r} = \hat{i}x + \hat{j}y = \hat{i}r\cos\theta_1 + \hat{j}r\sin\theta_1, \tag{3.2}$$

where $\hat{i}, \hat{j}$ denotes the unit vectors. Suppose we rotate this vector by an angle θ in the anti-clockwise direction, the rotated vector will be written as

$$\vec{r'} = \hat{i}x' + \hat{j}y' = \hat{i}r\cos\theta_2 + \hat{j}r\sin\theta_2. \tag{3.3}$$

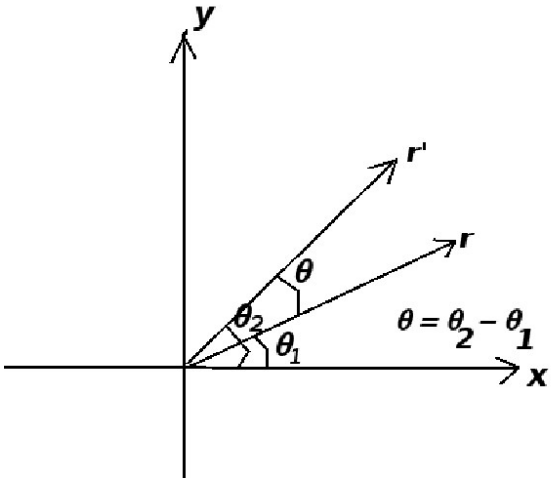


Figure 3.2: Schematic representation of two dimensional rotation

Writing in the component form we have, see Fig.(3.2)

$$x = r\cos\theta_1;\ \ y = r\sin\theta_1 \tag{3.4}$$

$$x' = r\cos\theta_2 = r\cos\theta_1\cos\theta - r\sin\theta_1\sin\theta = x\cos\theta - y\sin\theta. \tag{3.5}$$

$$y' = r\sin\theta_2 = r\sin\theta_1\cos\theta + r\cos\theta_1\sin\theta = x\sin\theta + y\cos\theta. \tag{3.6}$$

where $\theta_2 = \theta_1 + \theta$ and θ is the angle of rotation. Thus we have

$$x' = x\cos\theta - y\sin\theta$$

$$y' = x\sin\theta + y\cos\theta.$$

This is called active rotation. (Rotating the axes to represent the vector in two different sets of axes is called the passive rotation.) The angle θ can be varied continuously to obtain any desired orientation. This transformation may be written in the matrix form:

$$\begin{pmatrix} x' \\ y' \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} : \quad \vec{r'} = R(\theta)\vec{r}, \tag{3.7}$$

where we represent the two dimensional vector by a column and the rotational transformation through a 2×2 matrix R. This transformation is shown schematically in Fig.(3.2). This transformation is an example of a **Linear Transformation** on a vector space spanned by two real numbers (x,y). This applies to any arbitrary vector $\vec{A'} = R\vec{A}$ in two dimensions.

Consider two vectors $\vec{A}, \vec{B}$. While writing them as column vectors of components, we may drop the arrows on top for simplicity. After rotational transformation they are given by

$$A' = R(\theta)A; \quad B' = R(\theta)B \tag{3.8}$$

The scalar product

$$\begin{aligned} \vec{A'}.\vec{B'} &= A'_x B'_x + A'_y B'_y \\ &= (A_x\cos\theta - A_y\sin\theta)(B_x\cos\theta - B_y\sin\theta) \\ &+ (A_x\sin\theta + A_y\cos\theta)(B_x\sin\theta + B_y\cos\theta) \\ &= A_x B_x + A_y B_y = \vec{A}.\vec{B} \end{aligned} \tag{3.9}$$

Thus we say that the scalar product of two vectors is invariant under rotations. We write this in matrix notation as

$$A'_j = \sum_{k=1}^{2} (R)_{jk} A_k; \quad B'_j = \sum_{l=1}^{2} (R)_{jl} B_l; \tag{3.10}$$

such that

$$A'.B' = \sum_{j=1}^{2} (A')_j (B')_j = \sum_{j,k,l=1}^{2} (R)_{jk} A_k (R)_{jl} B_l = \sum_{j=1}^{2} (A)_j (B)_j = A.B \tag{3.11}$$

Therefore, the scalar product is preserved under rotations provided

$$\sum_j (R)_{jk} R_{jl} = \delta_{kl} \tag{3.12}$$

If we now define the matrix

$$(R^T)_{lj} = (R)_{jl} \tag{3.13}$$

then

$$\sum_j (R^T)_{kj} R_{jl} = \delta_{kl} \quad \Rightarrow R^T R = I \tag{3.14}$$

where I is the 2×2 unit matrix. The superscript denotes the **Transpose** of a matrix under consideration. Matrices with this property are called *Orthogonal Matrices* and the transformation is called orthogonal transformation.

We can now move from the specific example above, to the general properties of the Rotation matrices (orthogonal transformations):

- $$R^{-1} = R^T$$

  because

  $$R^T R = I$$

  .

- $$det(R^T) = det(R)$$

  Therefore

  $$det(R^T R) = det(R^T) det(R) = [det(R)]^2 = 1.$$

  and

  $$det(R) = \pm 1$$

- $det(R) = -1$ is rotation associated with inversion; this also includes combined rotation with inversion.

- $det(R) = 1$ is rotation and transformation associated with pure rotation as in the example above are called *Proper Orthogonal Transformations*. Such transformations may be continuously generated from unity. We are interested in these transformations here.

There is yet another, complex, representation using which we can characterise rotations in a plane. Let

$$\eta = x + iy = r(\cos\theta_1 + i\sin\theta_1) = re^{i\theta_1}$$

$$\eta' = x' + iy' = r(\cos\theta_2 + i\sin\theta_2) = re^{i\theta_2}$$

As we have seen the length of the vector is unchanged under rotations and $\theta_2 = \theta_1 + \theta$ as before. Thus we may write

$$\eta' = re^{i\theta_2} = re^{i(\theta+\theta_1)} = U(\theta)\eta,$$

where

$$U(\theta) = e^{i\theta}$$

is a one-dimensional complex representation of the rotational transformation in a plane (phase transformation). Furthermore we have the properties of the U as given by

$$U^\dagger U = 1; \quad U^{-1} = U^\dagger; \quad |U| = 1.$$

Here $U^\dagger = U^*$ but we use the $\dagger$ notation for future convenient.

Together both $R(\theta)$ and $U(\theta)$ represent the same rotation. Next we look at the properties of a set of such transformations.

3.1.2 Proper Orthogonal Group SO(2)

Let us now check if these 2×2 rotation matrices, with $0 \leq \theta < 2\pi$, form a group. The group operation $\star$ is simply matrix multiplication.

1. Consider a product of two rotations:

$$\begin{pmatrix} \cos\theta_1 & -\sin\theta_1 \\ \sin\theta_1 & \cos\theta_1 \end{pmatrix} \begin{pmatrix} \cos\theta_2 & -\sin\theta_2 \\ \sin\theta_2 & \cos\theta_2 \end{pmatrix} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} : \quad \theta = \theta_1 + \theta_2. \tag{3.15}$$

   Hence the product of two rotations is also a rotation.

2. The identity matrix is also a rotation but by angle $\theta = 0$, the identity I is contained in the set.

3. The inverse is also a rotation by angle $-\theta$ such that

$$\begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I. \tag{3.16}$$

4. The matrix multiplication is associative by definition. That is

$$R(\theta_1)[R(\theta_2)R(\theta_3)] = [R(\theta_1)R(\theta_2)]R(\theta_3) \tag{3.17}$$

Hence the set of matrices (transformations)

$$\mathbf{SO(2)} = \{\mathbf{Real\ 2x2\ matrices\ R};\ \mathbf{RR^T = R^TR = I},\ \mathbf{det(R) = +1}\}$$

form a group called *Special Orthogonal Group SO(2) or simply Group of Rotations in two dimensions*. The scalar product of any two vectors is invariant under the action of the group. As a result the *length of a vector is invariant under rotations*. Clearly SO(2)has infinitely many elements and it is a continuous group since all the elements are generated by varying the parameter θ continuously.

The group SO(2) has a special property, not shared by rotations in higher dimensions: The rotations in 2-dimensions commute, that is

$$R(\theta_1)R(\theta_2) = R(\theta_2)R(\theta_1)$$

It is called an *Abelian Group*. Rotations in higher dimensions

3.1.3 Unitary group in 1D: U(1)

As we have seen earlier all rotations in a plane (2D) may be written as transformations of the 2D vector expressed as complex function η where under rotations

$$\eta' = U(\theta)\eta,$$

where U is a unitary or phase transformation in a plane. As in the case of SO(2), the set of all phase transformation form a group, since

$$\begin{aligned} U(\theta_1)U(\theta_2) &= U(\theta_1+\theta_2) \\ U(0) = I \qquad & \qquad U^{-1}(\theta) = U(-\theta) \\ U(\theta_1)[U(\theta_2)U(\theta_3)] &= [U(\theta_1)U(\theta_2)]U(\theta_3). \end{aligned} \tag{3.18}$$

Further the group U(1), which is the set of all phase transformations $U(\theta)$ where $0 \leq \theta < 2\pi$ takes continuous values, is also abelian just as SO(2). Therefore the group SO(2) and U(1) are **Isomorphic** to each other. We say the unitary group U(1) in 1D provides a representation of the group SO(2). While the 2×2 dimensional representation is a natural representation of SO(2), there are other higher dimensional representation. We will discuss these as and when necessary.

In physics we are more interested in the representation than the abstract group itself.

3.1.4 Infinitesimal Transformation and its Generator

Since any rotation by θ can be obtained by combining many smaller rotations $\delta\theta = \theta/N$ applying it N times, we may parameterise an infinitesimal transformation by

$$\lim_{\delta\theta\to 0}\begin{pmatrix}\cos\delta\theta & -\sin\delta\theta\\ \sin\delta\theta & \cos\delta\theta\end{pmatrix} = I + \delta\theta\sigma + O(\delta\theta^2): \quad \sigma = \begin{pmatrix}0 & -1\\ 1 & 0\end{pmatrix}, \tag{3.19}$$

and

$$\sigma^2 = -I,\ Tr(\sigma) = 0.$$

An arbitrary rotation by θ is then generated by repeated application of the infinitesimal transformation, that is

$$R(\theta) = \lim_{N\to\infty}(I + \delta\theta\sigma)^N = \lim_{N\to\infty}(I + \frac{\theta}{N}\sigma)^N = \exp(\theta\sigma) \tag{3.20}$$

This reduces to the standard form when we expand the exponential

$$R(\theta) = (1 - \frac{\theta^2}{2} + \frac{\theta^4}{4!} + \cdots)I + \sigma(\frac{\theta}{1} - \frac{\theta^3}{3!} + \cdots) = \cos\theta I + \sin\theta\sigma, \tag{3.21}$$

where we used the fact that $\sigma^2 = -I$. We may write it using the well known Pauli matrix σ_y in the Hermitian form:

$$R(\theta) = \exp(-i\theta\sigma_y) = \cos\theta I - i\sigma_y\sin\theta\ ; \quad \sigma_y = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}. \tag{3.22}$$

We call σ_y the **Generator** of rotations in two dimensions. Since there is only one parameter θ, there is only one generator. In general the number of parameters of rotation is equal to the number of generators.

3.1.5 Rotations of functions

The rotations on coordinates of a two dimensional vector is given by

$$r' = R\ r,$$

where r is a two dimensional column vector and the set of 2D matrices R are elements of the group SO(2).

The action of the group on complex numbers constructed with the components of vectors is given by

$$\eta' = U\eta,$$

where now the the set of U's belong to the group U(1) and provide a representation of the group SO(2).

Now let us see how a $\psi(x, y)$, which may be a quantum mechanical wave function for example, change when the coordinates are rotated. Define

$$\psi'(x, y) = R\psi(x, y) \Rightarrow \psi(x', y')$$

Consider an infinitesimal transformation of coordinates, where

$$x' = x + \delta x = x - y\delta\theta; \quad y' = y + x\delta\theta,$$

$$R(\delta\theta)\psi(x, y) = \psi(x - y\delta\theta, y + x\delta\theta).$$

Taylor expanding the function on the right around (x,y) gives us

$$\psi(x - y\delta\theta, y + x\delta\theta) = \psi(x, y) + \frac{\partial\psi}{\partial x}\delta x + \frac{\partial\psi}{\partial y}\delta y + \cdots .$$

or

$$\psi(x', y') = \psi(x, y) + \delta\theta\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right]\psi + \cdots = \psi(x, y) + \frac{i}{\hbar}\delta\theta L\psi,$$

where L is the angular momentum operator in 2D given by

$$L = \vec{r} \times \hat{p} = -i\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right].$$

Note that angular momentum in two dimension is a pseudo-scalar. The rotation operator, integrated over the infinitesimal is given by

$$R(\theta) = \exp\left(\frac{i}{\hbar}L\theta\right)$$

The Planck's constant $\hbar = \frac{h}{2\pi}$ is introduced here for later convenience. It also ensures that L has the correct dimensions (angular momentum).

With these preliminaries, we now consider the rotational transformations in three dimensions which has a much richer structure as we shall see.

3.1.6 Rotations in three-dimensions

Consider the proper rotations in three dimensions following the template in two-dimensions given in the previous section. A three dimensional vector is specified by its Cartesian coordinates

$$\vec{r} = \hat{i}x + \hat{j}y + \hat{k}z \tag{3.23}$$

Most general rotation of the vector involves three angles which we may denote by $\vec{\theta}$ each of which may be varied continuously. Any such rotation in three dimensions

involves the modulus of θ and an axis of rotation $\hat{n}$. The axis is usually given by the right-hand thumb rule.

As in the case of two-dimensions we may write the transformation in the form

$$\vec{r'} = R(\vec{\theta})\vec{r}, \tag{3.24}$$

where R is now a 3×3 matrix. Writing in the component form we have,

$$x'_j = \sum_{k=1}^{3} (R)_{jk} x_k : \quad x_1 = x,\ x_2 = y,\ x_3 = z \tag{3.25}$$

Suppose now $\vec{A}, \vec{B}$ are two vectors, then the rotational transformation will preserve the scalar product, that is the scalar product of two vectors is invariant under rotations:

$$A'.B' = \sum_{j=1}^{3} (A')_j (B')_j = \sum_{j,k,l=1}^{3} (R)_{jk} A_k (R)_{jl} B_l = \sum_{j=1}^{3} (A)_j (B)_j = A.B \tag{3.26}$$

Obviously the norm (length) of the vector, which is the scalar product of the vector with itself, is unchanged under-rotations. As in the case of two-dimensions we have the following properties of R: Therefore, the scalar product is preserved under rotations provided

$$\sum_j (R)_{jk} R_{jl} = \delta_{kl} \tag{3.27}$$

If we now define the matrix transpose as

$$(R^T)_{lj} = (R)_{jl} \tag{3.28}$$

then

$$\sum_j (R^T)_{kj} R_{jl} = \delta_{kl} \quad \Rightarrow R^T R = I \tag{3.29}$$

where I is the 3×3 unit matrix.

The general properties of rotation in any dimension, extending from 2- and 3-dimensions, are given by

- $$R^{-1} = R^T$$

  because

  $$R^T R = I$$

  .

- $$det(R^T) = det(R)$$

  Therefore
  $$det(R^T R) = det(R^T) det(R) = [det(R)]^2 = 1.$$

- $$det(R) = \pm 1$$

- $det(R) = -1$ is rotation associated with inversion, that is parity.

- $det(R) = 1$ is rotation and transformation associated with pure rotation as in the example above are called *Proper Orthogonal Transformations*.In what follows we restrict to proper rotations.

These properties are unchanged for rotations in any dimension. We may specify rotations explicitly by specifying the axis of rotation. For example

- Rotation about the z-axis with $\vec{\theta} = (0, 0, \theta_3)$:
$$R_3 = \begin{pmatrix} \cos\theta_3 & -\sin\theta_3 & 0 \\ \sin\theta_3 & \cos\theta_3 & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{3.30}$$

- Rotation about the y-axis with $\vec{\theta} = (0, \theta_2, 0)$:
$$R_2 = \begin{pmatrix} \cos\theta_2 & 0 & \sin\theta_2 \\ 0 & 1 & 0 \\ -\sin\theta_2 & 0 & \cos\theta_2 \end{pmatrix} \tag{3.31}$$
  Note that there is sign change compared to R_3 due to the convention - right hand thumb rule that we have used.

- Rotation about the x-axis with $\vec{\theta} = (\theta_1, 0, 0)$:
$$R_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta_1 & -\sin\theta_1 \\ 0 & \sin\theta_1 & \cos\theta_1 \end{pmatrix} \tag{3.32}$$

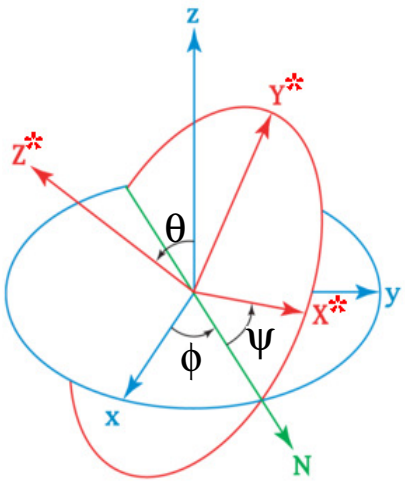
Note that each of the above representation of planar rotations about an axis forms a group by itself providing a 3D representation of the group SO(2). By Euler's theorem every rotation in 3D can be expressed as a product of three successive rotations about 3-independent axes. Hence each of three SO(2) representations forms a subgroup of the full 3D rotation group SO(3) which we will discuss below.

3.1.7 Euler angles: Representation of the most general rotation

Euler's Theorem: An arbitrary rotation can be expressed as a product of three successive rotations about 3-distinct axes.

Since we can choose any three distinct axes, following Euler we can represent an arbitrary rotation using the rotation of axes. Let us choose a vector that is represented in a frame S. We want to represent the same vector in a frame S* which has an arbitrary orientation wrt to S. This is done in the following way:

Let us assume the two origins to be the same located at the origin of a vector. The line ON denotes the *line of nodes* corresponding to the intersection of the XY plane in the space fixed system with the X^*Y^* plane of the body fixed system. The line of nodes is evidently perpendicular to the Z and Z^* axes. We take the positive direction along the vector product $\hat{Z} \times \hat{Z}^*$.



The orientation of $X^*Y^*Z^*$ axes with respect to XYZ is defined in terms of the Euler angles θ, ϕ, ψ. Here θ is the angle between Z and Z^* axes. Angle ϕ is the angle between the X axis and the line of nodes where as angle ψ denotes the X^* axis and the line of nodes ON. Angles ϕ, ψ are measured around the axes Z and Z^* respectively in the direction given by the corkscrew rule. Furthermore it is clear that

$$0 \leq \theta \leq \pi, \quad 0 \leq \phi, \psi \leq 2\pi.$$

Thus the most general rotation in Euler representation is given by

$$R(\psi,\theta,\phi) = R_3(\psi)R_1(\theta)R_3(\phi)$$

or equivalently

$$R(\psi,\theta,\phi) = R_3(\psi)R_2(\theta)R_3(\phi)$$

3.1.8 Proper Orthogonal Group SO(3)

Consider now the set of all matrices

$$\mathbf{SO(3)} = \{\mathbf{Real\ 3\times 3\ matrices\ R};\ \mathbf{RR^T = R^TR = I},\ \mathbf{det(R) = +1}\}$$

The set of matrices satisfy the following conditions:

1. Consider the product of two arbitrary rotations R_a, R_b:

$$R_a^T R_a = I, \quad R_b^T R_b = I; R_c = R_a R_b,\ R_c^T = R_b^T R_a^T, \Rightarrow R_c^T R_c = I \tag{3.33}$$

   Hence the product of two rotations is also a rotation.

2. The identity matrix is also a rotation but by angle $\theta = 0$. Hence Identity element is contained in the set.

3. the inverse is also a rotation since

$$(R_a^{-1})^T(R_a^{-1}) = (R_a^T)^{-1}(R_a)^{-1} = I \tag{3.34}$$

   The inverse is also contained in the set.

4. The matrix multiplication is associative by definition. That is

$$R(\vec{\theta}_a)[R(\vec{\theta}_b)R(\vec{\theta}_c)] = [R(\vec{\theta}_a)R(\vec{\theta}_b)]R(\vec{\theta}_c) \tag{3.35}$$

Hence the set of matrices defined by

$$\mathbf{SO(3)} = \{\mathbf{Real\ 3x3\ matrices\ R};\ \mathbf{RR^T = R^TR = I},\ \mathbf{det(R) = +1}\}$$

form a group called *Special Orthogonal Group SO(3) or simply Group of Rotations in three dimensions.*

Unlike the elements of the group SO(2), Rotations in three dimensions do not commute, that is

$$R(\vec{\theta}_1)R(\vec{\theta}_2) \neq R(\vec{\theta}_2)R(\vec{\theta}_1)$$

Hence it is a non-Abelian group of transformations.

3.1.9 Infinitesimal Transformations and Generators of SO(3)

Now let us consider infinitesimal rotations about the three axes separately: As before a rotation by θ_i is obtained by $\delta\theta_i = \theta_i/N$ rotation applying it N times. We may parameterise an infinitesimal transformation around z-axis by

$$\lim_{\delta\theta_3\to 0}\begin{pmatrix}\cos\delta\theta_3 & -\sin\delta\theta_3 & 0\\ \sin\delta\theta_3 & \cos\delta\theta_3 & 0\\ 0 & 0 & 1\end{pmatrix} = I + \delta\theta_3 l_3 : \quad l_3 = \begin{pmatrix}0 & -1 & 0\\ 1 & 0 & 0\\ 0 & 0 & 0\end{pmatrix}. \tag{3.36}$$

The matrix corresponding to a rotation about z-axis by an angle θ_3 is given by

$$R(\theta_3) = \lim_{N\to\infty}\left(I + \frac{\theta_3}{N} l_3\right)^N = \exp(\theta_3 l_3).$$

Similarly the infinitesimal transformations along y- and x-axes are given by

$$\lim_{\delta\theta_2\to 0}\begin{pmatrix}\cos\delta\theta_2 & 0 & \sin\delta\theta_2\\ 0 & 1 & 0\\ -\sin\delta\theta_2 & 0 & \cos\delta\theta_2\end{pmatrix} = I + \delta\theta_2 l_2 : \quad l_2 = \begin{pmatrix}0 & 0 & 1\\ 0 & 0 & 0\\ -1 & 0 & 0\end{pmatrix}, \tag{3.37}$$

$$\lim_{\delta\theta_1\to 0}\begin{pmatrix}1 & 0 & 0\\ 0 & \cos\delta\theta_1 & -\sin\delta\theta_1\\ 0 & \sin\delta\theta_1 & \cos\delta\theta_1\end{pmatrix} = I + \delta\theta_1 l_1 : \quad l_1 = \begin{pmatrix}0 & 0 & 0\\ 0 & 0 & -1\\ 0 & 1 & 0\end{pmatrix}, \tag{3.38}$$

where $l_i^2 = -1,\ Tr(l_i) = 0$ and I is the identity matrix in 3-dimensions. Corresponding finite rotations are given by

$$R(\theta_2) = \exp(\theta_2 l_2), \quad R(\theta_1) = \exp(\theta_1 l_1).$$

Most general infinitesimal transformation is then given by

$$R(\delta\theta_1, \delta\theta_2, \delta\theta_3) = I + \sum_{j=1}^{3} \delta\theta_i l_i = I + A \tag{3.39}$$

where A is in general an antisymmetric matrix given by

$$A = \begin{pmatrix}0 & -\delta\theta_3 & \delta\theta_2\\ \delta\theta_3 & 0 & -\delta\theta_1\\ -\delta\theta_2 & \delta\theta_1 & 0\end{pmatrix}, \tag{3.40}$$

As in the case of SO(2) we would like to exponentiate and write the general transformation as

$$R(\theta_1, \theta_2, \theta_3) = \lim_{N\to\infty}(I + A)^N = \lim_{N\to\infty}(I + \sum_i \frac{\theta_i l_i}{N})^N = \exp(\sum_i \theta_i l_i) \tag{3.41}$$

Note that

$$R(\theta_1, \theta_2, \theta_3) = \exp(\sum_i \theta_i l_i) \neq \exp(\theta_1 l_1) \exp(\theta_1 l_2) \exp(\theta_1 l_3) \tag{3.42}$$

In doing so, the closure property 1 of the group should be maintained by product of rotations. However this is non-trivial since matrices l_i are non-commuting, since in general the product of two rotations has the form

$$R_c = R_a R_b = e^A e^B = e^{A+B+\frac{1}{2}[A,B]+\frac{1}{12}[A,[A,B]]+\cdots}, \tag{3.43}$$

where A, B are some 3×3 anti-symmetric matrices given in-terms of l_i. This is called the *Baker-Campbell-Hausdorff Formula*. Thus if R_c is also a rotation then we should be able to write it in the exponential form, just as R_a, R_b then the commutator $[A, B]$ must have a specific form– the commutator must also be linear in the set of matrices that generates a rotation.

In the case of rotations we have the following property obeyed by l_i:

$$[l_1, l_2] = l_3; \quad [l_2, l_3] = l_1; \quad [l_3, l_1] = l_2; \quad [l_i, l_j] = \epsilon_{ijk} l_k \tag{3.44}$$

as can be easily checked. As a result all the commutators in the Baker-Campbell-Hausdorff formula are linear in l_i. Therefore the exponential form of rotation matrices obey the matrix multiplication rule of the group SO(3)

$$R_c(\vec{\psi}) = e^{\sum_i \psi_i l_i} = R_a(\vec{\theta}) R_b(\vec{\phi}) = e^{\sum_i \theta_i l_i} e^{\sum_i \phi_i l_i} \tag{3.45}$$

where every rotation is characterised by three-angles and are generated by the same set of matrices l_i. Thus we call l_i as generators of rotation.

Lie Groups and Lie algebras From the preceding discussion it is clear that the finite number of generators l_i, equal to the number of parameters (angles), determined from infinitesimal transformations completely determine all such group elements. Hence they are called *generators* of the group. Such groups are called *Lie Groups*. Rotation group is an example of this.

The group elements depend analytically on a finite number of parameters, in our case these are the angles. The number of linearly independent parameters define the *dimension* of the group (not necessarily the dimension of the matrices). The number of generators is equal to the dimension of the group.

The product of two such group elements are contained in the group is ensured by the fact that the *algebra* of generators is closed:

$$[l_i, l_j] = \epsilon_{ijk} l_k \tag{3.46}$$

which is called the *Lie Algebra* of generators- ϵ_{ijk} are called structure constants of the group.

Until now we have considered rotational transformations geometrically and its representations through the elements of SO(3) and the corresponding algebra of generators. The connection to Quantum Mechanics comes from the fact that we can represent the generators of SO(3) in the form

$$l_k = -\frac{i}{\hbar} L_k \tag{3.47}$$

so that rotation matrices are written in the form

$$R(\vec{\theta}) = \exp\left(-\frac{i}{\hbar}\vec{\theta}.\vec{L}\right) \tag{3.48}$$

and the algebra of matrices L_k obey the algebra

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k; \quad L_i^\dagger = L_i \tag{3.49}$$

which is precisely the algebra of *Angular Momentum Operators*. Unlike l_k the L_k are Hermitian generators of the group SO(3).

3.1.10 Representation: Rotation of functions

Until now we have considered the action of group SO(3) on the space of vectors represented by cartesian coordinates $(x, y, z) = (x_1, x_2, x_3)$. Let us now consider the transformation on functions. Following the example of SO(2), let

$$\psi'(x, y, z) = R\psi(x, y, z) \Rightarrow \psi(x', y', z').$$

Let us fix $z' = z$ which is equivalent to a rotation in the x-y plane where the rotation transformations form a 3D subgroup SO(2) of the full group SO(3).

Taylor expanding as in the 2D case when the transformation is infinitesimal we have

$$\psi(x', y', z) = \psi(x, y, z) + \frac{i}{\hbar}\delta\theta_3 L_3\psi,$$

where $\hbar$ is introduced to be consistent with the notation used in quantum mechanics and as before

$$L_3 = -i\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right].$$

Repeating the procedure with y and x axis fixed, we have

$$L_2 = -i\hbar\left[z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right],$$

$$L_1 = -i\hbar \left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right].$$

These are precisely expressions we obtain in quantum mechanics by replacing the classical angular momentum

$$\vec{L} = \vec{r} \times \vec{p}$$

by the corresponding operators for linear momentum components. We have deliberately used the same notation as in the case of generators of rotation group SO(3), namely L_i. The reason will become clear when we consider th commutators among these L_i. For example consider

$$\begin{aligned} [L_1, L_2]\psi &= (L_1L_2 - L_2L_1)\psi \\ &= -\hbar^2 \left(\left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y} \right] \left[z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z} \right] - ... \right) \psi \\ &= -\hbar^2 \left(y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y} \right) \psi = i\hbar L_3 \psi \end{aligned} \tag{3.50}$$

so that we have the operator equation

$$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k. \tag{3.51}$$

Thus the algebra of angular momentum operators L_i is the same as the algebra of the generators of the rotation group SO(3) in three dimensions. For arbitrary rotations of the function ψ we have

$$\psi(x', y', z') = \exp\left(\frac{i}{\hbar}\theta_i L_i \right) \psi(x, y, z).$$

Spherical Harmonics

We may now consider some explicit representations. In quantum mechanics we often consider a basis which is characterised by angular momentum quantum numbers, namely the so called spherical harmonics. This can be achieved by the following transformation of the basis where $(x, y, z) \Rightarrow (rY_{lm})$: Let us express the cartesian coordinates in terms of polar coordinates

$$\begin{aligned} x &= r\sin\theta\cos\phi \\ y &= r\sin\theta\sin\phi \\ z &= r\cos\theta \end{aligned} \tag{3.52}$$

where $r^2 = x^2 + y^2 + z^2$ which is an invariant under rotations. We may transform this basis as a complex basis given by

$$\begin{aligned} x + iy = r\sin\theta\exp(i\phi) &\Rightarrow rY_{11}(\theta,\phi) \\ z = r\cos\theta &\Rightarrow rY_{10}(\theta) \\ x - iy = r\sin\theta\exp(-i\phi) &\Rightarrow rY_{1-1}(\theta,\phi) \\ \vec{r} &\Rightarrow rY_{1m}(\theta,\phi) \end{aligned} \tag{3.53}$$

The arrows indicate equality apart from an overall normalisation of the functions Y_{lm} which are the so called Spherical Harmonic Functions (of rank 1). While this is a simple change of basis as far as rotations are concerned, the spherical harmonic basis has some nice properties which are used extensively in quantum theory of angular momentum.

The relation between angular momentum and spherical harmonics becomes clear once we look at the action of angular momentum operators or generators of rotations on the Y's. To see this let us express L_i in terms of polar coordinates:

$$\begin{aligned} \vec{L} &= i\hbar\left(\hat{\mathbf{i}}\left(\sin(\phi)\frac{\partial}{\partial\theta} + \cot(\theta)\cos(\phi)\frac{\partial}{\partial\phi}\right) + \hat{\mathbf{j}}\left(-\cos(\phi)\frac{\partial}{\partial\theta} + \cot(\theta)\sin(\phi)\frac{\partial}{\partial\phi}\right) - \hat{\mathbf{k}}\frac{\partial}{\partial\phi}\right) \\ L_+ &= L_1 + iL_2 = \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot(\theta)\frac{\partial}{\partial\phi}\right), \\ L_- &= L_1 - iL_2 = \hbar e^{-i\phi}\left(-\frac{\partial}{\partial\theta} + i\cot(\theta)\frac{\partial}{\partial\phi}\right), \\ L_3 &= -i\hbar\frac{\partial}{\partial\phi}, \\ L^2 &= \vec{L}.\vec{L} = -\hbar^2\left(\frac{1}{\sin(\theta)}\frac{\partial}{\partial\theta}\left(\sin(\theta)\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2(\theta)}\frac{\partial^2}{\partial\phi^2}\right). \end{aligned} \tag{3.54}$$

Note that in this spherical polar representation all the components L_i and L^2 involve derivatives of angles only.

It is easy to check the following properties of the spherical harmonics Y_{1m}:

$$L_3 Y_{1m} = \hbar m Y_{1m}$$

$$L^2 Y_{1m} = 2\hbar^2 Y_{1m}.$$

Thus the Y_{1m} are simultaneous eigenstates of L_3, L^2 and the eigenvalues of L^2 are independent of m, the projection or magnetic quantum number as it is called. We call the spherical harmonics Y_{1m} as tensors of rank 1 (vector) whose transformation under rotation group is then given by

$$Y_{1m'} = \sum_m D^1_{m'm}(R) Y_{1m}. \tag{3.55}$$

Just as x, y, z transform among themselves under rotations, the Y_{1m} also transform among themselves. The rank of the tensor is unchanged under rotations. The $D^1(R)$ matrices provide a representation of three dimensional rotations on the space of rank 1 spherical harmonics. We will not go into phase conventions involved in defining these matrices here.

We may now extend the arguement by constructing higher rank tensors by taking product of the cartesian components x, y, z. For example combining the three components of a position vector, we have

$$x^2, y^2, z^2, xy, yz, zx,$$

which constitute the components of a second-rank Cartesian tensor. Out of these six second order components only five are independent since under rotations we have

$$r^2 = x^2 + y^2 + z^2.$$

These five independent components of the second-rank tensor may be organised according to their properties under the action of L_3 and L^2 as in the case of Y_{1m}:

$$\begin{aligned}
(x+iy)^2 = r^2 \sin^2\theta \exp(2i\phi) &\Rightarrow r^2 Y_{22}(\theta,\phi) \\
z(x+iy) = r^2 \sin\theta\cos\theta\exp(i\phi) &\Rightarrow r^2 Y_{21}(\theta,\phi) \\
(3z^2-1) = r^2(3\cos^2\theta - 1) &\Rightarrow r^2 Y_{20}(\theta) \\
z(x-iy) = r^2 \sin\theta\cos\theta\exp(-i\phi) &\Rightarrow r^2 Y_{2-1}(\theta,\phi) \\
(x-iy)^2 = r^2 \sin^2\theta \exp(-2i\phi) &\Rightarrow r^2 Y_{2-2}(\theta,\phi)
\end{aligned} \tag{3.56}$$

It is easy to see that the following properties are satisfied:

$$L_3 Y_{2m} = m\hbar Y_{2m},$$

$$L^2 Y_{2m} = 6\hbar^2 Y_{2m}.$$

where $m = -2, -1, 0, 1, 2$.

We may continue the exercise to construct higher rank tensors- either Cartesian or spherical harmonics by taking higher powers of the basic components of the position vector x, y, z. Each such representation is organised by its properties under the action of L_3, L^2. An inspection of Y_{11}, Y_{22}, clearly indicates how the arbitrary rank spherical harmonics may be constructed. We may write

$$r^l Y_{ll} = (x+iy)^l = r^l \sin^l\theta e^{il\phi},$$

Similarly

$$r^l Y_{l-l} = (x+iy)^{-l} = r^l \sin^l\theta e^{-il\phi}.$$

All other spherical harmonic function may then be obtained using the properties of the operators L_+, L_-,

$$L_- Y_{lm} \propto Y_{lm-1}; \quad m = -l, \cdots, l$$

$$L_+ Y_{lm} \propto Y_{lm+1}; \quad m = -l, \cdots, l$$

Notice that the spherical harmonics generated in this manner are still un-normalised which needs to be done.

Finally we summarise the important properties of spherical harmonics of arbitrary rank as generated above. Following the convention used in quantum mechanics we write the normalised spherical harmonics as

$$Y_{\ell m}(\theta, \phi) = (-1)^m \sqrt{\frac{(2\ell+1)}{4\pi} \frac{(\ell-m)!}{(\ell+m)!}} \, P_{\ell m}(\cos\theta) \, e^{im\phi}, \tag{3.57}$$

where $P_{\ell,n}(\theta)$ are the associated Legendre Polynomials. The rank of the tensor representation is l with $2l+1$ independent components. The spherical harmonics as defined above are normalised such that

$$\int_{\theta=0}^{\pi} \int_{\phi=0}^{2\pi} Y_{\ell m} \, Y^*_{\ell' m'} \, d\Omega = \delta_{\ell\ell'} \, \delta_{mm'}, \tag{3.58}$$

which obey the eigenvalue equations

$$L_3 Y_{lm} = m\hbar Y_{lm}; \quad L^2 Y_{lm} = l(l+1)\hbar^2 Y_{lm}, \tag{3.59}$$

where $m = -l, -l+1, \cdots, l-1, l$ takes $2l+1$ values for $l = 0, 1, 2, \cdots$. Under rotations the spherical harmonics transform as

$$Y_{lm'} = \sum_m D^l_{m'm}(R) Y_{lm}, \tag{3.60}$$

where $D^l_{m'm}$, called Wigner D-matrices, provide a representation of Rotations R of vector components x, y, z acting on tensors in the basis given by spherical harmonics. Notice the D matrices transform the Y_{lm} with out changing the rank of the tensor given by l and the dimension of the representation is given by $(2l+1)$. Such a representation where the rank of the tensor remains the same is called an **Irreducible Representation**.

Finally we take a look at the property of spherical harmonics under parity transformation. In polar coordinates, the parity transformation is

$$r' = r; \quad \theta' = \theta - \pi; \quad \phi' = \phi + \pi$$

and

$$Y_{lm}(\theta', \phi') = (-1)^l Y_{lm}(\theta, \phi).$$

3.1.11 Summary: Lie Group and Lie Algebra

Every rotation in 3-D maps an ortho-normal basis in R^3 to another ortho-normal basis (passive rotation) equivalently every rotation R acting on the components of a vector rotates the vector (active) preserving the length of the vector. It is an example of a general linear transformation that may be represented as matrix of transformation with the property

$$R^T R = R R^T = I.$$

A subset of the transformations preserving the length of the vector with the property $det(R) = +1$ form a group called the **Special Orthogonal Group SO(3)**.

Every element of the group may be exponentiated and written in terms of the generators

$$R(\vec{\theta}) = exp(-\frac{i}{\hbar}\vec{\theta}.\vec{L}),$$

where

$$[L_i, L_j] = i\hbar L_k$$

defines the algebra of generators.

These properties define what is called a Lie Group with an associated Lie algebra- SO(3) is an example of this general class of groups.

- A **Lie group** is defined by group elements that are specified by one or more continuous parameter(s):

  SO(2): Continuous parameter Angle θ.

  SO(3): Continuous parameters Angles $\theta_1, \theta_2, \theta_3$.

  SO(n): Rotation group in n-dimensions with continuous parameters Angles $\theta_i,\ i = 1, \cdots, n(n-1)/2$.

  The self- or natural-representation of the group SO(n) is given by $n \times n$ orthogonal matrices R.

- **Lie Algebra** of the group is an algebraic structure that underlies the group. All elements of the group may be written as in the exponentiated form:

  SO(2): $R(\theta) = \exp(-i\theta\sigma_y)$- σ_y is the generator of the group.

  SO(3): $R(\theta) = \exp\left(-\frac{i}{\hbar}\theta_i L_i\right)$- such that

  $$[L_i, L_j] = i\hbar\epsilon_{ijk}L_k.$$

  SO(n): $R(\theta) = \exp(-i\theta_i L_i)$- such that

  $$[L_i, L_j] = i f_{ijk} L_k; \quad i, j, k = 1, \cdots, n(n-1)/2.$$

f_{ijk} are called the structure constants of the group.

Every representation of the group self- or higher dimensional representation is completely specified by the algebraic structure of the group.

- Casimir invariant of the group is defined as a quadratic operator in terms of the generators. For example for SO(3) it is defined as

$$L^2 = L_1^2 + L_2^2 + L_3^2$$

whose essential property if that it commutes with all the generators, that is

$$[L^2, L_i] = 0.$$

Without proof we may state that in any representation of the generators L_i of SO(3) at best we may diagonalise one of them and is usually chosen to be L_3. Therefore all states of an SO(3) group may be characterised by two quantum numbers corresponding the eigenvalues of L_3 and L^2. We have already seen an example of this in the case of spherical harmonics, Y_{lm}:

$$L_3 Y_{lm} = m Y_{lm}; \quad L^2 Y_{lm} = l(l+1) Y_{lm},$$

where the basis is characterised by the eigenvalues m and simply l for L^2.

In general the number of quadratic Casimirs of a group define what is called the **Rank** of the group.

Following the above considerations, we may now state that corresponding to every element R of SO(3), suppose there exists a unitary transformation $D(R)$ on the space of functions. Suppose the set of transformations $D(R)$ satisfy the same composition law of the group SO(3), that is

$$D(R_1)D(R_2) = D(R_1 R_2); \quad D(R^{-1}) = D^\dagger(R). \tag{3.61}$$

Then the set of matrices that satisfies these laws is a *Representation of the group SO(3).*

Chapter 4

Angular Momentum in Quantum Mechanics

A particle moving in a three dimensional space under the action of a potential $V(r,\theta,\phi) = V(r)$ is said to be moving in a central potential. The potential $V(r)$ is independent of the orientation or spherically symmetric.

$$V(r) = \frac{1}{2}m\omega^2(x^2+y^2+z^2) = \frac{1}{2}m\omega^2\ r^2 \tag{4.1}$$

and Coulomb potential $V(r) = e^2/r$. They constitute one of the simplest but useful application of Schroedinger equation.

Let us consider the non-relativistic motion of a particle moving in such a potential. The Hamiltonian is given by

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(r). \tag{4.2}$$

There is no explicit time dependent term, and the energy eigenvalue equation is given by

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(r)\right] u_E = E\ u_E. \tag{4.3}$$

Since the potential is spherical symmetric, central potential, it is useful to write this explicitly in spherical polar coordinates (r,θ,ϕ),

$$-\frac{\hbar^2}{2mr^2}\left[\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] u_E + V(r)u_E = E\ u_E. \tag{4.4}$$

By inspection, we see that the terms involving angular derivatives are familiar, in fact it is simply the operator $\hat{L}^2$. Therefore

$$-\frac{1}{2mr^2}\left[\hbar^2\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \hat{L}^2\right] u_E + V(r)u_E = E\ u_E. \tag{4.5}$$

It is easy to check

$$[\hat{H}, \hat{L}^2] = 0, \quad [\hat{H}, \hat{L}_z] = 0 \tag{4.6}$$

It is therefore possible to specify energy, angular momentum and its projection, simultaneously for a particle moving in a central potential. Since we already know the eigenstate of operator $\hat{L}^2$, without loss of generality we may write the general form of the solution as

$$u_{nlm}(r, \theta, \phi) = f_{nl}(r)\ Y_{lm}(\theta, \phi), \tag{4.7}$$

where n is an additional quantum number we introduce to account for radial excitations. The meaning of this will become clear soon. Consequently it is only the radial equation that needs to be solved

$$\left[-\frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\hbar^2 l(l+1)}{2mr^2}\right] f_{nl} + V(r) f_{nl} = E_{nl} f_{nl}, \tag{4.8}$$

where E_{nl} is now independent of the azimuthal quantum number m. We may use this equation to solve for a whole class of central potentials in principle. Here $0 \leq r < \infty$. A few points are to be noted here:

- The above analysis applies equally to any rotationally invariant Hamiltonian independent of the form of the potential.
- The invariance under rotations is sufficient to reduce the 3-dimensional partial differential equation system into an ordinary one-dimensional differential equation (on the half-line).

This is the power of symmetry. In fact even in classical systems with central potentials, we have seen the reduction of the number of variables using the symmetry properties. An example is the Kepler problem where using angular momentum conservation the equation for the orbit reduces to a one-dimensional equation.

4.1 Harmonic Oscillator in 3-dimensions

Consider the isotropic harmonic oscillator problem in three dimensions. The potential is spherical symmetric since

$$V(r) = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2) = \frac{1}{2}m\omega^2 r^2 \tag{4.9}$$

There is no angular dependence. We may introduce the dimensionless variable using the oscillator length

$$q = \sqrt{\frac{m\omega}{\hbar}}r = \frac{r}{l_\omega}. \tag{4.10}$$

The radial equation in terms of $q \geq 0$ may be written as

$$\frac{\hbar\omega}{2}\left[-\frac{1}{q^2}\frac{\partial}{\partial q}\left(q^2\frac{\partial}{\partial q}\right)+\frac{l(l+1)}{q^2}+q^2\right]f_{nl}=E_{nl}f_{nl}. \tag{4.11}$$

Here n refers to radial excitations and its meaning will become clear. The solutions may be obtained in terms of polar coordinates. The solution is straight forward in cartesian coordinates since the potential is separable. But it is instructive to obtain them in polar coordinates. We rewrite the basic equation as

$$\left[\frac{d^2}{dq^2}+\frac{2}{q}\frac{d}{dq}-\frac{l(l+1)}{q^2}+\lambda_{nl}-q^2\right]f_{nl}=0; \quad \lambda_{nl}=\frac{2E_{nl}}{\hbar\omega} \tag{4.12}$$

Let us look at the asymptotic properties of this equation. In the limit $q \to \infty$, we have

$$\left[\frac{d^2}{dq^2}-q^2\right]f_{nl}\approx 0. \tag{4.13}$$

Therefore we demand

$$f(q)\approx e^{\pm q^2/2}. \tag{4.14}$$

The solution with positive sign diverges in the asymptotic limit and is not normalisable, so we keep the solution with the negative sign- this should be a feature for all solutions,

$$f(q)\approx e^{-q^2/2}. \tag{4.15}$$

Unlike in the one dimensional problem, we have a problem of divergence as $q \to 0$ also since in this limit the equation is of the form

$$\left[\frac{d^2}{dq^2}+\frac{2}{q}\frac{d}{dq}-\frac{l(l+1)}{q^2}\right]f_{nl}\approx 0 \tag{4.16}$$

Let us then try a solution of the form q^s, in this limit. Substituting in the equation we obtain

$$s(s-1)+2s-l(l+1)=s(s+1)-l(l+1)=0 \implies s=l, \text{ or } s=-(l+1). \tag{4.17}$$

Again the normalisability condition implies that we choose $s = l$. Thus the most general solution that satisfies the asymptotic conditions has to have the form

$$f_{nl}(q)=q^l L_{nl}(q)e^{-q^2/2}, \tag{4.18}$$

where $L_{nl}(q)$ is a series in q which must terminate since we have already taken care of asymptotic behaviour at large q. Substituting this form in the full radial equation gives

$$\frac{d^2L_{nl}}{dq^2}+2\left(\frac{l+1}{q}-q\right)\frac{dL_{nl}}{dq}+(\lambda_{nl}-2l-3)L_{nl}=0. \tag{4.19}$$

N	n	l	E (d=3)	degeneracy (d=3)
0	0	0	3/2	1
1	0	1	5/2	3
2	2	0	7/2	1
2	0	2	7/2	5

Once again this may be reduced to a standard equation whose solutions are called Associated Laguarre Polynomials. We will deal with these functions later, but for now it suffices to say that this equation has meaningful solutions when

$$\lambda_{nl} - 2l - 3 = 2n \tag{4.20}$$

where n is an integer. This immediately yields the energy eigenvalues for the three dimensional oscillator in the form

$$E_{nl} = \hbar\omega(n + l + \frac{3}{2}) = \hbar\omega(N + \frac{3}{2}), \tag{4.21}$$

where n is called the radial quantum number which has appeared throughout this analysis but now acquires a definite meaning and N is the principle quantum number. The levels are equally spaced and states corresponding to each l are $(2l+1)$ degenerate. One can enumerate the states with their energies as follows:

In fact for arbitrary N, the degeneracy is

$$d_N = (N + 1)(N + 2)/2.$$

It is easy to check that the energies and degeneracies match with the ones calculated in Cartesian basis. This way, one may understand the degeneracies as associated with the symmetry of the problem, namely, rotational invariance. In fact this is an example of the intimate connection between symmetries and degenerate states in quantum mechanics. The states are now labelled by quantum numbers n, l, m instead of n_x, n_y, n_z. The energy for a given N is independent of the m quantum number.

We may also notice that the energy eigenstates alternate in Parity starting with the ground state which is even under mirror inversion. This again is a reflection of the invariance of the Hmiltonian under inversion.

The harmonic oscillator problem is almost ubiquitous in physics making its appearance in many physical situations. As an example, consider the simplest version of the nuclear shell model. As shown in figure below, the nuclear force is repulsive at short range (<0.7 fm) and is attractive (< 2-3 fermi) in the intermediate range and goes to zero in the long range. Close to the minimum of the potential at V_0 the

effective nuclear potential resembles an oscillator potential. This means that for low excitations from the ground state of a nucleus, we may use oscillator approximation. Furthermore in a nucleus each quantum state may be occupied, at a maximum, by two protons, $p^{\uparrow}p^{\downarrow}$ and two neutrons, $n^{\uparrow}n^{\downarrow}$, that is four nucleons per quantum state.

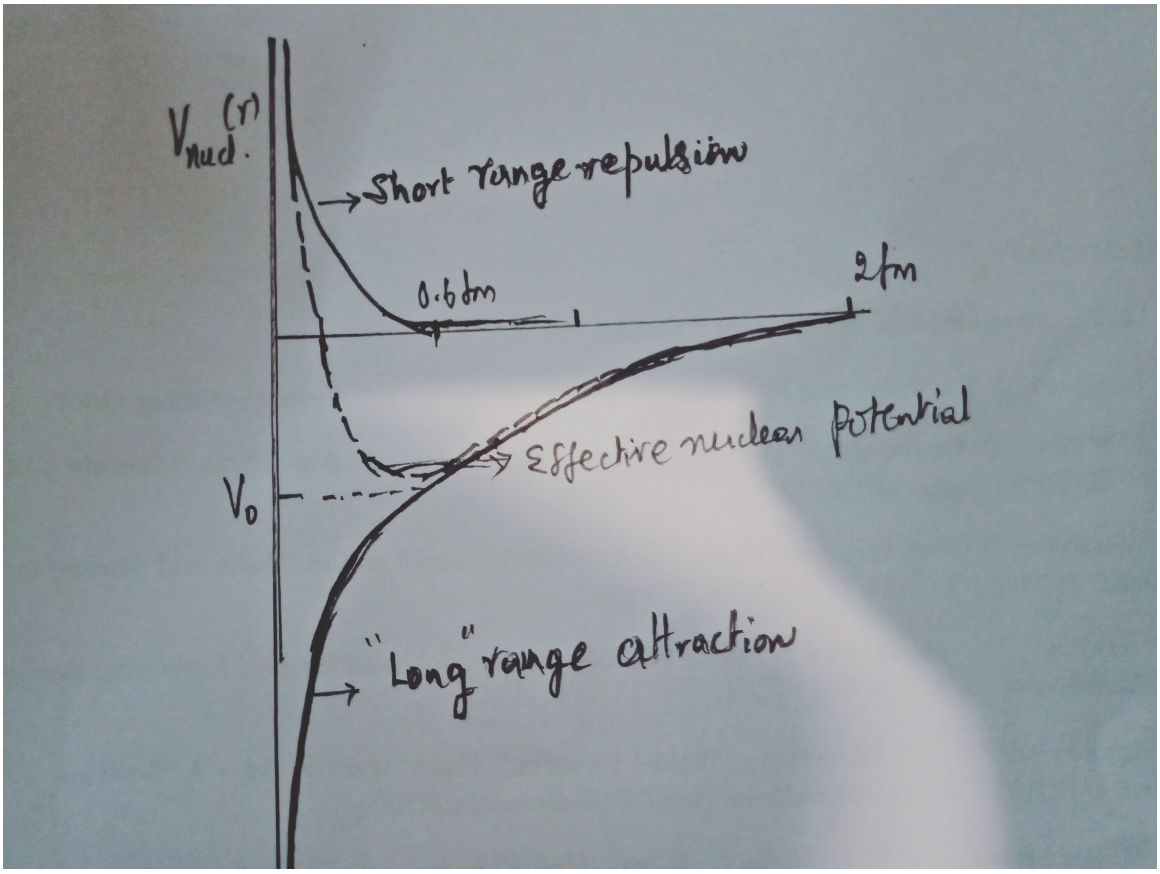


Figure 4.1: Sketch of Nuclear Potential

The ground state of the oscillator, which is non-degenerate, may be completely filled with two protons and two neutrons. This corresponds to the Helium nucleus. The first excited state has a degeneracy of three each of which may be completely filled with two protons and two neutrons as shown in the figure. Together with the ground state, the lowest two states may be completely filled with 16 nucleons which corresponds to Oxygen. Similarly, the when the third level with degeneracy 6 is completely filled we get Calcium at mass number 40. These three closed shell nuclei correspond to the first three "magic numbers" 2,8 and 20. The word magic refers to the stability of these nuclei. As they correspond to completely closed shell (states), addition of nucleons costs energy. The large energy gap, as opposed to the nuclei with partially filled shells, gives them the stability as observed.

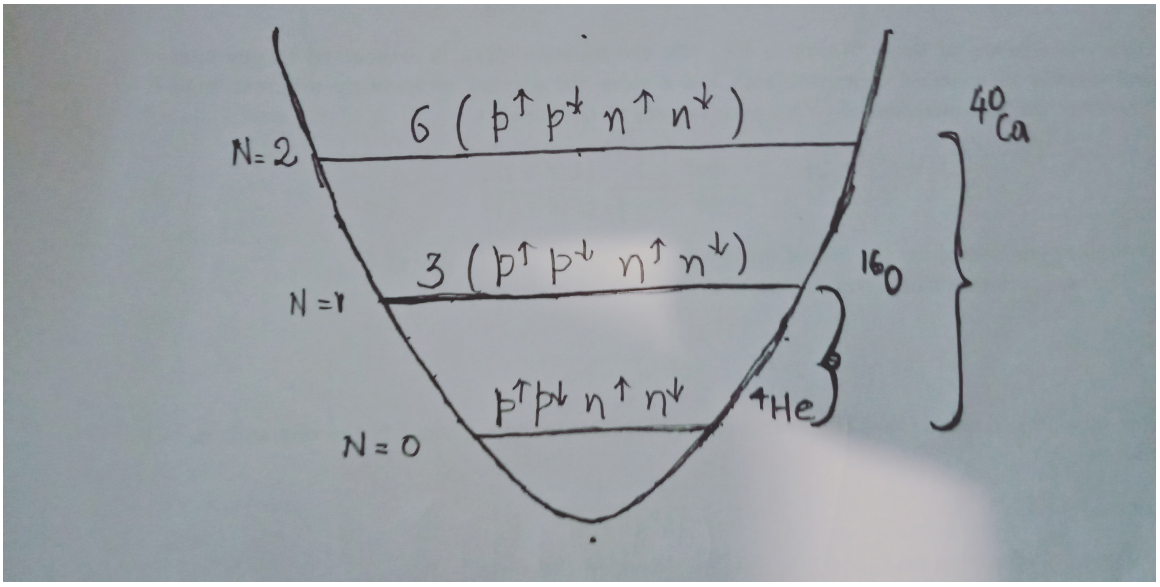


Figure 4.2: Sketch of Nuclear Potential

Since the oscillator potential is only an approximation that is valid only for a few lowest levels, we can not expect this simple shell model to work for heavier nuclei- in fact it does not as can be seen from the list of magic numbers beyond calcium. Also the model does not explain why nuclei like carbon, silicon are stable. That needs additional inputs to the nuclear potential including spin-orbit coupling etc. From our point of view here, this serves as an illustration of a simple model of a complex system like nuclei.

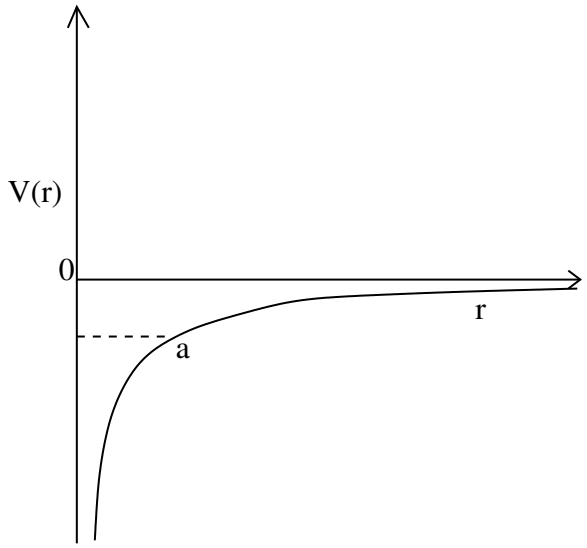
4.2 Hydrogen Atom

We now consider the crucial problem of the Hydrogen atom which ensuredthe applicability of Schroedinger equation in the beginning and allowed for detailed comparison with the observed spectrum of the Hydrogen atom. In general this is a two-body problem of electron moving around the nucleus. For simplicity let us assume that the nucleus is infinitely heavy. This reduces this to a one body problem- that of an electron moving under the action of a potential- Coulomb potential. We take this potential to be

$$V(r) = -\frac{Ze^2}{r}; \quad r = \sqrt{x^2 + y^2 + z^2} \tag{4.22}$$

where $Z = 1$ for the hydrogen atom and the sign ensures that the potential is attractive since the nucleus is positively charged. Classically this is very similar to the well-known Kepler problem-there are two distinct regions; negative energy eigenval-

ues indicate the electron is bound and is unbound for positive energies. Classically at a given energy the electron is confined to a finite region, say $0 \leq r \leq a$.



The potential is spherically symmetric, hence the eigenstates are simultaneous eigenfunctions of energy, $\hat{L}^2$ and $\hat{L}_z$. We focus on the negative energy region where the states are bound. The radial equation of motion given by

$$\left[-\frac{\hbar^2}{2mr^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{Ze^2}{r} + \frac{\hbar^2 l(l+1)}{2mr^2}\right] u_{nl} = E\ u_{nl}, \tag{4.23}$$

where l is as before the angular momentum eigenvalue and the equation is independent of the value of its projection m. The radial quantum number n will become clear later.

As in the case of the oscillator problem, we may transform the equation in terms of dimensionless variables using the following scaling transformations: Let

$$\epsilon = -E, \quad \alpha^2 = \frac{8m\epsilon}{\hbar^2}, \quad q = \alpha r, \quad \lambda = \frac{Ze^2}{\hbar}\sqrt{\frac{m}{2\epsilon}} \tag{4.24}$$

The radial equation in terms of $q \geq 0$ may be written as

$$\left[\frac{1}{q^2}\frac{\partial}{\partial q}\left(q^2\frac{\partial}{\partial q}\right) + \frac{\lambda}{q} - \frac{1}{4} - \frac{l(l+1)}{q^2}\right] u_{nl} = 0. \tag{4.25}$$

We expand the equation

$$\left[\frac{d^2}{dq^2} + \frac{2}{q}\frac{d}{dq} - \frac{l(l+1)}{q^2} + \frac{\lambda}{q} - \frac{1}{4}\right] u_{nl} = 0. \tag{4.26}$$

Let us look at the asymptotic properties of this equation. In the limit $q \to \infty$, we have

$$\left[\frac{d^2}{dq^2} - \frac{1}{4}\right] u_{nl} \approx 0. \tag{4.27}$$

Therefore we demand

$$u(q) \approx e^{\pm q/2}. \tag{4.28}$$

The solution with positive sign diverges in the asymptotic limit and is not normalisable, so we keep the solution with the negative sign- this should be a feature for all solutions,

$$u(q) \approx e^{-q/2}. \tag{4.29}$$

We also need to look as the asymptotic region as $q \to 0$ also since in this limit the equation is of the form

$$\left[\frac{d^2}{dq^2} + \frac{2}{q}\frac{d}{dq} - \frac{l(l+1)}{q^2}\right] u_{nl} \approx 0 \tag{4.30}$$

Let us then try a solution of the form q^s, in this limit. Substituting in the equation we obtain

$$s(s-1) + 2s - l(l+1) = s(s+1) - l(l+1) = 0 \implies s = l, \text{ or } s = -(l+1). \tag{4.31}$$

Again the normalisability condition implies that we choose $s = l$. Thus the most general solution that satisfies the asymptotic conditions has to have the form

$$u_{nl}(q) = q^l L_{nl}(q) e^{-q/2}, \tag{4.32}$$

where $L_{nl}(q)$ is a series in q which must terminate (we will show this below) since we have already taken care of asymptotic behaviour at $q \to 0$ and at $q \to \infty$. Substituting this form in the full radial equation gives

$$q\frac{d^2 L_{nl}}{dq^2} + (2(l+1) - q)\frac{dL_{nl}}{dq} + (\lambda - l - 1)L_{nl} = 0. \tag{4.33}$$

Now consider a series solution of the form

$$L_{nl}(q) = \sum_{k=0}^{\infty} a_k q^k. \tag{4.34}$$

Substituting this in the differential equation and equating coefficient of q^k, we get

$$(k+1)[k + 2(l+1)]a_{k+1} = [k + (l + 1 - \lambda)]a_k \tag{4.35}$$

It turns out that for large k, we have

$$a_{k+1} \approx \frac{a_k}{k} \tag{4.36}$$

so the $L(q) \approx e^q$ which is unacceptable as it diverges for large q. Therefore the series must terminate to satisfy the boundary conditions. The series termination may

n	l	m	-E	degeneracy
1	0	0	1	1
2	0,1	0,1,0,-1	1/4	4
3	0,1,2	0,1,0,-1,2,1,0,-1,-2	1/9	9

be ensured if $\lambda = n(> l)$, where n is an integer. Choice of n dictates the energy eigenvalue and the corresponding eigenfunction in terms of the Associated Laguarre Polynomials.

The energy eigenvalues are given by

$$E_n = -\frac{mZ^2e^4}{2\hbar^2}\frac{1}{n^2} = -\frac{Z^2e^2}{2a_0}\frac{1}{n^2}; \quad a_0 = \frac{\hbar^2}{me^2}, \tag{4.37}$$

where a_0 is the Bohr radius. The energy levels of hydrogen are recovered for $Z = 1$ which is essentially the Bohr formula. The energy levels are completely specified by a single quantum number n which is the *principal quantum number* which is positive and non-zero integer

$$n = 1, 2, 3, \cdots \tag{4.38}$$

For a given value of n we have $l = 0, 1, \cdots, (n-1)$ as allowed values. The eigenvalues of the square of the angular momentum is $\hbar^2 l(l+1)$ and for each l we have the azimuthal quantum number $m = \pm 0, \pm 1, \cdots, \pm l$ corresponding to $(2l+1)$ values. Thus corresponding to a given principle quantum number n with energy E_n, we have the degeneracy of the n-th level given by

$$D_n = \sum_{l=0}^{n-1}(2l+1) = n^2. \tag{4.39}$$

Some low lying states are given in the table below:

Notice that the degeneracies are different from those of the three dimensional oscillator. The eigenfunctions corresponding to each of these states labelled by quantum numbers $n, l.m$ are given by

$$u_{nlm}(r, \theta, \phi) = N_{nlm}u_{nl}(r)Y_{lm}(\theta, \phi), \tag{4.40}$$

where

$$u_{nl}(r) = r^l \; L_{nl}(r) \; e^{-Zr/a_0 n} \tag{4.41}$$

The normalised ground state and first excited are given by

$$u_{100} = \frac{1}{\pi^{1/2}} \left(\frac{Z}{a_0} \right)^{3/2} e^{-Zr/a_0} \tag{4.42}$$

$$u_{200} = \frac{1}{\pi^{1/2}} \left(\frac{Z}{2a_0} \right)^{3/2} \left(1 - \frac{Zr}{2a_0} \right) e^{-Zr/2a_0} \tag{4.43}$$

where the first excited is degenerate and only $l = 0, m = 0$ state is shown. These states are orthogonal as they are eigenstates.

Chapter 5

Spin and The group SU(2)

Having discussed rotational transformations and the group SO(3), let us look at other ways of representing rotational transformations. Basically any real three dimensional vector, say position vector $\vec{r}$ may be represented as a 2×2 matrix

$$A = \begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix} = \vec{r}.\vec{\sigma} \tag{5.1}$$

where σ_i are the well known Pauli matrices given by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}; \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \tag{5.2}$$

which are traceless and Hermitian. We summarise the properties of the Pauli matrices below:

- By definition
$$\sigma_i^2 = I; \quad Tr(\sigma_i) = 0$$
Here I is the 2×2 unit matrix.

- $$[\sigma_i, \sigma_j] = \sigma_i\sigma_j - \sigma_j\sigma_i = 2i\epsilon_{ijk}\sigma_k$$

- $$\{\sigma_i, \sigma_j\} = \sigma_i\sigma_j + \sigma_j\sigma_i = 2\delta_{ij}I$$

- Combining the above two properties
$$\sigma_i\sigma_j = i\epsilon_{ijk}\sigma_k, \ for\ i \neq j.$$

- Given any two three dimensional vectors $\vec{A}$ and $\vec{B}$

$$(\vec{\sigma}.\vec{A})(\vec{\sigma}.\vec{B}) = (\sum_{i=1}^{3}\sigma_i A_i)(\sum_{j=1}^{3}\sigma_j B_j) = \vec{A}.\vec{B}I + \sum_{i\neq j}\sigma_i\sigma_j(A_iB_j) = \vec{A}.\vec{B}I + i\vec{\sigma}.(\vec{A}\times\vec{B})$$

  where we have used both commutation and anti-commutation property of the Pauli matrices.

The vector A has the following properties

$$det(A) = -x^2 - y^2 - z^2 = -|A|^2; \quad Tr(A) = 0, \quad A = A^\dagger \tag{5.3}$$

which provides a representation of the vector in terms of Hermitian matrices. Thus any continuous transformation of $\vec{A}$ that leaves the determinant and trace unchanged while keeping it Hermitian is a rotation. Thus we can in-principle represent rotations too by 2×2 matrices.

Consider a bilinear **similarity** transformation of the form

$$A' = UAU^\dagger; \quad A'^\dagger = [UAU^\dagger]^\dagger = UA^\dagger U^\dagger = UAU^\dagger = A' \tag{5.4}$$

which leaves A' Hermitian if A is Hermitian. Furthermore, for this transformation to represent rotations, we require

$$Tr(A') = Tr(U^\dagger UA) = Tr(A); \quad det(A') = |det(U)|^2.det(A). \tag{5.5}$$

Thus if

$$UU^\dagger = U^\dagger U = I \tag{5.6}$$

all the above conditions of the transformation of A that correspond to rotations are satisfied. Matrices which satisfy the above condition are called Unitary matrices and the scalar product between two vectors,

$$A'.B' = \frac{1}{2}Tr(A'B') = \frac{1}{2}Tr(AB) = A.B$$

is preserved under these unitary transformations. Therefore the set of all unitary transformations provide a representation of rotations in 3-dimensional space. We may however note that in the space of vectors represented as two dimensional matrices, the transformations is not linear but bi-linear since it involves both U and $U^\dagger$.

In particular we may choose a subset of unitary matrices with the property

$$detU = 1$$

which implies we neglect the overall phase $e^{i\phi}$ since in QM such phases do not affect the observable properties. The transformation matrices U then are the elements of the set

$$\mathbf{SU(2)} = \{\mathbf{complex\ 2 \times 2\ matrices\ U} : \mathbf{UU^\dagger = U^\dagger U = 1},\ \mathbf{detU = 1}\}$$

It is straightforward to check that the set of 2×2 unitary-unimodular matrices form a group under matrix multiplication.

$$U_3 = U_1 U_2, \quad U_3^\dagger U_3 = U_2^\dagger U_1^\dagger U_1 U_2 = I.$$

$$U^{-1} = U^\dagger.$$

It is called the *Special Unitary Group SU(2)*. The group SU(2) provides the lowest dimensional non-trivial representation of the group SO(3).

5.1 Properties of the group SU(2)

Any complex matrix in 2-dimensions may be written in the form

$$U = \begin{pmatrix} a & b \\ c & d \end{pmatrix}, \tag{5.7}$$

where a, b, c, d are in general complex. We can always express this in the basis

$$U = q_0 I + i\sigma.\vec{q} = \begin{pmatrix} q_0 + iq_3 & iq_1 + q_2 \\ iq_1 - q_2 & q_0 - iq_3 \end{pmatrix}, \tag{5.8}$$

where we have simply expressed a, b, c, d in terms of q_0, q_1, q_2, q_3 and $I, \vec{\sigma}$ are a set of four linearly independent matrices which provide the basis for expansion of any 2×2 matrix. We have chosen σ to be the Pauli matrices. The linear independence of matrices is ensured since

$$Tr(I\sigma_i) = 0; \quad Tr(\sigma_i \sigma_j) = 0 \ i \neq j.$$

We demand U to be unitary which means

$$UU^\dagger = q_0^2 I + |\vec{q}|^2 I + i\sigma.(\vec{q}q_0^* - cc) + i\sigma.(\vec{q} \times \vec{q}^*) = I \tag{5.9}$$

where we have used the identity

$$(\sigma.\vec{A})(\sigma.\vec{B}) = \vec{A}.\vec{B} + i\sigma.(\vec{A} \times \vec{B}).$$

To satisfy unitarity, the coefficients of σ must vanish, hence the q_i are real. Furthermore we require the condition

$$q_0^2 + |\vec{q}|^2 = 1$$

which reduces the four real parameters to three. Thus any element of the group SU(2) can be parameterised by 3-real parameters just as in the case of the group SO(3). Clearly it is a representation of the rotation group SO(3). Using the above the most general representation of an element of SU(2) is given by

$$U = \begin{pmatrix} q_0 + iq_3 & iq_1 + q_2 \\ iq_1 - q_2 & q_0 - iq_3 \end{pmatrix}, = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}; \quad |a|^2 + |b|^2 = 1 \tag{5.10}$$

Geometry of the SU(2) Group Using the representation in terms of q_i given above, we can have a geometric interpretation of the elements of the group SU(2). Expanding the unimodularity condition we have

$$q_0^2 + q_1^2 + q_2^2 + q_3^2 = 1. \tag{5.11}$$

The representation in terms of $q's$ is known as the *quaternionic* representation of the elements of the group SU(2). The equation above immediately provides a geometric interpretation since it is the equation of a sphere S^3 in 4-dimensions. Since every element of the group SU(2) can be parameterized in terms of q_i, every such group element, represented by a matrix, is also represented by a point on the sphere S^3. Hence we have the following correspondence:

$$\begin{array}{ccc} SU(2) & \Longleftrightarrow & S^3 \\ U = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix} & \Longleftrightarrow & P = (q_0, q_1, q_2, q_3)\ , \\ Algebra & & geometry \end{array} \tag{5.12}$$

where P denotes a point on the sphere S^3. Every element of SU(2) now forms a point on the sphere S^3. We may choose a standard basis to represent the points on the

sphere:

$$\begin{aligned} I_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} &\iff (1,0,0,0) \\ J = \begin{pmatrix} i & 0 \\ 0 & -i \end{pmatrix} &\iff (0,1,0,0) \\ K = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} &\iff (0,0,1,0) \\ L = \begin{pmatrix} 0 & i \\ i & 0 \end{pmatrix} &\iff (0,0,0,1) \end{aligned} \tag{5.13}$$

where

$$J^2 = K^2 = L^2 = -I; \quad JK = -KJ = L$$

which are obtained directly from the properties of Pauli matrices. The four-dimensional space of real linear combinations of these four matrices is called the *quaternion algebra*. The north pole of the sphere may be identified with the identity matrix I.

The latitude is marked by the equation $q_0 = c$ and therefore

$$q_1^2 + q_2^2 + q_3^2 = 1 - c^2$$

which reduces to a point when $c = \pm 1$ corresponding to North and South poles and the equator is identified by $c = 0$.

The surface of S^3 is simply connected, that is any closed curve on the surface may be reduced to a point by smoothly contracting it.

Let us now consider an explicit representation of rotation in 3-dimensions about the z-axis by an angle θ. In Cartesian coordinates we have

$$x' = x\cos\theta - y\sin\theta; \quad y' = x\sin\theta + y\cos\theta; \quad , z' = z. \tag{5.14}$$

In terms of SU(2) transformation we may write this as

$$\begin{pmatrix} z & x' - iy' \\ x' + iy' & -z \end{pmatrix} = U(\theta) \begin{pmatrix} z & x - iy \\ x + iy & -z \end{pmatrix} U^\dagger(\theta) \tag{5.15}$$

The required rotation is achieved by choosing

$$U(\theta) = \begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix} \tag{5.16}$$

An important feature of matrices $U \in SU(2)$ is that it can be parameterised by an exponential form

$$U(\vec{\theta}) = \exp(-i\vec{\theta}.\vec{S}), \tag{5.17}$$

where $\vec{S}$ has three components since there are three angles as parameters. Since U is unitary S_k should be Hermitian,

$$UU^\dagger = \exp(-i(\vec{\theta}.\vec{S} - \vec{\theta}.\vec{S}^\dagger)) = I \Rightarrow S = S^\dagger \tag{5.18}$$

$$det(U) = 1 \Rightarrow Tr(S) = 0. \tag{5.19}$$

There exist many choices for these three linearly independent matrices with these properties. The simplest choice is given by the Pauli matrices:

$$S_1 = \frac{1}{2}\sigma_1;\ S_2 = \frac{1}{2}\sigma_2;\ S_3 = \frac{1}{2}\sigma_3 \tag{5.20}$$

The Pauli matrices provide a basis for all 2×2 Hermitian matrices. We can readily verify the *commutation property* of S_i using

$$[\sigma_i, \sigma_j] = 2i\epsilon_{ijk}\sigma_k \Rightarrow [S_i, S_j] = i\epsilon_{ijk}S_k. \tag{5.21}$$

This is identical to the Lie Algebra of the group SO(3) as it should be since SU(2) is a representation of the group SO(3).

To summarise, we have seen that the elements of group SU(2) provide a representation of rotations in 3-dimensions modulo the overall sign. It is a *double-valued lowest dimensional irreducible representation* of the group SO(3). This is often referred to as the $D^{1/2}$ representation of the group SO(3) where 1/2 refers to the property of the states on which the elements of SU(2) act in 2-dimensions. It is intimately connected to the properties of a spin 1/2 system as we shall see in the next section.

5.2 Construction of Spin 1/2 states

Notice that the algebra of the generators of SU(2) is given by

$$[S_i, S_j] = i\epsilon_{ijk}S_k. \tag{5.22}$$

which bears a close resemblance to the algebra of angular momentum operators in Quantum Mechanics. Using the properties of S_i represented in terms of Pauli Matrices, we have

$$S_k^2 = \frac{1}{4}I: \quad S^2 = \sum_k S_k^2 = \frac{3}{4}I = \frac{1}{2}(\frac{1}{2}+1)I \tag{5.23}$$

Suppose we choose the basis space spanned by these matrices as

$$\chi_+ = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \quad \chi_- = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{5.24}$$

which are linearly independent (orthogonal) by definition, then we have

$$S^2\chi_\pm = \frac{1}{2}(\frac{1}{2}+1)\chi_\pm, \tag{5.25}$$

and

$$S_3\chi_\pm = \pm\frac{1}{2}\chi_\pm. \tag{5.26}$$

Therefore the basis states are characterised by the eigenstates of the operator S_3 and S^2. It is therefore clear that the states $\chi_\pm$ behave precisely like the state with spin half, that is

$$\chi_m = |\frac{1}{2}, m\rangle; \quad m = \pm\frac{1}{2}; \quad \langle\frac{1}{2}, m'|\frac{1}{2}, m\rangle = \delta_{mm'}.$$

Thus the generators of the group SU(2) may be used to describe a spin-half system.

Using this notation, we can obtain a representation of an arbitrary rotation, given by

$$U(\alpha,\beta,\gamma) = \exp(-i\gamma S_3)\exp(-i\beta S_2)\exp(-i\alpha S_3) \tag{5.27}$$

in the space of states χ. Here we have used the Euler decomposition of an arbitrary rotation where the most general rotation is achieved by first rotating wrt to z-axis, then y-axiz and lastly wrt to the new z-axis. Thus we have the representation

$$\begin{aligned} D(\alpha,\beta.\gamma) &= \langle\frac{1}{2}m\,|\exp(-i\gamma S_3)\exp(-i\beta S_2)\exp(-i\alpha S_3)|\,\frac{1}{2}m'\rangle \\ &= \exp(-i\gamma m)\langle\frac{1}{2}m\,|\exp(-i\beta S_2)|\,\frac{1}{2}m'\rangle\exp(-i\alpha m') \\ &= \exp(-i\gamma m)[d^{(1/2)}_{mm'}](\beta)\exp(-i\alpha m'), \end{aligned} \tag{5.28}$$

where

$$d^{(1/2)}_{mm'} = \langle\frac{1}{2}m\,|\exp(-i\beta S_2)|\,\frac{1}{2}m'\rangle = \langle\frac{1}{2}m\left|\cos(\frac{\beta}{2})I - i\sin(\frac{\beta}{2})S_2\right|\frac{1}{2}m'\rangle. \tag{5.29}$$

Simplifying we get

$$d^{(1/2)} = \begin{pmatrix} \cos(\frac{\beta}{2}) & -\sin(\frac{\beta}{2}) \\ \sin(\frac{\beta}{2}) & \cos(\frac{\beta}{2}) \end{pmatrix} \tag{5.30}$$

and

$$D(\alpha,\beta,\gamma) = \begin{pmatrix} \cos(\frac{\beta}{2})\exp(-\frac{i}{2}(\alpha+\gamma)) & -\sin(\frac{\beta}{2})\exp(-\frac{i}{2}(\alpha-\gamma)) \\ \sin(\frac{\beta}{2})\exp(-\frac{i}{2}(\gamma-\alpha)) & \cos(\frac{\beta}{2})\exp(-\frac{i}{2}(-\alpha-\gamma)) \end{pmatrix} \tag{5.31}$$

An important point to note is that

$$d^{(1/2)}(2\pi) = -I \tag{5.32}$$

that is a 2π rotation changes the sign of the spin state. It requires two full rotations to bring back the original state- a character of the spin-1/2 representation.

Remark : The lowest representation of SO(3) that acts on the states χ is often denoted as $D^{1/2}$ representation referring to the spin identified by the eigenvalues of the states wrt the algebra of generators S_i. Once this identification is done, we can use this representation to construct higher dimensional representation by combining the irreducible spin-half representation $D^{1/2}$.

5.3 Many particle higher spin states

As we already know from quantum mechanics, many particle higher spin states may be composed using the spin-half states. For example the spin of the Deuteron nucleus is 1 which comes by combining the spins of individual nucleons. Similarly total electron spin in a Helium atom can be 0 or 1. We will now show how higher spin states may be constructed starting from an assembly of spin-half particles. At the heart of this is what is known as the Clebsch-Gordon Theorem.

Following the example of the SU(2) or $D^{(1/2)}$ representation, let us denote any general representation of the rotation group provided by the algebra of angular momentum operators

$$[J_i, J_j] = i\epsilon_{ijk}J_k; \quad i, j, k = 1, 2, 3.$$

by $D^{(j)}$. In general such a representation consists of matrices of dimension $(2j+1) \times (2j+1)$ which act on a space of dimension $(2j+1)$. When j is an integer the space is called **Tensorial** and j is half-odd integer the space of states is called **Spinorial**.

For example $D^{(1/2)}$ representation is a Spinorial representation characterised by spin-1/2. These spinors transform according to the elements of the group SU(2) whose representation is provided by $D^{(1/2)}$. The $D^{(1)}$ representation is vectorial (tensor of rank-1) and is the group SO(3) itself.

In general these need not form the basis of an irreducible representation. However, the basis of any irreducible representation contained in the product can be expanded in terms of the product tensors. The coefficients of such an expansion are called Clebsch-Gordon coefficients generalising from the example of the rotation group where they were formulated first.

Consider for example the D^j representation of the rotation group $SO(3)$. Combining two such representations corresponding to spin j_1, j_2 the product is written as

$$D^{j_1} \otimes D^{j_2} = D^{|j_1+j_2|} \oplus ... \oplus D^{|j_1-j_2|'} \tag{5.33}$$

where each irreducible representation D^j is characterised by well defined permutation symmetry. Here $\otimes$ denotes a **direct product** representation- such direct product representation of two irreducible representations is in general reducible. That means the direct product is expressible as a **direct sum**, denoted by $\oplus$, of irreducible representations. This in essence is the statement of the **Clebsch-Gordon Theorem** that the direct product of two **irreducible** representations may be written as a direct sum of **irreducible** representations. Any representation is said to be irreducible if it can not be further broken up as a sum of irreducible representations. The meaning of these terms and the statement will be clear soon when we consider the explicit examples below.

Let us start by combining a spin-half system with another spin-half system. The group of transformations on a spin 1/2 system is given by the representation $D^{1/2}$. For a system of two spin-half objects, we have

$$D^{1/2} \otimes D^{1/2} = D^1 \oplus D^0$$

which is simply a statement of the fact that the two spin half particles may be combined into a spin-1 or spin-0 system. In terms of dimensionalities this may also be written as,

$$2 \otimes 2 = 3 \oplus 1$$

We note that the representation $D^{1/2}$ defines the unitary irreducible representation of lowest dimension of the group SO(3) while it is also the self representation of the unitary-unimodular group SU(2). The above group theoretical statements may be illustrated easily by the following example. Consider explicitly the states of a spin half particle.

Let,

$$\begin{aligned} |\uparrow\rangle &= |S = 1/2, S_z = 1/2\rangle \\ |\downarrow\rangle &= |S = 1/2, S_z = -1/2\rangle \end{aligned}$$

be the basis vectors of the fundamental representation of SU(2) which is a group of Unitary-Unimodular 2×2 matrices. The product states are four in number,

$$|\uparrow\uparrow\rangle\,, \quad |\uparrow\downarrow\rangle\,, \quad |\downarrow\uparrow\rangle\,, \quad |\downarrow\downarrow\rangle\,.$$

Except the first and the last others do not have definite symmetry under permutation. There exists a transformation T acting on the basis above which projects these into states with definite permutation symmetry:

$$\begin{aligned} |1,1\rangle &= |\uparrow\uparrow\rangle \\ |1,0\rangle &= \frac{|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle}{\sqrt{2}} \\ |1,-1\rangle &= |\downarrow\downarrow\rangle \end{aligned}$$

which are fully symmetric and the other combination is antisymmetric and leads to the spin-0 representation of the two particle system.

$$|0,0\rangle = \frac{(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)}{\sqrt{2}}$$

Formally we write this as

$$|j,m\rangle = \sum_{m_1,m_2} C(\frac{1}{2},\frac{1}{2},j;m_1,m_2,m) \left|\frac{1}{2}m_1\right\rangle \left|\frac{1}{2}m_2\right\rangle$$

where $m_1 + m_2 = m$ and $j = 1, 0$. The coupling coefficient $C(j_1, j_2, j; m_1, m_2, m)$ is called the Clebsch-Gordon or angular momentum coupling coefficient. Specifically we have

$$|1,m\rangle = \sum_{m_1,m_2} C(\frac{1}{2},\frac{1}{2},1;m_1,m_2,m) \left|\frac{1}{2}m_1\right\rangle \left|\frac{1}{2}m_2\right\rangle$$

$$|0,0\rangle = \sum_{m_1,m_2} C(\frac{1}{2},\frac{1}{2},0;m_1,m_2,0) \left|\frac{1}{2}m_1\right\rangle \left|\frac{1}{2}m_2\right\rangle$$

Note that the spin- 1 representation is completely symmetric under the exchange of the two spins while spin-0 representation is completely antisymmetric under the exchange of the two spins. The Clebsch-Gordon (CG) Coefficients may be directly obtained from the explicit form given above:

$$\begin{aligned} C(\frac{1}{2},\frac{1}{2},0;\frac{1}{2},-\frac{1}{2},0) &= \frac{1}{\sqrt{2}} \\ C(\frac{1}{2},\frac{1}{2},0;-\frac{1}{2},+\frac{1}{2},0) &= -\frac{1}{\sqrt{2}} \\ C(\frac{1}{2},\frac{1}{2},0;\frac{1}{2},-\frac{1}{2},0)^2 + C(\frac{1}{2},\frac{1}{2},0;-\frac{1}{2},\frac{1}{2},0)^2 &= 1 \end{aligned} \tag{5.34}$$

Note that the overall sign in $\langle 00 \rangle$ is arbitrary. Hence we have assumed a sign convention here. For the spin-1 states we have

$$\begin{aligned} C(\frac{1}{2},\frac{1}{2},1;\frac{1}{2},\frac{1}{2},1) &= 1 \\ C(\frac{1}{2},\frac{1}{2},1;\frac{1}{2},-\frac{1}{2},0) = C(\frac{1}{2},\frac{1}{2},1;-\frac{1}{2},\frac{1}{2},0) &= \frac{1}{\sqrt{2}} \\ C(\frac{1}{2},\frac{1}{2},1;-\frac{1}{2},-\frac{1}{2},-1) &= 1 \end{aligned} \tag{5.35}$$

Note that

$$\begin{aligned} J^2 \left|j,m\right\rangle &= j(j+1)\left|j,m\right\rangle \\ J_z \left|j,m\right\rangle &= m \left|j,m\right\rangle \end{aligned}$$

While combining two spin 1/2 objects it is sufficient to look at the symmetry properties of CG coefficients to get the symmetry property of the state

$$C(j_1,j_2,j;m_1,m_2,m) = (-1)^{j_1+j_2-j} C(j_2,j_1,j;m_1,m_2,m)$$

Example of a physical system for two spin-1/2 objects is the Deuteron nucleus which is spin-1; the two electron system in Helium atom has both spin-0 and spin-1 states present.

5.3.1 A system of three spin-1/2 objects

Once the method of combining spin states is clear, we may proceed to construct the higher dimensional representations with 3 or more spin-1/2 objects.

Applying the CG theorem,

$$D^{1/2} \otimes D^{1/2} \otimes D^{1/2} = [D^1 \oplus D^0] \otimes D^{1/2} = [D^{3/2} \oplus D^{1/2}] \oplus D^{1/2}$$

or in terms of multiplicities we have

$$2 \otimes 2 \otimes 2 = [4 \oplus 2] \oplus \bar{2}$$

Thus there are two spin 1/2 representations (distinguished by their permutation symmetry and one spin 3/2 representation.

The states that span these representations may be constructed explicitly: The states in spin-3/2 representation are given by

$$\begin{aligned}
\left|\frac{3}{2}m\right\rangle &= \sum_{m_1,m_2} C(1,\frac{1}{2},\frac{3}{2};m_1,m_2,m)\,|1m_1\rangle\left|\frac{1}{2}m_2\right\rangle \\
\left|\frac{3}{2},\frac{3}{2}\right\rangle &= |\uparrow\uparrow\rangle\,|\uparrow\rangle = |\uparrow\uparrow\uparrow\rangle\,; \\
&\Rightarrow\ C(1,\frac{1}{2},\frac{3}{2};1,\frac{1}{2},\frac{3}{2}) = 1 \\
\left|\frac{3}{2},\frac{1}{2}\right\rangle &= \frac{|\uparrow\uparrow\downarrow\rangle+\sqrt{2}[|\uparrow\downarrow\uparrow\rangle+|\downarrow\uparrow\uparrow\rangle]/\sqrt{2}}{\sqrt{3}} = \frac{|\uparrow\uparrow\downarrow\rangle+|\uparrow\downarrow\uparrow\rangle+|\downarrow\uparrow\uparrow\rangle}{\sqrt{3}}; \\
&\Rightarrow\ C(1,\frac{1}{2},\frac{3}{2};1,-\frac{1}{2},\frac{1}{2}) = \frac{1}{\sqrt{3}};\quad C(1,\frac{1}{2},\frac{3}{2};0,\frac{1}{2},\frac{1}{2}) = \sqrt{\frac{2}{3}} \\
\left|\frac{3}{2},-\frac{1}{2}\right\rangle &= \frac{|\downarrow\downarrow\uparrow\rangle+\sqrt{2}[|\uparrow\downarrow\downarrow\rangle+|\downarrow\uparrow\downarrow\rangle]/\sqrt{2}}{\sqrt{3}} = \frac{|\downarrow\downarrow\uparrow\rangle+|\uparrow\downarrow\downarrow\rangle+|\downarrow\uparrow\downarrow\rangle}{\sqrt{3}}; \\
&\Rightarrow\ C(1,\frac{1}{2},\frac{3}{2};-1,\frac{1}{2},-\frac{1}{2}) = \frac{1}{\sqrt{3}};\quad C(1,\frac{1}{2},\frac{3}{2};0,-\frac{1}{2},-\frac{1}{2}) = \sqrt{\frac{2}{3}} \\
\left|\frac{3}{2},-\frac{3}{2}\right\rangle &= |\downarrow\downarrow\downarrow\rangle\,; \\
&\Rightarrow\ C(1,\frac{1}{2},\frac{3}{2};-1,-\frac{1}{2},-\frac{3}{2}) = 1
\end{aligned}$$

Collectively we refer to these states as χ_s and are explicitly symmetric - the intermediate step is given to show explicitly how the states have combined and to evaluate the appropriate CG coefficients.

The states in spin-1/2 representation obtained by coupling spin-1 and spin-1/2 are given by

$$\begin{aligned}
\left|\frac{1}{2}m\right\rangle &= \sum_{m_1,m_2} C(1,\frac{1}{2},\frac{1}{2};m_1,m_2,m)\,|1m_1\rangle\left|\frac{1}{2}m_2\right\rangle \\
\left|\frac{1}{2},\frac{1}{2}\right\rangle &= \frac{2\,|\uparrow\uparrow\downarrow\rangle-\sqrt{2}[|\uparrow\downarrow\uparrow\rangle+|\downarrow\uparrow\uparrow\rangle]/\sqrt{2}}{\sqrt{6}} = \frac{2\,|\uparrow\uparrow\downarrow\rangle-(|\uparrow\downarrow\uparrow\rangle+|\downarrow\uparrow\uparrow\rangle)}{\sqrt{6}}; \\
&\Rightarrow\ C(1,\frac{1}{2},\frac{1}{2};1,-\frac{1}{2},\frac{1}{2}) = \sqrt{\frac{2}{3}};\quad C(1,\frac{1}{2},\frac{1}{2};0,\frac{1}{2},\frac{1}{2}) = -\sqrt{\frac{1}{3}} \\
\left|\frac{1}{2},-\frac{1}{2}\right\rangle &= -\frac{2\,|\downarrow\downarrow\uparrow\rangle-\sqrt{2}[|\uparrow\downarrow\downarrow\rangle+|\downarrow\uparrow\downarrow\rangle]/\sqrt{2}}{\sqrt{6}} = -\frac{2\,|\downarrow\downarrow\uparrow\rangle-(|\uparrow\downarrow\downarrow\rangle+|\downarrow\uparrow\downarrow\rangle)}{\sqrt{6}}; \\
&\Rightarrow\ C(1,\frac{1}{2},\frac{1}{2};-1,\frac{1}{2},-\frac{1}{2}) = -\sqrt{\frac{2}{3}};\quad C(1,\frac{1}{2},\frac{1}{2};0,-\frac{1}{2},-\frac{1}{2}) = \sqrt{\frac{1}{3}}
\end{aligned}$$

Collectively we call these states χ_λ. Note that these states are not symmetric or antisymmetric under exchange of spins. These are called Mixed-symmetry states-symmetric in 1-2 with no particular symmetry with respect the third spin.

The states in spin-1/2 representation obtained by coupling spin-0 and spin-1/2 are given by

$$\begin{aligned}
\left|\frac{1}{2}m\right\rangle &= \sum_{m_1,m_2} C(0,\frac{1}{2},\frac{1}{2};0,m,m)\,|00\rangle\left|\frac{1}{2}m\right\rangle \\
\left|\frac{1}{2},\frac{1}{2}\right\rangle &= \frac{[|\uparrow\downarrow\uparrow\rangle - |\downarrow\uparrow\uparrow\rangle]}{\sqrt{2}} = \frac{[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle]}{\sqrt{2}}\,|\uparrow\rangle\,; \\
&\Rightarrow\ C(0,\frac{1}{2},\frac{1}{2};0,\frac{1}{2},\frac{1}{2}) = 1 \\
\left|\frac{1}{2},-\frac{1}{2}\right\rangle &= \frac{[|\uparrow\downarrow\downarrow\rangle - |\downarrow\uparrow\downarrow\rangle]}{\sqrt{2}} = \frac{[|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle]}{\sqrt{2}}\,|\downarrow\rangle\,; \\
&\Rightarrow\ C(0,\frac{1}{2},\frac{1}{2};0,-\frac{1}{2},-\frac{1}{2}) = 1
\end{aligned}$$

Collectively we call these states χ_ρ. These are again called Mixed-symmetry states- antisymmetric in 1-2 with no particular symmetry with respect to the third spin. We can not have complete symmetry or antisymmetry while combining three particles since the electron spin has only two states. However, when combined with spacial states, it is possible to have many electron states which are completely antisymmetric as required by the quantum statistics.

The precise number of states in each representation correspond to the multiplicities obtained from the CG theorem.

Chapter 6

Brief Review of Lorentz Group

This is a brief review of some aspects of special relativity and the Lorentz group. We begin with special theory of relativity.

6.1 Special theory of relativity: A brief review

This is going to be a very brief review just to give an idea of a group defined by the invariance of metric similar to the rotation group, apart from the basic framework for relativistic quantum mechanics . For details consult any book on special Relativity and Lorentz group. Let us start with a simple situation of a frame S' moving at uniform velocity v with respect to a from S along some direction, say along x-axis. In Newtonian mechanics, we use Galilean transformations to describe the motion in S or S':

$$x_1' = x_1 - vt;\ x_2' = x_2;\ x_3' = x_3 :\ , t' = t \tag{6.1}$$

The Newton's law appears in the same form in both S and S' and hence they are inertial by definition. The problem comes when you use these transformations to describe the motion of light waves as observed in S and S'. The velocity of light in vacuum appears to depend on the frame against all experimental evidence which states that the velocity of light is the same in all frames of reference.

We retrieve the situation using the two postulates of Special Theory or Relativity (STR):

- The laws of physics are the same in all inertial systems (uniformly moving frames) and
- The speed of light c in vacuum is the same for all observers independent of the state of the observers.

Using the second postulate of STR, we may reduce STR to the invariance of of the space-time distance between any two events viewed in any inertial frame of reference, namely

$$ds^2 = dx_1^2 + dx_2^2 + dx_3^2 - c^2dt^2. \tag{6.2}$$

All equations of STR may be derived using this symmetry. The transformations that preserve the line element are the Lorentz transformations. Corresponding to a boost in $x - direction$ we may write these transformations in the familiar form

$$x_1' = \gamma(x_1 - \beta x_0);\ x_2' = x_2;\ x_3' = x_3 :\ , x_0' = \gamma(x_0 - \beta x_1) \tag{6.3}$$

where

$$x_0 = ct;\quad \gamma = \frac{1}{\sqrt{1-\beta^2}};\quad \beta = \frac{v}{c}.$$

Yet another form in which we can express the Lorentz transformation along the x-axis is given by

$$\begin{aligned} x_1' &= \cosh\phi x_1 - \sinh\phi x_0 \\ x_0' &= -\sinh\phi x_1 + \cosh\phi x_0, \end{aligned} \tag{6.4}$$

where $\cosh\phi = \gamma,\ \sinh\phi = \beta\gamma$, ϕ is called the rapidity some times.

In general any Lorentz boost an be generated continuously from infinitesimal boost. This may be written as

$$\delta L_1 = I + i\delta\phi K_1 + \cdots \tag{6.5}$$

where $\delta\phi = \phi/N$ where N is large. The Lorentz boost above may then be written as

$$L_1 = \lim_{N\to\infty}(I + i\frac{\phi}{N}K_1)^N = \exp(i\phi K_1) \tag{6.6}$$

where K_1 is the generator of Lorentz boost in the $x - direction$ given by

$$K_1 = i\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{6.7}$$

We may also write these transformations in the 2- and 3- directions analogous to the above. The most general boost will consist of a combination of all the three.

The line element or space-time distance between any two events is now invariant under these transformations. In particular rotations about an axis with the origin fixed also leave the distance invariant. The set of all transformations which leave the space-time distance invariant form a group called the *Lorentz group*. In particular the transformations with determinant +1 form a subgroup called the *proper Lorentz group*.

6.2 4-vector notation

Let us begin by developing some notation. We define a four vector as

$$A^\mu \equiv (A^0, A^1, A^2, A^3) = (A^0, \vec{A}), \tag{6.8}$$

where $\vec{A} = (A^1, A^2, A^3)$ is the usual 3-vector. An example of a four-vector is the position vector encountered above

$$x^\mu \equiv (x^0, x^1, x^2, x^3) = (ct, \vec{x}) = (x^0, x, y, z) \tag{6.9}$$

where we have combined time and position into a four-vector. Here c is the velocity of light. We use the greek indices to denote the components of a four vector reserving the usual $i, j, k...$ for denoting the components of the three vector.

An observer in a frame that is boosted in the positive x^1 direction with a uniform velocity v, for example, will observe the same vector as

$$x'^\mu = L^\mu_\nu x^\nu, \tag{6.10}$$

(unless otherwise specified, repeated indices are summed over) where

$$\begin{pmatrix} ct' \\ x'^1 \\ x'^2 \\ x'^3 \end{pmatrix} = \gamma \begin{pmatrix} 1 & -\frac{v}{c} & 0 & 0 \\ -\frac{v}{c} & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} ct \\ x^1 \\ x^2 \\ x^3 \end{pmatrix}; \qquad \gamma = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}} \tag{6.11}$$

Similarly you may define the boost in the direction x^2 or x^3 by appropriately changing the above equation. Any boost in an arbitrary direction can always be written as a composition of three independent boosts in x^1, x^2, x^3 directions just as any arbitrary rotation of a three vector can always be written as a composition of three independent planar rotations.

Exercise: Show that the Lorentz in an arbitrary direction $\hat{n}$ may be written as

$$\begin{aligned} ct' &= \gamma \left(ct - \frac{v}{c} \hat{n}.\vec{r} \right) \\ \vec{x}' &= \vec{x} + (\gamma - 1)(\hat{n}.\vec{x})\hat{n} - \gamma ct \frac{v}{c} \hat{n} \end{aligned} \tag{6.12}$$

where $\hat{n}$ is the direction of the boost and v is the modulus of the velocity.

An important property of any Lorentz transformation is that it leaves the "length" of the four vector defined as

$$x^\mu x_\mu = (ct)^2 - \vec{x}.\vec{x} = x^\mu g_{\mu\nu} x^\nu, \tag{6.13}$$

invariant, where

$$g_{\mu\nu} = g^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{6.14}$$

is called the **metric tensor**. The metric tensor plays an important role not only special relativity but more so general theory of relativity. Because of this property, invariance of length, we have

$$x'^{\mu}x'_{\mu} = L^{\mu}_{\nu}L^{\nu}_{\mu}x^{\nu}x_{\nu} = x^{\nu}x_{\nu} \tag{6.15}$$

and therefore

$$L^{\mu}_{\nu}L^{\nu}_{\mu} = L^{T}L = I, \tag{6.16}$$

that is Lorentz transformations are orthogonal. Here I denotes an Unit matrix $I = diag(1, 1, 1, 1)$. Some times we simply write it as 1. We write this in general as

$$g_{\mu\nu}L^{\mu}_{\alpha}L^{\nu}_{\beta} = g_{\alpha\beta}. \tag{6.17}$$

Conversely we could have started with the property of orthogonality and shown that the four-length is invariant.

Digression on Lorentz group and algebra: We are already familiar with Orthogonal transformations namely rotations. The rotation of a three vector may be written as

$$\begin{pmatrix} x'^1 \\ x'^2 \\ x'^3 \end{pmatrix} = R \begin{pmatrix} x^1 \\ x^2 \\ x^3 \end{pmatrix} \tag{6.18}$$

where R is a rotation matrix which transforms the three dimensional vector with the property $R^T R = (R)^{-1}R = 1$. We may rewrite this in the four-vector language as

$$\begin{pmatrix} ct' \\ \vec{x'} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & R \end{pmatrix} \begin{pmatrix} ct \\ \vec{x} \end{pmatrix} \tag{6.19}$$

Since the rotations preserves the length of the vector and since we have not changed the time coordinate, these transformations also preserve the length of the four vector.

The set of all such linear orthogonal transformations which preserve the length of a four vector, or distance between any two points in the four-dimensional space is invariant, form a group which is called the proper-Lorentz group, denoted by L with the important property det(L)=+1.[1]

[1]We may define even more general transformations which leave the length invariant but whose determinant is -1. These are referred to as improper Lorentz transformations.

Under these transformations the kinematical laws of special relativity, the Klein-Gordon and Dirac equations as well as Maxwell equations are invariant. The Lorentz transformations that preserve the direction of time are also called **orthochronous** Lorentz transformations and have determinant +!.

Generators of Lorentz Group We already know that the elements of the rotation group may be generated by generators J_i acting on the space-time coordinators may be written as

$$R(\theta_i) = e^{-i\theta_i J_i}, \tag{6.20}$$

where θ_i are the three independent rotations necessary to change the orientation of a vector. Though the time coordinate does not change, we may write R and therefore J_i as acting on the space time coordinates as shown above. The three generators of the rotation group satisfy the commutation relation

$$[J_i, J_j] = J_i J_j - J_j J_i = i\epsilon_{ijk} J_k. \tag{6.21}$$

The generators are represented by the Hermitian matrices

$$J_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ 0 & 0 & i & 0 \end{pmatrix}; \quad J_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & i \\ 0 & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}; \quad J_3 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \tag{6.22}$$

The commutation relation determines the signs given above.

To this we add the generators of the Lorentz boosts. It is easy to verify that the generators of boosts may be represented by matrices corresponding to x_1, x_2, x_3 directions are given by

$$K_1 = i\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \quad K_2 = i\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}; \quad K_3 = i\begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \tag{6.23}$$

Exercise: Show that the six generators of the Lorentz group satisfy the following algebra:

$$[J_i, J_j] = i\epsilon_{ijk} J_k \tag{6.24}$$

$$[J_i, K_j] = i\epsilon_{ijk} K_k \tag{6.25}$$

$$[K_i, K_j] = -i\epsilon_{ijk} J_k \tag{6.26}$$

Note that the algebra of generators of the rotations closes on itself.

The advantage of dealing with the Lie algebra of the Lorentz group becomes clear when we have to transform not only the space-time vectors, but also functions of these coordinates. The representation of the Lorentz group acting on these functions, not necessarily one dimensional, may be obtained by generating such transformations using the Lie algebra of the group since the algebra remains the same no matter which representation we want.

A few important properties of Lorentz Group is summarised below without giving details:

- Note that the Lorentz transformations are linear coordinate transformations between two frames that move at constant velocity with respect to each other.
- Lorentz group is a group of transformations that preserve the length of a four vector. The elements of the group includes not only the Lorentz transformations but also rotations.
- Together Lorentz boost and rotations define the most general transformations from one frame to another.
- Since the set all rotations forms a group by themselves, it is a compact subgroup of the Lorentz group. Compact because all the rotation angles are bounded.
- Unlike the Rotation group- a subgroup, Lorentz group is a non-compact group. That is the parameters of boost are not bounded unlike the rotation angles.

Energy and Momentum The four-momentum is defined such that its time component is proportional to energy while the its three-space components correspond to the three momentum:

$$p^\mu = (E/c, p_x, p_y, p_z) = (E/c, \vec{p}) \tag{6.27}$$

The length of this four-momentum given by

$$p^\mu p_\mu = p^\mu g_{\mu\nu} p^\nu = E^2/c^2 - \vec{p}.\vec{p} \tag{6.28}$$

which is an invariant under Lorentz transformations (actually Lorentz group). It is simply the mass squared

$$p^\mu p_\mu = m^2 c^2. \tag{6.29}$$