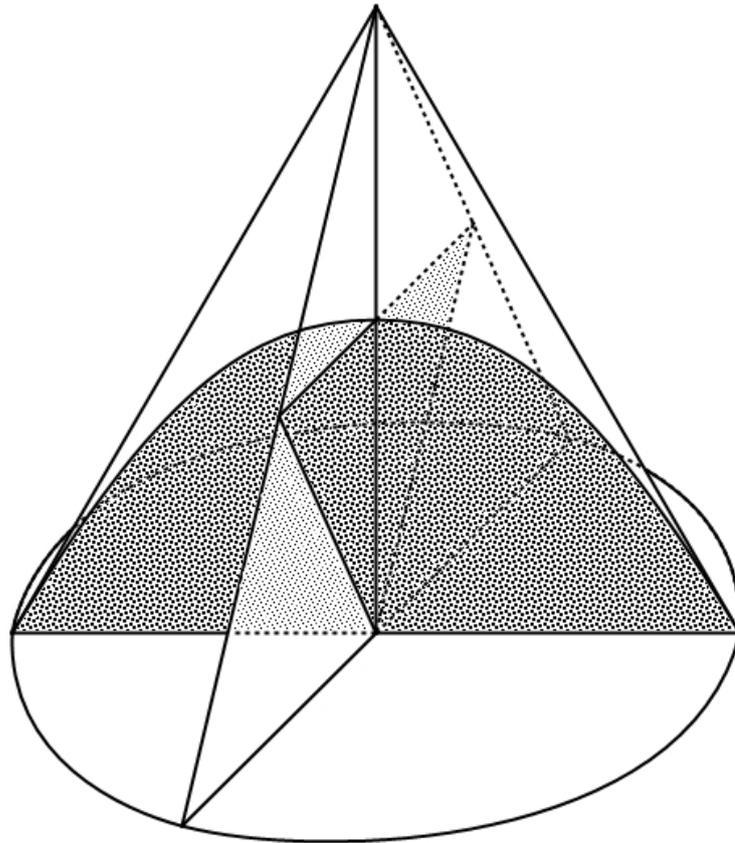

The Convex Hull of Spin Coherent States



Author:
Muhammad SADIQ

Supervisor:
Prof. Ingemar BENGTTSSON



Stockholm University
Fysikum, May 28, 2009.

Abstract

Pure coherent states are known as the most classical states in quantum mechanics. Similarly, pure spin coherent states based on the rotation group also exist in finite dimensions. We call these states pure classical states, and the mixed classical states are the statistical mixtures of these states. The set of all classical states is a subset of the set of all pure & mixed states. We present an essentially complete description of the geometry of this set for 3-dimensional Hilbert space. While studying its geometry we find a remarkable similarity between the geometry of this set and the geometry of the set of all classical probability distributions. This study also improves a recent work on this set done by Giraud et al [4] and relates it to an earlier work by Wootters [14].

Acknowledgements

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After this, my most humble thanks to my family and friends for their cooperation and extra support that provided me confidence to present this work in the best possible form.

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Contents

1	Introduction	1
2	Mixed States and Convex Bodies	5
2.1	Pure and Mixed States	5
2.2	The Density Matrix	6
2.3	Convex Set and Convex Bodies	7
2.4	The Set of Classical Probability Distributions	10
2.5	The set of Density Matrices	11
3	Spin Coherent States	17
3.1	Spin Coherent States	18
3.2	The Set of Spin Coherent States	21
3.3	The Set of Classical States	22
4	Magical Basis	25
4.1	State Vectors in Magical Basis	26
4.2	Angular Momentum Operator in Magical Basis	27
4.3	Spin Coherent States in Magical Basis	30
4.4	The Set of Classical States : A Review	32
5	Classicality of Spin States	33
5.1	The P-Representation	34
5.2	The Decomposition of a Density Matrix	35
5.3	The Z-Criterion For Classicality	37
5.4	The Rank of a Density Matrix in ϱ_{cl}	37
6	The Geometry of ϱ_{cl}	39
6.1	The Simplest Case.	40
6.2	The Second Simplest Case.	41

7	The Minimal Faces of ϱ_{cl}	45
7.1	Portion of the Minimal Faces of \mathcal{D} in ϱ_{cl}	45
7.2	Minimal Faces of ϱ_{cl}	47
8	Rank of States in ϱ_{cl}	51
8.1	States of Rank Three or Less	51
8.2	States of Rank Four	52
8.3	Finding the Four States	53
9	The End	57
	Bibliography	59

List of Figures

2.1	Mixtures of two points.	8
2.2	Convex sets and convex bodies.	9
2.3	Description of a face.	10
2.4	Geometry of classical probability distributions.	11
2.5	The Bloch Ball, with pure and mixed states.	14
3.1	An arbitrary unit vector in spherical coordinates.	19
3.2	Majorana description for spin states.	21
6.1	2–dimensional cross-section of \mathcal{D} containing diagonal density matrices in \mathbf{e}_{cl}	41
6.2	Another 2–dimensional cross-section of \mathcal{D} showing more matrices in \mathbf{e}_{cl}	42
6.3	The overlap between the two cross-sections.	43

Chapter 1

Introduction

The world at very small scale is quite non-intuitive. Quantum Mechanics provides the best known description for this world and hence it is based on a set of principles which are fundamentally different than our daily life experienced classical laws. Many things which are assumed to be impossible classically, becomes possible in the quantum domain. We are now, due to the advancement of the technology, capable of building systems, which can explore quantum oddities and hence able to perform classically impossible tasks, this is actually what we aim at Quantum information science.

In Quantum information, we usually require correlations stronger than classical and therefore, we are almost always looking for non-classical states; thus it becomes very important that we can distinguish between classical and non-classical states. This is why these are the currently hot topics of research. In this thesis we will concentrate on classical states and will study some geometrical aspects of the set of classical states for spin systems. Studying classical states becomes far more important in respect that the world we live in is undoubtedly classical at the large scale and it is still a mystery that how it emerges from the quantum origin. First of all, we will see in this chapter what these classical states are.

As you might know, one of the most distinguishing features of the quantum theory is the strange uncertainty principle. Which says, the uncertainty in position q and momentum p can be written as¹

$$\Delta q \cdot \Delta p \geq \frac{1}{2} \tag{1.1}$$

therefore, this principle clearly predicts that one can never make exact simultaneous measurements of non-commutating observables, no matter how perfect instruments one would have. The answer of the question, “Why this is so?” becomes a matter of on which interpretation one believes, hence it is

¹in a system of units where $\hbar = 1$

still controversial¹. Besides this contentious fact, one thing is quite clear; if this principle will ever be proved wrong the whole empire of quantum theory will collapse.

Nevertheless, the world we live in seems to obey classical laws, the laws of Newtonian or Hamiltonian mechanics; this is true, because one can deduce classical results from the quantum theory as a limiting case. Technically this implies there are states, whose dynamics very much resembles to the dynamics of classical systems. It does not mean that for these states uncertainty is zero, rather it implies that these are the states with minimum uncertainty.

In fact, there exists a whole class of states for which equality holds in Eq. (1.1) and therefore these states can rightfully be called *Minimum Uncertainty States*. The technical name for this class is *Squeezed States*. However the states, whose dynamics closely resembles to the dynamics of classical systems are those which not only minimize the uncertainty relation, but also for them the uncertainty of position and momentum becomes equal according to Eq. (1.1), i.e. $\frac{1}{\sqrt{2}}$ for each[1]. This means uncertainty in position and momentum form a circle in the phase space and hence this uncertainty is symmetric around the point represented by the center of this circle. Thus every classical phase space point corresponds to a state of this type and hence there is a one-to-one mapping of classical phase space points onto the space of these states. Therefore these states are, in fact, quantum analogues of points in classical phase space [3].

The fancy name for these special kind of states is *Coherent States*, which was given by Roy J. Glauber, who got the Nobel prize for his work on these states and hence sometimes these are also called *Glauber States*. His reason of calling these states coherent might be that in his work [5], these are referred to the most classical sort of states of light field corresponding to a single resonator mode. It is also true that the term coherent states means different things for different people but all are agree about the fact that these states are as classical as they can be.

In this thesis I shall talk about *Spin Coherent States*. These are also coherent states, but are referred to the spin systems. In fact, these are the coherent states of rotation group $\text{SU}(2)$. The nice thing about the spin systems is that their states can be represented by vectors in a finite dimensional Hilbert space. In this thesis, I study spin-1 systems, which mean eventually in this work we will restrict ourselves to the 3-dimensional Hilbert space.

For the spin systems, not only spin coherent states but all other states which can be represented as a weighted sum of spin coherent states with positive weights, provided that these weights sum to one, considered as *The*

¹All one can say according to standard Copenhagen interpretation is that this cannot be done, simplify because there does not exist such things like exact position together with momentum etc.

Most Classical States or *Classical States*. This means that any mixture of spin coherent states is classical; hence, these classical states form a convex set in the space of density matrices. Furthermore, as all pure points of this set are pure spin coherent states, therefore the set of all classical states is the convex hull of spin coherent states, the main object of the study in this work. We will study some geometrical aspects of this convex hull.

We will begin our study by defining pure and mixed states, density matrices, convex set, convex hull and etc in chapter 2, then in chapter 3 we will define spin coherent states and introduce the convex hull of these states. Chapter 4 will be devoted to a very useful basis —called magical basis— and we will discover that for this study, magical basis might be the best choice.

In chapter 5, we will look at some of the work [4] which has already been done by Giraud et al on this set, and translate this into magical basis, and then finally in chapter 6 we will start exploring some geometry of the convex hull of spin coherent states. Chapter 7, describe the minimal faces of this set and can be read independent of chapter 6. Chapter 8 will cover some more results and conclusions I made and in the last chapter 9, I will make some concluding remarks.

Chapter 2

Mixed States and Convex Bodies

In the previous chapter, we have seen what coherent states are. Like any other state of a system these states can be represented by vectors in Hilbert space. However, in general this is not necessarily true for a statistical system or ensemble. In such situations one has to use the density matrix or density operator formulation. Actually density matrices contain all the information of a system that one can reach and hence can be used to describe any quantum mechanical state of a system that may or may not be represented by a vector in Hilbert space. In this sense studying density matrices becomes more important.

In this chapter our main concern will be to develop necessary background for subsequent chapters. Therefore, in Sec.2.1, we shall start by explaining what we mean by pure and mixed states then I shall describe what density matrices are, in Sec.2.2. In Sec.2.3, we shall look at some important concepts and terms of the geometry of the convex bodies and in the light of these in Sec. 2.4 we see what geometry the set of classical probability distributions has. Finally, we will look at the geometry of the set of all density matrices in Sec.2.5.

2.1 Pure and Mixed States

Before looking at pure and mixed states, the reader should make it absolutely clear that quantum theory is a probabilistic theory and this probabilistic nature enters into the theory not because of our lack of knowledge, rather it is because of the lack of exact predictability inherent in the theory due to the uncertainty principle as discussed in chapter 1 and hence we cannot predict the exact outcome of any future measurement on any system, even when we have the maximal knowledge about its current state. Therefore, in quantum mechanics, whatever we can predict is always in probabilities.

However, most of the time, practically the situation is even worse; be-

cause we do not have as much knowledge about the system as we are allowed i.e. in case of statistical systems or ensemble. Hence another probability enters into our description of the system. We call these second probabilities as classical probabilities.

It will not be out of the context to mention here that, although we are distinguishing between classical and quantum probabilities but there are situations when these so called classical and quantum probabilities are mixed up together in a way that there remains no distinction e.g. in case of a system which has uncertain preparation history. Since, no measurement or observation can distinguish between these probabilities, thus, in such cases; one can regard both kinds of probabilities to have the same origin. Because of this fact, there are many people, who do not distinguish between these quantum and classical probabilities and treat them under the same roof provided by the density matrices. Maintaining such an attitude might be good because in a physical theory one should never try to compel a concept/thing which, in principle, cannot be verified directly or indirectly.

Now suppose, we have maximal knowledge about the state of a system i.e. there are no classical probabilities involved. This is usually true just after a suitable measurement, say, if we measure the position of a particle then just after the measurement, in principle, we can have exact knowledge of its position and we can represent it by a vector in Hilbert space. Such states are called *Pure States*.

On the other hand, in almost all practical situations, we usually have statistical systems or ensemble and we know the probabilities with which a given system or member could be find in a number of states. Such statistical states are called *Mixed States*. These states cannot be represented by vectors in Hilbert space. These are, in fact situations, where the density matrix formulation really shines.

Regarding mixed states, the reader should notice that these states do not represent quantum superposition, since superposition of any number of states can be represented by a vector in Hilbert space. Furthermore if we do not want to distinguish between classical and quantum probabilities, as I mentioned earlier, then the best definitions of the pure and mixed states are provided by density matrices, which is our next topic.

2.2 The Density Matrix

Imagine an ensemble in which the probability that a member can be found in a state $|\psi_i\rangle$ is p_i , then we can write the *Density Matrix* ρ for the ensemble as

$$\rho = \sum_{i=1}^k p_i |\psi_i\rangle \langle \psi_i| \quad (2.1)$$

Here, the reader should note a number of things. First of all, $|\psi_i\rangle$ represent pure states and hence are vectors in Hilbert space. Secondly, as p_i represent probability, therefore we must have

$$\sum_i p_i = 1 \quad \text{and} \quad p_i \geq 0 \quad (2.2)$$

Moreover, the decomposition shown in Eq. (2.1) is not unique and hence, we can mix different pure states to get the same density matrix. We will come to this point later in Sec. 2.5. For now, I just like to mention that when we decompose a given density matrix into the pure states, as done in Eq. (2.1), then it can turn out that these pure states, represented by $|\psi_i\rangle$ here, may or may not be orthonormal and hence the number of terms in the decomposition, i.e. k , need not be equal to the dimensionality, say N , of the Hilbert space. It can certainly exceed N , in such cases the pure states represented by $|\psi_i\rangle$ will obviously not be orthogonal [11].

In case of a pure state i.e. when we have maximal knowledge about the system, all $p_i = 0$, except one and hence there will be no classical probabilities involved and Eq. (2.1) becomes

$$\rho = |\psi\rangle\langle\psi| \quad (2.3)$$

This is also known as *Projection Operator*, as it can give the projection of any vector onto a 1-dimensional subspace $|\psi\rangle$.

Density matrices also provide us a way to distinguish between mixed and pure states. For pure states $\text{Tr } \rho^2 = 1$ and for mixed states $\text{Tr } \rho^2 < 1$. Also for mixed states there is no decomposition of a density matrix which leads to an equation similar to Eq. (2.3).

We can summarize this section by saying that; mathematically a density matrix is a Hermitian matrix with unit trace and positive eigenvalues. These positive eigenvalues represent probabilities of corresponding pure states and unit trace guarantees that these probabilities will sum up to 1.

2.3 Convex Set and Convex Bodies

In this section, we will equip with some geometrical terms like rank, convex sets, convex hull etc. which will be needed to discuss the set of density matrices, in Sec. 2.5, and also for the set of all classical states, the central object of study in this thesis, in the following chapters. To understand the meaning of these terms we will also look at the geometry of the set of classical probability distributions in the next section.

To define a convex set, first I have to tell you what we mean by mixtures in convex geometry. The *Mixture* of two points is a point which we obtain by weighted sum of these points provided that the weights are positive and

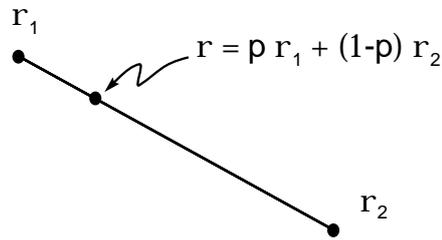


Figure 2.1: Mixtures of two points. Any point ρ , on the line segment shown, can be regarded as a mixture of two points ρ_1 and ρ_2 for a particular value of p . The line segment itself is a convex set.

add up to one [3]. Mathematically if ρ_1 and ρ_2 represent two points in a flat space and p and $1 - p$ are the weights then

$$\rho = p\rho_1 + (1 - p)\rho_2 \quad \text{with} \quad 0 \leq p \leq 1 \quad (2.4)$$

Here ρ is the resultant point and is called mixture of ρ_1 and ρ_2 , figure (2.1) shows a line segment which is the set of all possible mixtures of the two points ρ_1 and ρ_2 . In the same way we can form the mixture of any number of points.

Now, in a flat space, a *Convex Set* is a set of points such that if we mix any pair of these points the resultant mixture, a point, also belongs to this set. Hence in this sense, the line segment shown in the figure (2.1) is a convex set. Figure (2.2) shows some more examples of convex sets. Intuitively one can imagine a convex set as a collection of points such that while sitting on anyone of these points, one can watch all other points in the set.

In this thesis we will mainly be concerned with *Convex Bodies*; these are convex sets which are closed and bounded and have an interior [3]. Figure (2.2) also shows some convex bodies.

In convex sets, all points can be obtained by mixing some special points. These special points are special in the sense that anyone of these points cannot be represented as a mixture of other points in the convex body. These points are called *Pure Points*. Another important term in this regard is the rank. In convex geometry the minimum number of pure points that are needed to mix up to get a given point, as a mixture, is called the *Rank* of that point. Therefore, the rank of a pure point is one, as it is a mixture only of itself.

We can also define the *Convex Hull* or *Convex Cover* of a convex set. This is the minimal or smallest convex set that contains a given convex set. In 2-dimensional case, we can imagine a convex hull as a convex set, which is formed by a rubber band and its interior, while enclosing a set. This intuitive picture can be extended to higher dimension by imagining a perfect rubber sheet or balloon, but only if it does not have any dent across

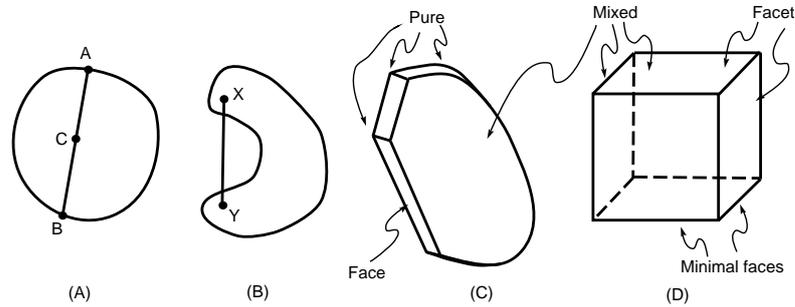


Figure 2.2: Convex sets and convex bodies. (A) A convex set, the whole boundary is consist of pure points. Points mark as A and B are pure with rank one, whereas point C is a mixture with rank two as it can be obtain by mixing two points A and B. (B) it is not a convex set, as many points which are mixtures of X and Y, and lie on the line segment \overline{XY} , are not belongs to the set. (C) A convex body, a Face is also shown. (D) A cube is a convex body with corners as pure points and all other points are mixtures of these pure points. Sides of a cube are Facets and edges represent minimal faces formed by special pure points.

its whole surface, in which case, it is not even a convex set.

The next important term that we need is the face. The *Face* of a convex body is a subset which is stable under mixture and purification. A set is stable under mixture, if the mixture of any pair of points in the set is also belongs to this set, which means a set has to be a convex set in order to be stable under mixture. Therefore, as a first requirement, a subset of a convex body must be a convex set itself in order to be a face. Furthermore a subset of a convex set is called stable under purification if no point in this subset can be a mixture of points that do not belong to it. Therefore, as a second requirement, a face must also include some pure point of the body such that other points in the face are mixtures of these pure points. Thus, one can also say that a *Face* is a convex hull of pure points, which form a subset of pure points of the body, such that no point in this convex hull can be represented by mixture of other point in the body [3]. Figure (2.3) explain the concept of a face clearly.

Furthermore, a face of $(d - 1)$ dimension, where d is the dimensionality of the convex body, is called a *Facet*. In contrast to this, we can also define *Minimal Faces* of a convex set; these are the smallest convex subsets, formed by a given pair of pure points such that they are stable under mixture and purification. An example of convex body is a cube. Its extreme points or corner are pure points, we can also call these pure point as 0-faces. Minimal faces, in this case, do not have a clear answer for the whole body, rather it depends on the choice of the pair of pure points which are chosen to get a minimal face. For some special selection of points we get 1-faces or edges of the cube as minimal faces. Sides of the cube are 2-faces and we can also call them facet as the cube is 3-dimensional body. This is shown in figure

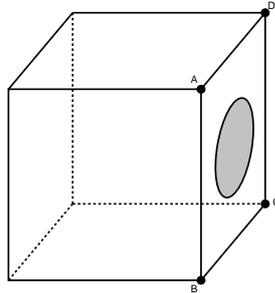


Figure 2.3: A face is stable under mixture and purification. A circle shown in the figure is stable under mixture, as it is a convex set itself, but all points, in this case, are mixtures of four point marked as A,B,C and D, therefore it is not stable under purification. Conversely we can consider the set consist of point A, B, C and D as a candidate for a face. While it is stable under purification, it is not stable under mixture and therefore is not a face. However each side is stable under mixture and purification and hence represents a face of the cube.

(2.2-D).

2.4 The Set of Classical Probability Distributions

Having defined these geometrical terms of convex sets, we are now ready to analyze the shape of the set of classical probability distributions. We will look at the discrete probability distributions in which the possible outcomes will be represented by N .

First, consider a case in which we have only two possible outcomes i.e. $N = 2$ e.g. tossing a coin. If we assume that the probability of one outcome is p then the probability of the other outcome will be $1 - p$. We can represent these probabilities by an ordered pair $(p, 1 - p)$, which can also be considered as the coordinate of a point on a plane. Hence, all values of p will give us a line segment represented by $\overline{P_1 P_2}$ in the figure (2.4-A). Clearly this line segment is a convex hull of two pure points P_1 and P_2 , and all other points on it will have the rank two. Also note that in this case minimal face, which is the whole segment itself, is an edge.

Now suppose $N = 3$ i.e. when there are three possible outcomes. In this case we can represent all allowed probabilities by a tuple with three numbers and hence this can also be represented by the coordinate of a point in 3-dimensional flat space. In this case, all possible combinations of different probabilities define an equilateral triangle shown in figure (2.4-B). This is the convex hull of three pure points P_1 , P_2 and P_3 , and all other points have the rank three except those which lies on the edges where rank is two. The minimal face in this case is also 1-face which is an edge.

Now If we consider four possible outcomes i.e. $N = 4$, then any possible values of the probabilities of all four outcomes can be represented by a

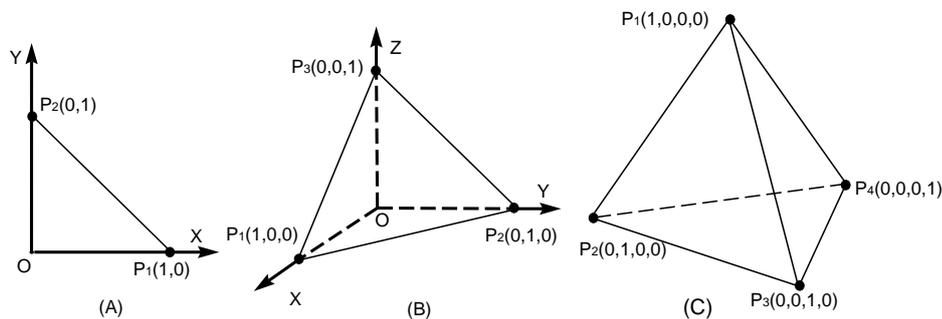


Figure 2.4: Geometry of classical probability distributions. when (A) outcomes = $N = 2$, a line or 1–simplex. (B) $N = 3$, a triangle or 2–simplex. (C) $N = 4$, a 3–simplex or tetrahedron.

4–tuple. We can also imagine this 4–tuple as coordinate of a point on a tetrahedron in 4–dimensional space. The whole probability distribution in this case, is a convex hull of four pure points, which are represented by P_1 , P_2 , P_3 and P_4 in figure (2.4-C). Again, here, minimal faces are 1–faces which are edges of the tetrahedron.

If we analyze these three cases, we can easily conclude that in all these case the shape of the set of classical probability distributions is a simplex or d –simplex, because a line, triangle and tetrahedron are all d –simplexes with $d = 1, 2, 3$.

A simplex or d –simplex is a d –dimensional analogue of a triangle, which is itself a 2–simplex. More precisely, in a d –dimensional flat space, a d –simplex is a convex hull of $(d + 1)$ points such that no m –plane, in this convex hull (where $m \leq d$), contains more than $(m + 1)$ pure points. Also note that the minimal face of a simplex is always a 1–face or an edge.

Therefore, one can generalize this result to the case of N outcomes and can say that the set of classical probability distributions are convex sets with the shape of d –simplexes, which are d –dimensional convex bodies, where $d = N - 1$. The minimal faces of this body are always edges. Also note that every point at or inside these simplexes can be represented by a $(d + 1)$ –tuple, which is unique to this point and hence can also be regarded as the coordinates of this point, only if we consider the d –simplex in a $(d + 1)$ –dimensional space.

2.5 The set of Density Matrices

In this section we will discuss the set of all density matrices which is the quantum analogue of the classical probability distributions. Therefore we also compare the geometry of this set to the geometry of the set of classical probability distributions that we just have discussed in the last section.

Each member of the set of all $N \times N$ Hermitian matrices can be regarded as a vector, since this set fulfill all the axioms of a vector space. However here, we are only interested in density matrices, which are Hermitian matrices with unit trace and positive eigenvalues; therefore, we will be confined to a sub-space of this vector space, which will not be a linear sub-space (or vector space) as the origin i.e. zero matrix will not be included. We call this sub-space \mathcal{V} , it is a space of $N \times N$ Hermitian matrices with unit trace. As there are $(N^2 - 1)$ independent parameters in a $N \times N$ Hermitian matrix with unit trace, therefore we can regard \mathcal{V} as a space with $(N^2 - 1)$ real dimensions. Each point in \mathcal{V} corresponds to a Hermitian matrix of unit trace.

We can also define distances in this space. The distance $D(\rho_1, \rho_2)$ between two matrices ρ_1 and ρ_2 is given by

$$D^2(\rho_1, \rho_2) = \frac{1}{2} \text{Tr} (\rho_1 - \rho_2)^2 \quad (2.5)$$

Hence \mathcal{V} is a flat space [3].

The set of density matrices, which are Hermitian matrices with unit trace and positive eigenvalues, is a sub-set of \mathcal{V} , we call it \mathcal{D} here. \mathcal{D} , actually is the set of all density matrices which can describe states of a N -dimensional quantum system, this include pure as well as mixed states. Here, by dimension of a quantum system I mean, whenever possible the state of the system can be represented by vectors in Hilbert space, span by at most N orthonormal vectors.

As you might know, the mixture of any two density matrices is also a density matrix i.e. density matrices also obey an equation exactly as Eq. (2.4) —where ρ now represent a density matrix— therefore the set of density matrices is a convex set. Hence the set \mathcal{D} is a convex body in \mathcal{V} . Note that the set \mathcal{D} is an $(N^2 - 1)$ dimensional convex body.

Now, As \mathcal{D} is an $(N^2 - 1)$ dimensional body therefore, imagining any case when $N > 2$ is quite hard. Here, to understand the geometry of the set \mathcal{D} , we will consider the case when $N = 2$ i.e. we will consider the case of 2×2 density matrices, which can describe a 2-dimensional quantum system completely.

We can write a general 2×2 Hermitian matrix with unit trace as

$$\rho = \begin{pmatrix} \frac{1}{2} + z & x - iy \\ x + iy & \frac{1}{2} - z \end{pmatrix} \quad (2.6)$$

where x, y and z are real numbers. Now, in order that the above matrix represents a density matrix, we further demand that it has positive eigenvalues. This leads to the condition

$$x^2 + y^2 + z^2 \leq \left(\frac{1}{2}\right)^2 \quad (2.7)$$

This implies that \mathcal{D} , in 2-dimensional case, is a ball with diameter equal to 1 unit. This ball is called *Bloch Ball*. This is a convex body and it is a convex hull of all pure points which make the surface of this ball. These pure points are, in fact, represent pure quantum states. All other points inside this ball have the rank two, as they can be obtained by mixing two pure points lies on the surface. This is shown in figure (2.5). Hence all points inside the ball represent mixed states. The minimal face, in this case, is a 2-face, which is entire ball itself.

At the center of this Bloch ball x, y and z are all zero, and this point represents a density matrix ρ_0 given as

$$\rho_0 = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix} \quad (2.8)$$

This is the *Totally Mixed Density Matrix*. Physically, this represents a situation when any outcome of every measurement is equally likely. As it is a multiple of unit matrix, therefore, it remains diagonal in every basis and can be obtained by mixing any two pure points on the surface of this ball, which are opposite to each other. Such opposite pure points represent orthogonal pure states.

After taking this example we can, now, conclude that the set of all density matrices is quite different from the set of classical probability distributions. Here, one can observe two big differences between these two sets.

1. When there are N outcomes the convex set, in case of the set of classical probability distributions, forms a $(N-1)$ dimensional convex body, whereas in case of \mathcal{D} , it is a $(N^2 + 1) = (N+1)(N-1)$ dimensional convex body.
2. For the set of classical probability distributions, the minimal faces are edges of the simplexes, as we have seen in the last section whereas for the set \mathcal{D} , minimal faces are 2-faces, which are Bloch balls.

Regarding second difference, we just have observed this for 2×2 density matrices and this is also true in general. This can easily be seen if we note that any two given states in a N -dimensional Hilbert space, belong to a 2-dimensional subspace of this space, and in this subspace we can always found a pair of orthogonal states which span this 2-dimensional sub-space, therefore all states in this sub-space can be described by 2×2 density matrices and we have already seen that the set of such matrices always forms a Bloch ball. Thus in the set \mathcal{D} any two orthogonal states corresponds to a minimal face which is a Bloch ball.

I want the reader to notice one more thing, there is a theorem on convex sets, named as *Caratheodory's theorem*, which says, any point, which belongs to a d -dimensional convex set, can be represented by a mixture of $d+1$

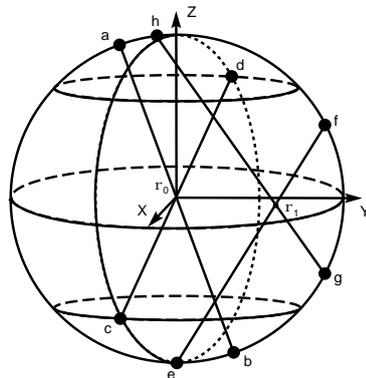


Figure 2.5: The Bloch Ball. Pure states marked as a, b and c, d are two different decomposition of the same density matrix ρ_0 . Similarly, pure states marked as e, f and g, h are two different decomposition of a mixed density matrix ρ_1 .

pure points [10]. This can be seen very easily in case of the set of classical probability distributions i.e. in simplexes. Thus using this theorem, we can also conclude that any $N \times N$ density matrix can, in general, be decompose into at most N^2 pure states or in other words the maximum rank of a point in the set \mathcal{D} can be N^2 . What is special about the set \mathcal{D} is that we never need N^2 states, rather we can always decompose a density matrix in only N pure states, which will be the eigenstates of this density matrix and hence will diagonalize it.

Before ending this chapter, I also like to mention a consequence of the first difference between the two sets. Actually, this difference implies that there can be many different decompositions of a density matrix while this is not true for the set of classical probability distributions. For example as we have seen, for the set of classical probability distributions (which are simplexes), when outcomes $N = 2$ we get a line segment as a convex body and any possible values of the probabilities of the two outcomes can be denoted by a unique coordinate of a point on this segment, this is shown in fig (2.4-A). Similarly this is true for any d -simplex by regarding it in $N = (d + 1)$ dimensions. Whereas, for the same value of $N = 2$, every member of the set \mathcal{D} is 2×2 density matrix and the whole set is a ball which is a 3-dimensional object. Therefore it turns out that there is no unique decomposition of the density matrix except when it is also a projection operator. We can get the same density matrix by mixing different pure states. This is shown in figure (2.5). The situation is even worse for higher values of N , because then \mathcal{D} will be $(N^2 - 1)$ dimensional convex body, thus any $N \times N$ density can be decompose in many different ways. This important fact was first noted by Schrödinger and he coded it in a theorem called Schrödinger mixture theorem [3].

Schroödinger's Mixture Theorem

According to this theorem any density matrix which has the diagonal form

$$\rho = \sum_{i=1}^N \lambda_i |e_i\rangle \langle e_i| \quad (2.9)$$

where $|e_i\rangle$ are orthonormal vectors and λ_i are eigenvalues, can also be written as

$$\rho = \sum_{i=1}^m p_i |\psi_i\rangle \langle \psi_i| \quad , \quad \sum_i p_i = 1 \quad , \quad p_i \geq 0 \quad (2.10)$$

if and only if there exist a unitary $m \times m$ matrix U such that

$$|\psi_i\rangle = \frac{1}{\sqrt{p_i}} \sum_{j=1}^N U_{ij} \sqrt{\lambda_j} |e_j\rangle \quad , \quad i = 1, \dots, m \quad , \quad m \geq N \quad (2.11)$$

Here note that U is not an operator in Hilbert space, rather it is a matrix whose first row, when multiplied by the list of vectors $|e_i\rangle$ gives a vector $|\psi_1\rangle$ and similarly by the multiplication of other row we can get other vectors $|\psi_i\rangle$. This theorem clearly says, density matrices do not have unique decomposition, except when they are also projectors, But there is a preferred decomposition which diagonalize a given density matrix, such a decomposition is given in Eq. (2.9).

Chapter 3

Spin Coherent States

In the previous chapter, we have seen that the set of density matrices (\mathcal{D}) is quite different from the set of classical probability distributions, consequently, despite the fact that quantum theory is a probabilistic theory, it is fundamentally different from the classical probability theory. In chapter 1, we have also seen that the pure coherent states are the most classical states in quantum mechanics; however the mixtures of these coherent states can also be treated as classical. Therefore these mixed states together with pure coherent states form the set of classical states and we expect that this set may have some resemblance with the set of classical probability distributions; actually this investigation is the main theme of this thesis.

Having said this, now our goal in this thesis is quite clear. After acquiring necessary background in the last chapter we will now introduce the set of classical states in this chapter. However, as we know from the last chapter that the set \mathcal{D} is an $(N^2 - 1)$ dimensional convex body in the space (\mathcal{V}) of $N \times N$ Hermitian matrices with unit trace —where N denotes the number of possible outcomes— therefore considering the geometry of the set of classical states, which is a subset of \mathcal{D} , for all general values of N is quite difficult. Hence, in this chapter we will eventually restrict ourselves to the case when $N = 3$. The most common examples of such discrete or finite dimensional quantum systems are spin-1 systems, therefore, from now on we shall talk in the language of these spin systems only.

Coherent states for these spin systems are known as spin coherent states, hence, first of all I will tell you what spin coherent states are in Sec. 3.1 and then we will look at the set of these coherent states in Sec. 3.2. At the end of this chapter in Sec. 3.3, I will introduce the set of classical states, the central object of study in this thesis.

3.1 Spin Coherent States

Spin Coherent States are simply the coherent states of spin systems. In the first chapter I mentioned that the coherent states are those states which minimize the uncertainty relation of position and momentum. However they do so in a certain way¹ that there is one-to-one mapping of classical phase space onto the space of these states. In a similar manner, spin coherent states are those states which minimize an uncertainty relation and form a set that can also be mapped onto the classical phase space, but this time the uncertainty relation is rather special and such that it is only minimized by these spin coherent states [3]. If we define Δ as

$$\Delta^2 \equiv (\Delta J_x)^2 + (\Delta J_y)^2 + (\Delta J_z)^2 = \langle \hat{J}^2 \rangle - \sum_{i=1}^3 \langle \hat{J}_i \rangle^2 \quad (3.1)$$

where \hat{J}_x, \hat{J}_y and \hat{J}_z are the components of angular momentum operator with eigenvalues j , then this Δ^2 obeys the inequality

$$j \leq \Delta^2 \leq j(j+1) \quad (3.2)$$

To arrive at this result note that the $\langle \hat{J}^2 \rangle = j(j+1)$ and as Eq. (3.1) is invariant under rotation group $\text{SU}(2)$ therefore we can always bring the vector $\langle \hat{J}_i \rangle$ to the form

$$\langle \hat{J}_i \rangle = \langle \hat{J}_z \rangle \delta_{i3} \quad (3.3)$$

Now any state $|\psi\rangle$ can be expanded as

$$|\psi\rangle = \sum_{m=-j}^j c_m |m\rangle \quad \Rightarrow \quad \langle \hat{J}_z \rangle = \sum_{m=-j}^j m |c_m|^2 \quad (3.4)$$

therefore we lead to the inequality

$$0 \leq \langle \hat{J}_z \rangle \leq j \quad (3.5)$$

Now this inequality together with Eq. (3.1) leads to Eq. (3.2) and completes the proof.

Now, we can define spin coherent states as precisely those states for which relation given in Eq. (3.2) saturates, i.e. for only spin coherent states $\Delta^2 = j$.

Also note that there are other uncertainty relations for spin systems like

$$\Delta J_x \Delta J_y \geq \frac{|\langle \hat{J}_z \rangle|}{2} \quad (3.6)$$

¹see chapter 1, for details

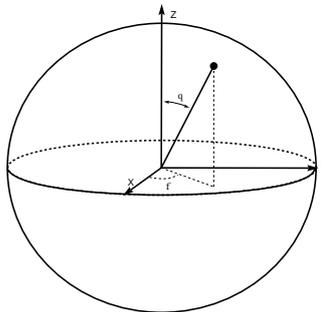


Figure 3.1: An arbitrary unit vector in spherical coordinates.

but this is not the one which is only minimized by spin coherent states e.g. in spin-1 systems, spin-0 states also minimize the above inequality, but these are not coherent states. Another reason of why this is not a relevant uncertainty relation, in our case, is the fact that the right hand side of this relation is frame dependent— as it contains $|\langle \hat{J}_z \rangle|$ —whereas Eq. (3.1) is frame invariant. This is important, because, as we will see later in this chapter, the spin coherent states are invariant under $SU(2)$ rotations, which suggest that a relevant uncertainty relation must also be invariant [2].

As we have noted that Eq. (3.1) is invariant under rotation group $SU(2)$ and hence under $SO(3)$ also, therefore we can also regard spin coherent states as the coherent states of the rotation group $SO(3)$. This provides us another simple definition for these states. We can define spin coherent states as the eigenstates of an operator

$$\hat{\mathbf{z}} \cdot \hat{\mathbf{J}} = \sum_{i=1}^3 z_i \hat{J}_i \quad (3.7)$$

with eigenvalues j , where $\hat{\mathbf{z}}$ is an arbitrary unit vector represented in spherical coordinates and $\hat{\mathbf{J}}$ is the angular momentum operator as before, with components $\hat{J}_i = \hat{J}_x, \hat{J}_y$ and \hat{J}_z . With polar angle θ and azimuth ϕ , as shown in figure (3.1), $\hat{\mathbf{z}}$ can be written as

$$\hat{\mathbf{z}} = \begin{pmatrix} \sin \theta \cos \phi \\ \sin \theta \sin \phi \\ \cos \theta \end{pmatrix} \quad (3.8)$$

We can summarize the above definition by saying that a state $|\psi\rangle$ will be a spin coherent state if

$$(\hat{\mathbf{z}} \cdot \hat{\mathbf{J}})|\psi\rangle = |\psi\rangle \quad (3.9)$$

This means, physically for some unit vector $\hat{\mathbf{z}}$ a spin coherent state, (called only “coherent state” in the following for short) represents a spin up state in some direction.

Now, if we consider the example of spin $-\frac{1}{2}$ systems, then according to Eq. (3.9), a state $|\psi\rangle$ will be a coherent state if it is an eigenstate of an operator $(\hat{\mathbf{z}} \cdot \hat{\boldsymbol{\sigma}})$ where $\hat{\boldsymbol{\sigma}}$ is the angular momentum operator, whose components in this case are also known as *Pauli Matrices* [11] and are written as

$$\hat{\sigma}_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \hat{\sigma}_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \hat{\sigma}_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (3.10)$$

However for every pure state, in this case, there exist a unit vector $\hat{\mathbf{z}}$ such that it is a an eigenstate of $(\hat{\mathbf{z}} \cdot \boldsymbol{\sigma})$ and represents a spin up state in $\hat{\mathbf{z}}$ direction. Therefore, for spin $-\frac{1}{2}$ systems all pure states are coherent states.

Similarly, for spin -1 systems, any state $|\psi\rangle$ will be a spin coherent state if it is an eigenstates of $(\hat{\mathbf{z}} \cdot \hat{\mathbf{J}})$, and in this case a possible representation for the component of angular momentum operator $\hat{\mathbf{J}}$ is

$$\begin{aligned} \hat{J}_x &= \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} & \hat{J}_y &= \frac{\hbar}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix} \\ \hat{J}_z &= \hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \end{aligned} \quad (3.11)$$

Now for this case, all pure states are not coherent, because there are pure spin -0 states which do not satisfy Eq. (3.9). In fact the situation is even worse because in this case, there also exist pure states which are neither spin -1 nor spin -0 states —namely those states that can be regarded as the superposition of these spin -1 and spin -0 states— these states will also not be coherent. Notice that any superposition of spin up and down state is also a spin up state in a different direction and thus will be a coherent state. This is also true in spin $-\frac{1}{2}$ systems. In this thesis we will not go beyond spin -1 systems.

Before ending this section, I like to tell you that the most intuitive picture of the spin coherent states can be provided by the *Majorana Description* of the spin states [9]. In this description any spin of $\frac{1}{2}n\hbar$, where n is a positive integer, can be represented by a set of n unordered points on the surface of a sphere. Each such point provides an amount $\frac{1}{2}\hbar$ of spin. This is shown in figure (3.2).

Now in this description, coherent states are those states which correspond to minimum spread and maximum coherence of these points. Therefore for these states all points coincide at one position. The question, why such states are regarded as the most classical states, can be answered if we try to think about quantum mechanical spin as the same phenomenon as the familiar concept of the spin in classical mechanics, and consider the points in Majorana description as arrows or axis around which the particle can rotate. This means that a quantum particle can able to rotate about

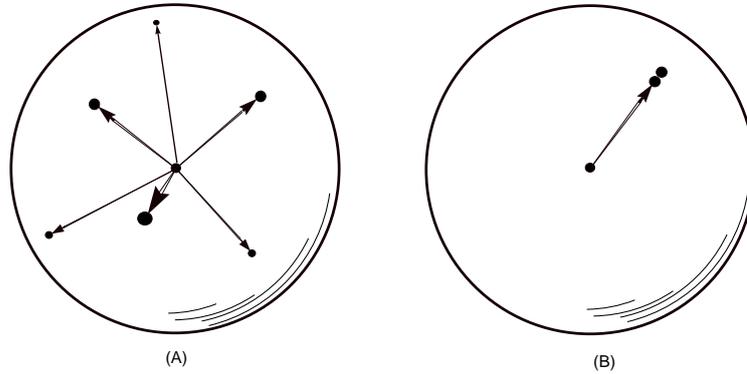


Figure 3.2: Majorana description for spin states. (A) A spin-3 particle, can be represented by six independent points on a sphere. (B) Similarly a spin-1 particle is represented by two independent points and for a spin coherent states both points coincide.

various axes at once. Clearly the most classical situation is the one when all such axes coincide; this is exactly what happens in the case of spin coherent states.

3.2 The Set of Spin Coherent States

Before discussing this set, I would like to define what we call an orbit in group theory. Using the language of vectors we can define an *Orbit* as a set of all vectors that can be obtained by the action of a group on a *Reference Vector*. Therefore, if we choose our reference vector as a unit vector in the z-direction and our relevant group is $SO(3)$, then the orbit in this case will be S^2 or the surface of the sphere. We need this concept because spin coherent states form an $SO(3)$ orbit. Let's see how.

In the last section we have seen that a spin coherent state is a spin up state in some direction. Since every point on the surface of a sphere represents a unique direction, therefore each such point corresponds to a pure coherent state and thus the set of all pure coherent states forms the surface of a sphere and we say that the set of these coherent states is an $SO(3)$ orbit. The reader should note that this sphere or orbit resides in the state space i.e. in the space of density matrices. Any temptation to think of this sphere as embedded in a 3-dimensional ordinary space must be resisted. This become obvious if one notice that a point can represent a *State* only if it is in the state space which, in this case, is the space of density matrices. Actually any spin up state $|\psi\rangle$, in the direction of $\hat{\mathbf{z}}$, is a vector in Hilbert space and although its associated unit vector $\hat{\mathbf{z}}$ is a vector in 3-dimensional ordinary space, however its state is represented by its projection operator which is a density matrix in the space \mathcal{V} . As every $\hat{\mathbf{z}}$ vector corresponds

to a state, therefore, this also implies that the set of spin coherent states is always a sphere or $\mathbb{S}\mathbb{O}(3)$ orbit whatever be the value of j .

Now, before ending this chapter I will introduce the set of classical states in the last section, which is the convex hull of spin coherent states in the space of density matrices.

3.3 The Set of Classical States

We know that the coherent states are the most classical states in quantum mechanics. However, for spin systems, as I have already mentioned in the first chapter, not only coherent states but all other states, which can be represented as a mixture of these coherent states, are considered as classical, therefore the set of these classical states form a convex set [4]. Here, we will call this set \mathfrak{e}_{cl} .

The set \mathfrak{e}_{cl} resides in the space of $N \times N$ Hermitian matrices (\mathcal{V}), which is an $(N^2 - 1)$ dimensional space. As this set is bounded and has some interior also, therefore it is a convex body and contained in a much bigger convex body of density matrices \mathcal{D} in the space \mathcal{V} . Note that this body contains all the mixtures of spin coherent states, which means, all pure points in this body are spin coherent states and thus one can regard \mathfrak{e}_{cl} as the convex hull of these coherent states.

This is also true that the dimension of the convex body formed by all classical states (\mathfrak{e}_{cl}) is $(N^2 - 1)$. However this is not obvious, because, if one keep in mind the fact that coherent states form an $\mathbb{S}\mathbb{O}(3)$ orbit and \mathfrak{e}_{cl} being a convex hull of coherent states contained in the body \mathcal{D} —which is itself $(N^2 - 1)$ dimensional—, then one can only expect that the dimensionality of this body can take any value between 3 and $(N^2 - 1)$. In the next chapter, we will see how one can arrive at this result.

As the set \mathfrak{e}_{cl} is an $(N^2 - 1)$ dimensional convex body therefore imagining its shape, in general, is quite hard. The $N = 2$ case or spin- $\frac{1}{2}$ systems, provides the simplest example. In this case \mathfrak{e}_{cl} is a $(2^2 - 1) = 3$ dimensional convex body. Since all pure states of a spin- $\frac{1}{2}$ system are coherent states, therefore the convex hull of these coherent states is the convex hull of pure states. However we have seen in Sec. 2.5 that when $N = 2$ the convex hull of pure states is the entire Bloch ball, therefore the whole ball represents classical states or in other words every state in spin- $\frac{1}{2}$ systems is a classical state. Hence for $N = 2$,

$$\mathfrak{e}_{cl} = \mathcal{D}$$

When $N = 3$, i.e. for spin-1 systems, \mathfrak{e}_{cl} is a convex body in an 8-dimensional space of 3×3 density matrices. In contrast to spin- $\frac{1}{2}$ case, here all pure states are not coherent states. This is because there are pure states with spin-0, which are neither coherent nor their convex sum, therefore these states are not considered as classical. Furthermore any pure state

which involve superposition of these spin-0 states are not classical as well. Hence convex hull of coherent states (ρ_{cl}) is the subset of \mathcal{D} i.e.

$$\rho_{cl} \subset \mathcal{D}$$

In this thesis, we will study the convex geometry of this set. This means, in the following chapters we will be restricted to 3×3 density matrices, which can describe all pure and mixed states of a spin-1 system or a qutrit. This also implies that from now on our Hilbert space will be 3-dimensional, which we represented as \mathcal{H}^3 .

Chapter 4

Magical Basis

In quantum mechanics, we represent states of a system by vectors in Hilbert space. However not every vector in Hilbert space represents a unique state, instead all vectors that are complex multiple of a given vector represent the same physical state. This fact provides us more freedom than only normalizing states vectors. Using it we can also write our state vectors in a way that its real and imaginary parts become orthogonal. Soon we will see that this representation is useful in our case. The second very useful fact that we need in this chapter is about spin coherent states, namely that they are the coherent states of the rotation group $SU(2)$. Using these facts and taking the advantage of our restriction in this thesis to the 3-dimensional Hilbert space (\mathcal{H}^3), in this chapter I shall introduce a representation or basis, known as *Magical Basis*, which considerably simplifies our formulae as well as calculations in the later chapters.

In the light of the first fact, described above, the idea behind the magical basis can be expressed nicely, as the spin coherent states are the coherent states of the rotation group $SU(2)$, and fortunately —due to the fact that $SU(2) \sim SO(3)$ which I explain later— there exist a real 3-dimensional representation for this group, therefore we can use this real representation for the description of our spin coherent states. The advantage of using this representation is that it will preserve the split between real and imaginary parts of the state vectors which in turn simplifies the representation of the spin coherent states and hence can also simplify our calculation and formulae.

This chapter is divided into three sections. In Sec. 4.1, I shall explain, how one can split state vectors into real and imaginary parts that represent two orthogonal vectors. Then in Sec. 4.2 we will see what will be the components of angular momentum operator— the generators of the rotations— which preserve this split. Then in the Sec. 4.3, we will see how coherent states look like in this basis. In the end, in Sec. 4.5, we will briefly reconsider the set of all classical states in the light of this new basis.

4.1 State Vectors in Magical Basis

In quantum mechanics the states of a system are represented by vectors in Hilbert space. This is a complex vector space, which means every vector in it has some real and imaginary parts. However not every vector in Hilbert space corresponds to a unique quantum state, rather we can say that each direction or a ray in this space represents only one quantum state. Mathematically this means, a vector $|\psi\rangle$ and its complex multiple $c|\psi\rangle$ where $c \in \mathbb{C}$, represents the same physical state. Note also that we can always split the complex multiple c into two parts i.e.

$$|\psi\rangle \sim c|\psi\rangle = Ae^{i\phi}|\psi\rangle \quad (4.1)$$

where A is a real number and $e^{i\phi}$ is a complex phase factor. We usually choose the real number A such that it normalizes our state vector. Then the only freedom left is due to the phase factor. Now, we will use this freedom to write our state vectors in such a way that its real and imaginary parts become multiple of two orthonormal vectors [8].

Suppose $|\psi\rangle$ represents a normalized vector in Hilbert space then we can write it in real and imaginary parts as

$$|\psi\rangle = \mathbf{a} + i\mathbf{b} \quad (4.2)$$

Since $|\psi\rangle$ is normalized therefore we can write $\mathbf{a} = \cos \sigma \hat{\mathbf{x}}$, and $\mathbf{b} = \sin \sigma \hat{\mathbf{y}}$ where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit vectors in the direction of \mathbf{a} and \mathbf{b} , then Eq. (4.2) becomes

$$|\psi\rangle = \cos \sigma \hat{\mathbf{x}} + i \sin \sigma \hat{\mathbf{y}} \quad (4.3)$$

Now normalization of $|\psi\rangle$ means

$$\langle\psi|\psi\rangle = |\mathbf{a}|^2 + |\mathbf{b}|^2 = \cos^2 \sigma + \sin^2 \sigma = 1 \quad (4.4)$$

Here we have used the fact that $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are unit vectors.

In general $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ need not be orthogonal. If they are orthogonal then our task to split $|\psi\rangle$ into desired form has been accomplished. Otherwise, we can always make them orthogonal by multiplying $|\psi\rangle$ by a phase factor. To see this, consider $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are not orthogonal then using phase freedom we can write Eq. (4.3) as

$$\begin{aligned} |\psi\rangle \sim e^{i\phi}|\psi\rangle &= (\cos \phi + i \sin \phi)(\cos \sigma \hat{\mathbf{x}} + i \sin \sigma \hat{\mathbf{y}}) \\ \Rightarrow |\psi\rangle &= (\cos \phi \cos \sigma \hat{\mathbf{x}} - \sin \phi \sin \sigma \hat{\mathbf{y}}) + i(\sin \phi \cos \sigma \hat{\mathbf{x}} + \cos \phi \sin \sigma \hat{\mathbf{y}}) \end{aligned} \quad (4.5)$$

if we suppose

$$\mathbf{X} = (\cos \phi \cos \sigma \hat{\mathbf{x}} - \sin \phi \sin \sigma \hat{\mathbf{y}}) \quad (4.6a)$$

$$\mathbf{Y} = (\sin \phi \cos \sigma \hat{\mathbf{x}} + \cos \phi \sin \sigma \hat{\mathbf{y}}) \quad (4.6b)$$

and demand that $\mathbf{X} \cdot \mathbf{Y} = 0$ then it will lead to the condition

$$\tan \phi - \frac{1}{\tan \phi} = \frac{\cos^2 \sigma - \sin^2 \sigma}{\sin \sigma \cos \sigma (\hat{\mathbf{x}} \cdot \hat{\mathbf{y}})} \quad (4.7)$$

This equation can be solved to get a value of ϕ which make \mathbf{X} and \mathbf{Y} orthogonal. Now using unit vectors in the direction of \mathbf{X} and \mathbf{Y} we can write $|\psi\rangle$ as in Eq. (4.3) such that real vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ will now be the unit vectors of \mathbf{X} and \mathbf{Y} and orthonormal. Hence using this procedure we can always write a state vector $|\psi\rangle$ in a way that its real and imaginary parts are orthogonal.

In this representation we can also restrict σ as, $0 \leq \sigma \leq \frac{\pi}{4}$. With this restriction our state vectors will be such that their real parts will always be greater than their imaginary parts. Note that if one restrict σ as said then he will never come across to purely imaginary state vectors, however purely real vectors are allowed. Having done this the phase factor is thereby fixed up to a sign, except when $\sigma = \frac{\pi}{4}$ in which case the phase ambiguity still remains.

4.2 Angular Momentum Operator in Magical Basis

First of all note that we can define spin coherent states of spin-1 systems, as the eigenstates of an operator $(\hat{\mathbf{z}} \cdot \hat{\mathbf{J}})$ with eigenvalues $j = 1$, therefore it is quite clear that if we want some nice properties in our representation of spin coherent states then we not only choose a better representation for our state vectors, but we will do this for the operator $\hat{\mathbf{J}}$ also. In the previous section we learnt how to split a state vector into real and imaginary parts that are multiple of orthonormal vectors, now in this section we will introduce a representation of the operator $\hat{\mathbf{J}}$ which will preserve this split.

In general unitary transformations in \mathcal{H}^3 mixed up real and imaginary parts of the state vectors, however as the spin coherent states are the coherent states of the rotation group $\text{SU}(2)$, therefore we are interested in only $\text{SU}(2)$ rotations and thus by using real representation of this group we can restrict ourselves to only those unitary transformations which do not mix up real and imaginary parts of the state vectors. This all could be quite confusing for some readers. Does this mean that we are going to perform some unitary transformations? —to understand things better and answer such questions we have to go in some details and try to understand how the operator $\hat{\mathbf{J}}$ is associated with unitary transformations.

We know that the state vector of a system carries all the information about its state; therefore we expect that if we rotate an entire system in our reference frame then its state vector should also undergo a change. However the state vector does not reside in the ordinary 3-dimensional space, rather it is a vector in Hilbert space; therefore the state vector for rotated system

cannot be obtained by just replacing old unrotated position vectors with the new rotated position vectors. It turns out that the state vector of the rotated system can be obtained by a unitary transformation of the old unrotated state vector.

Mathematically, if $|\psi\rangle$ represent the state vector of unrotated system and $|\psi\rangle_R$ of the rotated system, while rotation take place around $\hat{\mathbf{n}}$ with an angle of ϕ then

$$|\psi\rangle_R = \hat{\mathcal{R}}(\hat{\mathbf{n}}, \phi)|\psi\rangle \quad (4.8)$$

where

$$\hat{\mathcal{R}}(\hat{\mathbf{n}}, \phi) = \exp\left(\frac{-i\phi(\hat{\mathbf{J}} \cdot \hat{\mathbf{n}})}{\hbar}\right) \quad (4.9)$$

where $\hat{\mathbf{J}}$ is as usual angular momentum operator. Now if $\hat{\mathbf{J}}$ is Hermitian—which is always be the case, because it represents the operator of angular momentum and in quantum mechanics all observables are represented by Hermitian operators—then $\hat{\mathcal{R}}$ will be unitary. Hence we can conclude that if we rotate a system in ordinary 3–dimensional space then its state vector undergoes a unitary transformation in the Hilbert space, which is given in Eq. (4.8) [11].

The reader should also notice that, for N dimensional quantum system, $\hat{\mathbf{J}}$ and $\hat{\mathcal{R}}$ are actually $N \times N$ matrices, which act on the Hilbert space of the system. The components of $\hat{\mathbf{J}}$ are also called generator of rotations, as using them we can obtain the state vector of a system which undergoes any general rotation in ordinary 3–dimensional space. Therefore, they obey the commutation relation of $SO(3)$ group i.e.

$$[\hat{J}_i, \hat{J}_j] = i\hbar\epsilon_{ijk}\hat{J}_k \quad (4.10)$$

and can be described using the same Lie algebra as of $SO(3)$. In our case i.e. for spin–1 systems $\hat{\mathbf{J}}$ and $\hat{\mathcal{R}}$ are 3×3 matrices.

Some reader might still be confused and could ask why we are interested in rotations here at all. The reason for this, is that we are interested in spin coherent states, which form an $SU(2)$ orbit in Hilbert space. This means if we start with a *Reference State* — which can be a spin up state in z-direction — then all other spin coherent states can be obtained by this state through $SU(2)$ rotations. In other words spin coherent states are in fact has $SU(2)$ rotational symmetry and our representation of $\hat{\mathbf{J}}$ will be interesting or advantageous only if the action of an operator ($\hat{\mathbf{z}} \cdot \hat{\mathbf{J}}$) on all spin coherent states will be similar i.e. if it preserves the split between real and imaginary part for one coherent state, for a particular vector $\hat{\mathbf{z}}$, then it should also preserves this split for all other coherent states for some other vectors $\hat{\mathbf{z}}$.

Now, as we are interested in spin–1 systems, where the components of angular momentum are 3×3 matrices, therefore we can take the advantage of the fact that there exist a real representation of the group $SU(2)$ in terms

of 3×3 matrices, and hence we can use this representation to reach all spin coherent states from our reference state. The benefit of using real representation is quite clear, in this representation all elements of the group $\mathbb{S}\mathbb{U}(2)$ are real unitary matrices—which are then called orthogonal matrices—and thus all unitary transformation using such matrices preserve our split in real and imaginary parts, which is a nice achievement.

The reason why we are able to find a real representation here is the fact that the group we are interested in i.e. $\mathbb{S}\mathbb{U}(2)$ is homomorphic¹ to the group $\mathbb{S}\mathbb{O}(3)$ i.e. $\mathbb{S}\mathbb{U}(2) \sim \mathbb{S}\mathbb{O}(3)$. Note that all $\mathbb{S}\mathbb{O}(N)$ groups have real representations. Hence we can always find such a real representation when our group of interest is equivalent to any $\mathbb{S}\mathbb{O}(N)$ group. This idea was first introduced by William K Wootters [14], who is actually interested in the entanglement of two qubits, i.e. he is interested in the group $\mathbb{S}\mathbb{U}(2) \times \mathbb{S}\mathbb{U}(2)$ which is equivalent to the group $\mathbb{S}\mathbb{O}(4)$ i.e. $\mathbb{S}\mathbb{U}(2) \times \mathbb{S}\mathbb{U}(2) \sim \mathbb{S}\mathbb{O}(4)$ and hence magical basis is advantageous for him.

Now we can come to the main objective of this section that is, to suggest a representation of the angular momentum components. A possible representation is given in Eq. (3.11) which clearly not leads to the real unitary matrices through Eq. (4.9). If we carefully observe Eq. (4.9) then we can easily conclude that our components of angular momentum should be purely imaginary, in order that they lead to real unitary matrices $\hat{\mathcal{R}}$. Obviously, first of all they should be Hermitian, as they are the operator of quantum observables. Another property that they should possess is that they must obey the commutation relation given in Eq. (4.10).

In the light of the above discussion and keeping in mind the fact that $\mathbb{S}\mathbb{U}(2) \sim \mathbb{S}\mathbb{O}(3)$, it is quite clear that we are now seeking for a real representation of the group $\mathbb{S}\mathbb{U}(2)$ in terms of the group elements of $\mathbb{S}\mathbb{O}(3)$. Therefore, it is advantageous to look at the generator of the group $\mathbb{S}\mathbb{O}(3)$. The generators of the group $\mathbb{S}\mathbb{O}(3)$ are in fact matrices which generates infinitesimal rotations in ordinary 3-dimensional space and hence, can be obtained by differentiation of the rotation matrices [13]. These rotation matrices, which represent rotation around x, y and z-axis are written as

$$\begin{aligned}
 R_x &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos \gamma & -\sin \gamma \\ 0 & \sin \gamma & \cos \gamma \end{pmatrix} & R_y &= \begin{pmatrix} \cos \beta & 0 & \sin \beta \\ 0 & 1 & 0 \\ -\sin \beta & 0 & \cos \beta \end{pmatrix} \\
 R_z &= \begin{pmatrix} \cos \alpha & -\sin \alpha & 0 \\ \sin \alpha & \cos \alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}
 \end{aligned} \tag{4.11}$$

¹Means it has many-to-one correspondence with the other group. In this case the correspondence is 2-to-1.

A generator G_x corresponding to R_x can be obtained by

$$G_x = \left. \frac{dR_x}{d\gamma} \right|_{\gamma=0} \quad (4.12)$$

In the same way one can also write formulae for the generator of R_y and R_z . The reader can check that these generators are turn out to be

$$\begin{aligned} G_x &= \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} & G_y &= \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \\ G_z &= \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{aligned} \quad (4.13)$$

However, these are neither Hermitian nor purely imaginary, although one can check that they obey the commutation relation given in Eq. (4.10), therefore we cannot use them as it is. Now we suggest that the three matrices which are purely imaginary, Hermitian and obey the commutation relation of Eq. (4.10), could be

$$\begin{aligned} \hat{L}_x &= i \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} & \hat{L}_y &= i \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix} \\ \hat{L}_z &= i \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \end{aligned} \quad (4.14)$$

The careful reader might have noticed that I just have placed an i in front of previous generators. We can write these three matrices in a compact form, using Einstein summation convention as

$$(\hat{L}_i)_{ab} = i\epsilon_{aib} \quad (4.15)$$

It is easy to check that these are purely imaginary, Hermitian and obey the commutation relation

$$[\hat{L}_i, \hat{L}_j] = i\epsilon_{ijk}\hat{L}_k \quad (4.16)$$

that is we have accomplished our task in this section. Now in the last section we will see how our magical representation simplifies the representation of spin coherent states.

4.3 Spin Coherent States in Magical Basis

First of all note that when we write our state vector in the form

$$|\psi\rangle = \cos\sigma \hat{\mathbf{x}} + i \sin\sigma \hat{\mathbf{y}}$$

then it is clear that we are writing $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ using following basis vectors,

$$\hat{\mathbf{e}}_{\mathbf{x}} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \hat{\mathbf{e}}_{\mathbf{y}} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \hat{\mathbf{e}}_{\mathbf{z}} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (4.17)$$

Another important thing is that in magical basis σ is invariant. We can see this if we calculate $\langle \psi^* | \psi \rangle$ —where ψ^* is the complex conjugate of ψ — as follows

$$\begin{aligned} \langle \psi^* | \psi \rangle &= (\cos \sigma \hat{\mathbf{x}} + i \sin \sigma \hat{\mathbf{y}})(\cos \sigma \hat{\mathbf{x}} + i \sin \sigma \hat{\mathbf{y}}) \\ &= \cos^2 \sigma \hat{\mathbf{x}} \cdot \hat{\mathbf{x}} + i \sin^2 \sigma \hat{\mathbf{y}} \cdot \hat{\mathbf{y}} + 2(\hat{\mathbf{x}} \cdot \hat{\mathbf{y}}) \cos \sigma \sin \sigma \end{aligned}$$

Now if we use the fact that $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are orthonormal vectors then

$$\begin{aligned} \langle \psi^* | \psi \rangle &= \cos^2 \sigma - \sin^2 \sigma \\ &= \cos 2\sigma \end{aligned} \quad (4.18)$$

As all unitary transformations preserved inner product therefore this product will also be preserved which implies that σ will be invariant.

In this representation we have restricted σ as, $0 \leq \sigma \leq \frac{\pi}{4}$, therefore our state vectors will either always be real or— whenever complex —have non-zero real and imaginary parts that are orthogonal.

Now take a purely real state vector, say $|\psi\rangle = \hat{\mathbf{x}}$ and form the operator $\hat{\mathbf{x}} \cdot \hat{\mathbf{L}}$ and calculate $(\hat{\mathbf{x}} \cdot \hat{\mathbf{L}})\hat{\mathbf{x}}$. In the index notation we can write it as

$$\begin{aligned} (x_i \hat{L}_i)_{ab} x_b &= i x_i \epsilon_{aib} x_b \\ &= i \epsilon_{aib} x_i x_b \\ &= 0 \end{aligned} \quad (4.19)$$

here, in the last line we used the fact that the cross product of a vector with itself is zero. This is actually eigenvalue equation with eigenvalue zero, and hence we can conclude that all pure spin-0 states are, in fact, represented as real vectors in this representation.

Now, for spin coherent state, the reader can check that

$$(\hat{\mathbf{z}} \cdot \hat{\mathbf{L}}) \left(\frac{1}{\sqrt{2}} (\hat{\mathbf{x}} + i \hat{\mathbf{y}}) \right) = \frac{1}{\sqrt{2}} (\hat{\mathbf{x}} + i \hat{\mathbf{y}}) \quad (4.20)$$

Where $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$ and $\hat{\mathbf{z}}$ are three orthonormal vectors which form a right handed system. This means, in this representation spin coherent states always have $\sigma = \frac{\pi}{4}$ and represent spin up state in a direction which is perpendicular to both the vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$.

In the light of this simplified representation of our state vectors, we can now take a brief review of the set of all classical states $\boldsymbol{\rho}_{cl}$.

4.4 The Set of Classical States : A Review

As we have already seen, in the space of Hermitian matrices \mathcal{V} , the set of all density matrices formed a convex body \mathcal{D} . All pure points of this body are actually pure density matrices or projectors which represent pure states. Spin coherent states form a subset of these pure states. We have also defined classical states as those states that can be represented as a convex sum of these coherent states, therefore convex hull of these spin coherent states formed another convex body \mathcal{Q}_{cl} , which is contained in \mathcal{D} . To study the geometry of this body for $N = 3$ is our task in this thesis.

All pure points of \mathcal{Q}_{cl} represent pure coherent states and using magical basis we can represent such pure states by their corresponding $\hat{\mathbf{z}}$ vectors. This $\hat{\mathbf{z}}$ vector—which is perpendicular to both $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ that constitute the state vector, as shown in Eq. (4.3), where $\sigma = \frac{\pi}{4}$ for pure coherent states— together with $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ form an orthonormal triad.

For spin-1 systems, \mathcal{Q}_{cl} is an 8-dimensional body. In the 3rd chapter I promised you to show that how one can see this. Using magical basis this is trivial. First, lets take an example of spin-0 states, we can ask what will be the dimension of the convex body formed by the convex hull of spin-0 states. To answer this question, notice that in magical basis we represent spin-0 states by real vectors. This means their corresponding density matrices will be real symmetric 3×3 matrices with unit trace. All such matrices can be written by using five independent variables and hence we can conclude that all spin-0 states form a 5-dimensional convex body in \mathcal{D} . We can use same procedure for spin coherent states, however notice that in magical basis these states are represented by complex vectors and in general there is no way of writing them as real vectors, therefore their corresponding density matrix will be complex Hermitian matrices with unit trace. Such 3×3 matrices can be written by using 8 real variables, thus the set \mathcal{Q}_{cl} is an 8-dimensional convex body.

Chapter 5

Classicality of Spin States

Our main task in this thesis is to study the geometry of the set of all classical states for spin-1 systems. For this study we have developed the necessary background in the first four chapters and now, in the rest of the chapters we will explore this geometry.

We know from Sec. 3.4, that a state is called classical state if it is in the convex hull of the spin coherent states. Moreover, as any state of a quantum system can be described by a density matrix, therefore, we defined the set of all classical states as a set of all density matrices (ρ_{cl}) which represent these states. As the set ρ_{cl} is a convex body contained in a much bigger convex body of the set of density matrices (\mathcal{D}) —whose each point represents a density matrix— therefore to study its geometry it becomes necessary that we can recognize when a density matrix represents a classical state. To do this, we will follow the line of Giraud et al [4] and will introduce the Glauber-Sudarshan P-representation [6, 12] for the spin coherent states in this chapter. Using the fact that the projectors of coherent states form an informationally complete basis, in this representation we actually expand a density matrix as a sum of these projectors and when in this expansion all coefficients are positive, we say that the decomposed density matrix represents a classical state. We will also discuss a more direct criterion due to Giraud et al, to find out whether a given density matrix represents a classical state or not.

First of all we will define the Glauber-Sudarshan P-representation in Sec. 5.1, then we will see how one can decompose a density matrix into projectors of coherent states in Sec. 5.2, this decomposition will show us how a density matrix of a classical state will look like. Then in Sec. 5.3 we derive the Giraud's Z-criterion for P-representability of a density matrix [4]. In the last Sec. 5.4 we will discuss the rank of a density matrix as a point in the convex set ρ_{cl} , for spin-1 system. In this chapter our discussion is similar to Giraud et al [4], however it is much simpler because of the use of

magical basis.

5.1 The P-Representation

Like coherent states of other systems, spin coherent states also form an over-complete basis in the Hilbert space. This means, we can write any Hilbert space vector in terms of these coherent states. However this all does not mean that we can also write a density matrix in terms of these states, because a density matrix resides in a different space, which in general has much higher dimensionality than the corresponding Hilbert space. For example in our case, when $N = 3$, our Hilbert space has 3 complex or 6 real dimensions whereas the set all density matrices \mathcal{D} is an 8-dimensional body. Fortunately the set of spin coherent states is also informationally complete, which means these states can also provide us sufficient numbers of projectors, that can be used to expand any density matrix. Therefore any density matrix, when expanded in terms of these projectors, can be written as

$$\rho = \int d\alpha P(\alpha) |\alpha\rangle\langle\alpha| \quad (5.1)$$

Where $|\alpha\rangle$ represent coherent states and P-function $P(\alpha)$ is real and normalized as

$$\text{Tr } \rho = \int d\alpha P(\alpha) = 1 \quad (5.2)$$

For spin-1 system, as discuss in chapter 2, we need at most $N^2 = (3)^2 = 9$ coherent states. Therefore we can write Eq. (5.1) for spin-1 systems as

$$\rho = \sum_{i=1}^9 p_i |\alpha_i\rangle\langle\alpha_i| \quad \text{where} \quad \sum_{i=1}^9 p_i = 1 \quad (5.3)$$

This decomposition of a density matrix in terms of projectors of coherent states is called *Glauber -Sudarshan P-Representation*.

Now, using this P-representation we can define when a given density matrix represents a classical state. As we have seen in chapter 2 that decomposition of a density matrix is not unique, therefore we can say that if there exist a decomposition of a density matrix in terms of the coherent states¹ —as given in Eq. (5.3)— for which all p_i are non negative then we can regard ρ as a convex sum of pure coherent states. In this case the point represented by this density matrix in the body \mathcal{D} will be in the convex hull of spin coherent states and hence represents a classical state. Here, we follow Giraud, and call such a density matrix as *P-Representable* or *P-Rep* for

¹Here, we need not to say “in terms of the projectors of coherent states”, as it is clear from the context. Whenever, it is clear from the context, I will choose this way.

short. In the next section we will see how such a decomposition looks like for spin-1 systems.

5.2 The Decomposition of a Density Matrix into The Coherent States

In this section first of all we will write the density matrix in a form which we will find useful later. Then, using magical basis we will expand a density matrix in terms of pure coherent states.

As we have seen in chapter 2, a density matrix is a Hermitian matrix with unit trace and positive eigenvalues, therefore we can also write it as

$$\rho = \rho_{Re} + i\rho_{Im} \quad (5.4)$$

where ρ_{Re} and ρ_{Im} are respectively real and imaginary parts of the density matrix. ρ_{Re} is a symmetric matrix with unit trace and ρ_{Im} is an anti-symmetric, traceless matrix. ρ_{Im} can always be expressed using an arbitrary vector \mathbf{u} and our components of angular momentum operator $\hat{\mathbf{L}}$ as

$$\rho_{Im} = -\frac{i}{2} (\mathbf{u} \cdot \hat{\mathbf{L}}) \quad (5.5)$$

We can also write the real part ρ_{Re} as

$$\rho_{Re} = \frac{1}{2} (\mathbf{I} - \mathbf{W}) \quad (5.6)$$

where, \mathbf{I} is 3×3 unit matrix and \mathbf{W} is a 3×3 , symmetric matrix with unit trace. The reason why we introduce \mathbf{W} here, will be clear later. Now using Eq. (5.5) and Eq. (5.6) we can write Eq. (5.4) as

$$\rho = \frac{1}{2} (\mathbf{I} - \mathbf{W} + \mathbf{u} \cdot \hat{\mathbf{L}}) \quad (5.7)$$

or in index notation,

$$\rho_{ab} = \frac{1}{2} (\delta_{ab} - W_{ab} + (\mathbf{u} \cdot \hat{\mathbf{L}})_{ab}) \quad (5.8)$$

Now consider a pure density matrix

$$\rho = |\psi\rangle\langle\psi| \quad (5.9)$$

In magical basis $|\psi\rangle$ can be written as

$$|\psi\rangle = \cos \sigma \hat{\mathbf{x}} + i \sin \sigma \hat{\mathbf{y}} \quad (5.10)$$

Where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are orthonormal vectors in \mathbb{R}^3 . Now, using Eq. (5.10), we can write Eq. (5.9) as

$$\rho_{ab} = \cos^2 \sigma x_a x_b + \sin^2 \sigma y_a y_b - i \sin \sigma \cos \sigma (x_a y_b - y_a x_b)$$

If we consider a vector $\hat{\mathbf{z}}$ perpendicular to both $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ then $x_a y_b - y_a x_b = \sum_c \epsilon_{abc} z_c$ and using Eq. (4.15) we get

$$\rho_{ab} = \cos^2 \sigma x_a x_b + \sin^2 \sigma y_a y_b + \sin \sigma \cos \sigma (\hat{\mathbf{z}} \cdot \hat{\mathbf{L}})_{ab} \quad (5.11)$$

Now, as we have restricted σ as, $0 \leq \sigma \leq \frac{\pi}{4}$, therefore we can consider two special cases here, when $\sigma = 0$, Eq. (5.11) becomes

$$\rho_{ab} = x_a x_b \quad (5.12)$$

As we know that $\sigma = 0$, correspond to spin-0 states therefore we can say that the density matrices which represent spin-0 states will all be real matrices. Now, for a coherent states we know that $\sigma = \frac{\pi}{4}$, in this case Eq. (5.11) becomes

$$\rho_{ab} = \frac{1}{2} \left(x_a x_b + y_a y_b + (\hat{\mathbf{z}} \cdot \hat{\mathbf{L}})_{ab} \right) \quad (5.13)$$

Using completeness relation in \mathbb{R}^3 i.e. $\delta_{ab} = x_a x_b + y_a y_b + z_a z_b$ this can be written as

$$\rho_{ab} = \frac{1}{2} \left(\delta_{ab} - z_a z_b + (\hat{\mathbf{z}} \cdot \hat{\mathbf{L}})_{ab} \right) \quad (5.14)$$

This is a density matrix for a pure coherent state. Now we can compare it with Eq. (5.8), and for a pure coherent state we get

$$\mathbf{W} = z_a z_b \quad \text{and} \quad \mathbf{u} = \hat{\mathbf{z}} \quad (5.15)$$

This justifies why we have written a density matrix as in Eq. (5.7) and introduced \mathbf{W} .

This all is about a pure density matrix. However, as we know that any mixture of density matrices is also a density matrix therefore, we can form a general density matrix in the convex hull of coherent states as

$$\rho = \sum_{k=1}^n p_k |\alpha\rangle \langle \alpha| \quad (5.16)$$

where all $|\alpha\rangle$ represent coherent states, p_k are positive numbers which sum up to 1 and n is the number of density matrices we mixed up. Using Eq. (5.14) this can be written as

$$\rho_{ab} = \frac{1}{2} \left(\delta_{ab} - \sum_{k=1}^n p_k z_a^{(k)} z_b^{(k)} + \left(\sum_{k=1}^n p_k \hat{\mathbf{z}}^{(k)} \cdot \hat{\mathbf{L}} \right)_{ab} \right) \quad (5.17)$$

Comparing it with Eq. (5.8) we get

$$W_{ab} = \sum_{k=1}^n p_k z_a^{(k)} z_b^{(k)} \quad \text{and} \quad \mathbf{u} = \sum_{k=1}^n p_k \hat{\mathbf{z}}^{(k)} \quad (5.18)$$

Therefore any density matrix which represents a classical state can be written as given in Eq. (5.17). Note that the point represented by this density matrix (Eq. 5.17) in the body \mathcal{D} has the rank n .

5.3 The Z-Criterion For Classicality

In this section we will derive a more direct way of finding when a given density matrix represents a classical state or is P-rep. This criterion is proposed by Giraud et al [4].

Using \mathbf{W} and \mathbf{u} as describe in the last section, we can form a matrix \mathbf{Z} given as

$$Z_{ab} = W_{ab} - u_a u_b \quad (5.19)$$

Suppose Eq. (5.18) do have a solution then Eq. (5.19) becomes

$$Z_{ab} = \sum_{ij} p_i z_a^{(i)} z_b^{(j)} \delta_{ij} - \sum_{ij} p_i p_j z_a^{(i)} z_b^{(j)} \quad (5.20)$$

For an arbitrary vector $\mathbf{y} \in \mathbb{R}^3$ we get

$$\mathbf{y}^t \mathbf{Z} \mathbf{y} = \sum_i p_i \left(\mathbf{y} \cdot \hat{\mathbf{z}}^{(i)} \right)^2 - \left(\sum_i p_i \mathbf{y} \cdot \hat{\mathbf{z}}^{(i)} \right)^2 \quad (5.21)$$

Now if we consider $(\mathbf{y} \cdot \hat{\mathbf{z}}^{(i)}) = \lambda^{(i)}$ then this can be written as

$$\mathbf{y}^t \mathbf{Z} \mathbf{y} = \sum_i p_i \left(\lambda^{(i)} \right)^2 - \left(\sum_i p_i \lambda^{(i)} \right)^2 \quad (5.22)$$

As p_i are positive numbers which sum up to 1 therefore we can write it as

$$\mathbf{y}^t \mathbf{Z} \mathbf{y} = \langle \lambda^2 \rangle - \langle \lambda \rangle^2 = \langle (\lambda - \langle \lambda \rangle)^2 \rangle \geq 0 \quad (5.23)$$

Therefore we can conclude that a density matrix is P-rep if and only if Z is non-negative.

5.4 The Rank of a Density Matrix in \mathcal{D}_{cl}

Here, we need to distinguish between the two different concepts referred by the same term *the rank*. In matrix theory, the rank is the number of linearly independent eigenvectors a matrix has. Whereas in convex geometry it is the minimum number of pure points that must be mixed to get a given point as a mixture. Although sometimes both concepts referred to the same number —namely when discussing the body \mathcal{D} , the set of all density matrices— but one should keep in mind that in this work the relevant concept is the later one i.e. the one which we use in convex geometry.

Here we are interested in the rank of a density matrix i.e. how many coherent states do we need, to form any general density matrix in the convex hull of spin coherent states. This number is referred by n in Eq. (5.17). According to *Caratheodory's theorem* —which has been discuss in Sec. 2.5—

for any general density matrix — i.e. any point in the body \mathcal{D} — we only need 9 pure states. However, for the set \mathcal{D}_{cl} which is much smaller than \mathcal{D} , according to Giraud et al [4] the answer is “at most 8” i.e. we need at most 8 pure coherent states to form any density matrix in this convex hull (\mathcal{D}_{cl}). However, we expect that the rank of any density matrix in the convex hull of spin coherent states may have a value much less than this. Hence in the later chapter we will try to improve this answer.

Chapter 6

The Geometry of \mathcal{Q}_{cl}

In this thesis we are representing the space of all $N \times N$ Hermitian matrices by \mathcal{V} . In this space the set of all density matrices forms a convex body \mathcal{D} and the set of all classical states (\mathcal{Q}_{cl}) is a subset of this body. This subset is itself a convex body and our aim here is to explore the geometry of this body for spin-1 systems. Every point of the body \mathcal{D} represents a density matrix and from the knowledge of the chapter 5, we are now able to recognize when a given density matrix belongs to the set \mathcal{Q}_{cl} . Therefore, from this chapter, we can start exploring the geometry of this set.

A possible and simple way to explore this set would be to take a density matrix from the set \mathcal{D} and ask whether it belongs to the set \mathcal{Q}_{cl} or not. To answer this question, we can use the Z-criterion introduced in the last chapter. We will in fact employ this strategy here, however as the set \mathcal{D} is an 8-dimensional body, therefore considering the points or matrices from the whole set \mathcal{D} at once will be a difficult task. Instead we will keep the things simpler in this chapter and only consider 2-dimensional cross-sections of \mathcal{D} , that can be represented by much simpler density matrices. Actually, we will consider only two simple cases here.

As our first case, in Sec. 6.1 we will consider a general diagonal density matrix and see for what choice of the diagonal elements, all point represented by this matrix will belong to the set \mathcal{Q}_{cl} . After this in Sec. 6.2, we will apply this same procedure to a set of points in \mathcal{D} that can be represented by another simple but not diagonal density matrix. In the end we will also see that there is a set of points which is common in both cross-sections, this means that they intersect each other.

6.1 The Simplest Case: Diagonal Matrices in \mathcal{Q}_{cl}

In this section we will consider a general diagonal density matrix and see what restrictions on its elements we should impose, such that all points represented by this matrix in the body \mathcal{D} belong to the set \mathcal{Q}_{cl} .

Some reader here may think that this is the only case I need to consider, because density matrices are Hermitian matrices and like all other Hermitian matrices we can always diagonalize our 3×3 density matrices using $SU(3)$ rotations. However, as explained in the 4th chapter, we are interested here in spin coherent states which are the coherent states of the rotation group $SU(2)$, therefore we will restrict ourselves to only those transformation which transform spin coherent states among themselves. These transformation will precisely be the $SU(2)$ transformations and thus, we cannot diagonalize every density matrix. Therefore, while considering diagonal matrices we are looking only on a subset of \mathcal{D} .

To build such a diagonal density matrix, we will use three orthogonal states which actually represent spin-0 states as shown below

$$|\psi_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad |\psi_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad |\psi_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad (6.1)$$

A general density matrix, formed by the convex sum of three states can be written as

$$\rho = \sum_{i=1}^3 p_i |\psi_i\rangle\langle\psi_i| \quad \text{where} \quad \sum_{i=1}^3 p_i = 1 \quad (6.2)$$

Now, using the projectors of the above states this equation will lead to the matrix

$$\rho = \begin{pmatrix} p_1 & 0 & 0 \\ 0 & p_2 & 0 \\ 0 & 0 & p_3 \end{pmatrix} \quad (6.3)$$

If we compare it with Eq. (5.7) we get

$$\mathbf{W} = \begin{pmatrix} 1-2p_1 & 0 & 0 \\ 0 & 1-2p_2 & 0 \\ 0 & 0 & 1-2p_3 \end{pmatrix} \quad \text{and} \quad \mathbf{u} = 0 \quad (6.4)$$

As $\mathbf{u} = 0$ here, therefore, for a diagonal density matrix the condition for P-rep i.e. $Z \geq 0$ reduces to $W \geq 0$. In the space of Hermitian matrices, the set of all density matrices that can be represented by the matrix given in Eq. (6.3) for all possible values of p_1 , p_2 and p_3 , is a triangle as shown in fig. (6.1). The condition $W \geq 0$ will tell us that only the portion represented by inner triangle in this figure is included in the set \mathcal{Q}_{cl} .

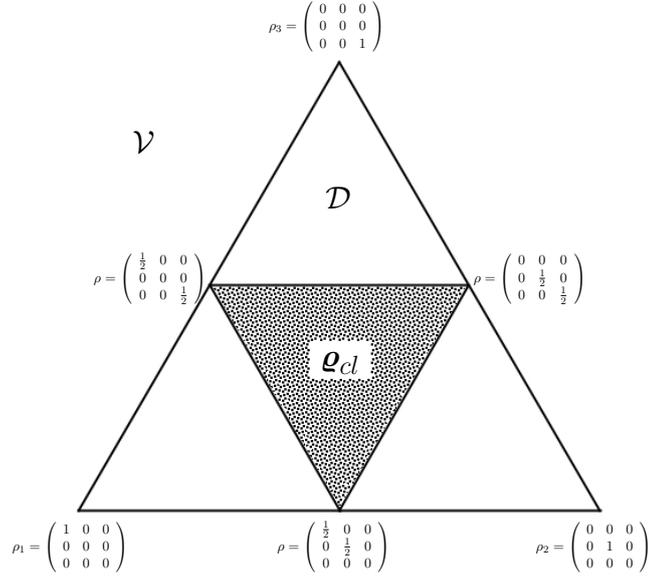


Figure 6.1: 2–dimensional cross-section of \mathcal{D} showing diagonal density matrices in \mathcal{D}_{cl} . The outer triangle shows the set of all diagonal density matrices formed by convex sum of the states given in Eq. (6.1) and inner triangle represents that portion of this set which belongs to set \mathcal{D}_{cl} .

6.2 The Second Simplest Case: More Matrices in \mathcal{D}_{cl}

In this case, we will again form a density matrix by using three orthogonal states, however this time we will take two coherent or spin–1 states and one spin–0 state. The reason why we are taking only three states at once is that only three orthogonal states can be shown on a 2–dimensional plot. This will be much clearer if you imagine a triangle formed by these orthogonal states as a 2–simplex which resides in a 3–dimensional space, as explained in chapter 2.

Now, if we choose our coherent states as spin up and spin down states in z-direction, then the reader can check that their state vectors in the magical basis can be written as

$$|\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \\ 0 \end{pmatrix}, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ -i \\ 0 \end{pmatrix} \quad (6.5)$$

because, both the real vectors $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ of these states vectors — when written

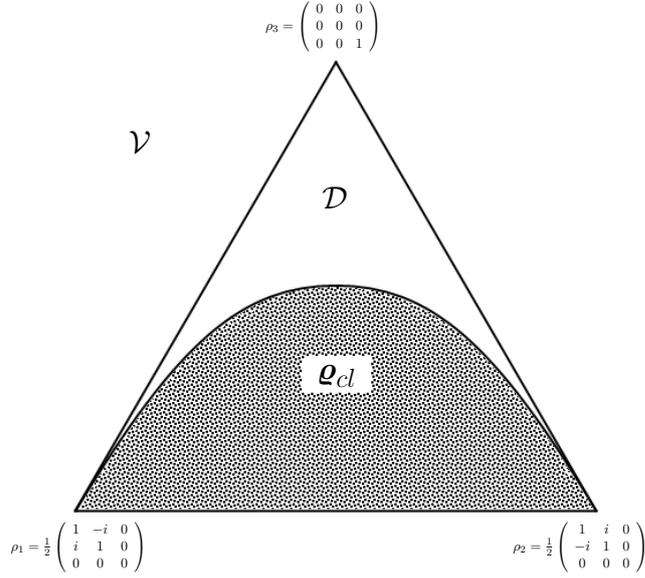


Figure 6.2: Another 2–dimensional cross-section of \mathcal{D} showing more matrices in \mathfrak{Q}_{cl} . The whole triangle represents the set of all points in the set \mathcal{D} that can be represented by the density matrices given in Eq. (6.7) and the shaded region of this figure is that portion of this set which belongs to set \mathfrak{Q}_{cl} .

as in Eq. (4.20)— will be perpendicular to a vector

$$\hat{\mathbf{z}} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (6.6)$$

This $\hat{\mathbf{z}}$ vector is actually the vector which use to refer a coherent state in the formulas like Eq. (5.17). As $\hat{\mathbf{z}}$ is also perpendicular to both $|\psi_1\rangle$ and $|\psi_2\rangle$ and real, therefore, our third state, a spin–0 state, can be $|\psi_3\rangle = \hat{\mathbf{z}}$.

Now, a general density matrix which represents the convex sum of the projectors of these three states, can be written by using Eq. (6.2) again and leads to a ρ given as

$$\rho = \frac{1}{2} \begin{pmatrix} p_1 + p_2 & -i(p_1 - p_2) & 0 \\ i(p_1 - p_2) & p_1 + p_2 & 0 \\ 0 & 0 & 2p_3 \end{pmatrix} \quad (6.7)$$

Comparing it with Eq. (5.7) gives

$$\mathbf{W} = \begin{pmatrix} 1 - (p_1 + p_2) & 0 & 0 \\ 0 & 1 - (p_1 + p_2) & 0 \\ 0 & 0 & 1 - 2p_3 \end{pmatrix} \quad (6.8)$$

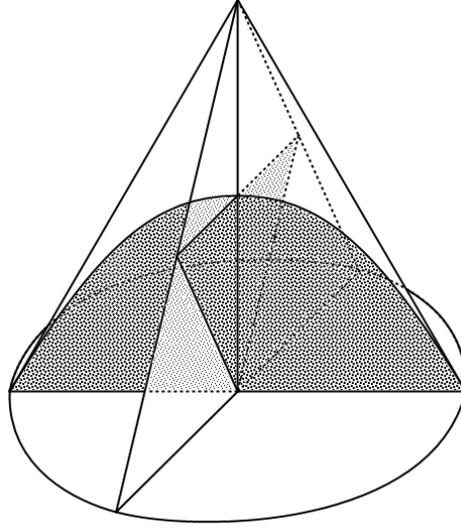


Figure 6.3: The overlap between the two cross-sections.

and

$$\mathbf{u} \cdot \hat{\mathbf{L}} = \begin{pmatrix} 0 & -i(p_1 - p_2) & 0 \\ i(p_1 - p_2) & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (6.9)$$

which implies

$$\mathbf{u} = \begin{pmatrix} 0 \\ 0 \\ p_1 - p_2 \end{pmatrix} \quad (6.10)$$

Therefore, \mathbf{Z} will be

$$\mathbf{Z} = \begin{pmatrix} 1 - (p_1 + p_2) & 0 & 0 \\ 0 & 1 - (p_1 + p_2) & 0 \\ 0 & 0 & 1 - 2p_3 - (p_1 - p_2)^2 \end{pmatrix} \quad (6.11)$$

Now, again we can depict the set of all points which are represented by the matrix ρ —given in Eq. (6.7)—in the space of Hermitian matrices as a 2-dimensional plot. This is shown in fig. (6.2). In this figure, we have also shade off the region of this triangle which is according to \mathbf{Z} -criterion belongs to the set \mathcal{Q}_{cl} . This figure shows that the set \mathcal{Q}_{cl} touches the boundaries of the set \mathcal{D} in case of pure coherent states.

Now, as we have taken a non-coherent state common in both the cross-sections therefore it leads to a set of common points or an overlap in both of these cross-sections. This overlap can be seen in fig. (6.3). The circle in the bottom of this figure is that portion of the space \mathcal{V} which belongs to the set \mathcal{D} . The portion of this circle which belongs to the set \mathcal{Q}_{cl} is just the straight

line which join the two pure coherent states. In the next chapter we will see that this circle is the projection of a Bloch ball which extend in a different dimension (4th dimension, note that the set \mathfrak{q}_{cl} is an 8th dimensional body.) and the straight line which join the two pure coherent states on this ball is the minimal face of \mathfrak{q}_{cl} .

Chapter 7

The Minimal Faces of \mathfrak{e}_{cl}

After sketching the plots of the set of all classical states for the two simplest cases in the last chapter, we will now consider the minimal faces of this set in this chapter instead of considering some more involved cases first.

From chapter 2, we know that a face is a subset of a convex body which is stable under mixture and purification and the minimal face generated by a pair of given pure points is the smallest face which contain these points. We have also seen that the minimal faces of the set of all classical probability distributions, which are simplexes, actually form edges. This fact motivated us to investigate the minimal faces of \mathfrak{e}_{cl} , which is the set of all classical states. Note that if we keep in mind that the minimal faces of the set of all density matrices \mathcal{D} are actually *Bloch Balls* then, it is not obvious at all whether the minimal faces of \mathfrak{e}_{cl} , which is a subset of \mathcal{D} will form edges or not. This is true or not, actually this investigation is the main theme of this chapter.

In the light of the fact that \mathfrak{e}_{cl} is a subset of \mathcal{D} , the definition of the minimal face suggest that all points of a minimal face of \mathfrak{e}_{cl} must be a subset of a minimal face of \mathcal{D} therefore, we can simply start this investigation by asking what portion of the minimal face of the set \mathcal{D} , which is a Bloch Ball, belongs to the set \mathfrak{e}_{cl} . We will consider this question in Sec. 7.1. Then in Sec. 7.2 we will present a general proof which indeed shows that the minimal faces of \mathfrak{e}_{cl} are in fact edges, which in a sense provides additional motivations for calling \mathfrak{e}_{cl} the set of all classical states.

7.1 Portion of the Minimal Faces of \mathcal{D} in \mathfrak{e}_{cl}

In this section, we will see what portion of the minimal faces of the set \mathcal{D} belongs to the set \mathfrak{e}_{cl} for spin-1 systems. In chapter 2, for $N = 2$ we showed that the minimal face of \mathcal{D} is a Bloch Ball. To see that this is also true for $N = 3$, one can form minimal faces of \mathcal{D} by taking two arbitrary states

from this set. These states will always belong to a 2-dimensional subspace of \mathcal{H}^3 . In this subspace one can find two orthonormal states that can be used as basis and, hence all other states in this subspace can be written using them. Now the projector of a general state in this subspace will give a density matrix and the condition of the positivity of its eigenvalues always give a sphere, a Bloch ball. Applying the \mathbf{Z} -criterion on this density matrix will give the portion of the Bloch ball, which belongs to the set \mathcal{Q}_{cl} .

By applying the above procedure we can generate all possible minimal faces in \mathcal{D} . However, instead of considering two arbitrary pure states from \mathcal{D} we will keep the things simple in this section and consider two orthogonal states. Let them be the pure coherent states in z -direction. States vectors of these states are shown in Eq. (6.5). Now a general state in the subspace span by these states will be

$$|\psi\rangle = \alpha|\psi_1\rangle + \beta|\psi_2\rangle \quad (7.1)$$

The projector of this state will lead to the following density matrix.

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + (\alpha\beta^* + \alpha^*\beta) & (\alpha\beta^* - \alpha^*\beta)i - (\alpha^2 - \beta^2)i & 0 \\ (\alpha\beta^* - \alpha^*\beta)i + (\alpha^2 - \beta^2)i & 1 - (\alpha\beta^* + \alpha^*\beta) & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

This can also be parameterized as

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + z & x - iy & 0 \\ x + iy & 1 - z & 0 \\ 0 & 0 & 0 \end{pmatrix} \quad (7.2)$$

where x , y and z are real parameters. Now, the condition for positive eigenvalues will lead to the same equation as Eq. (2.7) with only difference that the diameter of the Bloch ball is 2 units now and therefore we conclude that the minimal faces of the set \mathcal{D} for $N = 3$ are Bloch balls as well. In fact this is true for any N . To see what portion of this minimal face belongs to the set \mathcal{Q}_{cl} we have to calculate \mathbf{Z} . To do this, we need \mathbf{W} and \mathbf{u} which can be obtained by comparing Eq. (7.2) to Eq. (5.7). The reader can check that this comparison gives

$$\mathbf{W} = \begin{pmatrix} -z & -x & 0 \\ -x & z & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \mathbf{u} = \begin{pmatrix} 0 \\ 0 \\ y \end{pmatrix} \quad (7.3)$$

Therefore, using Eq. (5.19) \mathbf{Z} becomes

$$\mathbf{Z} = \begin{pmatrix} -z & -x & 0 \\ -x & z & 0 \\ 0 & 0 & 1 - y^2 \end{pmatrix} \quad (7.4)$$

Now calculating the eigenvalues of this matrix, and applying the \mathbf{Z} -criterion i.e. $\mathbf{Z} \geq 0$ gives

$$1 - y^2 \geq 0 \quad \text{and} \quad z = x = 0 \quad (7.5)$$

To arrive at this result one should also keep in mind that values of x , y and z are restricted already by Eq. (2.7) with the only difference that the diameter of the Bloch ball is 2 units now. Now we can ask what portion of the Bloch ball is represented by the condition of Eq. (7.5). Yes! This represents the diameter of the Bloch Ball on y -axis, which connects the projectors of our pure coherent states¹ $|\psi_1\rangle$ and $|\psi_2\rangle$. You can also recognize this line as the base of the triangle shown in fig. (6.2) which connect projectors of our states $|\psi_1\rangle$ and $|\psi_2\rangle$. As this is the only portion of the Bloch ball which belongs to the set \mathfrak{e}_{cl} , therefore we can conclude that in this case the minimal face of \mathfrak{e}_{cl} is actually an edge. In the next section we will prove this assertion in general.

7.2 Minimal Faces of \mathfrak{e}_{cl} : A General Proof

Concluding from the discussion of the last section we can say that some of the pure points of the body \mathcal{D} are pure coherent states, these states lie on the boundaries of this body and belong to its minimal faces which, as we have seen, are actually Bloch balls. From the last section we also know that if the coherent states on a Bloch ball are orthogonal then the portion of this Bloch ball, that belongs to the set \mathfrak{e}_{cl} , form an edge which joins these two pure coherent states. Therefore, as it is also seen in fig. (6.2), in this case the set \mathfrak{e}_{cl} touches the boundaries of \mathcal{D} , however, this is true in general for all pure coherent states, because these states are just a subset of the pure points of \mathcal{D} which all lie on the boundaries.

Now, to see that the minimal faces of the set \mathfrak{e}_{cl} for every pair of pure points are edges we can look at the different Bloch balls and try to find a ball which contains more than two coherent states, because if a Bloch ball only contains two coherent states —orthogonal or not— then the convex hull of these coherent states will always be a straight line segment which joins these two states and hence will always be an edge. Whereas, if we can find a third coherent state on a Bloch ball which already contains two coherent states, then the convex hull of all of these coherent states will not be an edge and the statement that “The minimal faces of the set \mathfrak{e}_{cl} are in general edges.” will not be true.

¹you might think that this should be the z -axis not the y -axis in order that it connects the projectors of the pure coherent states in z -direction. This ambiguity is produced because the way we parametrized Eq. (7.2) and if we exchange y and z in this equation we will get $1 - z^2 \geq 0$ as the relevant condition.

Now, to prove that “The minimal faces of the set \mathfrak{q}_{cl} are in general edges.” we only need to show that there is no Bloch ball in the set \mathcal{D} or no 2–dimensional sub-space (\mathcal{H}^2) of the space \mathcal{H}^3 which contains three coherent states. If we can prove this, then it will mean that any Bloch ball will contain at most two coherent states and these can always be joined to get an edge as minimal face.

To start this proof we need three pure coherent states and we can always make them lie on a latitude circle. Then the three $\hat{\mathbf{z}}$ vectors corresponding to these states will be

$$\hat{\mathbf{z}}^{(1)} = \begin{pmatrix} \sin \theta \\ 0 \\ \cos \theta \end{pmatrix}, \quad \hat{\mathbf{z}}^{(2)} = \begin{pmatrix} \sin \theta \cos \phi_1 \\ \sin \theta \sin \phi_1 \\ \cos \theta \end{pmatrix}, \quad \hat{\mathbf{z}}^{(3)} = \begin{pmatrix} \sin \theta \cos \phi_2 \\ \sin \theta \sin \phi_2 \\ \cos \theta \end{pmatrix} \quad (7.6)$$

and the states vectors associated with these $\hat{\mathbf{z}}$ vectors will be

$$|\psi_1\rangle = \begin{pmatrix} -\cos \theta \\ -i \\ \sin \theta \end{pmatrix} \quad |\psi_2\rangle = \begin{pmatrix} -\cos \theta \cos \phi_1 - i \sin \phi_1 \\ \cos \theta \sin \phi_1 - i \cos \phi_1 \\ \sin \theta \end{pmatrix} \quad (7.7)$$

$$|\psi_3\rangle = \begin{pmatrix} -\cos \theta \cos \phi_2 - i \sin \phi_2 \\ \cos \theta \sin \phi_2 - i \cos \phi_2 \\ \sin \theta \end{pmatrix}$$

To prove that these vectors are linearly independent and hence does not lie on a sub-space (\mathcal{H}^2) of \mathcal{H}^3 , we can evaluate the determinant, formed by these vector, given as

$$\begin{vmatrix} -\cos \theta \cos \phi_2 - i \sin \phi_2 & -\cos \theta \cos \phi_1 - i \sin \phi_1 & -\cos \theta \\ \cos \theta \sin \phi_2 - i \cos \phi_2 & \cos \theta \sin \phi_1 - i \cos \phi_1 & -i \\ \sin \theta & \sin \theta & \sin \theta \end{vmatrix} \quad (7.8)$$

Evaluating this and equating it to zero gives

$$(\sin \phi_1 - \sin \phi_2 - \sin(\phi_1 - \phi_2)) (\cos^2 \theta - 1) = 0 \quad (7.9)$$

This equation has only trivial solutions like $\theta = 0$ or $\phi_1 = \phi_2$ etc. which shows that these three vectors are in fact linearly independent and hence does not lie on any sub-space (\mathcal{H}^2) of \mathcal{H}^3 . Therefore minimal faces of \mathfrak{q}_{cl} are, in general, actually edges.

In short, \mathfrak{q}_{cl} being a convex hull of coherent states—which are supposed to be the most classical states—we expect that this set may have some resemblance with the set of all classical probability distributions, which are

simplexes and have edges as their minimal faces. In this chapter, we have seen that these resemblances are actually present and both sets have edges as their minimal faces, this is a remarkable fact.

Chapter 8

Rank of States in \mathcal{Q}_{cl}

In the 5th chapter, we have seen how one can decompose any density matrix in the convex hull of spin coherent states into a convex sum of n projectors of the coherent states. Such a decomposition is shown in Eq. (5.17), here, n is called the rank¹ of this density matrix ρ . In this chapter, we will investigate what the maximum rank is for all of the states in the convex body \mathcal{Q}_{cl} .

As we have seen in chapter 5, Giraud et al [4] have also considered this question and actually proved that the answer is at most 8 in this case, however, using Wootters' work [14]—which is, in fact, about entanglement of qubits— we will conclude that the maximum rank of any state in \mathcal{Q}_{cl} is actually 4 i.e. any density matrix in the set \mathcal{Q}_{cl} can be written as a convex sum of the projectors of only 4 coherent states.

Before discussing this, here, we will first give some supportive proofs for this claim. We will give two proofs before discussing Wootters' work. In Sec. 8.1, we will prove that all states of rank three or less will lie on the boundaries of the set \mathcal{Q}_{cl} . Then in Sec. 8.2, we will show that all states which have rank 4, are actually lie inside the body \mathcal{Q}_{cl} . In the last Sec. 8.3, using Wootters work [14] we will conclude that the maximum rank will be 4 for any state which belongs to \mathcal{Q}_{cl} and we also discuss the method which lead us to such a set of four states.

8.1 States of Rank Three or Less

Here, our claim is, “*All states which have rank three or less lie on the boundaries of the set \mathcal{Q}_{cl}* ”. To prove this, we will take three coherent states, which will be represented by their corresponding $\hat{\mathbf{z}}$ vectors, then we will calculate \mathbf{u} and \mathbf{W} using Eq. (5.18). Then we can use Z-criterion to see whether these states lie on the boundaries or inside the body \mathcal{Q}_{cl} .

¹in the convex geometrical sense.

First of all, we need three coherent states. If we note the fact that we can always make them lie on the same latitude circle on a sphere as we did in chapter 7, then again the $\hat{\mathbf{z}}$ vectors corresponding to these states will be same as given in Eq. (7.6), with states vectors shown in Eq. (7.7). A general density matrix that can be decomposed into these three states can be written by mixing the projectors of these states using weights p_1, p_2 and p_3 . Note that here,

$$p_1 + p_2 + p_3 = 1 \quad (8.1)$$

As, we are interested to calculate \mathbf{Z} only, therefore, instead of calculating density matrix, we can directly calculate \mathbf{u} using Eq. (5.18), this will be

$$\mathbf{u} = \begin{pmatrix} \sin \theta (p_1 + p_2 \cos \phi_1 + p_3 \cos \phi_2) \\ \sin \theta (p_2 \sin \phi_1 + p_3 \sin \phi_2) \\ \cos \theta \end{pmatrix} \quad (8.2)$$

and one can also calculate \mathbf{W} using formula given in Eq. (5.18), this will be

$$W = \begin{bmatrix} S_\theta^2(p_1 + p_2 C_{\phi_1}^2 + p_3 C_{\phi_2}^2) & S_\theta^2(p_2 C_{\phi_1} S_{\phi_1} + p_3 C_{\phi_2} S_{\phi_2}) & S_\theta C_\theta (p_1 + p_2 C_{\phi_1} + p_3 C_{\phi_2}) \\ S_\theta^2(p_2 C_{\phi_1} S_{\phi_1} + p_3 C_{\phi_2} S_{\phi_2}) & S_\theta^2(p_2 S_{\phi_1}^2 + p_3 S_{\phi_2}^2) & S_\theta C_\theta (p_2 S_{\phi_1} + p_3 S_{\phi_2}) \\ S_\theta C_\theta (p_1 + p_2 C_{\phi_1} + p_3 C_{\phi_2}) & S_\theta C_\theta (p_2 S_{\phi_1} + p_3 S_{\phi_2}) & C_\theta^2 \end{bmatrix} \quad (8.3)$$

here, we represent sin and cos by S and C and subscripts denote the arguments of these functions. Now, \mathbf{Z} is given by

$$Z_{ij} = W_{ij} - u_i u_j \quad (8.4)$$

Using \mathbf{u} and \mathbf{W} one can easily calculate the matrix \mathbf{Z} . The reader can check that the determinant of this \mathbf{Z} will be

$$|\mathbf{Z}| = p_1 p_2 p_3 \sin^4 \theta \cos^2 \theta (\cos \phi_1 - 1) (\cos \phi_2 - 1) (\cos \phi_1 \cos \phi_2 + \sin \phi_1 \sin \phi_2 - 1) (1 - p_1 - p_2 - p_3) \quad (8.5)$$

This is identically zero, because $p_1 + p_2 + p_3 = 1$ for any values of p_1, p_2 and p_3 . Now according to Z-criterion, any density matrix that belongs to \mathfrak{q}_{cl} must have $Z \geq 0$, i.e. we are inside the body of \mathfrak{q}_{cl} if $Z > 0$ and $Z = 0$ represent the boundaries of the set \mathfrak{q}_{cl} . As in this case $Z = 0$, therefore we can conclude that all states with rank three lies on the boundaries.

8.2 States of Rank Four

Here, our claim is “All states which have rank 4 will lie inside the boundaries of \mathfrak{q}_{cl} .” In the light of the discussion of the last section, to prove this we only need to show that in this case $Z \neq 0$, and equality holds for only trivial

cases, meaning only when some of these four states overlap or have zero weight in the convex sum.

To prove this, we need to consider four coherent states. Again as before, we can make three of these four states to lie on a latitude circle then the $\hat{\mathbf{z}}$ vectors of these states can be written as

$$\begin{aligned} \hat{\mathbf{z}}^{(1)} &= \begin{pmatrix} \sin \theta_1 \\ 0 \\ \cos \theta_1 \end{pmatrix}, & \hat{\mathbf{z}}^{(2)} &= \begin{pmatrix} \sin \theta_1 \cos \phi_1 \\ \sin \theta_1 \sin \phi_1 \\ \cos \theta_1 \end{pmatrix} \\ \hat{\mathbf{z}}^{(3)} &= \begin{pmatrix} \sin \theta_1 \cos \phi_2 \\ \sin \theta_1 \sin \phi_2 \\ \cos \theta_1 \end{pmatrix}, & \hat{\mathbf{z}}^{(4)} &= \begin{pmatrix} \sin \theta_2 \cos \phi_3 \\ \sin \theta_2 \sin \phi_3 \\ \cos \theta_2 \end{pmatrix} \end{aligned} \quad (8.6)$$

Now, we can mix these states using weights p_1, p_2, p_3 and p_4 such that

$$p_1 + p_2 + p_3 + p_4 = 1 \quad (8.7)$$

then using Eq. (5.18), we can write \mathbf{u} as

$$\mathbf{u} = \begin{pmatrix} \sin \theta_1 (p_1 + p_2 \cos \phi_1 + p_3 \cos \phi_2) + p_4 \sin \theta_2 \cos \phi_3 \\ \sin \theta_1 (p_2 \sin \phi_1 + p_3 \sin \phi_2) + p_4 \sin \theta_2 \sin \phi_3 \\ \cos \theta_1 (p_1 + p_2 + p_3) + p_4 \cos \theta_2 \end{pmatrix} \quad (8.8)$$

One can also calculate \mathbf{W} using Eq. (5.18) and then the matrix \mathbf{Z} can also be calculated using Eq. (8.4). All of these calculations can be performed easily on Maple. The reader can check that the determinant of this matrix will \mathbf{Z} be

$$|\mathbf{Z}| = 2 p_1 p_2 p_3 p_4 \sin^4 \theta_1 (\cos \phi_1 - 1) (\cos \phi_2 - 1) (\cos \theta_1 - \cos \theta_2)^2 (1 - \cos(\phi_1 - \phi_2)) \quad (8.9)$$

This does not identically vanish, meaning that there are some states in the interior of \mathcal{Q}_{cl} which have rank 4. Now, if we analyze the determinant of \mathbf{Z} then it reveals that all the factors here indicate that they are zero only when either the weight for a particular state is zero or if two or more states overlap, which in any case leads to trivial solutions. Thus we can conclude that all states with rank 4 must lie inside the body of \mathcal{Q}_{cl} .

8.3 Finding the Four States

Giraud et al [4] prove that any state belonging to \mathcal{Q}_{cl} can have a maximum rank of 8. However, in the last two section we see that no states with

rank 4 lie at the boundaries of the set \mathfrak{Q}_{cl} , this fact together with an easily established fact that the totally mixed density matrix has rank four give us slight indication that the maximum rank of a state inside \mathfrak{Q}_{cl} would be 4. This is in fact true and there exists a proof due to Wootters [14]. In his work, one can also find a criterion for P-rep. Wootters' criterion is more difficult and tedious to deal with than Giraud's Z-Criterion [4], but it is more powerful in the sense that it deals with other things as well. Actually Wootters deals with a different problem, he is interested in the entanglement of two qubits and dealing with the group $SO(4) \sim SU(2) \times SU(2)$ and it turns out that the problem we are interested in, is a special case of his problem.

As Wootters' criterion for P-rep is more difficult to use in our case, therefore, here we will only show that the maximum rank of any state in \mathfrak{Q}_{cl} is indeed 4 and how one can find these states. Let's see how one can find these four coherent states for a given density matrix ρ .

To do this, first of all find out all eigenvectors $|e_i\rangle$ of ρ with non-zero eigenvalues, then

$$\rho = \sum_{i=1}^N \zeta_i |e_i\rangle \langle e_i| \quad (8.10)$$

where ζ_i are the eigenvalues of ρ and $N = 3$, in our case. Now sub-normalize these eigenvectors such that

$$|v_i\rangle = \sqrt{\zeta_i} |e_i\rangle \quad \Rightarrow \quad \langle v_i | \tilde{v}_i \rangle = \zeta_i \quad (8.11)$$

where \tilde{v} represent complex conjugation of a state vector in magical basis. Then ρ becomes

$$\rho = \sum_{i=1}^N |v_i\rangle \langle v_i| \quad (8.12)$$

Now according to Schrödinger mixture theorem, described in the chapter 2, any legitimate decomposition of ρ can be written as

$$\rho = \sum_{i=1}^m |w_i\rangle \langle w_i| \quad (8.13)$$

such that

$$|w_i\rangle = \sum_{j=1}^N U_{ij}^* |v_j\rangle \quad (8.14)$$

Here, m can be greater than N and $*$ represent complex conjugation which is introduced for later convenience. Note also that, as described in the 2nd chapter, U is not a Hilbert space operator.

Now, define a new basis $|x_i\rangle$ via unitary matrix \mathbf{U} such that

$$|x_i\rangle = \sum_{j=1}^N U_{ij}^* |v_j\rangle \quad (8.15)$$

then

$$\langle x_i| = \sum_{l=1}^N U_{il} \langle v_l| \quad (8.16)$$

and

$$|\tilde{x}_j\rangle = \sum_{k=1}^N U_{jk} |\tilde{v}_k\rangle \quad (8.17)$$

Hence

$$\langle x_i|\tilde{x}_j\rangle = \sum_{l,k=1}^N U_{il} \langle v_l|\tilde{v}_k\rangle U_{jk} \quad (8.18)$$

where $\langle v_l|\tilde{v}_k\rangle$ is a symmetric but not necessarily Hermitian matrix. If we define

$$\langle v_i|\tilde{v}_j\rangle = \tau_{ij} \quad (8.19)$$

then

$$\langle x_i|\tilde{x}_j\rangle = (U\tau U^T)_{ij} \quad (8.20)$$

and we want it to be

$$\langle x_i|\tilde{x}_j\rangle = \lambda_i \delta_{ij} \quad (8.21)$$

where, λ_i are square root of the eigenvalues of the non-Hermitian matrix $\rho\tilde{\rho}$. This can be achieved, if $(U\tau U^T)_{ij}$ is diagonal. The reader must note that it is a well known fact that for a Hermitian matrix τ_{ij} we can always find a unitary \mathbf{U} which diagonalize τ_{ij} as $(U\tau U^\dagger)_{ij}$, but here our requirement is different. Our τ_{ij} is need not be a Hermitian matrix, moreover we want it be diagonalized by a unitary \mathbf{U} as $(U\tau U^T)_{ij}$. However, it is true that for a symmetric matrix τ_{ij} one can always choose a unitary matrix \mathbf{U} such that $(U\tau U^T)_{ij}$ is diagonal [7]. Moreover, the diagonal elements of $(U\tau U^T)_{ij}$ can be made real and non-negative, in which case they are the square root of the eigenvalue of $\tau\tau^*$. Now, if we note that $\langle v_i|\tilde{v}_j\rangle = \tau_{ij}$ then it is clear that the eigenvalues of $\tau\tau^*$ are same as the eigenvalues of $\rho\tilde{\rho}$, therefore we can achieve desired relation as in Eq. (8.21).

Now the desired four states $|z_i\rangle$ can be calculated using vectors $|x_i\rangle$ as

$$\begin{aligned} |z_1\rangle &= \frac{1}{2} \left(e^{i\theta_1} |x_1\rangle + e^{i\theta_2} |x_2\rangle + e^{i\theta_3} |x_3\rangle \right) \\ |z_2\rangle &= \frac{1}{2} \left(e^{i\theta_1} |x_1\rangle + e^{i\theta_2} |x_2\rangle - e^{i\theta_3} |x_3\rangle \right) \\ |z_3\rangle &= \frac{1}{2} \left(e^{i\theta_1} |x_1\rangle - e^{i\theta_2} |x_2\rangle + e^{i\theta_3} |x_3\rangle \right) \\ |z_4\rangle &= \frac{1}{2} \left(e^{i\theta_1} |x_1\rangle - e^{i\theta_2} |x_2\rangle - e^{i\theta_3} |x_3\rangle \right) \end{aligned} \quad (8.22)$$

where phase factor should be chosen so that

$$\sum_{k=1}^3 e^{2i\theta_k} \lambda_k = 0 \quad (8.23)$$

Such phase factors can always be found when $\lambda_1 \leq \lambda_2 + \lambda_3$, where λ_1 is the greatest eigenvalue among these three. This condition can be fulfilled easily if one tries to think each term in the above sum as a line segments in a complex plane and whenever one can make a triangle with these segments by choosing appropriate angles θ_i then this condition can be fulfilled.

With this method, one not only see that there really exist four states which can be used to write any density matrix in ρ_{cl} in P-rep form but can also find these four states.

Chapter 9

The End

Before ending this thesis, I would like to summarize the main facts and results which we have presented in this work and using these we will see, what conclusions one can draw.

In general, quantum states reveal non-intuitive phenomena and therefore the geometry of these states, which is the geometry of the set of density matrices, is far more complicated than its classical counterpart. However, there exists a set of states called classical states, whose description is much closer to the classical description of the systems. The idea of this thesis is to explore the geometry of this set.

In the first chapter, it is said that the most classical states are known as the coherent states and such states corresponding to spin systems are called spin coherent states. These spin coherent states are the coherent states of the rotation group $SU(2)$ and hence they form a 2-sphere (S^2). Each such state, is a spin up state in a certain direction in the ordinary 3-dimensional space, therefore we can also represent these states by corresponding vectors in that direction.

The convex hull of spin coherent states is the set of all classical states. Although, each spin coherent state corresponds to a unique vector in a real 3-dimensional ordinary space but the convex hull of these states is not a ball. This is because, each point in this ball though represents a unique \mathbf{u} —according to Eq. (5.7)—but not a unique \mathbf{W} . However, each \mathbf{u} and \mathbf{W} correspond to a density matrix which is represented by a unique point in the convex body \mathcal{D} of the set of all density matrices.

For spin-1 systems, the set of all classical states i.e. the convex hull of spin coherent states, form an 8-dimensional convex body \mathcal{Q}_{cl} , which is contained in a much bigger convex body of density matrices \mathcal{D} . All points in the body \mathcal{Q}_{cl} , represent density matrices that are P-rep. One can use the Z-criterion proposed by Giraud et al [4], to see when a given density matrix belongs to the body \mathcal{Q}_{cl} . We also presented two 2-dimensional cross-sections

of this set in two simpler cases. We have also discovered the remarkable fact that the minimal faces of \mathcal{Q}_{cl} are also edges, like the set of classical probability distributions, and this in a sense provides additional motivations for calling \mathcal{Q}_{cl} the set of all classical states.

We also present the proofs that all states of rank three or less which belongs to \mathcal{Q}_{cl} , are lie on the boundaries, moreover all states with rank four lie inside this body. In the end, using Wootters work [14], we concluded that the maximum rank of a state in \mathcal{Q}_{cl} is actually four, and presented the method to find such states.

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