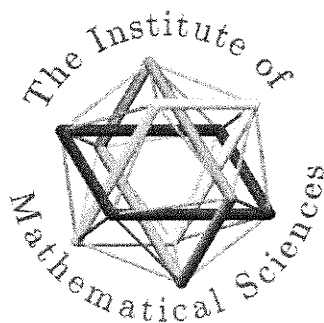


Geometry Of Quantum States

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BONAFIDE CERTIFICATE

Certified that this dissertation titled **GEOMETRY OF QUANTUM STATES** is the bonafide work of **Mr. Sandeep K Goyal** who carried out the project under my supervision.



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Abstract

Understanding the geometry of state space is of fundamental interest in the field of quantum information, in particular to study entanglement. The states of a d dimensional system form a convex set in the $d^2 - 1$ dimensional Euclidean space \mathbf{R}^{d^2-1} . For a two dimensional system this convex set is nothing but a solid unit sphere (Bloch sphere) with centre at the origin. The surface S^2 of this unit sphere consists of all the pure states of the system. Every unitary transformation $U \in SU(2)$ of the Hilbert space corresponds to an associated $SO(3)$ rotation of this space. This kind of correspondence becomes much richer when we go to higher dimension. For example, in the $d = 3$ case the corresponding unitary group is the eight parameter group $SU(3)$ whereas the rotation group in \mathbf{R}^8 is the 28 parameter group $SO(8)$. Therefore, not every point on or inside the sphere S^7 in \mathbf{R}^8 will correspond to a state of the system. So, not every rotation in \mathbf{R}^8 will correspond to a valid unitary transformation of the 3 dimensional Hilbert space. This gives us a fairly complex convex object as the set of all states.

In order to gain insight into the structure of this state space, we study its two dimensional and three dimensional cross-sections. In particular, we describe in detail the discrete symmetries of a non-trivial 3-section of the convex set of states (density matrices) for three dimensional systems. This group turns out to be the same as that of a tetrahedron.

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Chapter 1

Introduction

1.1 Quantum Systems

“ *A quantum system is a useful abstraction, which frequently appears in the literature, but does not exist in nature.*” Asher Peres.

State of a quantum system is an important concept in quantum mechanics. This provides us the full ‘available’ information regarding the system. A state is characterised by the probabilities of the various outcomes of every conceivable experiment.

In principle we can assign a state to any individual particle. But assigning state to an individual does not make any sense, because there is no way of verifying the claims. And unless there is a room for falsification, no theory can be accepted. So one can say that ‘in practice’ the state is a statistical property.

If we have every possible information about the system (as permitted by the framework of the theory), then the system is said to be in a *pure state*. Ignorance about the state of quantum system costs us the lack of full information about the system. Then we say the system is in a *mixed state*.

In quantum theory a pure state of a system is represented by a vector $|\psi\rangle$ in a *Hilbert Space* \mathcal{H} characteristic of the given system. It is almost impossible in Nature to find pure states. Because every system interacts with its surrounding, so only the entire universe can have pure state for all times. The systems prepared in lab are the exceptions, for times immediately after preparation. Interaction with the surrounding introduces unknown and uncontrollable phases in the state, and increases lack of information. This gives rise to mixed states.

One cannot represent a mixed state by a state vector in Hilbert Space. In 1932 *J.von Neumann* gave a method of representing any mixed state by a corresponding positive operator which we call *density matrix* and denote by ρ . This operator satisfies the following three defining conditions:

- $\rho \geq 0$ Positivity,
- $\rho^\dagger = \rho$ Hermiticity,

- $\text{Tr}(\rho) = 1$ Normalisation.

Any and every operator meeting these three requirements is a valid density operator. These conditions have important implications for the family of all possible density matrices. We shall refer to this family as the ‘state space’. We mention a few of these implications:

- The positivity condition implies convexity of the state space: if ρ_1 and ρ_2 are density matrices of a quantum system, then

$$\rho = p\rho_1 + (1 - p)\rho_2$$

is again a density matrix of the system, for all $p \in [0, 1]$.

- Positivity and Trace condition together imply that the spectrum of any density matrix is a valid probability distribution, and
- The trace condition implies that the set of density matrices, or state space, is a bounded set.

Now we explore these implications in some more detail.

1.2 Convexity Property Of Density Matrix

“What picture does one see, looking at a physical theory from a distance, so that the detail disappears? Since quantum mechanics is a statistical theory, the most universal picture which remains after the details are forgotten is that of a convex set.” Bogdon Mielnik.

We always use the word state space but states (density matrices) do not form a linear space because of positivity: General linear combinations of two or more density matrices need not be a density matrix. But density matrices form a convex set. This means that any convex combination, i.e, linear combination with positive coefficients adding to unity, of two or more density matrices will always be a density matrix. This last requirement of the coefficients adding to unity arises because we want the trace to be preserved. The density matrices which cannot be written as convex combination of other density matrices are called *extremal states*. Any state can be written as the convex combination of pure states, and pure states cannot be written as convex sum of other states, so the pure states are the extremal states. But if we are looking at a convex subset of the state space, then the extremals (of the subset) need not be just pure states!

1.3 Positivity of Density matrices

Density matrices are ‘positive semidefinite’ operators acting on the Hilbert space appropriate for the system. We recall that positivity is the requirement

$$\langle \psi | \rho | \psi \rangle \geq 0, \quad \text{for all } |\psi\rangle \in \mathcal{H}.$$

In other words, all the eigenvalues of density matrix should be greater than or equal to zero. Positivity and trace condition together imply that the set of eigenvalues of a density matrix constitutes a valid probability distribution. No matrix with a negative eigenvalue can be a density matrix.

Positive semidefiniteness of density matrices is very important from the point of view of geometry. It is because of this property that the state space becomes a convex region of all hermitian matrices. Clearly, the boundary surface of the state space is such that all positive semidefinite matrices are inside or on the surface, and all non-positive matrices are outside this closed surface. Further, all density matrices of less than maximal rank are in the interior.

1.4 Density matrix:

Any matrix can be additively split into a multiple of identity (the trace part) and a traceless part. So we can write any density matrix as:

$$\rho = \frac{1}{d}[I + \Lambda],$$

where d is the dimension of the Hilbert space under consideration, I is the identity matrix and Λ is a traceless hermitian matrix. Thus, the density operator is fully described by its traceless part Λ . It may be noted that the number of independent parameters in Λ is equal to the number of independent parameters in ρ . This is so because both matrices are Hermitian, their traces being fixed: in the case of ρ the trace is 1, and in the case of Λ the trace is 0.

Hermitian matrices need d^2 real independent parameters to describe them, and if we fix the trace then we are reducing the number of parameters by one. On the other hand positivity is an inequality. In positivity we are only demanding that all eigenvalues of ρ should be ≥ 0 . This does not reduce the number of independent parameters. Thus we are left with $d^2 - 1$ parameters. That is, the state space is a $(d^2 - 1)$ -dimensional family.

The Λ matrix can be written as a real linear combination of $d^2 - 1$ orthogonal hermitian traceless matrices. These traceless hermitian matrices can be chosen to be the generators of the $SU(d)$ group in its defining representation [10, 11]. So we can write the Λ matrix as:

$$\Lambda = \sum_{i=1}^{d^2-1} r_i \lambda_i,$$

where r_i are real coefficients, and the λ -matrices are the generators of the $SU(d)$ algebra. The latter are orthogonal in the sense that

$$\text{Tr}(\lambda_i \lambda_j) = \delta_{ij}.$$

For the two dimensional case the generators of the algebra are the Pauli matrices. In a following Section we will see how these give rise to the Bloch sphere.

We can represent any density matrix uniquely in this fashion once the basis (λ matrices) is fixed. One can see that the ordered set r_i form a vector in \mathbb{R}^{d^2-1} . So we can conclude that one density matrix will occupy exactly one point in this Euclidean space. The set of density matrices is a compact and convex set. So the region this set occupies in this space will be closed and convex. This is the property which we will explore in our study of the geometry of state space.

1.5 Motivation

In 1976, F. J. Bloore[1] wrote a paper which reads:

“This paper offers a geometrical description of the convex set of states for a spin-1/2 and spin-1 quantum system. The purpose is pedagogical; the descriptions probably have no direct usefulness, but they illustrate aspects of the convexity property of state, which is now an important concept in statistical mechanics.”

Thus the study of the geometry of state space is interesting in its own right. But in recent years the geometry of state space has started acquiring a central position in many contexts. For example in Quantum Information Theory (QIT) we have the pivotal problem of separability: how can we say if a given mixed state of a bipartite or multipartite system is entangled or separable? In this problem geometry of state space can play an important role. The set of density matrices form a convex set, as already noted. Separable states form a subset of the space of density matrices. And the convex combination of two or more separable states is also a separable state, by definition. So among density matrices (which already form a convex set) separable states form a convex subset. So, if we can geometrically characterize this later convex set of separable states in a convenient manner, we will be able to identify whether a given state is entangled or not.

An attempt to solve the problem of separability was initiated by S.L. Braunstein et al.[9] in 1999. They proved that all mixed states of N qubits in a sufficiently small neighbourhood of the maximally mixed state are separable, i.e, we can always find a sphere of nonzero radius around the origin in \mathbb{R}^{d^2-1} , with $d = 2^N$ (for N qubits), in which all states are separable. This result was improved by L. Gurvits and H. Barnum [8] in 2002 by giving the exact bound. They gave the radius $\epsilon = \sqrt{\frac{d}{d-1}}$ for d -dimensional density matrix which is the radius of the largest ball inside the state space. And demonstrated that inside this ball every state is separable.

The above discussion gives a hint of the importance of geometry in some physically interesting problems. We have some more examples. Characterization of positive maps is also a well known problem in QIT. One can relate this problem also to the geometry of state space. There are two recent papers by O. Gühne and N. Lütkenhaus [6, 7] on nonlinear entanglement witnesses. The geometry of separable states plays a central role in this context as well.

Geometry also helps in state determination from experimental data. We can write any density

matrix as:

$$\rho = \frac{1}{N} \left[I + \sum_{i=1}^{N^2-1} \alpha_i \lambda_i \right],$$

where λ_i are traceless, orthogonal, and Hermitian and so they are eligible to be physical observables. The coefficients α_i are their corresponding expectation values.

$$\alpha_i = \langle \rho \lambda_i \rangle = \text{Tr}[\rho \lambda_i].$$

The α_i 's form a $N^2 - 1$ dimensional real vector, or an element of \mathbb{R}^{N^2-1} . Positivity condition on ρ gives restriction on the α_i 's, and thus we get the convex structure of the state space.

All these factors prompt us to study the geometry of state space. The outline of this thesis is as follows. We end this introductory Chapter with a discussion of 2-dimensional Hilbert space and the associated geometry of state space, which turns out to be both simple and beautiful. We get a sphere embedded in \mathbb{R}^3 . This is often called the 'Bloch Sphere'. We discuss in detail in Chapter 2, which constitutes the bulk of the thesis, the 3-dimensional Hilbert space and the associated 8-dimensional state space with the help of 2-sections and 3-sections. There we present one theorem on arbitrary 2-section. We conclude in Chapter 3 with some final remarks.

1.6 Bloch Sphere

The two-dimensional case is the most simple case and gives rise to a very beautiful structure, a solid sphere of unit radius in \mathbb{R}^3 . Diametrically opposite points on the surface of the sphere turn out to be orthogonal pure states.

Let us begin with the pure states. Any vector in the two dimensional Hilbert space has only two complex components, or four real parameters. We restrict our vector to have unit norm, and a common phase factor will not affect our state, so we are left with just two real parameters. Any such vector can be written as:

$$|\psi\rangle = \begin{bmatrix} \cos(\theta/2) \\ \sin(\theta/2)e^{i\varphi} \end{bmatrix}.$$

All values in the range $0 \leq \theta \leq \pi$ and $0 \leq \varphi < 2\pi$ are possible. It is understood that $\varphi = 0$ and $\varphi = 2\pi$ are identified, and that for $\theta = 0, \pi$ all values of φ are identified. The corresponding density matrix is

$$\begin{aligned} \rho \equiv |\psi\rangle\langle\psi| &= \frac{1}{2} \begin{bmatrix} 1 + \cos\theta & \sin\theta \cos\varphi - i \sin\theta \sin\varphi \\ \sin\theta \cos\varphi + i \sin\theta \sin\varphi & 1 - \cos\theta \end{bmatrix} \\ &= \frac{1}{2} (I + \hat{r} \cdot \vec{\sigma}), \end{aligned}$$

where \hat{r} is the unit vector in \mathbb{R}^3 specified by its polar and azimuthal angles (θ, φ) . Thus pure states correspond to points on the surface of the unit sphere S^2 in three dimension. Given a mixed state density matrix ρ , it can always be written as:

$$\rho = \begin{bmatrix} p & \alpha^* \\ \alpha & 1-p \end{bmatrix},$$

where $0 \leq p \leq 1$ is a real number, or, equivalently, as

$$\rho = \frac{1}{2} [I + r_1 \sigma_1 + r_2 \sigma_2 + r_3 \sigma_3],$$

where

$$r_3 = \frac{p - (1 - p)}{2},$$

$$r_1 = 2\text{Re}(\alpha) = \alpha + \alpha^*,$$

$$r_2 = 2\text{Im}(\alpha) = (\alpha - \alpha^*).$$

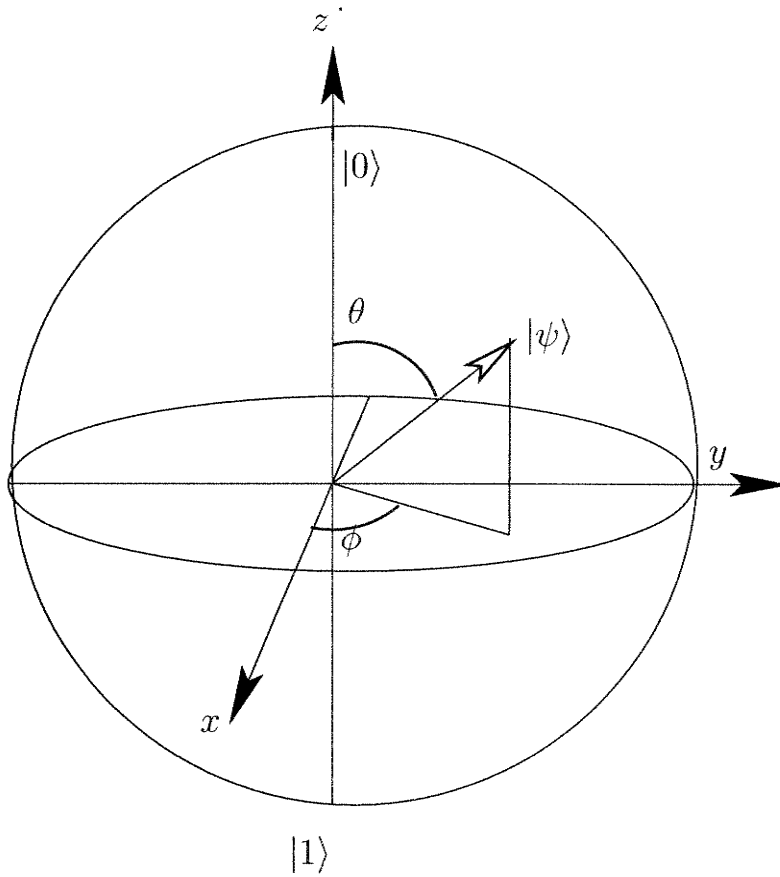


Figure 1.1: Bloch Sphere. Here $|\psi\rangle$ represents a pure state, a unit vector with component $(\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)$ which gives rise to the density matrix ρ . $|0\rangle$ and $|1\rangle$ are the points on the north and south pole res. Being the diametrically opposite points, they represent the orthogonal states.

And the condition for positivity of ρ simply reads $\|\mathbf{r}\|_2^2 = r_1^2 + r_2^2 + r_3^2 \leq 1$, which is the equation for the solid unit sphere in \mathbb{R}^3 .

We may summarize our discussion of pure and mixed states thus: the states of a two-dimensional system, or qubit, can be represented by points on or inside this unit solid sphere: the points on the

surface represent pure states, and points in the interior correspond to mixed states. Diametrically opposite points on the surface correspond to orthogonal pure states, and the point at the origin to the maximally mixed state.

Chapter 2

3-dimensional Hilbert space

The geometry of state space associated with the 3-dimensional Hilbert space is a deceptively simple looking problem in quantum mechanics. However, it is far from being trivial. The difficulty of this problem lies in the structure of the geometry in 8-dimensions. Not much work has been done on this problem. To our knowledge, one of the earliest attempts to address this problem was in 1976 by Bloore [1]. It appears he was possibly not aware of the importance of his own work. However, renewed interest in this problem in recent years has convincingly demonstrated its importance.

The operators acting on 3-dimensional Hilbert space \mathcal{H} (and taking \mathcal{H} into itself) form a 9-dimensional complex vector space. Among these, the positive operators with unit trace represent the state of a physical system. They form an 8-dimensional convex set. And we can always write them as:

$$\rho = \frac{1}{3} [I + \Lambda],$$

where Λ is a traceless Hermitian matrix.

The space of 3×3 traceless Hermitian matrices forms an 8-dimensional real vector space. We can choose an orthogonal basis for this vector space, and write Λ as

$$\Lambda = \sum r_i \lambda_i,$$

where r_i are real numbers such that ρ is positive. To define orthogonality we use the notion of inner product in the vector space of operators. Given two operators A and B , their inner product is defined through

$$\langle A, B \rangle = \text{Tr}[A^\dagger B].$$

This inner product is called *Hilbert-Schmidt* inner product. The norm of an operator follows from this definition:

$$\|A\| = \sqrt{\langle A, A \rangle} = \sqrt{\text{Tr}[A^\dagger A]}.$$

Thus if two operators A, B satisfy $\text{Tr}[A^\dagger B] = 0$, they are said to be orthogonal.

Without loss of generality we can choose the generators of $SU(3)$ algebra in the defining representation as the orthogonal basis for the vector space of traceless matrices. These are

$$\begin{aligned} \lambda_1 &= \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, & \lambda_2 &= \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, & \lambda_3 &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \\ \lambda_4 &= \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, & \lambda_5 &= \begin{bmatrix} 0 & 0 & -i \\ 0 & 0 & 0 \\ i & 0 & 0 \end{bmatrix}, & \lambda_6 &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \\ \lambda_7 &= \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{bmatrix}, & \lambda_8 &= \frac{1}{\sqrt{3}} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -2 \end{bmatrix}. \end{aligned}$$

We will refer to these matrices as the λ -matrices. They are orthogonal and have norm $\sqrt{2}$: $\text{Tr}(\lambda_i \lambda_j) = 2\delta_{ij}$. Thus the state space is a convex set embedded in \mathbb{R}^8 and the boundary (upper layer) of this 8-dimensional object is 7 dimensional. We now attempt to find the structure of this 8-dimensional object.

This problem can be approached in multiple ways. One can consider different slices of this 8-dimensional object and study them. These slices can range from 1-dimensional to 7-dimensional. We will discuss the 1-dimensional, 2-dimensional, and 3-dimensional cases. Because of the large number of sections of different dimensions, it is customary to consider only standard sections. To get a t -dimensional standard section, we fix the orthogonal basis and allow t among the eight r_i 's vary and set the other r_i 's to zero. We will discuss these standard sections in the following sections in great detail. But before going into those details, let us first find the equations that describe the surface of the 8-dimensional state space.

The equation of the surface can be obtained from the positivity requirement on the density matrix. We can write

$$\rho = I + \Lambda$$

(This is not a density matrix, but if we make its trace one by multiplying it by $\frac{1}{3}$ and put the restriction on Λ such that ρ be positive, we will get a density matrix. Overall positive factor cannot affect the positivity of a matrix. So if this matrix is positive then its normalized form will also be positive, and vica versa.) We can diagonalize this matrix ρ . Here I and Λ commute so we can diagonalize them simultaneously. Now if the smallest eigenvalue of Λ is greater than -1 then ρ is positive.

We can write:

$$\Lambda = \frac{1}{\sqrt{2}} \sum_{i=1}^{d^2-1=8} r_i \lambda_i = \frac{1}{\sqrt{2}} \begin{bmatrix} r_3 + \frac{1}{\sqrt{3}}r_8 & r_1 - ir_2 & r_4 - ir_5 \\ r_1 + ir_2 & -r_3 + \frac{1}{\sqrt{3}}r_8 & r_6 - ir_7 \\ r_4 + ir_5 & r_6 + ir_7 & -\frac{2}{\sqrt{3}}r_8 \end{bmatrix}$$

where the factor of $\frac{1}{\sqrt{2}}$ is to normalize the basis operators. Now the eigenvalue equation of Λ matrix is

$$\det \begin{bmatrix} r_3 + \frac{1}{\sqrt{3}}r_8 - \alpha & r_1 - ir_2 & r_4 - ir_5 \\ r_1 + ir_2 & -r_3 + \frac{1}{\sqrt{3}}r_8 - \alpha & r_6 - ir_7 \\ r_4 + ir_5 & r_6 + ir_7 & -\frac{2}{\sqrt{3}}r_8 - \alpha \end{bmatrix} = 0$$

where the solutions of this equation for α will give the eigenvalues. If the rank of ρ is less than 3 then we can see that the state must be on the boundary of the state space, and we are interested only in the boundary of the state space. So we can just substitute $\alpha = -\sqrt{2}$ to make ρ a matrix on the surface:

$$2\sqrt{2} - \sqrt{2}(r_1^2 + r_2^2 + r_3^2 + r_4^2 + r_5^2 + r_6^2 + r_7^2 + r_8^2) + \frac{2r_8}{\sqrt{3}}(r_1^2 + r_2^2 - \frac{r_4^2}{2} - \frac{r_5^2}{2} - \frac{r_6^2}{2} - \frac{r_7^2}{2} + r_3^2 - \frac{r_8^2}{3}) + r_3(r_4^2 + r_5^2 - r_6^2 - r_7^2) + 2(r_1r_4r_6 + r_1r_5r_7 + r_2r_5r_6 - r_2r_4r_7) = 0.$$

While this condition ensures that $I + \Lambda$ is singular, the additional condition

$$\sum_{j=1}^8 r_j^2 \leq 6,$$

ensures that $I + \Lambda$ has no negative eigenvalue. Thus these two conditions together completely specify the boundary of the state space.

2.1 One-dimensional Sections

We begin our analysis with consideration of one-dimensional cross-sections of the 8-dimensional convex body. Imagine a line passing through the centre: $r_j = 0$, $j = 1, 2, \dots, 8$. This line will intersect the surface at two points. Let these points be called *opposite points*. If we assemble all such pairs of points corresponding to all possible lines through the origin, we will obtain, in principle, the boundary surface of the state space.

Now every density matrix can be diagonalized by a unitary transformation, and unitary transformations preserve the norm. If

$$\rho = \frac{1}{3}[I + \Lambda],$$

after diagonalization we will get

$$\rho' = \frac{1}{3}[I + \Lambda'],$$

where Λ' is a real diagonal traceless matrix. Diagonal traceless hermitian matrices themselves form a subspace of dimension $n - 1$ in the real vector space of $n \times n$ hermitian matrices. So Λ' can be written as a real linear combination of the basis of diagonal traceless matrices of this subspace:

$$\Lambda' = \sum_i r_i \lambda_{T_i},$$

where r_i 's are real and λ_{T_i} form a basis for the diagonal traceless subspace. For the 3×3 case, λ_3 and λ_8 constitute the diagonal traceless basis. So

$$\rho' = \frac{1}{3} \left[I + \frac{1}{\sqrt{2}}(r_3 \lambda_3 + r_8 \lambda_8) \right] = \frac{1}{3} \begin{bmatrix} 1 + \frac{1}{\sqrt{2}}r_3 + \frac{1}{\sqrt{6}}r_8 & 0 & 0 \\ 0 & 1 - \frac{1}{\sqrt{2}}r_3 + \frac{1}{\sqrt{6}}r_8 & 0 \\ 0 & 0 & 1 - \frac{\sqrt{2}}{3}r_8 \end{bmatrix}.$$

It is easily seen that positive diagonal matrices of this kind are necessarily convex sums of the three projections $\text{diag}(0, 0, 1)$, $\text{diag}(1, 0, 0)$, and $\text{diag}(0, 1, 0)$, which correspond respectively to the parameter values $(r_3, r_8) = (0, -\sqrt{6})$, $(\pm\frac{3}{\sqrt{2}}, \sqrt{\frac{3}{2}})$, or equivalently to the pure states

$$\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}, \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}.$$

Such positive matrices fill an equilateral triangle in the (r_3, r_8) plane, the vertices being in one-to-one correspondence with the above three pure states or projections.

The 1-sections of the triangle are the only distinct 1-sections of the state space. All others are unitarily equivalent to these 1-sections. While the possible distinct 1-sections are simply characterized in this manner, a corresponding characterization of unitarily inequivalent 2-sections proves to be much more complex.

Now we will exhibit some interesting properties of state space geometry for N dimensional Hilbert Space. In the $(N^2 - 1)$ -dimensional object which represents our convex state space, we can find r_{max} and r_{min} such that every point inside the $(N^2 - 1)$ -dimensional sphere of radius r_{min} represents a valid density matrix, and every point outside the sphere of radius r_{max} represents a non-positive matrix. These spheres will be called in-sphere and out-sphere respectively. By non-positive matrix we mean those matrices which have atleast one negative eigenvalue. [In the shell between these two spheres, some points correspond to positive matrices and some do not. This is precisely where the complexity of the state space is located].

These spheres are very important in some contexts. As we have said, if the system is composite, so that N is not a prime, then if any given density matrix lies inside the in-sphere we can be sure that the state is separable and if the matrix lies outside the out-sphere then it is not a state at all. Any ρ can be written as:

$$\rho = \frac{1}{N} [I + \Lambda]$$

where N is the dimension of the Hilbert space on which ρ acts, and Λ is a Hermitian traceless matrix. Now

$$\text{Tr}[\rho^2] = \frac{1}{N^2} [\text{Tr}(I) + \text{Tr}(\Lambda^2) + 2\text{Tr}(\Lambda)]$$

The requirement that ρ is a state implies that

$$\text{Tr}[\rho^2] \leq 1,$$

and since Λ is traceless, this requirement is equivalent to

$$\frac{1}{N^2} [N + \|\Lambda\|_2^2] \leq 1.$$

Here $\text{Tr}[I] = N$ and $\|\Lambda\|_2^2 = \text{Tr}[\Lambda^2]$ is the square of the Hilbert-Schmidt norm of Λ . Pure states are the farthest points at distance r_{max} from the origin of the state space, because in the case of

pure states the above inequality gets saturated. Pure states satisfy:

$$\text{Tr}[\rho^2] = 1.$$

So

$$\begin{aligned} N + r_{max}^2 &= N^2, \\ r_{max} &= \sqrt{N(N-1)}. \end{aligned}$$

Thus we get the radius of the out-sphere of the generalised 'Bloch sphere'. [The generalized Bloch sphere is not a sphere; it is just the convex state space].

Let us examine the above calculation in some more detail. In the following sections we will represent ρ as:

$$\rho = \frac{1}{N} \left[I + \frac{1}{\sqrt{2}} \sum_i r_i \lambda_i \right]$$

where λ_i are the generators of $SU(N)$ (orthogonal basis for the vectors space of traceless matrices), and $\frac{1}{\sqrt{2}}\lambda_i$ has unit Hilbert Schmidt norm. So

$$\|\Lambda\|_2^2 = \text{Tr}[\Lambda^2] = \text{Tr} \left[\frac{1}{\sqrt{2}} \sum_i r_i \lambda_i \right]^2 = |\mathbf{r}|^2,$$

where $\mathbf{r} \in \mathbb{R}^{N^2-1}$ so from previous calculation we will get $|\mathbf{r}|_{max}^2 = N(N-1)$.

Now let us consider two different density matrices ρ and ρ' . clearly, $\text{Tr}[\rho\rho']$ is positive, since both ρ and ρ' are positive operators:

$$\begin{aligned} \text{Tr}[\rho\rho'] &= \frac{1}{N^2} \left[\text{Tr}(I) + \frac{1}{2} \sum_{i,j} r_i r_j \text{Tr}(\lambda_i \lambda_j) + \frac{1}{\sqrt{2}} \text{Tr} \left(\sum_i r_i \lambda_i + \sum_j r'_j \lambda_j \right) \right] \\ &= \frac{1}{N^2} \left[N + \frac{1}{2} (\mathbf{r} \cdot \mathbf{r}') \text{Tr} \left[\sum_i \lambda_i^2 \right] + \text{Tr}[\text{some trace less part}] \right] \\ &= \frac{1}{N^2} [N + (\mathbf{r} \cdot \mathbf{r}')]. \end{aligned}$$

Since \mathbf{r} and \mathbf{r}' are just two vectors in \mathbb{R}^{N^2-1} , and we can always find a 2-dimensional plane which contains these two vectors. Thus $\mathbf{r} \cdot \mathbf{r}'$ can be written as $|\mathbf{r}||\mathbf{r}'| \cos \theta$, where θ is the angle between \mathbf{r} and \mathbf{r}' in that specific plane. The positivity condition $\text{Tr}(\rho\rho') \geq 0$ thus become

$$N + |\mathbf{r}||\mathbf{r}'| \cos \theta \geq 0.$$

Let us choose ρ to be a pure state so that $|\mathbf{r}| = r_{max} = \sqrt{N(N-1)}$ and thus we get the restriction

$$|\mathbf{r}'| \cos(\theta) \geq -\sqrt{\frac{N}{N-1}}.$$

The positivity condition is reduced to this equation in the \mathbb{R}^{N^2-1} space. That is, this condition must be satisfied by every positive ρ' . For all positive $\cos \theta$ this condition is automatically satisfied. For negative value of $\cos \theta$, we obtain a limit on $|\mathbf{r}'|$. Let us say $\cos \theta = -x$, where x is positive. So

$$|\mathbf{r}'| \leq \frac{1}{x} \sqrt{\frac{N}{N-1}}.$$

Here x can never be more than one and we are interested in only positive x . So the minimum values of $|\mathbf{r}'|$ is when $x = 1$ which is $\sqrt{\frac{N}{N-1}}$. This is the minimum possible value of $|\mathbf{r}'|$, denoted r_{min} . This shows that every point inside the sphere of radius $\sqrt{\frac{N}{N-1}}$ is a valid state. Thus, r_{min} is the radius of the in-sphere of the generalized Bloch sphere.

We are thus presented with two spheres. One is the smallest outer sphere (out-sphere) of radius $r_{max} = \sqrt{N(N-1)}$ such that every state is inside this sphere. And we have another sphere which is the largest inner sphere (in-sphere) of radius $r_{min} = \sqrt{\frac{N}{N-1}}$ such that every point inside it is a state.

Again, consider the equation

$$|\mathbf{r}'| \cos \theta \geq -\sqrt{\frac{N}{N-1}}$$

This reveals a very important property of state space, i.e, if any state is on the out-sphere, the opposite point will be on the in-sphere. This property is one of the most important aspects of the geometry of our state space. This property gives us the maximum distance between two opposite points which is $\sqrt{N(N-1)} + \sqrt{\frac{N}{N-1}}$. Clearly, for 3-Dimensional Hilbert Space the value of r_{max} is $\sqrt{6}$ and $r_{min} = \sqrt{3/2}$.

2.2 Standard 2-dimensional Sections

To define a 2-dimensional arbitrary cross-section we need two independent vectors in \mathbb{R}^8 , which we denote Λ_1, Λ_2 . Using the unitary freedom, we can choose with out loss of generality Λ_1 to be diagonal:

$$\Lambda_1 = \frac{1}{\sqrt{2}} (\cos \theta \lambda_3 + \sin \theta \lambda_8).$$

Then Λ_2 is arbitrary except for the requirement that it needs to be orthogonal to Λ_1 :

$$\Lambda_2 = \frac{1}{\sqrt{2}} \left[\cos \varphi (\sin \theta \lambda_3 - \cos \theta \lambda_8) + \sin \varphi \sum_{j \neq 3, 8} r_j \lambda_j \right]$$

Here j runs over all off-diagonal λ matrices. For a fixed Λ_1 , Λ_2 has 6 independent parameters (φ and five from the r_i 's) and Λ_1 and Λ_2 define the whole family of 2-sections. This shows that unitarily inequivalent 2-sections form a 7-parameter family. Λ_1 and Λ_2 may not commute so we can-not in general diagonalize them simultaneously. That is the origin of the difference between the family of 1-sections and the family of 2-sections in respect of proliferation.

Instead of studying this entire 7-parameter family of 2-sections, we restrict attention to what may be called “standard 2-sections”. Let us clarify what we mean by a standard 2-section. These are the sections obtained by linear combinations of any two λ -matrices. For 8-dimensional object we will thus get ${}^8c_2 = 28$ standard 2-sections. Among these twenty eight 2-sections, it turns out that we only have four distinct type of 2-sections: and each of the twenty eight sections is unitarily equivalent to one of these four types.

The four distinct types of 2-sections may be tabulated as follows, with 12 standing for the (λ_1, λ_2) -plane, 13 for the (λ_1, λ_3) -plane and so on:

<i>Circle</i>	<i>Triangle</i>	<i>Parabola</i>	<i>Ellipse</i>
<i>area = 6.28</i>	<i>area = 7.8</i>	<i>area = 7.5</i>	<i>area = 8.6</i>
12, 13, 23	18	34	48
14, 15, 16	28	35	58
17, 24, 25	38	36	68
26, 27, 45		37	78
46, 47, 56			
57, 67			

Figure 2.1: List of all 2-sections, arranged according to their types. Here 12 stands for the (λ_1, λ_2) section, and 13 for the (λ_1, λ_3) section, and so on.

Circle

Seventeen out of the twenty eight standard 2-sections turn out to be circles of radius $\sqrt{2}$. A list of them are provided in the first column of the above table. Consider, for instance, the 16 section. The corresponding matrix is

$$\rho = \frac{1}{3} \left[I + \frac{1}{\sqrt{2}} (r_1 \lambda_1 + r_6 \lambda_6) \right],$$

$$r_1 \lambda_1 + r_6 \lambda_6 = \begin{bmatrix} 0 & r_1 & 0 \\ r_1 & 0 & r_6 \\ 0 & r_6 & 0 \end{bmatrix}.$$

Clearly, the eigenvalue equation for this Λ matrix is:

$$\alpha(\alpha^2 - r_1^2 - r_6^2) = 0.$$

If and only if α , the eigenvalues of this Λ matrix obeys $\alpha \geq -\sqrt{2}$, our density matrix ρ will be positive. Thus the restriction on (r_1, r_6) is

$$r_1^2 + r_6^2 \leq 2,$$

a disk of radius $\sqrt{2}$. This section have no pure states.

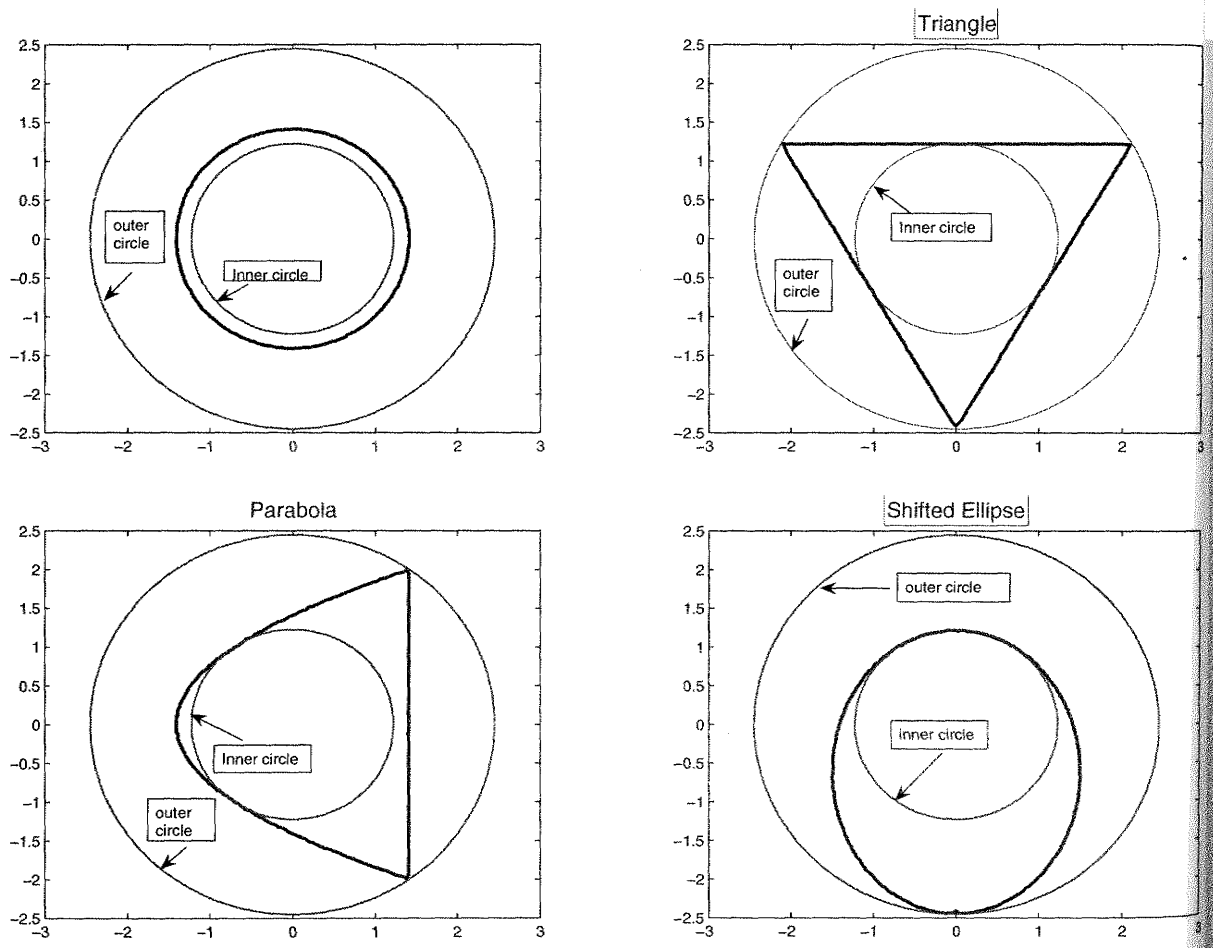


Figure 2.2: In all the diagram we showed the smallest larger circle (outer circle), largest smaller circle (inner circle), and the standard 2-section. First one on the top left is circle with radius $\sqrt{2}$. Top right is triangle. Bottom left is the parabola and the bottom right is Shifted ellipse. The radius of the outer circle is $\sqrt{6}$ and the radius of inner circle is $\sqrt{3/2}$ and the surface of state space will always be in between these two circles.

Triangle

The 2-sections are triangles in the three cases (18), (28), (38). These cases are distinguished from the others by the fact that the λ -matrices involved in each pair, commute with one another:

$$[\lambda_1, \lambda_8] = [\lambda_2, \lambda_8] = [\lambda_3, \lambda_8] = 0.$$

In each case the three vertices corresponds to pure states. The triangle touches the out-sphere at three points and the in-sphere at the corresponding three opposite points, as shown in the figure.

Parabola

In four cases, (34), (35), (36), (37) we obtained as 2-section truncated parabola, i.e, parabola bounded by a straight line. The section has two pure states: these are the intersection points of the parabola with the straight line. The section touches the out-sphere at two points (pure state) and the in-sphere at the corresponding two opposite points.

For the purpose of illustration, consider the case (34). The positivity requirement reads:

$$\det \begin{bmatrix} \sqrt{2} + r_3 & 0 & r_4 \\ 0 & \sqrt{2} - r_3 & 0 \\ r_4 & 0 & \sqrt{2} \end{bmatrix} = 0 = [(\sqrt{2} + r_3)\sqrt{2} - r_4^2](\sqrt{2} - r_3),$$

which is clearly the product of the straight line $r_3 = \sqrt{2}$ and the equation for a shifted parabola.

Ellipse

This one is also an interesting 2-section. This is actually called a shifted ellipse because its centre is not the centre of the state space (origin of \mathbb{R}^8). We get four such cases, namely (48), (58), (68) and (78). These sections have only one pure state, and have the maximum area among all the twenty eight standard 2-sections. The equation of this 2-section can be written by considering, for example, the (48) case. The positivity equation is:

$$\det \begin{bmatrix} \sqrt{2} + \frac{r_8}{\sqrt{3}} & 0 & r_4 \\ 0 & \sqrt{2} + \frac{r_8}{\sqrt{3}} & 0 \\ r_4 & 0 & \sqrt{2} - 2\frac{r_8}{\sqrt{3}} \end{bmatrix} = \left[\left(\sqrt{2} + \frac{r_8}{\sqrt{3}} \right) \left(\sqrt{2} - 2\frac{r_8}{\sqrt{3}} \right) - r_4^2 \right] \left(\sqrt{2} + \frac{r_8}{\sqrt{3}} \right) = 0.$$

This is clearly product of the ellipse

$$\left[\left(\sqrt{2} + \frac{r_8}{\sqrt{3}} \right) \left(\sqrt{2} - 2\frac{r_8}{\sqrt{3}} \right) - r_4^2 \right] = 0$$

and a straight line tangent to the out-sphere.

2.3 Special Cross-Sections

Having discussed standard 2-sections, we now wish to briefly address the issue of cross-sections with minimum and maximum areas.

2.3.1 Minimum area Cross-section

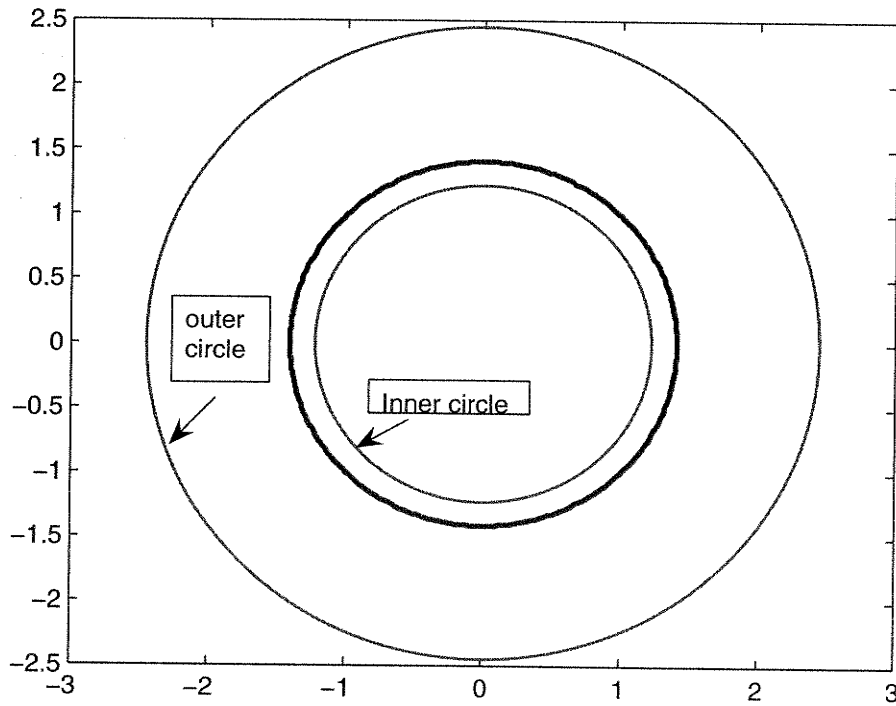


Figure 2.3: Here the bold circle shows the minimum area cross-section and this is the same circle which is also a standard 2-section.

The process of finding the minimum area cross-section is helped by first finding the smallest distance between two opposite points of the state space. Consider a one-dimensional section (line) through the origin. It will intersect the surface of our convex body at two points. These are called *opposite points*, as noted earlier.

As we have already discussed, one-dimensional cross-sections are fully captured by diagonal density matrices, and the associated Λ matrix is a convex combination of (λ_3, λ_8) . We know that such density matrices form a triangle in the (λ_3, λ_8) plane (figure 2.2). The minimum distance between opposite point is easily seen to be $2\sqrt{2}$, it is one of the line segments parallel to a side of the triangle (and passing through the origin).

Incidentally, we have earlier presented a set of circular 2-sections of radius $\sqrt{2}$ among the standard 2-sections. Hence this circular 2-section will be expected to be the section of smallest area. The claim is that this is the minimum area 2-section not only among the standard 2-section, but also among all the seven-parameter family of 2-section. This circular cross section with radius $\sqrt{2}$ plays a very significant role in understanding the geometry of state space, and this turns out to be true in higher dimensions as well.

In the 2-dimensional case, the radius of the Bloch sphere is also $\sqrt{2}$ (due to our normalisation convention), and so any 2-section of the Bloch sphere will qualify to be 'this' minimum area cross-section. In the 3-dimensional case, we have five standard 3-sections which are spherical, and four 4-sections which are also spherical, all of the same radius $\sqrt{2}$ [see Sec. 2.4.1]. Any 2-dimensional cross-section of spherical 3-section or 4-sections will be a circular 2-section. Thus we get infinitely many 2-dimensional circular cross-section with diameter $2\sqrt{2}$.

As we have already proved, if we have a pure state or a point on the out-sphere the corresponding opposite point will be on the in-sphere. A result similar in spirit applies to the smallest area cross-section.

Theorem 1 *If a 2-section crosses the circle of radius $\sqrt{2}$, then it will necessarily cross this circle also at the diametrically opposite point.*

Proof: Any density operator in the 2-plane can be written as

$$\rho = \frac{1}{3} [I + r_1 X_1 + r_2 X_2]$$

where X_1 and X_2 are two real orthogonal traceless matrices: $\text{tr}(X_i X_j) = \delta_{ij}$.

If ρ is on the boundary of the 2-section, it will have rank ≤ 2 . So among three eigenvalues of operator $r_1 X_1 + r_2 X_2$ one must have value -1 . If α_i are the eigenvalues of this operator, the condition that ρ is on circle of radius $\sqrt{2}$ reads

$$\alpha_1^2 + \alpha_2^2 + \alpha_3^2 = 2.$$

Since

$$\alpha_1 + \alpha_2 + \alpha_3 = 0,$$

the only solution is this: one of the α 's is 0, and the others equal ± 1 . That is, eigenvalues of ρ are $\frac{2}{3}, \frac{1}{3}, 0$.

It is clear from this structure that

$$\rho' = \frac{1}{3} [I - r_1 X_1 - r_2 X_2]$$

which corresponds to the diametrically opposite point of the circle has the same set of eigenvalues, and hence fall on the boundary of the state space. Thus this is the opposite point corresponding to ρ . Hence our theorem is proved. \square

It should be appreciated that the above result is not really one to do with 2-sections, but a property of 1-sections. We know that 1-sections form a one parameter family and all density matrices corresponding to a given 1-section can be simultaneously diagonalized to the form

$$\rho' = \frac{1}{3} \left[I + \frac{1}{\sqrt{2}} (r_3 \lambda_3 + r_8 \lambda_8) \right].$$

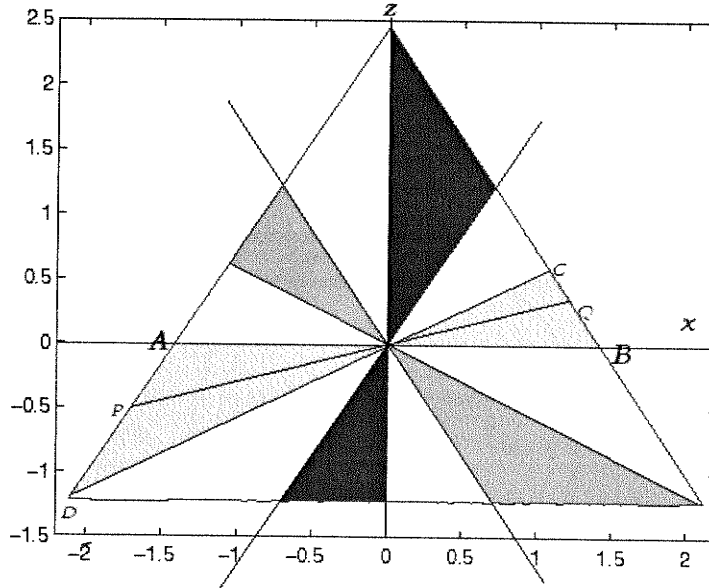


Figure 2.4: Here x axis represents λ_3 and z axis is $-\lambda_8$. AB is the smallest one-section, CD is the largest one-section, and PQ is the general one-section. The shaded (shaded in one shade only) is the region of inequivalent one-sections.

Thus all distinct properties of 1-sections are captured in the (λ_3, λ_8) plane. In particular the shaded region of figure (2.4) describes all possible unitarily inequivalent 1-sections. Incidentally, the shaded region has one-sixth the area of the triangle, consistent with the fact that the symmetry of the triangle is the six-element group $S_3 \sim C_{3v}$, and this group is unitarily realized on the state space.

2.3.2 Maximum Area Cross-Section

We have attempted to find the maximum area 2-section using the computer. And what we have obtained in this process is a section of the cone (cone is one of the 3-sections to be discussed below).

To describe a 2-section we need two traceless hermitian orthogonal matrices. We may choose, without loss of generality one to be diagonal

$$\chi_1 = \frac{1}{\sqrt{2}}[\cos \theta \lambda_3 + \sin \theta \lambda_8],$$

and the other to be orthogonal to it:

$$\chi_2 = \frac{1}{\sqrt{2}}[\cos \varphi (\sin \theta \lambda_3 - \cos \theta \lambda_8) + \sin \varphi (\sum_i r_i \lambda_i)].$$

Here i runs over all the off-diagonal operators, and r_i are such that $\sum_{i \neq 3,8} r_i^2 = 1$. Thus we need 7 parameters to specify a 2-section.

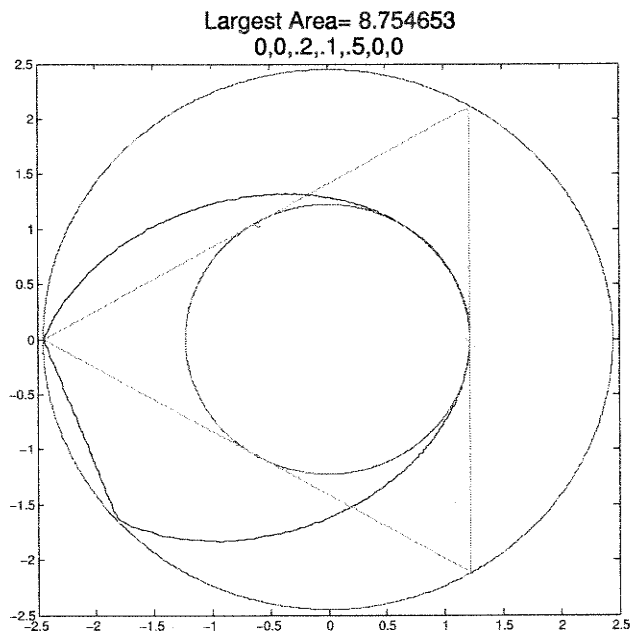


Figure 2.5: Here we showed the inner circle outer circle and triangle. The fourth cross-section is the maximum area cross section. The numbers on the top tells us about the cross-section parameters. First number is the value of $\cos\theta$, second is r_1 , next is r_2 , 4th is $\cos\varphi$, 5th, 6th, and 7th are r_4 , r_5 , r_6

2.4 Standard 3-Sections

The twenty eight standard 2-sections cannot give us a full description of the structure of the state space. And therefore now we turn our attention to the standard 3-sections, spanned by triplets of the λ -matrices. It should, however, be noted that the set of all possible three-sections constitute a 12-parameter family of equivalence classes. The ${}^{\delta}c_3 = 56$ standard 3-sections we study is just a tiny part of this family. It should also be appreciated that in studying one 3-section we are implicitly studying a continuum of 2-sections.

These fifty six 3-sections separate into seven unitarily inequivalent types. Though these sections cannot give us a complete description of the state space, the information they yield adds to the insight gained from the standard 2-sections. The list of all seven types of 3-section and their corresponding planes are listed below:

Sphere, ellipsoid, cone, and paraboloid are familiar shapes. However the others are shapes which are not so familiar. These are Obese Tetrahedron (OT), RS1, and RS2. We give a brief description of these 3-sections.

<i>Sphere</i>	<i>Ellipsoid</i>	<i>cone</i>	<i>Obese Tetrahedron</i>	<i>RS1</i>	<i>RS2</i>	<i>Paraboloid</i>
123, 245	458	128	146	134	148	345
124, 246	468	138	157	135	158	367
125, 257	478	238	247	136	168	
126, 267	568	348	256	137	178	
127, 456	578	358	346	234	248	
145, 457	678	368	347	235	258	
147, 467		378	356	236	268	
156, 567			357	237	278	
167						

Figure 2.6: List of all 3-sections, arranged according to their types. Here 123 stands for the $(\lambda_1, \lambda_2, \lambda_3)$ plane, and so on.

2.4.1 Sphere

Among the fifty six 3-sections seventeen are spheres. We can understand these in the following way:

- We get one sphere in (123) three-plane. This plane is spanned by the “generators of $SU(2)$ ” within $SU(3)$, namely

$$\lambda_1 = \begin{bmatrix} & & 0 \\ \sigma_1 & & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \lambda_2 = \begin{bmatrix} & & 0 \\ \sigma_2 & & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad \lambda_3 = \begin{bmatrix} & & 0 \\ \sigma_3 & & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

where $\sigma_1, \sigma_2, \sigma_3$ are the Pauli matrices. In this sense, this sphere is essentially the Bloch sphere which we encountered in the 2-dimensional case. It is clear that the radius of this sphere is $\sqrt{2}$.

- Of the four spheres (257), (147), (156) and (246), the first one namely (257) is spanned by the $SO(3)$ generators $\lambda_2, \lambda_5, \lambda_7$.

$$\rho = \frac{1}{3} \left[I + \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -ir_2 & -ir_5 \\ ir_2 & 0 & -ir_7 \\ ir_2 & ir_7 & 0 \end{pmatrix} \right]$$

The other three cases are conjugate to this case by diagonal $SU(3)$ elements.

- The third type of three-dimensional spheres are the 3-sections of the three 4-dimensional sphere (1245), (1267) and (4567). We can have ${}^4c_3 = 4$ standard 3-sections of a 4-dimensional object, hence we have twelve 3-dimensional spheres of the same kind. They all add up to 17.

2.4.2 Cone

Among the standard 3-sections, of familiar shape, the cone is probably the most important and interesting one. It is important in the sense that when we searched for the maximum area 2-section

using the computer, we got the maximum area 2-section as one of the 2-sections of the cone. It is interesting in the sense that we get the cone by rotating the triangle (one of the standard 2-sections) about one of its symmetry axes, and that all standard 2-sections are 2-sections of the cone. In particular, the minimum area 2-section is a cross-section of the cone.

Positivity of the density matrix $\rho = I + \Lambda$ will give us the equation of the cone. Here the eigenvalues of the Λ should not be less than -1 . Let us consider the $(\lambda_1, \lambda_2, \lambda_8)$ plane. and the associated Λ matrix:

$$\Lambda = \frac{1}{\sqrt{2}} \begin{bmatrix} \frac{1}{\sqrt{3}}z & x - iy & 0 \\ x + iy & \frac{1}{\sqrt{3}}z & 0 \\ 0 & 0 & -\frac{2}{\sqrt{3}}z \end{bmatrix}.$$

The positivity requirement reads

$$\det \begin{vmatrix} \frac{1}{\sqrt{3}}z + \sqrt{2} & x - iy & 0 \\ x + iy & \frac{1}{\sqrt{3}}z + \sqrt{2} & 0 \\ 0 & 0 & -\frac{2}{\sqrt{3}}z + \sqrt{2} \end{vmatrix} = 0,$$

Thus, the equation of the surface is

$$x^2 + y^2 = \frac{1}{3}[z + \sqrt{6}]^2,$$

and

$$z \leq \sqrt{\frac{3}{2}}.$$

The first equation is the equation of cone whose apex is at $z = -\sqrt{6}$ with half angle $\pi/6$. The second equation is the equation of the plane which truncates the cone.

The following seven standard 3-sections turn out to be cones: 128, 138, 238, 348, 358, 368, 378.

2.4.3 Ellipsoid

Ellipsoid is a familiar shape, and it turns out to be one of the standard 3-sections. Among the fifty six standard 3-sections, six are ellipsoids. These are listed in the table above. This 3-section has only one pure state and λ_8 axis is common among all the ellipsoids.

For the purpose of illustration, let us consider the $(4, 6, 8)$ plane. The corresponding λ matrix is:

$$\Lambda = \frac{1}{\sqrt{2}} \begin{bmatrix} \frac{1}{\sqrt{3}}z & 0 & x \\ 0 & \frac{1}{\sqrt{3}}z & y \\ x & y & -\frac{2}{\sqrt{3}}z \end{bmatrix}.$$

The demand that the eigenvalues of Λ should not be less than -1 , for positivity of the density matrix, gives us the equation:

$$\det \begin{bmatrix} \frac{1}{\sqrt{3}}z + \sqrt{2} & 0 & x \\ 0 & \frac{1}{\sqrt{3}}z + \sqrt{2} & y \\ x & y & -\frac{2}{\sqrt{3}}z + \sqrt{2} \end{bmatrix} = 0,$$

so the equation of the surface is:

$$x^2 + y^2 + \frac{2}{3} \left(z + \sqrt{\frac{3}{2\sqrt{2}}} \right)^2 = 0,$$

and

$$z \leq -\sqrt{6}.$$

The first equation is the equation of ellipsoid. And the other equation is the equation of a plane tangent to the out-sphere.

2.4.4 Paraboloid

The fourth familiar shape for the 3-section is the paraboloid. There are only two paraboloids among standard 3-sections. These are (3, 4, 5) and (3, 6, 7). Each has a continuum of pure states.

To get the equation of this 3-section, consider (3, 4, 5) plane. The corresponding Λ matrix is:

$$\Lambda = \frac{1}{\sqrt{2}} \begin{bmatrix} z & 0 & x - iy \\ 0 & -z & 0 \\ x + iy & 0 & 0 \end{bmatrix},$$

and following the same procedure as in the ellipsoid case, the equation of the surface is:

$$\det \begin{bmatrix} z + \sqrt{2} & 0 & x - iy \\ 0 & -z + \sqrt{2} & 0 \\ x + iy & 0 & \sqrt{2} \end{bmatrix} = 0,$$

which we may write as

$$\sqrt{2}(z + \sqrt{2}) = x^2 + y^2,$$

and

$$z \leq \sqrt{2}.$$

The equation is the equation for paraboloid with vertex at $z = -\sqrt{2}$, and the other equation is the equation of the plane $z = \sqrt{2}$ which truncates the paraboloid. The intersection of the paraboloid and the plane turns out to be the circle of pure states.

2.4.5 Obese Tetrahedron (OT)

This is the 3-section with possibly the most interesting structure in this state space. It is the first of the three less familiar 3-sections. It can be seen as a tetrahedron which is swollen without losing its symmetry: it is a tetrahedron with curved faces. It has 4-vertices and 6-edges which resemble with tetrahedron. All the 4-vertices represent pure states, and these are the only pure states in the 3-section. All 6-edges contain rank-2 density matrices. On the face also we have rank-2 matrices, but in the bulk of the body all points are rank 3 states.

There are eight OT 3-sections, related to one another through simple $SU(3)$ transformations. We may conveniently group them into two subsets of 4 elements each: $\{(146), (157), (247), (256)\}$ and $\{(346), (347), (356), (367)\}$. For illustration, consider the case (146):

$$\rho = \frac{1}{3} \left[I + \frac{1}{\sqrt{2}}(x\lambda_1 + y\lambda_4 + z\lambda_6) \right] = \frac{1}{3} [I + \Lambda],$$

where

$$\Lambda = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & x & y \\ x & 0 & z \\ y & z & 0 \end{bmatrix}.$$

Positivity of ρ demands that the eigenvalues of Λ must be no less than -1 . So if one or more of the eigenvalues equal -1 , we will get the equation of the surface through:

$$\det \begin{bmatrix} \sqrt{2} & x & y \\ x & \sqrt{2} & z \\ y & z & \sqrt{2} \end{bmatrix} = 0.$$

So the equation of the surface is:

$$\sqrt{2}[2 - x^2 - y^2 - z^2] + 2xyz = 0$$

The property of this equation is that this gives equal importance to each of the three variable. We call this surface OT. This structure has a large number of symmetry elements (as compared to the standard 3-sections of other less familiar shapes).

The other three 3-sections in this subset lead to identical equations. The four 3-sections corresponding to the other subset is simply a rotated version of this surface:

$$\sqrt{2}[2 - x^2 - y^2 - z^2] + [x^2 - y^2]z = 0$$

Evidently, the OT described by the two equations are connected by a $\pi/4$ rotation in the xy plane. Note that for the second subset λ_3 corresponds to the z -axis.

The first type of OT describes the sections (146), (157), (247), (256) and second type describes (346), (347), (356), (357). Now we will give the specific $SU(3)$ matrices which transform the OT within each subset:

$$\begin{array}{ccccc} (157) & \xleftarrow{A_1} & (146) & \xrightarrow{A_3} & (256), \\ & & \downarrow A_2 & & \\ & & (247) & & \end{array}$$

where

$$A_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & i \end{bmatrix}, \quad A_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad A_3 = \begin{bmatrix} i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

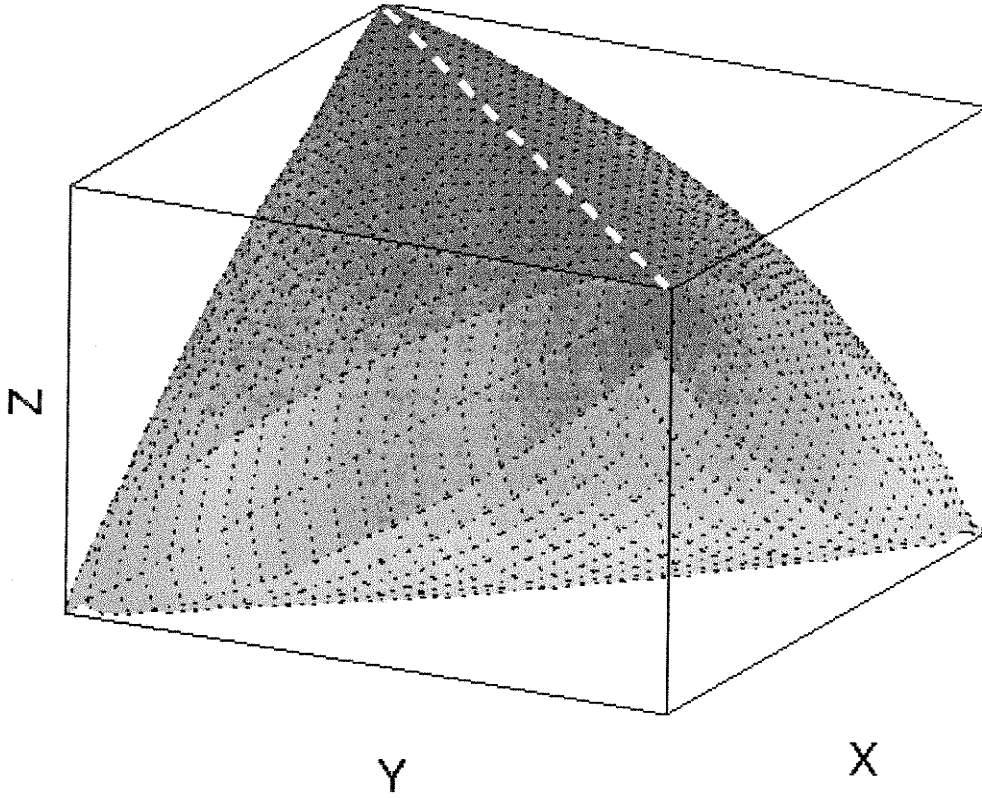


Figure 2.7: Obese Tetrahedron

Here $(146) \xrightarrow{A_3} (156)$ means $(256) = A_3(146)A_3^\dagger$. For the second subset we have:

$$\begin{array}{ccc} (347) & \xleftarrow{B_1} & (346) \xrightarrow{B_3} (355), \\ & & \downarrow B_2 \\ & & (356) \end{array}$$

where

$$B_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -i & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad B_2 = \begin{bmatrix} -i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad B_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -i \end{bmatrix}.$$

Finally, the matrix which transforms one subset to the other is

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & \sqrt{2} \end{bmatrix},$$

as can be verified easily.

The symmetry group of OT turns out to be the same as the tetrahedral group T_d . It is for this reason that we have called this structure obese tetrahedron. Consider, for instance, the case (146)

again. The associated Λ matrices have the form

$$\Lambda = \begin{bmatrix} 0 & x & y \\ x & 0 & z \\ y & z & 0 \end{bmatrix}.$$

We wish to enumerate the $U(3)$ elements which leave this form invariant. It is clear that such $U(3)$ elements will form a subgroup. The fact that x, y, z are constrained to be real implies that we are indeed confined to $O(3)$, rather than the full $U(3)$. Writing out the form-invariance

$$R\Lambda R^T = \Lambda'$$

in detail, we have

$$\begin{bmatrix} r_{11} & r_{12} & r_{13} \\ r_{21} & r_{22} & r_{23} \\ r_{31} & r_{32} & r_{33} \end{bmatrix} \begin{bmatrix} 0 & x & y \\ x & 0 & z \\ y & z & 0 \end{bmatrix} \begin{bmatrix} r_{11} & r_{21} & r_{31} \\ r_{12} & r_{22} & r_{32} \\ r_{13} & r_{23} & r_{33} \end{bmatrix} = \begin{bmatrix} 0 & x' & y' \\ x' & 0 & z' \\ y' & z' & 0 \end{bmatrix}.$$

By comparing the left hand side and the right hand side we get the following set of equations:

$$2x r_{12}r_{11} + 2y r_{13}r_{11} + 2z r_{13}r_{12} = 0, \quad (2.1)$$

$$2x r_{22}r_{21} + 2y r_{23}r_{21} + 2z r_{23}r_{22} = 0, \quad (2.2)$$

$$2x r_{32}r_{31} + 2y r_{33}r_{31} + 2z r_{33}r_{32} = 0; \quad (2.3)$$

$$x(r_{12}r_{21} + r_{11}r_{22}) + y(r_{13}r_{21} + r_{11}r_{23}) + z(r_{13}r_{22} + r_{12}r_{23}) = x', \quad (2.4)$$

$$x(r_{12}r_{31} + r_{11}r_{32}) + y(r_{13}r_{31} + r_{11}r_{33}) + z(r_{13}r_{32} + r_{12}r_{33}) = y', \quad (2.5)$$

$$x(r_{22}r_{31} + r_{21}r_{32}) + y(r_{23}r_{31} + r_{21}r_{33}) + z(r_{23}r_{32} + r_{22}r_{33}) = z'. \quad (2.6)$$

The first three equations correspond to the demand that the diagonal elements remain zero. The next three equations are the equations which will give us the transformation matrix between x, y, z and x', y', z' .

Note that we are dealing with two kinds of matrices. One is the transformation matrix R acting on the matrix Λ through conjugation, and the other is the transformation matrix T acting on the three-component vector (x, y, z) .

$$\begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = T \begin{pmatrix} x \\ y \\ z \end{pmatrix},$$

$$T(R) = \begin{bmatrix} r_{12}r_{21} + r_{11}r_{22} & r_{13}r_{21} + r_{11}r_{23} & r_{13}r_{22} + r_{12}r_{23} \\ r_{12}r_{31} + r_{11}r_{32} & r_{13}r_{31} + r_{11}r_{33} & r_{13}r_{32} + r_{12}r_{33} \\ r_{22}r_{31} + r_{21}r_{32} & r_{23}r_{31} + r_{21}r_{33} & r_{23}r_{32} + r_{22}r_{33} \end{bmatrix}. \quad (2.7)$$

In $O(3)$ there are 48 real solutions to the above six coupled linear equations. Of these 24 are proper rotations. The other 24 are improper rotations. The latter are simply the negative of the 24 proper rotations, and hence do not lead to any new T matrices. For this reason, we consider

only the proper R matrices, 24 in number. We divide these 24 elements of $SO(3)$ into two subsets of 12 elements each. The reason for this division will become clear later. The 12 elements in the first subset of R matrices are:

$$\begin{aligned} & \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \\ & \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}, \\ & \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}. \end{aligned}$$

The corresponding T matrices acting on the three-dimensional subspace of traceless hermitian matrices are computed from eq.(2.7):

R	\rightarrow	T		R	\rightarrow	T
$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$		$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$		$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 1 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$		$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$
$\begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}$		$\begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}$
$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$		$\begin{bmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix}$
$\begin{bmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{bmatrix}$		$\begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix}$

The R -matrices in the second subset are:

$$\begin{aligned} & \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}, \begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}, \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \\ & \begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \\ & \begin{bmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix}. \end{aligned}$$

The corresponding T-matrices are:

R	\rightarrow	T	R	\rightarrow	T
$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$
$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$
$\begin{bmatrix} 0 & -1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$
$\begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}$
$\begin{bmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 0 & -1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$
$\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ -1 & 0 & 0 \end{bmatrix}$	$\begin{bmatrix} 0 & 0 & 1 \\ 0 & -1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$	\rightarrow	$\begin{bmatrix} 0 & 0 & -1 \\ 0 & 1 & 0 \\ -1 & 0 & 0 \end{bmatrix}$

While the T matrices in the first set are proper rotations, those in the second are improper rotations. And this is the reason for dividing the R matrices into two subsets.

The eight-dimensional matrices corresponding to any $U(3)$ matrix and acting on the space of traceless matrices will always be elements of $SO(8)$, this being the adjoint representation. We present these 8-dimensional matrices in the Appendix. Whenever the rotation in the $(\lambda_1, \lambda_4, \lambda_6)$ plane is improper, the rotation in the (λ_3, λ_8) plane is also improper [the rotation in the $(\lambda_2, \lambda_5, \lambda_7)$ plane is always proper], thus rendering the 8-dimensional matrix proper.

2.4.6 RS1

$RS1$ is the second of our less familiar 3-sections. There are eight of these. We consider the case (134) first. The positivity requirement reads:

$$\det \begin{bmatrix} z + \sqrt{2} & x & y \\ x & \sqrt{2} - z & 0 \\ y & 0 & \sqrt{2} \end{bmatrix} = 0,$$

or, equivalently,

$$\sqrt{2}(x^2 + y^2 + z^2 - 2) - y^2z = 0.$$

The surface described by the latter is what we call $RS1$. It has only two pure states.

It is easy to see that there are only four elements in the symmetry group of $RS1$. These are generated by reflection in the xz and yz planes. Though it has a small symmetry group, it has a very beautiful shape. This can be appreciated from the projections in different directions, but we have shown only three projections, respectively in the x , y , and z directions.

It should be noted that the y -projection is a circle, and coincides with the standard 2-section in the (1, 4) plane. Similarly the x -projection is a parabola, and coincides with the 2-section in the (3, 4) plane. But the z -projection does not coincide with the 2-section in the (1, 3) plane, the latter being a circle.

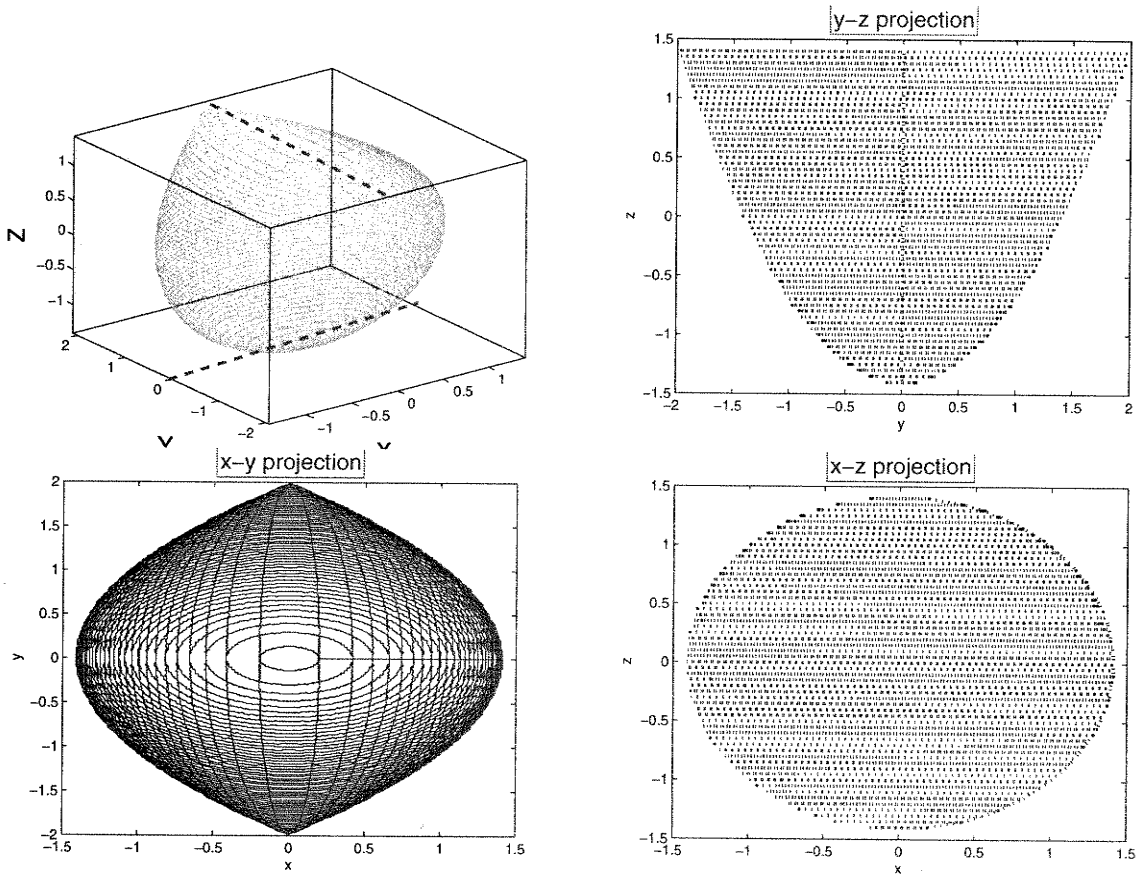


Figure 2.8: The top left is our 3-section RS1. It is not easy to see what shape it has so I give these three projections also. The top right projection is in yz plane. The bottom left and bottom right are the xy and xz projection.

The following eight 3-sections lead to $RS1$: (134, 135, 136, 137, 234, 235, 236 and 237). We can conveniently divide them into two subsets: (134, 135, 234, 235) and (136, 137, 236, 237). The transformation matrices which connect the four 3-sections in the first subset are:

$$\begin{array}{ccc}
 (135) & \xleftarrow{C_1} & (134) \xrightarrow{C_2} (234), \\
 & & \downarrow C_3 \\
 & & (235)
 \end{array}$$

where

$$C_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & i \end{bmatrix}, \quad C_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad C_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & i \end{bmatrix}.$$

Similarly, the transformation matrices connecting the second subset of *RS1* sections are:

$$(137) \xleftarrow{D_1} (136) \xrightarrow{D_2} (236),$$

$$\downarrow D_3$$

$$(237)$$

where

$$D_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & i \end{bmatrix}, \quad D_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & i \end{bmatrix}, \quad D_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & -1 \end{bmatrix}.$$

It is easy to see that $U(3)$ matrix which connects two subsets through conjugation

$$U = \begin{bmatrix} & & 0 \\ \sigma_j & & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

where σ_j is any of the two Pauli matrices σ_1 or σ_2 .

2.4.7 RS2

RS2 is the third and the last of our less-familiar shape for the 3-sections. There are 8 of these type listed in the table above. Consider, for instance, the (1, 4, 8) plane. The positivity requirement reads:

$$\det \begin{bmatrix} \sqrt{2} + \frac{z}{\sqrt{3}} & x & y \\ x & \sqrt{2} + \frac{z}{\sqrt{3}} & 0 \\ y & 0 & \sqrt{2} - 2\frac{z}{\sqrt{3}} \end{bmatrix} = 0,$$

so the equation of the surface is

$$\sqrt{2}(x^2 + y^2 + z^2 - 2) + \frac{z}{\sqrt{3}}(2x^2 - y^2 - \frac{2z^2}{3}) = 0$$

The surface described by this equation is what we call *RS2*.

In this 3-section we have only three pure states, but there are only four elements in the symmetry group of *RS2*: The symmetry groups of *RS1* and *RS2* are same. This symmetry group is generated by reflections in the xy and yz planes. The persence of λ_8 instead of λ_3 in *RS2* is the key difference between *RS2* and *RS1*.

Similar to the case of *RS1*, we can divide the eight *RS2* 3-sections into two subsets. These are: (148, 158, 248, 258) and (168, 178, 268, 278). The transformation matrices connecting the four *RS2* sections in the first subset are:

$$(158) \xleftarrow{E_1} (148) \xrightarrow{E_2} (248),$$

$$\downarrow E_3$$

$$(258)$$

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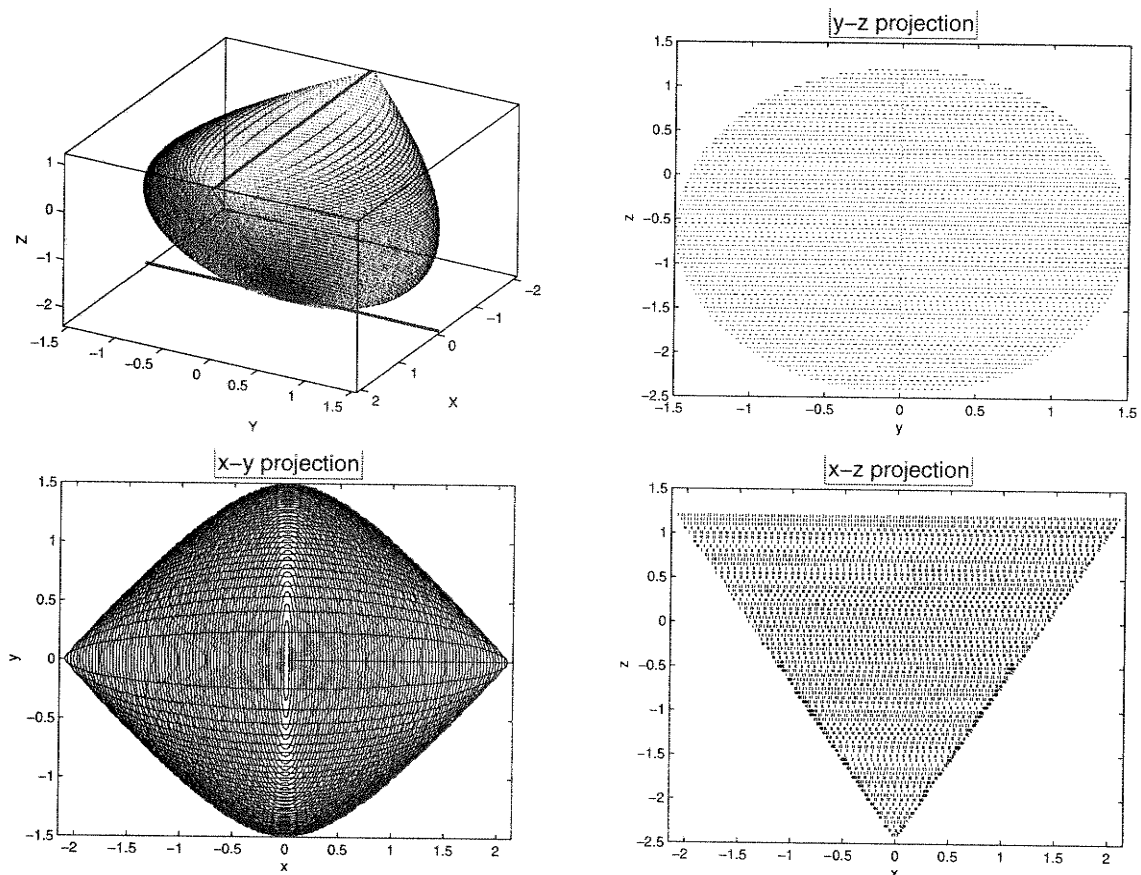


Figure 2.9: The top left is our 3-section RS2. Top right bottom left and bottom right are yz, xy and xz projections.

where

$$E_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & i \end{bmatrix}, \quad E_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad E_3 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & i & 0 \\ 0 & 0 & i \end{bmatrix}.$$

Similarly, the transformation matrices connecting the four elements in the second subset are:

$$\begin{array}{ccc} (178) & \xleftarrow{F_1} & (168) \xrightarrow{F_2} (268), \\ & & \downarrow F_3 \\ & & (278) \end{array}$$

where

$$F_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & i \end{bmatrix}, \quad F_2 = \begin{bmatrix} i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad F_3 = \begin{bmatrix} i & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & i \end{bmatrix}.$$

Finally, the $U(3)$ element which connect through conjugation the two subsets is

$$U = \begin{bmatrix} \sigma_j & 0 \\ 0 & 0 & 1 \end{bmatrix},$$

where σ_j could be σ_1 or σ_2 .

Chapter 3

Conclusion

In this thesis, we have tried to give glimpses of the geometry of the convex body of density matrices [the state space] corresponding to a given finite dimensional Hilbert space. Our attention was restricted to 2 and 3-dimensional Hilbert spaces, the corresponding dimensions of the state space being 3 and 8. We have studied in detail the standard 2-sections as well as 3-sections for the 3-dimensional Hilbert space case, described their symmetry group in the interesting cases, analytically found the smallest-area 2-section and numerically estimated the largest-area 2-section.

We would like to continue this study in two different directions. In the three-dimensional case we would like to classify the 4-sections to the same level of exhaustive detail as we have done with 3-sections. In the four-dimensional case our study of the geometry of state space is fine-tuned towards understanding the problem of separability. In both directions our preliminary result [not included in this thesis] are encouraging. In particular, we may mention the extremely interesting four-dimensional analogue of the obese tetrahedron. By studying the geometry in lower dimensional Hilbert space, we would like to infer the general geometrical structure of the convex set of density matrices in higher dimension. The ultimate goal is to characterize the geometry of the sets of separable and entangled states in tensor product Hilbert spaces. This thesis is but a beginning towards this end.

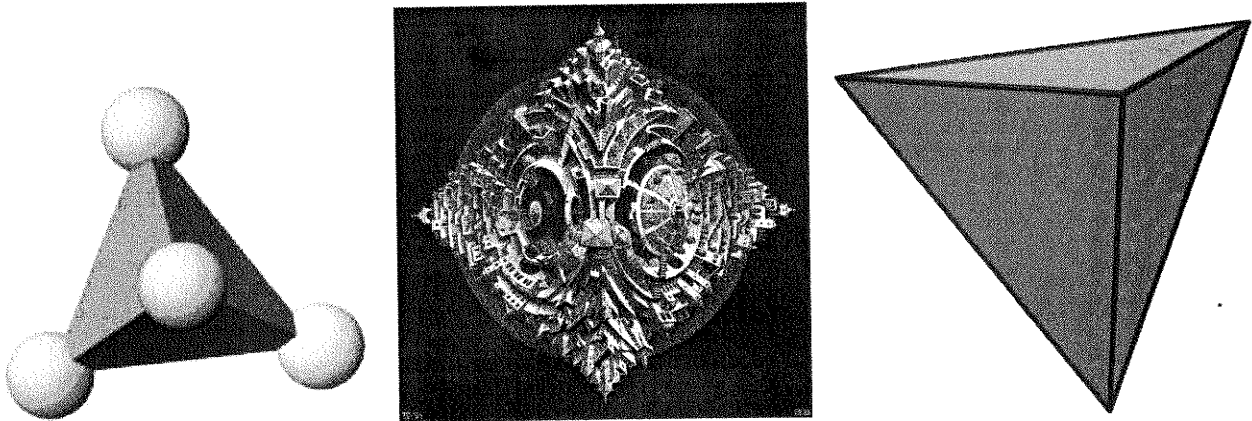


Figure 3.1: Here we showed some tetrahedrons. First and third one are the usual tetrahedrons. And the central one is a piece of art. This is the tetrahedron when we look at it from its one edge.

$$\begin{aligned}
 \begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{bmatrix} &\rightarrow \begin{bmatrix} 1 & 0 & 0 & & & \\ 0 & -1 & 0 & & & \\ 0 & 0 & -1 & & & \\ & & & 1 & 0 & 0 \\ & & & 0 & -1 & 0 \\ & & & 0 & 0 & -1 \\ & & & & & & 1 & 0 \\ & & & & & & 0 & 1 \end{bmatrix} \\
 \begin{bmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} &\rightarrow \begin{bmatrix} -1 & 0 & 0 & & & \\ 0 & 1 & 0 & & & \\ 0 & 0 & -1 & & & \\ & & & -1 & 0 & 0 \\ & & & 0 & 1 & 0 \\ & & & 0 & 0 & -1 \\ & & & & & & 1 & 0 \\ & & & & & & 0 & 1 \end{bmatrix} \\
 \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} &\rightarrow \begin{bmatrix} 0 & 0 & 1 & & & \\ 1 & 0 & 0 & & & \\ 0 & 1 & 0 & & & \\ & & & 0 & 0 & 1 \\ & & & -1 & 0 & 0 \\ & & & 0 & -1 & 0 \\ & & & & & & -1/2 & \sqrt{3}/2 \\ & & & & & & -\sqrt{3}/2 & -1/2 \end{bmatrix} \\
 \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \end{bmatrix} &\rightarrow \begin{bmatrix} 0 & 0 & -1 & & & \\ -1 & 0 & 0 & & & \\ 0 & 1 & 0 & & & \\ & & & 0 & 0 & -1 \\ & & & 1 & 0 & 0 \\ & & & 0 & -1 & 0 \\ & & & & & & -1/2 & \sqrt{3}/2 \\ & & & & & & -\sqrt{3}/2 & -1/2 \end{bmatrix}
 \end{aligned}$$

$$\begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \\ & & & 0 & 0 & 1 \\ & & & 1 & 0 & 0 \\ & & & 0 & 1 & 0 \\ & & & & & & -1/2 & \sqrt{3}/2 \\ & & & & & & -\sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$\begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \\ & & & 0 & 0 & -1 \\ & & & -1 & 0 & 0 \\ & & & 0 & 1 & 0 \\ & & & & & & -1/2 & \sqrt{3}/2 \\ & & & & & & -\sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \\ & & & 0 & -1 & 0 \\ & & & 0 & 0 & -1 \\ & & & 1 & 0 & 0 \\ & & & & & & -1/2 & -\sqrt{3}/2 \\ & & & & & & \sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & 1 \\ -1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & -1 \\ 1 & 0 & 0 \\ & & & 0 & 1 & 0 \\ & & & 0 & 0 & 1 \\ & & & 1 & 0 & 0 \\ & & & & & & -1/2 & -\sqrt{3}/2 \\ & & & & & & \sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & -1 \\ -1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & -1 \\ -1 & 0 & 0 \\ & & & 0 & -1 & 0 \\ & & & 0 & 0 & 1 \\ & & & -1 & 0 & 0 \\ & & & & & & -1/2 & -\sqrt{3}/2 \\ & & & & & & \sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 & -1 \\ 1 & 0 & 0 \\ 0 & -1 & 0 \end{bmatrix} \rightarrow \begin{bmatrix} 0 & -1 & 0 \\ 0 & 0 & 1 \\ -1 & 0 & 0 \\ & & & 0 & 1 & 0 \\ & & & 0 & 0 & -1 \\ & & & -1 & 0 & 0 \\ & & & & & & -1/2 & -\sqrt{3}/2 \\ & & & & & & \sqrt{3}/2 & -1/2 \end{bmatrix}$$

$$\begin{aligned}
\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} & \begin{bmatrix} r_3 + \frac{r_8}{\sqrt{3}} & r_1 - ir_2 & r_4 - ir_5 \\ r_1 + ir_2 & -r_3 + \frac{r_8}{\sqrt{3}} & r_6 - ir_7 \\ r_4 + ir_5 & r_6 + ir_7 & -\frac{2r_8}{\sqrt{3}} \end{bmatrix} \begin{bmatrix} a^*_{11} & a^*_{21} & a^*_{31} \\ a^*_{12} & a^*_{22} & a^*_{32} \\ a^*_{13} & a^*_{23} & a^*_{33} \end{bmatrix} \\
& = \begin{bmatrix} r'_3 + \frac{r'_8}{\sqrt{3}} & r'_1 - ir'_2 & r'_4 - ir'_5 \\ r'_1 + ir'_2 & -r'_3 + \frac{r'_8}{\sqrt{3}} & r'_6 - ir'_7 \\ r'_4 + ir'_5 & r'_6 + ir'_7 & -\frac{2r'_8}{\sqrt{3}} \end{bmatrix}
\end{aligned}$$

The above equation can be written as $RX = X'$ where R is a 8×8 real orthogonal matrix. And X is the column vector $X = [r_i]$, obtained by arranging r_1, r_2, \dots, r_8 into a column. Naturally, the r'_i are linear combinations of the r'_j and can be determined by the following expressions:

$$\begin{aligned}
r'_1 &= \frac{1}{2} [\vec{x} \cdot \lambda^T (P_{12} + P_{21})], \\
r'_2 &= \frac{i}{2} [\vec{x} \cdot \lambda^T (P_{12} - P_{21})], \\
r'_3 &= \frac{1}{2} [\vec{x} \cdot \lambda^T (P_{11} - P_{22})], \\
r'_4 &= \frac{1}{2} [\vec{x} \cdot \lambda^T (P_{13} + P_{31})], \\
r'_5 &= \frac{i}{2} [\vec{x} \cdot \lambda^T (P_{13} - P_{31})], \\
r'_6 &= \frac{1}{2} [\vec{x} \cdot \lambda^T (P_{23} + P_{32})], \\
r'_7 &= \frac{i}{2} [\vec{x} \cdot \lambda^T (P_{23} - P_{32})], \\
r'_8 &= -\frac{\sqrt{3}}{2} [\vec{x} \cdot \lambda^T (P_{33})]
\end{aligned}$$

where

$$\begin{aligned}
P_{12} + P_{21} &= \begin{bmatrix} a^*_{21}a_{11} + a^*_{11}a_{21} & a^*_{21}a_{12} + a^*_{11}a_{22} & a^*_{21}a_{13} + a^*_{11}a_{23} \\ a^*_{22}a_{11} + a^*_{12}a_{21} & a^*_{22}a_{12} + a^*_{12}a_{22} & a^*_{22}a_{13} + a^*_{12}a_{23} \\ a^*_{23}a_{11} + a^*_{13}a_{21} & a^*_{23}a_{12} + a^*_{13}a_{22} & a^*_{23}a_{13} + a^*_{13}a_{23} \end{bmatrix} \\
P_{12} - P_{21} &= \begin{bmatrix} a^*_{21}a_{11} - a^*_{11}a_{21} & a^*_{21}a_{12} - a^*_{11}a_{22} & a^*_{21}a_{13} - a^*_{11}a_{23} \\ a^*_{22}a_{11} - a^*_{12}a_{21} & a^*_{22}a_{12} - a^*_{12}a_{22} & a^*_{22}a_{13} - a^*_{12}a_{23} \\ a^*_{23}a_{11} - a^*_{13}a_{21} & a^*_{23}a_{12} - a^*_{13}a_{22} & a^*_{23}a_{13} - a^*_{13}a_{23} \end{bmatrix} \\
P_{11} - P_{22} &= \begin{bmatrix} a^*_{11}a_{11} - a^*_{21}a_{21} & a^*_{11}a_{12} - a^*_{21}a_{22} & a^*_{11}a_{13} - a^*_{21}a_{23} \\ a^*_{12}a_{11} - a^*_{22}a_{21} & a^*_{12}a_{12} - a^*_{22}a_{22} & a^*_{12}a_{13} - a^*_{22}a_{23} \\ a^*_{13}a_{11} - a^*_{23}a_{21} & a^*_{13}a_{12} - a^*_{23}a_{22} & a^*_{13}a_{13} - a^*_{23}a_{23} \end{bmatrix} \\
P_{13} + P_{31} &= \begin{bmatrix} a^*_{31}a_{11} + a^*_{11}a_{31} & a^*_{31}a_{12} + a^*_{11}a_{32} & a^*_{31}a_{13} + a^*_{11}a_{33} \\ a^*_{32}a_{11} + a^*_{12}a_{31} & a^*_{32}a_{12} + a^*_{12}a_{32} & a^*_{32}a_{13} + a^*_{12}a_{33} \\ a^*_{33}a_{11} + a^*_{13}a_{31} & a^*_{33}a_{12} + a^*_{13}a_{32} & a^*_{33}a_{13} + a^*_{13}a_{33} \end{bmatrix} \\
P_{13} - P_{31} &= \begin{bmatrix} a^*_{31}a_{11} - a^*_{11}a_{31} & a^*_{31}a_{12} - a^*_{11}a_{32} & a^*_{31}a_{13} - a^*_{11}a_{33} \\ a^*_{32}a_{11} - a^*_{12}a_{31} & a^*_{32}a_{12} - a^*_{12}a_{32} & a^*_{32}a_{13} - a^*_{12}a_{33} \\ a^*_{33}a_{11} - a^*_{13}a_{31} & a^*_{33}a_{12} - a^*_{13}a_{32} & a^*_{33}a_{13} - a^*_{13}a_{33} \end{bmatrix} \\
P_{23} + P_{23} &= \begin{bmatrix} a^*_{31}a_{21} + a^*_{21}a_{31} & a^*_{31}a_{22} + a^*_{21}a_{32} & a^*_{31}a_{23} + a^*_{21}a_{33} \\ a^*_{32}a_{21} + a^*_{22}a_{31} & a^*_{32}a_{22} + a^*_{22}a_{32} & a^*_{32}a_{23} + a^*_{22}a_{33} \\ a^*_{33}a_{21} + a^*_{23}a_{31} & a^*_{33}a_{22} + a^*_{23}a_{32} & a^*_{33}a_{23} + a^*_{23}a_{33} \end{bmatrix}
\end{aligned}$$

$$P_{23} - P_{23} = \begin{bmatrix} a_{31}^* a_{21} - a_{21}^* a_{31} & a_{31}^* a_{22} - a_{21}^* a_{32} & a_{31}^* a_{23} - a_{21}^* a_{33} \\ a_{32}^* a_{21} - a_{22}^* a_{31} & a_{32}^* a_{22} - a_{22}^* a_{32} & a_{32}^* a_{23} - a_{22}^* a_{33} \\ a_{33}^* a_{21} - a_{23}^* a_{31} & a_{33}^* a_{22} - a_{23}^* a_{32} & a_{33}^* a_{23} - a_{23}^* a_{33} \end{bmatrix}$$

$$P_{33} \begin{bmatrix} |a_{31}|^2 & a_{31}^* a_{32} & a_{31}^* a_{33} \\ a_{32}^* a_{31} & |a_{32}|^2 & a_{32}^* a_{33} \\ a_{33}^* a_{31} & a_{33}^* a_{32} & |a_{33}|^2 \end{bmatrix}$$

Using these matrices and the expressions given for the r_i' 's, we can find the 8×8 matrices.

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