Stratificational and antipodean properties of boundary states for \( N \times N \) density matrices

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Abstract. We investigate the space of \( N \times N \) dimensional density matrices. We show that there exist strata such that boundary states \( \rho_p \) with \( p \) zero eigenvalues lie on or outside the spheres with radii \( r_p = \sqrt{p/N(N-p)} \). Moreover, we show that if in a certain direction there is a boundary state with \( q = N - p \) equal eigenvalues, then in the opposite (antipodean) direction exists a boundary state with \( p = N - q \) equal eigenvalues.

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1. Introduction

The present renewed interest in the geometry of density matrices describing \( N \)-level quantum systems is largely due to the advances in the fundamentals of quantum mechanics and in quantum information theory [1]. The recent monograph by Bengtsson and Życzkowski [2] gives an excellent review of the subject and also very extensive bibliography. Nevertheless, there are still many important open questions. It is relatively easy to account for the required hermiticity and normalization of density matrices. But the requirement of positivity (strictly speaking: semi-positivity) causes serious problems. One of the methods of investigation of density matrices uses a concept of generalized Bloch vectors. This is due to the fact that the space of density matrices is in one-to-one correspondence with the space of these vectors (see, for example [3, 4, 5, 6]). The recent paper by Kimura and Kossakowski [7] proceeds along these lines. These authors construct the spherical-coordinate point of view in the space of Bloch vectors. To our minds, perhaps the term directional would be better. Kimura and Kossakowski derive inequalities which must be satisfied by the lengths of Bloch vectors in the specific directions. Moreover, they show that if there is a pure state in certain direction then in the opposite one there occur states with at most one zero eigenvalue.
The aim of this work is to simplify and generalize the results of Kimura and Kossakowski. We stress that we deal only with $N$-dimensional quantum systems described by $N \times N$ density matrices.

In the next section we briefly present the basic theoretical notions necessary in our analysis. We will formulate the expressions giving the metric in the space of density operators and hence the tool to measure distances which can also be expressed in terms of lengths of Bloch vectors. In the third section we will apply introduced ideas and show that the space of density matrices is stratified (that is possesses, colloquially speaking, onion-like structure). The fourth section is devoted to a presentation of the directional representation of density matrices. This is a brief review of some results of Kimura and Kossakowski \cite{7} which seem to be essential for the completeness of this work. In the fifth section we discuss and generalize the antipodean properties anticipated in \cite{7}. In the last section we give some additional comments and remarks.

For further convenience, we present here a very simple lemma which is due to Harriman \cite{8} and is quite useful in further discussion.

**Lemma.** Let $a_j \in \mathbb{R}, (j = 1, 2, \ldots, n)$ and $\sum_{j=1}^{n} a_j = 1$ (note that numbers $a_j$ need not be positive). Denoting $\sum_{j=1}^{n} a_j^2 = A$, one has:

\begin{align}
(i) & \quad A \geq 1/n; \\
(ii) & \quad A = 1/n \iff a_j = 1/n, \quad (j = 1, 2, \ldots, n). \quad (1b)
\end{align}

**Proof:** Consider the sum $S$ defined as follows

$$S = \sum_{j=1}^{n} \left( a_j - \frac{1}{n} \right)^2 = \sum_{j=1}^{n} \left( a_j^2 - \frac{2a_j}{n} + \frac{1}{n^2} \right) = A - \frac{1}{n}, \quad (2)$$

where we used the condition imposed upon the sum of numbers $a_j$. Then, we have $A = S + 1/n$. Sum $S$ is a sum of squares so it is nonnegative, then $A \geq 1/n$, which proves (1a). Let us now assume that $A = 1/n$. Then relation (2) entails $S = 0$, which means that all $a_j = 1/n$. Conversely, taking $a_j = 1/n$ we see that (2) gives $A = 1/n$. This completes the proof of the lemma.

2. Theoretical framework

Let us denote the maximally mixed state as

$$\rho_{\text{max}} = \text{diag} \left( \frac{1}{N}, \frac{1}{N}, \ldots, \frac{1}{N} \right) = \frac{1}{N} 1_N, \quad (3)$$

where $1_N$ is a unit $N \times N$ matrix. Hilbert-Schmidt distance between an arbitrary density matrix and $\rho_{\text{max}}$ is given as

$$d^2(\rho, \rho_{\text{max}}) = \text{Tr} \left\{ (\rho - \rho_{\text{max}})^2 \right\}. \quad (4)$$

The trace is invariant with respect to unitary transformations and so is $\rho_{\text{max}}$. Then we choose such a representation in which $\rho = \text{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N)$, where $\lambda_j$ are the eigenvalues of the density matrix and satisfy the requirements: (i) $\lambda_j \in \mathbb{R}$
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(hermiticity), (ii) $\sum_{j=1}^{N} \lambda_j = 1$ (normalization), (iii) $\lambda_j \geq 0$ (semi-positivity). Using this representation we have

$$d^2(\rho, \rho_{\text{max}}) = \sum_{j=1}^{N} \left( \lambda_j - \frac{1}{N} \right)^2 = \sum_{j=1}^{N} \lambda_j^2 - \frac{1}{N}.$$  \hspace{1cm} (5)

Since $\text{Tr}\{\rho^2\} \leq 1$ we immediately get

$$d^2(\rho, \rho_{\text{max}}) \leq \frac{N - 1}{N}.$$  \hspace{1cm} (6)

This means that all density matrices lie on or within a sphere (in the space of $N \times N$ hermitian and normalized matrices) with the center at $\rho_{\text{max}}$ and radius

$$R_L = \sqrt{\frac{N - 1}{N}}.$$  \hspace{1cm} (7)

We will call this sphere a large one. On the other hand, it is well known that for $N \geq 3$, not all matrices within this sphere are true density ones. The sphere also contains hermitian and normalized but nonpositive matrices. It is also known (see [8]) that there exists a small sphere (centered also at $\rho_{\text{max}}$) with a radius

$$R_S = \sqrt{\frac{1}{N(N-1)}},$$  \hspace{1cm} (8)

inside which there are only density matrices. The nonpositive ones can be found only outside a small sphere.

Above considerations were made by reference to the eigenvalues of the density matrices. Similar ones can be done in terms of the generalized Bloch vectors which are introduced as follows.

The basis in the space of hermitian $N \times N$ matrices consists of $N^2$ elements. We take the one consisting of the unit matrix $\hat{1}_N$ and of $N^2 - 1$ traceless, hermitian and orthonormal matrices $\{T_j\}_{j=1}^{N^2-1}$. There are various possibilities of the choice of such a basis, see the review [6]. We assume that orthogonality holds in the Hilbert-Schmidt sense, i.e., $\text{Tr}\{T_j T_k\} = \delta_{jk}$. Then, an arbitrary density operator for a $N$-level system can be written as

$$\rho = \frac{1}{N} \hat{1}_N + \sum_{i=1}^{N^2-1} V_i T_i = \frac{1}{N} \hat{1}_N + \vec{V} \cdot \vec{T},$$ \hspace{1cm} (9)

where $(V_1, V_2, \ldots, V_{N^2-1}) \in \mathbb{R}^{N^2-1}$ is called a generalized Bloch vector. Representation (9) ensures normalization and hermiticity. Requirement of positivity imposes restrictions upon vector $\vec{V}$. To our knowledge, their general form is not known although some particular cases [3, 4, 5] were studied in much detail. Discussion of this point, however, goes beyond the scope of the present work.

Bloch vector can be used to express the distance between an arbitrary density matrix and the maximally mixed one

$$d^2(\rho, \rho_{\text{max}}) = \text{Tr}\{(\rho - \rho_{\text{max}})^2\} = \sum_{i,j=1}^{N^2-1} V_i V_j \delta_{ij} = |\vec{V}|^2.$$ \hspace{1cm} (10)
as it follows from tracelessness and orthonormality of matrices $T_j$. Comparing this relation with (5) and (6) we can write

$$|\vec{V}|^2 = \sum_{j=1}^{N} \lambda_j^2 - \frac{1}{N} \leq \frac{N-1}{N}. \quad (11)$$

Therefore, the length of the Bloch vector is not arbitrary. Bloch vectors $\vec{V} \in \mathbb{R}^{N^2-1}$ lie on or within a sphere with radius $R_L$. Note that the space of Bloch vectors is different from the space of density matrices, although relation (9) establishes a one-to-one mapping between these spaces.

3. Stratification of the Bloch space

Boundary states are specified as such density matrices which possess at least one eigenvalue equal to zero. Let $\rho_p$ denote a boundary state with $p$ zero eigenvalues and with $q = N - p$ nonzero positive ones: $\lambda_1, \ldots, \lambda_q$ (obviously $\sum_{j=1}^{q} \lambda_j = 1$, due to normalization). For such a boundary state relation (5) gives

$$d^2(\rho_p, \rho_{\text{max}}) = \sum_{j=1}^{q} \lambda_j^2 - \frac{1}{N}. \quad (12)$$

Due to lemma (1a) we know that $\sum_{j=1}^{q} \lambda_j^2 \geq 1/q$. Therefore

$$d^2(\rho_p, \rho_{\text{max}}) \geq \frac{1}{q} - \frac{1}{N} = \frac{N-q}{Nq} = \frac{p}{N(N-p)}. \quad (13)$$

This inequality allows us to draw several conclusions. Some of them are obvious and well known, but we quote them just for completeness of the reasoning. Some other seem to be new.

Boundary states with just one zero eigenvalue ($p = 1$) lie on or outside the small sphere (centered at $\rho_{\text{max}}$) of radius $R_S = \sqrt{1/N(N-1)}$. In other words, the small sphere contains density matrices with all $N$ eigenvalues greater than zero. It is worth noting, that nonpositive but hermitian and normalized matrices can also be found just outside this sphere [8].

Pure states (with $\lambda_1 = 1$, all other eigenvalues are zeroes, so that $p = N - 1$) satisfy

$$d^2(\rho_{\text{pure}}, \rho_{\text{max}}) \geq \frac{N-1}{N}. \quad (14)$$

Obviously, this result together with relation (6) imply that pure states must lie strictly on the surface of a large sphere [8], so inequality (14) becomes an equality. This explains why pure states are also extremal. Pure states must lie on the surface of the large sphere (which is a very well-known result) but the converse is not true. There are (on the large sphere) matrices which are not positive definite [8].

It seems to be a new conclusion that relation (13) implies that the space of density matrices is stratified by concentric spheres $S_p$ (centered at $\rho_{\text{max}}$) of radii

$$r_p = \sqrt{\frac{p}{N(N-p)}}, \quad p = 1, 2, \ldots, N-1, \quad (15)$$
and boundary states $\rho_p$ (with $p$ zero eigenvalues) lie on or outside these spheres. We also note that for large and small spheres, we have $R_S = r_1$ and $R_L = r_{N-1}$.

Lemma (14) allows us also to say that inequality (13) is minimized for the boundary state of the form

$$\rho_p = \text{diag}\left(\frac{1}{q}, \frac{1}{q}, \ldots, \frac{1}{q}, 0, \ldots, 0\right) \equiv R(q),$$

so only boundary states $R(q = N - p)$ lie on the spheres $S_p$. Other boundary states with $p$ zero eigenvalues lie outside these spheres.

The discussed properties of the space of density matrices can easily be translated into the language of Bloch vectors. Firstly, density matrices with all nonzero eigenvalues correspond to Bloch vectors with the length

$$|\vec{V}|^2 < \frac{1}{N(N-1)}.$$  \hspace{1cm} (17)

Secondly, boundary states with $p$ zero eigenvalues correspond to Bloch vectors such that

$$|\vec{V}|^2 \geq \frac{p}{N(N-p)}.$$  \hspace{1cm} (18)

For boundary states $R(q)$ defined in Eq. (16) the above inequality becomes an equality and we have

$$|\vec{V}_{R(q)}|^2 = d^2(R(q), \rho_{\text{max}}) = \frac{N - q}{qN} = \frac{p}{N(N-p)}.$$  \hspace{1cm} (19)

All these lengths increase with growing number $p$. Finally, pure states correspond to $|\vec{V}|^2 = (N - 1)/N$ on the large sphere.

We have shown that the space of density matrices has stratified structure. With the growth of the number of zero eigenvalues the minimal distance of the given density matrix from the maximally mixed state also increases.

4. Directional representation

In any vector space, a vector can be represented by its direction and length. This is done writing

$$\vec{V} = |\vec{V}| \vec{n},$$

with directional vector $\vec{n}$ being normalized: $\sum_{j=1}^{N^2-1} n_j^2 = 1$. Then, instead of representation (9) we can take

$$\rho = \frac{1}{N} \hat{1}_N + |\vec{V}| \vec{n} \cdot \hat{T} = \frac{1}{N} \hat{1}_N + |\vec{V}| T_{\vec{n}},$$

where $T_{\vec{n}} = \sum_{j=1}^{N^2-1} n_j T_i$. Representation (21) may be called a directional (or spherical) one. It was introduced and investigated by Kimura and Kossakowski [7]. Let us note that matrix $T_{\vec{n}}$ is hermitian and has the following properties

$$\text{Tr}\{T_{\vec{n}}\} = 0, \quad \text{Tr}\{T_{\vec{n}}^2\} = 1,$$  \hspace{1cm} (22)
which follow from the tracelessness and orthonormality of $T_j$ matrices. From the above relations it follows that matrix $T_{\vec{n}}$ possesses positive and negative eigenvalues which we will denote by $\{\mu_k\}_{k=1}^N$. They can be ordered in a natural way

$$0 < \mu_1 \geq \mu_2 \geq \ldots \geq \mu_N < 0.$$  \hspace{1cm} (23)

Subsequently, we can take the diagonal representation of the $T_{\vec{n}}$ matrix in Eq. (21). The corresponding density matrix becomes also diagonal and its matrix elements become

$$\rho_{jj} = \frac{1}{N} + |\tilde{V}|\mu_j \quad j = 1, 2, \ldots, N,$$  \hspace{1cm} (24)

which must be nonnegative. The most restrictive relation is obtained for the smallest (negative) eigenvalue $\mu_N = -|\mu_N|$ (according to (23)). Inserting this eigenvalue into relation (24) one finds that

$$|\tilde{V}| \leq \frac{1}{N|\mu_N|}.$$  \hspace{1cm} (25)

This estimate for the length of the generalized Bloch vector constitutes one of the main results of the work by Kimura and Kossakowski [7]. This is obtained here in a manner which seems to be simpler and more intuitive. Next, these authors investigated the minimal and maximal possible values of $\mu_k$. They have obtained two cases

$$\mu_1 = \mu_{max} = \sqrt{\frac{N - 1}{N}}, \quad \text{and} \quad \mu_k = -\frac{1}{\sqrt{N(N - 1)}} \quad k = 2, 3, \ldots, N.$$  \hspace{1cm} (26)

$$\mu_k = \frac{1}{\sqrt{N(N - 1)}}, \quad k = 1, 2, \ldots, N - 1 \quad \text{and} \quad \mu_N = \mu_{min} = -\sqrt{\frac{N - 1}{N}}.$$  \hspace{1cm} (27)

In the first case (26), from inequality (25) we obtain

$$|\tilde{V}| \leq \sqrt{\frac{N - 1}{N}},$$  \hspace{1cm} (28)

which is not unexpected. Next, from relations (24) and (26) we get

$$\rho_{11} = \frac{1}{N} + |\tilde{V}|\sqrt{\frac{N - 1}{N}},$$

$$\rho_{kk} = \frac{1}{N} - |\tilde{V}|\sqrt{\frac{1}{N(N - 1)}}, \quad (k = 2, \ldots, N).$$  \hspace{1cm} (29)

Allowing for maximum value of $|\tilde{V}|$ as implied by (28) we have

$$\rho_{11} = 1, \quad \rho_{kk} = 0, \quad (k = 2, \ldots, N),$$  \hspace{1cm} (30)

which corresponds to a pure state.

The second case described by eigenvalues (27) yields

$$|\tilde{V}| \leq \sqrt{\frac{1}{N(N - 1)}},$$  \hspace{1cm} (31)
so it corresponds to density matrices on or within a small sphere. Then, from relations (24) we find
\[
\rho_{kk} = \frac{1}{N} + |\vec{V}| \sqrt{\frac{1}{N(N-1)}}, \quad (k = 1, \ldots, N-1),
\]
\[
\rho_{NN} = \frac{1}{N} - |\vec{V}| \sqrt{\frac{N-1}{N}}.
\]
(32)

Taking maximum value of $|\vec{V}|$ from inequality (31) we have now
\[
\rho_{kk} = \frac{1}{N-1}, \quad (k = 1, \ldots, N-1), \quad \rho_{NN} = 0.
\]
(33)

So we arrive at a boundary state with one zero eigenvalue lying on the surface of the small sphere. This summarizes the basic results of Kimura and Kossakowski [7]. On the other hand one may ask what interesting facts can be inferred. The answer is in the antipodean properties. This will be discussed in the next section. But before doing this, let us make two additional remarks.

Firstly, we note that when inequality (25) becomes an equality then the corresponding density matrix (21) is a boundary state. Indeed, in such a case, relation (24) for $j = N$ gives $\rho_{NN} = 0$. Moreover, eigenvalue $\mu_N$ may be degenerate (see, for example (26)).

Secondly, let us construct a directional matrix $T_{\vec{n}}$ which describes the boundary state $R(q)$ (Eq.(16)). According to representation (21) we now write
\[
R(q) = \frac{1}{N} \hat{1}_N + |\vec{V}_{R(q)}| T_{\vec{n}}.
\]
(34)

Taking the length of Bloch vector as in (19) and by definition (16) we get
\[
T_{\vec{n}} = \text{diag}(\sqrt{\frac{N-q}{qN}}, \ldots, \sqrt{\frac{N-q}{qN}}, -\sqrt{\frac{N(N-q)}{N}}, \ldots, -\sqrt{\frac{N(N-q)}{N}}),
\]
(35)

as a directional matrix corresponding to the boundary state $R(q)$. Note that the first $q$ elements of this matrix are equal to $|\vec{V}_{R(q)}|$ as given in (19).

5. Antipodean properties

The antipodes are defined as follows. If a unit vector $\vec{n}$ defines certain direction, then vector $(-\vec{n})$ specifies the opposite – an antipodean direction. Therefore, if a density matrix is given by its directional representation as in (21), then its antipodean counterpart is of the form
\[
\rho_a = \frac{1}{N} \hat{1}_N + |\vec{V}| T_{-\vec{n}} = \frac{1}{N} \hat{1}_N - |\vec{V}| T_{\vec{n}},
\]
(36)
because it seems obvious that $T_{-\vec{n}} = -T_{\vec{n}}$. 
Let us consider a state $\rho_a(q)$ which is, by definition, antipodean to the boundary state $R(q)$. Thus, we can write

$$\rho_a(q) = \frac{1}{N} \hat{1}_N - |\vec{V}_a| T_{\vec{a}},$$

where $T_{\vec{a}}$ is given in (35) and $|\vec{V}_a|$ is a suitably chosen length of the Bloch vector. Thus, matrix $\rho_a(q)$ is of the form

$$\rho_a(q) = \text{diag}\left(\frac{1}{N} - |\vec{V}_a| \sqrt{\frac{N-q}{qN}}, \ldots, \frac{1}{N} + |\vec{V}_a| \sqrt{\frac{q}{N(N-q)}}, \ldots\right).$$

The requirement of positivity entails a restriction on the allowed lengths of the Bloch vector. This implies

$$|\vec{V}_a| \leq \sqrt{\frac{q}{N(N-q)}}.$$  

Taking the maximal allowed value of $|\vec{V}_a|$, from (38) we get

$$R_a(q) = \text{diag}\left(0, \ldots, 0, \frac{1}{N-q}, \ldots, \frac{1}{N-q}\right) = R(p).$$

which is antipodean with respect to the boundary state $R(q)$. We note that any matrix of the form of (38), with $|\vec{V}_a|$ satisfying inequality (39) is antipodean to $R(q)$, while $R_a(q) = R(p)$ given by Eq.(40) is the one most distant from the center, that is from the maximally mixed state $\rho_{\text{max}}$.

This is a generalization of the conclusions derived by Kimura and Kossakowski [7] from the sets (26) and (27) of the eigenvalues of directional matrices. These two sets (up to numbering) clearly correspond to antipodal directions. In one direction there is a pure state ($p = N - 1$ or $q = 1$) while in the opposite one we find at most the state (33) with $p = 1$ or $q = N - 1$.

6. Final remarks

We have shown that in the space of $N \times N$-dimensional density matrices there are concentric spheres $S_p$ (centered at the maximally mixed state) with increasing radii $r_p = \sqrt{p/N(N-p)}$. These spheres characterize the stratification of boundary states $\rho_p$ with $p$ zero eigenvalues. States $\rho_p$ lie on the surface $S_p$ or outside them. We have also shown, that only special boundary states $R(q = N - p)$ defined in (16) are on $S_p$. When a density matrix possesses $q = N - p$ nonzero and unequal eigenvalues it must be outside the sphere $S_p$. The states situated inside spheres $S_p$ have less than $p$ zero eigenvalues, perhaps even none (all nonzero). In particular, $p = 1$ corresponds to a small sphere which contains only those density matrices which have all nonzero eigenvalues. Conversely, $p = N - 1$ correspond to pure states which lie only on the surface of the
large sphere. This shows that the space of density matrices has a complex stratified structure.

The complexity of this structure is amplified by antipodean properties. If we assume that in a certain direction $\vec{n}$ we have a boundary state $R(q)$, then in the antipode the corresponding density matrix $\rho_a(q)$ is given by expression (38). As long as the Bloch vector $\vec{V}_a$ has the length satisfying the sharp inequality (39) we may expect that $\rho_a(q)$ has all nonzero eigenvalues. When (39) becomes an equality, the antipodal matrix $\rho_a(q)$ attains the form of a boundary state $R(p = N - q)$ as given by Eq.(40). So the point $R(q = N - p)$ on the surface $S_p$ corresponds to the antipodean point $R(p = N - q)$ on the surface $S_q$.

As yet, we are not fully aware what are potential consequences of the presented stratification of the space of $N \times N$ dimensional density matrices. Nevertheless, we feel that our findings are interesting and deserving further investigations.

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