Geometry for separable states and construction of entangled states with positive partial transposes

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We construct faces of the convex set of all $2 \otimes 4$ bipartite separable states, which are affinely isomorphic to the simplex Δ_9 with 10 extreme points. Every interior point of these faces is a separable state which has a unique decomposition into 10 product states, even though the ranks of the state and its partial transpose are 5 and 7, respectively. We also note that the number 10 is greater than 2×4 , to disprove a conjecture on the lengths of qubit-qudit separable states. This face is inscribed in the corresponding face of the convex set of all PPT states so that subsimplices Δ_k of Δ_9 share the boundary if and only if $k \leq 5$. This enables us to find a large class of $2 \otimes 4$ PPT entangled edge states with rank 5.

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I. INTRODUCTION

One of the fundamental question in the theory of quantum entanglement is how to distinguish and construct entangled states. Even though the Positive Partial Transpose (PPT) criterion [1,2] gives us a simple and powerful necessary condition for separability together with the range criterion [3], it is not clear how to distinguish entanglement satisfying these two criteria. One possible way to overcome this difficulty is to compare the geometries for separable states and PPT states, as suggested in a recent work [4].

We note that the set of all separable states (with respect to PPT states) makes a convex set, which is denoted by \mathbb{S} (with respect to \mathbb{T}). In order to understand the geometry of a convex set, we need to characterize the facial structures. The facial structures for the convex set \mathbb{T} are relatively well understood [5]. It is also known [6] that a given PPT state ϱ satisfies the range criterion if and only if the face of \mathbb{T} determined by ϱ has a separable state in its interior. If we understand the facial structures of the corresponding face of \mathbb{S} , then it is easy to distinguish and construct entangled states within the face of \mathbb{T} . This is the case when the corresponding face of \mathbb{S} is affinely isomorphic to a simplex.

The authors [4] exploited this idea for the $3 \otimes 3$ case, to construct faces of \mathbb{S} which are isomorphic to the simplex Δ_5 with six extreme points and to understand how PPT entangled edge states of rank 4 arise. This construction also gives examples of separable states whose lengths are greater than the maximum of ranks of themselves and their partial transposes. The main idea was to begin with generic five-dimensional subspaces of $\mathbb{C}^3 \otimes \mathbb{C}^3$ which have six product vectors and exploit the fact that the number of product vectors is greater than the dimension.

In this paper, we pursue the same idea for the 2 \otimes 4 case, which is the smallest dimension in which PPT entangled states arise. But the above idea for the 3 \otimes 3 case does not work for this case, because the number *d* is the dimension for generic subspaces of $\mathbb{C}^2 \otimes \mathbb{C}^d$ with finitely many product vectors, and generic *d*-dimensional subspaces have just *d* product vectors.

To overcome this difficulty, we consider the equation

$$|x \otimes y\rangle \in D, \quad |\bar{x} \otimes y\rangle \in E$$
 (1)

for a given pair (D, E) of subspaces of $\mathbb{C}^2 \otimes \mathbb{C}^4$, where $|x \otimes y\rangle := |x\rangle \otimes |y\rangle$ and $|\bar{x}\rangle$ denotes the conjugate of $|x\rangle$. We construct five-dimensional spaces *D* and seven-dimensional spaces *E*, for which the above equations have exactly 10 solutions. This enables us to construct faces of S isomorphic to the simplex Δ_9 with 10 extreme points.

Any interior point of the face Δ_9 is a separable state with a unique decomposition into 10 product states and has the length 10. This disproves the conjecture [7] which claims that lengths of $2 \otimes d$ separable states are at most $2 \times d$. We note that this conjecture has been proved [8] recently for d = 3. We recall that a PPT state ρ is of type (p,q) if the ranks of ρ and ρ^{Γ} are p and q, respectively. We also note that the boundary of this face Δ_9 consists of simplices Δ_k with k + 1 extreme points, for $k \leq 8$. By the construction, every interior point of the face Δ_9 is a separable state of type (5,7). We show that any choice of 7 product vectors $|\bar{x} \otimes y\rangle$ among 10 solutions are linearly independent. From this, we conclude that if a boundary point ϱ_1 of Δ_9 is in the interior of Δ_k with $6 \leq k \leq 8$ then the line segment from an interior point ρ_0 of Δ_9 to ρ_1 can be extended within the convex set \mathbb{T} , to get PPT entangled states of rank five. For known examples of $2 \otimes 4$ PPT entangled states, see [3] and [9].

In the next section, we briefly review the material behind the above idea we have just explained, and in Sec. III we give the construction.

II. BACKGROUND

A density matrix ρ in the tensor product $M_m \otimes M_n$ of matrix algebras is said to be separable if it is the convex combination of product states, and so it is of the form

$$\varrho = \sum_{i=1}^{k} \lambda_i |x_i \otimes y_i\rangle \langle x_i \otimes y_i |, \qquad (2)$$

with unit product vectors $|x_i \otimes y_i\rangle$ in the space $\mathbb{C}^m \otimes \mathbb{C}^n$ and positive numbers λ_i with $\sum_{i=1}^k \lambda_i = 1$. A nonseparable state is called entangled. Because the partial transpose ρ^{Γ} of state

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 ρ in (2) is given by

$$\varrho^{\Gamma} = \sum_{i=1}^{k} \lambda_i |\bar{x}_i \otimes y_i\rangle \langle \bar{x}_i \otimes y_i |,$$

we see that the partial transpose of a separable state is also positive. This is the PPT criterion [1,2]. Furthermore, we also see that if ρ is separable, then there must exist product vectors $|x_i \otimes y_i\rangle$ satisfying

$$\mathcal{R}\varrho = \operatorname{span}\{|x_i \otimes y_i\rangle\}, \quad \mathcal{R}\varrho^{\Gamma} = \operatorname{span}\{|\bar{x}_i \otimes y_i\rangle\}, \quad (3)$$

as the range criterion [3] says, where $\mathcal{R}\rho$ denotes the range space of state ρ .

A convex subset F of a convex set C is said to be a face if it satisfies the following condition: If a point in F is a convex combination of two points in C, then they must be points of F. A face consisting of a single point is called an extreme point. A point x in a convex set C is said to be an interior point of C if it is an interior point of C with respect to the relative topology of the affine manifold generated by C. It is well known that every convex set is completely partitioned into interiors of faces. In this sense, a point x in a convex set determines a unique face in which x is an interior point. This is the smallest face containing x. A point of C is called a boundary point if it is not an interior point.

Any face of \mathbb{T} is determined [5] by a pair (D, E) of subspaces of $\mathbb{C}^m \otimes \mathbb{C}^n$ and is of the form

$$f(D,E) = \{ \varrho \in \mathbb{T} : \mathcal{R}\varrho \subset D, \, \mathcal{R}\varrho^1 \subset E \}.$$

Conversely, the set $\tau(D, E)$ is a face unless it is empty. The interior of $\tau(D, E)$ is given by

int
$$\tau(D, E) = \{ \varrho \in \mathbb{T} : \mathcal{R} \varrho = D, \mathcal{R} \varrho^{\Gamma} = E \}.$$

It was also shown in [6] that a PPT state ρ satisfies the range criterion if and only if the interior of the face $\tau(D, E)$ of \mathbb{T} determined by ρ has a separable state. In this case, the face $\mathbb{S} \cap \tau(D, E)$ of \mathbb{S} shares interior points with the face $\tau(D, E)$ of \mathbb{T} . Therefore, it is crucial to understand the facial structures of $\mathbb{S} \cap \tau(D, E)$ in order to determine whether or not ρ is separable.

A study of facial structures of S was initiated by Alfsen and Schultz [10], where they searched for faces of S which are affinely isomorphic to a simplex. Suppose that a convex set C is on the hyperplane of codimension 1 in the (d + 1)-dimensional real vector space which does not contain the origin. Then C is a simplex if and only if it is the convex hull of d + 1 linearly independent points on the hyperplane. This simplex is denoted by Δ_d . Therefore, if a separable state in (2) determines a face, then it is isomorphic to a simplex if and only if the product states in the expression are linearly independent in the real vector space of Hermitian matrices. For further progress on the facial structures of separable states, see [4], [6], and [11–13]. The length of the separable state ρ is defined by the smallest number k with which expression (2) is possible. It is clear that if a separable state determines the face isomorphic to the simplex Δ_k , then it has the length k + 1.

Now we are ready to explain the main idea of the construction in the next section. We construct a five-dimensional space D and a seven-dimensional space E of $\mathbb{C}^2 \otimes \mathbb{C}^4$ and show the following: (i) Equation (1) has exactly 10 solutions.

(ii) The corresponding 10 product states are linearly independent.

(iii) Any choice of five product vectors $|x \otimes y\rangle$ spans the space *D*.

(iv) Any choice of seven product vectors $|\bar{x} \otimes y\rangle$ spans the space *E*.

We conclude that the face $\tau(D, E)$ has a separable state in the interior by (iii) and (iv), and the face $\tau(D, E) \cap S$ is affinely isomorphic to the simplex Δ_9 by (i) and (ii).

We take an interior point ρ_0 in the face $\tau(D, E) \cap \mathbb{S}$, which is denoted just Δ_9 and take a boundary point ρ_1 which determines the face isomorphic to Δ_k with $k \leq 8$. This means that ρ_1 is the convex combination of k + 1 product states. Consider $\rho_t = (1 - t)\rho_0 + t\rho_1$ for t > 1. If $k + 1 \leq 6$, then $\mathcal{R}\rho_1^{\Gamma}$ is a proper subspace of $\mathcal{R}\rho_0^{\Gamma}$, and so we see that ρ_t is never positive for t > 1. If $k + 1 \geq 7$, then we see that the range spaces of ρ_0 and ρ_1 coincide by (iii), and the same for the range spaces of ρ_0^{Γ} and ρ_1^{Γ} by (iv). Therefore, we see that there exist t > 1 such that ρ_t is of PPT. It is clear that this is an entangled state. If we take the largest t such that ρ_t is of PPT, then ρ_t is of type (p,q) with p < 5 or q < 7. But it is not possible to have p < 5 by [14], because ρ_t is an entangled state. Therefore, we conclude that ρ_t is of type (5,5) or (5,6).

III. CONSTRUCTION

Let *D* be the five-dimensional subspace of $\mathbb{C}^2 \otimes \mathbb{C}^4$ which is orthogonal to the following three vectors:

$$|v_1\rangle = (0,1,0,0,-1,0,0,0)^{t}, |v_2\rangle = (0,0,1,0,0,-1,0,0)^{t}, |v_3\rangle = (0,0,0,1,0,0,-1,0)^{t}.$$

We note that these three vectors span a completely entangled space which has no product vectors. It is easy to see that every product vector $|z\rangle = |x\rangle \otimes |y\rangle$ in space *D* is one of the following forms:

$$|z_1\rangle = (0,1)^t \otimes (0,0,0,1)^t, \quad |z(\alpha)\rangle = (1,\alpha)^t \otimes (1,\alpha,\alpha^2,\alpha^3)^t$$
(4)

for a complex number α . Note that the partial conjugate of $|z(\alpha)\rangle$, which is denoted $|\bar{z}(\alpha)\rangle$, is given by

$$\begin{aligned} |\bar{z}(\alpha)\rangle &= (1,\bar{\alpha})^{\mathsf{t}} \otimes (1,\alpha,\alpha^2,\alpha^3)^{\mathsf{t}} \\ &= (1,\alpha,\alpha^2,\alpha^3,\bar{\alpha},|\alpha|^2,|\alpha|^2\alpha,|\alpha|^2\alpha^2)^{\mathsf{t}}. \end{aligned}$$

For given real numbers *a* and *b* with the relation $0 < b < 4a^3/27$, we consider the vector

$$|w\rangle = (b,0,0,1,0,-a,0,0)^{t},$$
 (5)

and let *E* be the *seven*-dimensional subspace of $\mathbb{C}^2 \otimes \mathbb{C}^4$ orthogonal to the vector $|w\rangle$.

Now, we proceed to solve Eq. (1) for the above *D* and *E*. We note that the partial conjugate of $|z_1\rangle$ belongs to *E*, and so $|z_1\rangle$ is a solution. In order to find complex numbers α so that $|z(\alpha)\rangle$ is a solution, we solve the equation $\langle \overline{z}(\alpha) | w \rangle = 0$; that is,

$$b + \alpha^3 - a|\alpha|^2 = 0.$$
 (6)

We first note that α^3 must be a real number, and so we have $\alpha = re^{i\theta}$ with $3\theta = n\pi$ and r > 0. If *n* is an even integer, then Eq. (6) is reduced to

$$r^3 - ar^2 + b = 0,$$

and we get two distinct positive roots, r_1 and r_2 , from the condition $0 < b < 4a^3/27$. In the case of an odd integer *n*, we get one positive root r_3 of the equation $r^3 + ar^2 - b = 0$ by the same condition. We also note that r_1 , r_2 , r_3 are mutually distinct. Therefore, we have the following nine solutions of the equation (6):

$$r_1, r_1\omega, r_1\omega^2, r_2, r_2\omega, r_2\omega^2, -r_3, -r_3\omega, -r_3\omega^2,$$
 (7)

where ω is the third root of unity. For the notational convenience, we rewrite the normalizations of the product vectors $|z(\alpha)\rangle$ in (4) for the above nine α 's by $|z(\alpha_i)\rangle$ for i = 2, 3, ..., 10.

In order to show item (ii) from the last section, suppose that

$$a_1|z_1\rangle\langle z_1| + \sum_{i=2}^{10} a_i|z(\alpha_i)\rangle\langle z(\alpha_i)| = O,$$

where *O* is the 8×8 zero matrix. Note that $|z(\alpha)\rangle\langle z(\alpha)|$ is given by

 $|z(\alpha)\rangle\langle z(\alpha)|$

$$= \begin{pmatrix} 1 & \bar{\alpha} & \bar{\alpha}^2 & \bar{\alpha}^3 & \bar{\alpha} & \bar{\alpha}^2 & \bar{\alpha}^3 & \bar{\alpha}^4 \\ \alpha & |\alpha|^2 & & \cdots & & |\alpha|^2 \bar{\alpha}^3 \\ \vdots & \vdots & & \ddots & & \vdots \\ \alpha^4 & |\alpha|^2 \alpha^3 & & \cdots & & |\alpha|^8 \end{pmatrix},$$

which is an 8 × 8 matrix. Therefore, we get 64 linear equations with respect to a_i (i = 1, 2, ..., 10) by comparing the entries on both sides. If we write

$$C = \begin{pmatrix} 0 & 1 & 1 & \cdots & 1 & 1 \\ 0 & \bar{\alpha}_2 & \bar{\alpha}_3 & \cdots & \bar{\alpha}_9 & \bar{\alpha}_{10} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & |\alpha_2|^6 & |\alpha_3|^6 & \cdots & |\alpha_9|^6 & |\alpha_{10}|^6 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & |\alpha_2|^8 & |\alpha_3|^8 & \cdots & |\alpha_9|^8 & |\alpha_{10}|^8 \end{pmatrix},$$

which is a 64 × 10 matrix, and $A = (a_1, a_2, ..., a_{10})^t$, then we have the equation

$$CA = O.$$

We note that entries in the first column in C are all 0 except the last entry. Since we have

$$|\alpha_i|^8 = a^2 |\alpha_i|^6 - 2ab|\alpha_i|^4 + b^2 |\alpha_i|^2, \quad i = 2, 3, \dots, 10$$

from Eq. (6), we can conclude that the row vector $(0, |\alpha_2|^8, |\alpha_3|^8, ..., |\alpha_{10}|^8)$ is the linear combination of three rows of the above matrix *C*. Therefore, we have $a_1 = 0$. Since any nine product states corresponding to the nine product vectors are linearly independent by Proposition 2.2 in [4], we have $a_2 = a_3 = \cdots = a_{10} = 0$. Proposition 2.1 of [4] also tells

us that any choice of 5 product vectors among 10 solutions is linearly independent.

It remains to show item (iv) from the last section. Without loss of generality, it suffices to consider the following five cases:

$$\{|z_1\rangle, |z(r_1)\rangle, |z(r_1\omega)\rangle, |z(r_1\omega^2)\rangle, |z(r_2)\rangle, |z(r_2\omega)\rangle, |z(r_2\omega^2)\rangle\}, \\ \{|z_1\rangle, |z(r_1)\rangle, |z(r_1\omega)\rangle, |z(r_1\omega^2)\rangle, |z(r_2)\rangle, |z(r_2\omega)\rangle, |z(-r_3)\rangle\}, \\ \{|z_1\rangle, |z(r_1)\rangle, |z(r_1\omega)\rangle, |z(r_2)\rangle, |z(r_2\omega)\rangle, |z(-r_3)\rangle, |z(-r_3\omega)\rangle\}, \\ \{|z(r_1)\rangle, |z(r_1\omega)\rangle, |z(r_1\omega^2)\rangle, |z(r_2)\rangle, |z(r_2\omega)\rangle, |z(r_2\omega^2)\rangle, |z(r_3)\rangle\}, \\ \{|z(r_1)\rangle, |z(r_1\omega)\rangle, |z(r_1\omega^2)\rangle, |z(r_2)\rangle, |z(r_2\omega)\rangle, |z(r_3)\rangle, |z(r_3\omega)\rangle\}.$$

For each case, we form the 7×8 matrix whose rows are given by the seven product vectors identified with row vectors in \mathbb{C}^8 . Then, in any case, it is easy to see that the reduced row echelon form of the matrix is given by

(1)	0	0	0	0	b/a	0	0)
0	1	0	0	0	0	0	0
0	0	1	0	0	0	0	0
0	0	0	1	0	1/a	0	0
0	0	0	0	1	0	0	0
0	0	0	0	0	0	1	0
0	0	0	0	0	0	0	1/

Therefore, for any choice of 7 product vectors among 10 solutions, we see that the corresponding 7 partial conjugates are linearly independent, and so they span the space E.

Finally, we illustrate the above discussion with an explicit example. We consider the case where a = 2 and b = 1 in (5). From the equation $r^3 - 2r^2 + 1 = 0$, we get two positive solutions, $r_1 = 1$ and $r_2 = (1 + \sqrt{5})/2$. We also get one positive solution, $r_3 = (\sqrt{5} - 1)/2$, from the equation $r^3 + 2r^2 - 1 = 0$.



FIG. 1. In both graphs, each curve represents distinct eigenvalues. (a) $\lambda_i(t)$'s are the eigenvalues of ρ_t . (b) $\mu_i(t)$'s are the eigenvalues of ρ_t^{Γ} . The thick line denotes the smallest eigenvalue of ρ_t^{Γ} except 0. So, the rank of ρ_v is 5 and the rank of ρ_v^{Γ} is 6.

By a direct computation, we have an interior point ρ_0 of Δ_0 :

$$\begin{split} & \overset{\Lambda_9:}{\varrho_0} = \frac{1}{10} \left(|z_1\rangle \langle z_1| + \sum_{i=2}^{10} |z(\alpha_i)\rangle \langle z(\alpha_i)| \right) \\ & = \frac{1}{400} \begin{pmatrix} 71 & 0 & 0 & 7 & 0 & 0 & 7 & 0 \\ 0 & 39 & 0 & 0 & 39 & 0 & 0 & 23 \\ 0 & 0 & 31 & 0 & 0 & 31 & 0 & 0 \\ 7 & 0 & 0 & 39 & 0 & 0 & 39 & 0 \\ 0 & 39 & 0 & 0 & 39 & 0 & 0 & 23 \\ 0 & 0 & 31 & 0 & 0 & 31 & 0 & 0 \\ 7 & 0 & 0 & 39 & 0 & 0 & 39 & 0 \\ 0 & 23 & 0 & 0 & 23 & 0 & 0 & 111 \end{pmatrix}, \end{split}$$

where $|z(\alpha_i)\rangle$ is the normalized product vectors with α_i 's in (7). We consider the eight-simplex Δ_8 determined by these nine product vectors $|z(\alpha_i)\rangle$'s. An interior point ρ_1 of this face is given by

$$\begin{split} \varrho_1 &= \frac{1}{9} \sum_{i=2}^{10} |z(\alpha_i)\rangle \langle z(\alpha_i)| \\ &= \frac{1}{360} \begin{pmatrix} 71 & 0 & 0 & 7 & 0 & 0 & 7 & 0 \\ 0 & 13 & 0 & 0 & 13 & 0 & 0 & 23 \\ 0 & 0 & 31 & 0 & 0 & 31 & 0 & 0 \\ 7 & 0 & 0 & 13 & 0 & 0 & 13 & 0 \\ 0 & 13 & 0 & 0 & 13 & 0 & 0 & 23 \\ 0 & 0 & 31 & 0 & 0 & 31 & 0 & 0 \\ 7 & 0 & 0 & 13 & 0 & 0 & 13 & 0 \\ 0 & 23 & 0 & 0 & 23 & 0 & 0 & 71 \end{pmatrix}. \end{split}$$

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We put $\rho_t = (1 - t)\varrho_0 + t\varrho_1$ and explore eigenvalues of ρ_t and ρ_t^{Γ} (see Fig. 1). We denote by $\lambda_i(t)$ and $\mu_i(t)$ the eigenvalues of ρ_t and ρ_t^{Γ} , respectively. Then we see that there exist $\nu \approx 1.48192$ so that ρ_{ν} is on the boundary of the face $\tau(D, E)$, which is a PPT entangled edge state of type (5,6). We note that ρ_t is a PPT entangled state of type (5,7) for $1 < t < \nu$.

IV. CONCLUSION

In this paper, we have constructed faces of the convex set of all $2 \otimes 4$ separable states, which are isomorphic to the simplex Δ_9 . The boundary of this face consists of simplices Δ_k with $k \leq 8$. Note that the number of faces isomorphic to Δ_k is $_{k+1}^{10}$. The discussion in Sec. II tells us that the interior of Δ_k is located in the interior of the face $\tau(D, E)$ if and only if $k \ge 6$. If $k \le 5$, then Δ_k is located on the boundary of $\tau(D, E)$. Since every interior point of Δ_5 is a separable state of type (5,6), it is very plausible that the boundary point ϱ_t of $\tau(D, E)$ is also of type (5,6). Actually, we got a PPT entangled state of type (5,6) in the last numerical examples. It is clear that the PPT entangled states which are located on the boundary of the face $\tau(D, E)$ must be edge states, but it is not clear whether or not they are extreme. It would be interesting if we could get PPT entangled states of type (5,5) by a similar construction.

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