PROBABILITY
AND
MATHEMATICAL STATISTICS
Vol. 33, Fasc. 2 (2013), pp. 385–400

FACES FOR TWO-QUBIT SEPARABLE STATES AND THE CONVEX HULLS OF TRIGONOMETRIC MOMENT CURVES

BY

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Abstract. We analyze the facial structures of the convex set consisting of all two-qubit separable states. One of the faces is a four-dimensional convex body generated by the trigonometric moment curve arising from polyhedral combinatorics. Another one is an eight-dimensional convex body, which is the convex hull of a homeomorphic image of the two-dimensional sphere. Extreme points consist of points on the surface, and any two of them determine an edge. We also reconstruct the trigonometric moment curve in any even-dimensional affine space using the qubit-qudit systems, and characterize the facial structures of the convex hull.

2000 AMS Mathematics Subject Classification: Primary: 81P16, 52B11, 15A30, 46L30.

Key words and phrases: Separable state, entanglement, trigonometric moment curve, face, extreme point.

1. INTRODUCTION

Let M_n denote the C^*-algebra of all $n \times n$ matrices over the complex field. A state on M_n is a unital positive linear functional on M_n, and is represented by a density matrix which is a positive semidefinite matrix with trace one. A state on the tensor product $M_m \otimes M_n = M_{mn}$ is said to be *separable* if it is the convex sum of rank one projections onto simple tensors of the form $x \otimes y \in \mathbb{C}^m \otimes \mathbb{C}^n$, which are called *product vectors*. A state which is not separable is said to be *entangled*. The notion of entanglement arising from quantum mechanics turns out to be very useful in the current quantum information and quantum communication theory.

The convex structures for the convex set $\mathbb{S}_{m\times n}$ of all separable states on $M_m \otimes M_n$ are highly nontrivial, and have begun to be studied very recently. See [1], [2], [6], [7], [11], [12], for examples. For the simplest case of $m = n = 2$, all faces of the convex set $\mathbb{S}_{2\times 2}$ have been classified in [10]. The first purpose of this note is to analyze convex sets arising as faces of $\mathbb{S}_{2\times 2}$, and to report relations with polyhedral combinatorics. The convex set $\mathbb{S}_{2\times 2}$ itself is a 15-dimensional convex body whose

* Partially supported by NRF 2009-0083521 funded by MSIP.

extreme points are parameterized by the 4-dimensional manifold $\mathbb{CP}^1 \times \mathbb{CP}^1$. Two extreme points represented by (x, y) and (z, w) on the manifold make an edge if and only if $x \neq y$ and $z \neq w$. Otherwise, they determine a face of $\mathbb{S}_{2\times 2}$ which is affinely isomorphic to the three-dimensional solid sphere whose extreme points are parameterized by just $\mathbb{CP}^1$.

There are two kinds of maximal faces. One kind of them consists of eight-dimensional convex sets whose extreme points are parameterized by two-dimensional sphere $\mathbb{CP}^1$. The convex combination of any two extreme points is an edge. If we take three extreme points, then the corresponding points on the sphere determine a circle. It turns out that this circle determines a maximal face of the maximal face, and is four-dimensional. In this way, we have an embedding of the circle into the four-dimensional convex body C^4 with the following property: A point of C^4 is an extreme point if and only if it is on the image of the circle, and any two extreme points make an edge. This embedding is exactly the trigonometric moment curve studied in polyhedral combinatorics.

The moment curve had been studied in [9] to realize four-dimensional polytopes with the property that convex combinations of any two extreme points are edges. It was shown that any finite distinct points on the moment curve

$$(t, t^2, r^3, \dots, t^{2p}) \in \mathbb{R}^{2p}, \qquad t \in \mathbb{R},$$

give rise to a convex body, called a *cyclic polytope*, with the property that any choice of p extreme points makes a face. The trigonometric moment curve

$$(\cos t, \sin t, \cos 2t, \sin 2t, \dots, \cos pt, \sin pt) \in \mathbb{R}^{2p}, \qquad t \in [0, 2\pi), \tag{1.1}$$

has the same property. The convex hull, denoted by C^{2p}, of the whole trigonometric moment curve has been studied in [22] for the case of $p = 2$. Extreme points of C^4 are those on the curve, and the convex hull of any two extreme points is an edge. There are no more nontrivial faces of C^4. The convex hull of the moment curve has been studied in [20].

The second purpose of this note is to investigate the convex structures for the convex hull C^{2p} of trigonometric moment curve, in terms of separable states, for arbitrary $p = 3, 4, \dots$ We show that C^{2p} arises as a face of the convex set $\mathbb{S}_{2\times p}$, and has the similar property to that of C^4. It is possible to express any point in C^{2p} by the convex combination of k extreme points with $k \leqslant p + 1$, and it is an interior point of C^{2p} if and only if we need $p + 1$ extreme points for the expression. We can also characterize elements of the convex body C^{2p} in $\mathbb{C}^p$ by a finite set of inequalities involving p complex variables. The convex hull of the trigonometric moment curve has been studied in [3], [21], [23], and parts of the above-mentioned results might be known to combinatorial theorists. See also Chapter 6 of [14].

In the next section we briefly review the classification of faces of the convex set $\mathbb{S}_{2\times 2}$, and in Section 3 we consider the intersections of maximal faces.

We examine four-dimensional faces of $\mathbb{S}_{2\times 2}$ in Section 4 to recover various moment and trigonometric moment curves for the case of $p = 2$. In the final section, we construct the trigonometric moment curve for arbitrary $p = 1, 2, 3, \dots$, which generates a face of the convex set $\mathbb{S}_{2\times p}$. With this machinery, we characterize the whole facial structure of the convex hull generated by the trigonometric moment curve. Throughout this note, we will identify vectors of the vector space $\mathbb{C}^2$ and points of $\mathbb{CP}^1$. Two points x and y of $\mathbb{CP}^1$ coincide if and only if they are parallel to each other, $x \parallel y$ in notation, as vectors in $\mathbb{C}^2$.

The author is grateful to Lin Chen, Kil-Chan Ha, and Woong Kook for useful comments on the draft.

2. FACES

For $\varrho = \varrho_1 \otimes \varrho_2 \in M_m \otimes M_n$, we define the partial transpose ϱ^Γ by $\varrho^\Gamma = \varrho_1^{\rm t} \otimes \varrho_2$, where $\varrho_1^{\rm t}$ denotes the usual transpose of ϱ_1. This operation can be extended to the whole $M_m \otimes M_n$. It was observed by Choi [8] and rediscovered by Peres [19] that if ϱ is separable, then ϱ^Γ is still positive semidefinite. In other words, we have $\mathbb{S}_{m\times n} \subset \mathbb{T}_{m\times n}$, if we denote by $\mathbb{T}_{m\times n}$ the set of all states ϱ on $M_m \otimes M_n$ with positive semidefinite partial transposes ϱ^Γ. It was also shown in [8], [13], and [24] that $\mathbb{S}_{m\times n} = \mathbb{T}_{m\times n}$ if and only if $mn \leqslant 6$. We exploit this result to investigate the structures of $\mathbb{S}_{2\times 2} = \mathbb{T}_{2\times 2}$.

It was shown in [10] that every face of $\mathbb{T}_{m\times n}$ is determined by a pair (D, E) of subspaces in $\mathbb{C}^m \otimes \mathbb{C}^n$, and is of the form

$$\tau(D, E) = \{\varrho \in \mathbb{T}_{m\times n} : \mathcal{R}\varrho \subset D,\ \mathcal{R}\varrho^\Gamma \subset E\},$$

where $\mathcal{R}\varrho$ denotes the range space of ϱ. The pair (D, E) is uniquely determined if we require that D and E are minimal. It is very difficult in general to characterize pairs (D, E) for which $\tau(D, E)$ is nonempty. In the case of $\mathbb{S}_{2\times 2}$, we have the complete list [10] of such pairs. We will identify a vector $(a, b, c, d) \in \mathbb{C}^2 \otimes \mathbb{C}^2$ with the 2×2 matrix by

$$(a, b, c, d) \leftrightarrow \begin{pmatrix} a & b \\ c & d \end{pmatrix}. \tag{2.1}$$

In this way, we can say about the rank of a vector in $\mathbb{C}^2 \otimes \mathbb{C}^2$. A vector in $\mathbb{C}^2 \otimes \mathbb{C}^2$ is a product vector if and only if it is of rank one. In the following, we list up all faces of the convex set $\mathbb{S}_{2\times 2}$, where two natural numbers in the subscripts denote $\dim D$ and $\dim E$ for $\tau(D, E)$, respectively.

- $G_{4,4}$: the full convex set $\mathbb{S}_{2\times 2}$.
- $G_{3,4}(V) = \tau(V^\perp, \{0\}^\perp)$, with a rank two vector $V \in \mathbb{C}^2 \otimes \mathbb{C}^2$.
- $G_{4,3}(W) = \tau(\{0\}^\perp, W^\perp)$, with a rank two vector $W \in \mathbb{C}^2 \otimes \mathbb{C}^2$.
- $H_{3,3}(x, y) = \tau\big((x \otimes y)^\perp, (\bar{x} \otimes y)^\perp\big)$, with $x, y \in \mathbb{C}^2$.

• $G_{3,3}(V, W) = \tau(V^{\perp}, W^{\perp})$, with rank two vectors $V, W \in \mathbb{C}^2 \otimes \mathbb{C}^2$ with a suitable relation, which will be given in the next section.

• $H_{2,2}(x, y, z, w) = \tau(\text{span}\,\{x \otimes y, z \otimes w\}, \text{span}\,\{\bar{x} \otimes y, \bar{z} \otimes w\})$, with $x, y, z,$ and w in $\mathbb{C}^2$ satisfying $x \parallel z$ or $y \parallel w$.

• $G_{2,2}(x, y, z, w) = \tau(\text{span}\,\{x \otimes y, z \otimes w\}, \text{span}\,\{\bar{x} \otimes y, \bar{z} \otimes w\})$, with $x, y, z,$ and w in $\mathbb{C}^2$ satisfying $x \nparallel z$ and $y \nparallel w$.

• $G_{1,1}(x, y) = \tau(\text{span}\,\{x \otimes y\}, \text{span}\,\{\bar{x} \otimes y\})$, with $x, y \in \mathbb{C}^2$.

We note that $G_{1,1}(x, y)$ is an extreme point of $\mathbb{S}_{2\times 2}$ which is nothing but the rank one projection $P_{x\otimes y}$ onto a unit product vector $x \otimes y$. The face $G_{2,2}(x, y, z, w)$ is an edge which is the convex hull of two extreme points $G_{1,1}(x, y)$ and $G_{1,1}(z, w)$. On the other hand, $G_{3,4}(V)$, $G_{4,3}(W)$, and $H_{3,3}(x, y)$ are maximal faces.

For $V \in \mathbb{C}^2 \otimes \mathbb{C}^2$, we note that $P_{x\otimes y} \in G_{3,4}(V)$ if and only if $x \otimes y \perp V$ if and only if $x \perp V\bar{y}$. Here, we consider V as a 2×2 matrix by (2.1), and $\bar{y}$ denotes the vector whose entries are given by the complex conjugates of the corresponding entries. We also note that $x \perp V\bar{y}$ if and only if $(VW^{-1})^* x \perp W\bar{y}$. Therefore, the affine isomorphism

$$\varrho \mapsto \big((VW^{-1})^* \otimes I_2\big)\varrho\big((VW^{-1}) \otimes I_2\big)$$

sends the face $G_{3,4}(V)$ onto the face $G_{3,4}(W)$, where $I_2 = (1, 0, 0, 1) \in \mathbb{C}^2 \otimes \mathbb{C}^2$. The operation of partial transpose sends $G_{3,4}(V)$ onto $G_{4,3}(V)$. Therefore, all the faces of types $G_{3,4}$ and $G_{4,3}$ are affinely isomorphic to each other. For given $x, y, z, w \in \mathbb{C}^2$, take nonsingular matrices V and W with $Vz = x$ and $Ww = y$. Then we see that the affine isomorphism

$$\varrho \mapsto (V^* \otimes W^*)\varrho(V \otimes W)$$

maps the face $H_{3,3}(x, y)$ onto the face $H_{3,3}(z, w)$.

Now, we find extreme points for a given maximal face (see Figure 1). We first note that all extreme points are parameterized by the four-dimensional manifold $\mathbb{CP}^1 \times \mathbb{CP}^1$. We see that an extreme point $G_{1,1}(z, w)$ belongs to the face $H_{3,3}(x, y)$ if and only if $x \perp z$ or $y \perp w$. Therefore, extreme points of the face $H_{3,3}(x, y)$ are parameterized by the union of two $\mathbb{CP}^1$'s in $\mathbb{CP}^1 \times \mathbb{CP}^1$. On the other hand, we see that extreme points of the face $G_{3,4}(V)$ are parameterized by $\mathbb{CP}^1$. Indeed, for each $z \in \mathbb{CP}^1$, there is a unique $w \in \mathbb{CP}^1$ such that $z \perp V\bar{w}$, and so $P_{z\otimes w} \in G_{3,4}(V)$.

3. INTERSECTION OF MAXIMAL FACES

In this section, we consider intersections of maximal faces. We recall [10] that every face of $\mathbb{T}_{m,n}$ is exposed, and so it is the intersection of a family of maximal faces. It is clear that the intersection of any two maximal faces of the form $H_{3,3}$ has two or infinitely many extreme points. The intersection $H_{3,3}(x, y) \cap H_{3,3}(z, w)$ has infinitely many extreme points if and only if $x = z$ or $y = w$ as

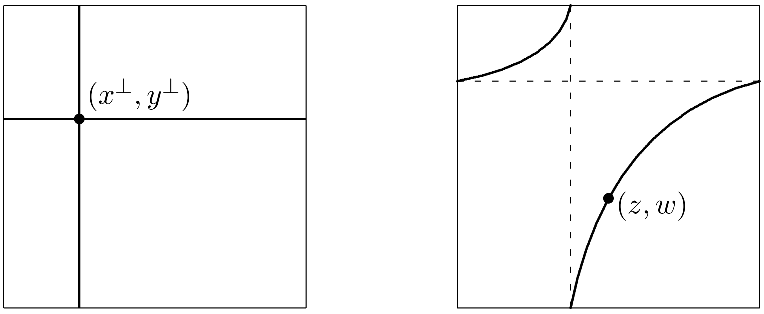

FIGURE 1. Points of $\mathbb{CP}^1 \times \mathbb{CP}^1$ whose associated extreme points belong to the faces $H_{3,3}(x, y)$ and $G_{3,4}(V)$. Both horizontal and vertical axes represent $\mathbb{CP}^1$

elements of $\mathbb{CP}^1$. In this case, we have $H_{3,3}(x, y) \cap H_{3,3}(z, w) = H_{2,2}(x, y, z, w)$. This is affinely isomorphic to the convex set $\mathbb{S}_{1,2}$ which is realized as the three-dimensional solid sphere whose extreme points are parameterized by $\mathbb{CP}^1$. If $x \neq z$ or $y \neq w$, then the intersection is an edge.

It is also apparent that the intersection $H_{3,3}(x, y) \cap G_{3,4}(V)$ has one or two extreme points. It has a single extreme point if and only if $(x^\perp, y^\perp)$ is an extreme point of $G_{3,4}(V)$. The intersection $H_{3,3}(x, y) \cap G_{4,3}(W)$ is similar. As for the intersection $G_{3,4}(V) \cap G_{3,4}(W)$, we have the following:

PROPOSITION 3.1. *Let V and W be nonsingular matrices which are different up to scalar multiplication. Then $G_{3,4}(V) \cap G_{3,4}(W)$ is a single point or a line segment. It is a single point if and only if $W^{-1}V = (a, b, c, d)$ satisfies the following two conditions*:

(i) $b \neq 0$ *or* $c \neq 0$;

(ii) $(a - d)^2 + 4bc = 0$.

Proof. An extreme point $P_{x \otimes y}$ belongs to $G_{3,4}(V) \cap G_{3,4}(W)$ if and only if $x \perp V\bar{y}$ and $x \perp W\bar{y}$ if and only if

$$W^{-1}V\bar{y} \parallel \bar{y}. \tag{3.1}$$

We first consider the case $b = c = 0$. In this case, we have $a \neq d$, and $\bar{y} = (1, 0)$ and $\bar{y} = (0, 1)$ are always two solutions of (3.1). Hence, the assertion is true. If $b = 0$ and $c \neq 0$, then $\bar{y} = (0, 1)$ is always a solution of (3.1). Furthermore, (3.1) has a solution of the form $\bar{y} = (1, \xi)$ if and only if such a solution is unique if and only if $a - d \neq 0$. Therefore, we get the required conclusion. The same reasoning may be applied to the case $b \neq 0$ and $c = 0$. Finally, suppose that $bc \neq 0$. In this case, any solution of (3.1) must be of the form $\bar{y} = (1, \xi)$, and this is a solution if and only if $b\xi^2 + (a - d)\xi - c = 0$. Thus, we get the conclusion. ∎

We have a similar result for the intersection $G_{4,3}(V) \cap G_{4,3}(W)$, and it remains to consider the intersection $G_{3,4}(V) \cap G_{4,3}(W)$. We first note that the extreme point $P_{x\otimes y}$ belongs to the intersection if and only if

$$x \perp V\bar{y}, \qquad \bar{x} \perp W\bar{y}, \tag{3.2}$$

because $(P_{x\otimes y})^\Gamma = P_{\bar{x}\otimes y}$. This is equivalent to $V\bar{y} \parallel \bar{W}y$ or $\bar{W}^{-1}V\bar{y} \parallel y$. The matrix of the form determined in the statement (v) of the following lemma appears in Proposition 3.6 of [4], to classify faces of the convex cone of all positive linear maps from M_2 into M_2.

LEMMA 3.1. *Let A be a 2×2 nonsingular matrix. Then the possible numbers of the solutions of*

$$A\bar{y} \parallel y \tag{3.3}$$

in $\mathbb{CP}^1$ are $0, 1, 2, \infty$, and the following are equivalent:

(i) *The equation* (3.3) *has infinitely many solutions in $\mathbb{CP}^1$.*
(ii) *The set of solutions of* (3.3) *in $\mathbb{CP}^1$ is a circle.*
(iii) *A is of the form $BJ\bar{B}^{-1}$ for a nonsingular B, where*

$$J = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.$$

(iv) *A is of the form $C\bar{C}^{-1}$ for a nonsingular C.*
(v) *A is of the form*

$$\begin{pmatrix} \alpha & r \\ s & -\bar{\alpha} \end{pmatrix},$$

where $\alpha \in \mathbb{C}$ and $r, s \in \mathbb{R}$ with the relation $|\alpha|^2 + rs > 0$.

Furthermore, for a given circle on the sphere $\mathbb{CP}^1$, there is a unique nonsingular matrix A up to scalar multiplication such that the solution of the equation (3.3) *consists of the circle.*

Proof. We denote by a_{ij} the ij-entry of A. We first note that the equation (3.3) with $y = (\xi, 1)^{\mathrm{t}}$ becomes

$$a_{21}|\xi|^2 + a_{22}\xi - a_{11}\bar{\xi} - a_{12} = 0. \tag{3.4}$$

We also note that $y = (1, 0)^{\mathrm{t}}$ is a solution of (3.3) if and only if $a_{21} = 0$. In this case, both real and imaginary parts of (3.3) with $y = (\xi, 1)^{\mathrm{t}}$ represent lines on the complex planes. If $a_{21} \neq 0$ then both real and imaginary parts of (3.3) with $y = (\xi, 1)^{\mathrm{t}}$ represent lines or circles. In any case, the solution of the equation (3.3) in the sphere $\mathbb{CP}^1$ is the intersection of two circles on the sphere. This tells us that the possible numbers of the solutions in $\mathbb{CP}^1$ are $0, 1, 2, \infty$, and shows the implication (i) $\Rightarrow$ (ii).

For the implication (ii) $\Rightarrow$ (iii), suppose that the solution of (3.3) is the circle on the sphere $\mathbb{CP}^1$, which is represented by the Möbius transform

$$\omega \mapsto \left(\frac{a\omega + b}{c\omega + d}, 1\right)^{\mathrm{t}} = (a\omega + b, c\omega + d)^{\mathrm{t}} \in \mathbb{CP}^1, \quad |\omega| = 1,$$

where

$$B = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$$

is nonsingular. This means that $A\bar{B}(\bar{\omega}, 1)^{\mathrm{t}} \parallel B(\omega, 1)^{\mathrm{t}}$ or, equivalently, the relation $B^{-1}A\bar{B}(\bar{\omega}, 1)^{\mathrm{t}} \parallel (\omega, 1)^{\mathrm{t}}$ holds for each ω with $|\omega| = 1$. Consequently, it is easy to see that $B^{-1}A\bar{B} = J$, up to scalar multiplication.

The implication (iii) $\Rightarrow$ (v) can be seen by direct calculation. Indeed, we have

$$A = BJ\bar{B}^{-1} = (\det \bar{B})^{-1} \begin{pmatrix} -a\bar{c} + b\bar{d} & |a|^2 - |b|^2 \\ -|c|^2 + |d|^2 & \bar{a}c - \bar{b}d \end{pmatrix}.$$

Put $\alpha = -a\bar{c} + b\bar{d}$, $r = |a|^2 - |b|^2$, and $s = -|c|^2 + |d|^2$. Then we see that $|\alpha|^2 + rs = |ad - bc|^2 > 0$, since B is nonsingular.

For (ii) $\Rightarrow$ (iv), we represent the circle by the image of the Möbius transform

$$t \mapsto \left(\frac{at + b}{ct + d}, 1\right)^{\mathrm{t}} = (at + b, ct + d)^{\mathrm{t}} \in \mathbb{CP}^1, \quad t \in \mathbb{R},$$

on the real line, with a nonsingular matrix

$$C = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

By exactly the same argument as above we can show that $C^{-1}A\bar{C} = I_2$, up to scalar multiplication. The implication (iv) $\Rightarrow$ (v) can be seen as (iii) $\Rightarrow$ (v).

It remains to show (v) $\Rightarrow$ (i). Suppose that A is of the form as in (v). Then we see that $A(\bar{\xi}, 1)^{\mathrm{t}} \parallel (\xi, 1)$ if and only if

$$s|\xi|^2 - \bar{\alpha}\xi - \alpha - \bar{\xi} - r = 0.$$

If $s \neq 0$, then this is the circle

$$\left|\xi - \frac{\alpha}{s}\right|^2 = \frac{|\alpha|^2 + rs}{s^2}.$$

If $s = 0$, then this the line $2\mathrm{Re}(\bar{\alpha}\xi) = s$. Therefore, (3.3) has infinitely many solutions.

For the last claim, we note that three mutually distinct points $(\xi_i, 1)^{\mathrm{t}}$ on the sphere, $i = 1, 2, 3$, determine a circle. We consider the vectors

$$\Xi_i = (\xi_i, -1) \otimes (\bar{\xi}_i, 1) = (|\xi_i|^2, \xi_i, -\bar{\xi}_i, -1) \in \mathbb{C}^4.$$

By Proposition 2.1 of [11], we see that $\{\Xi_1, \Xi_2, \Xi_3\}$ is linearly independent. Therefore, the matrix A is determined by (3.4) up to scalar multiplication. ∎

If $r = s = 0$ then we have

$$e^{-i\theta} \begin{pmatrix} e^{i\theta} & 0 \\ 0 & -e^{-i\theta} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & -e^{-2i\theta} \end{pmatrix}.$$

Therefore, any diagonal matrix satisfies the conditions of Lemma 3.1, whenever two diagonals have the same absolute values (it satisfies condition (v) of that lemma).

The relation between the matrices B and C in Lemma 3.1 is now clear. We denote by ϕ_B the Möbius transformation given by B. Then we see that the following are equivalent:

(i) The image of the unit circle under ϕ_B coincides with the image of the real axis under ϕ_C.

(ii) $\phi_{C^{-1}B} = \phi_C^{-1} \circ \phi_B$ sends the unit circle onto the real axis.

(iii) $BJ\bar{B}^{-1} = C\bar{C}^{-1}$ or, equivalently, $B^{-1}C\,\overline{B^{-1}C}^{-1} = J$, up to scalar multiplication.

As a byproduct, we see that ϕ_D sends the unit circle onto the real axis if and only if $D^{-1}\bar{D} = J$ up to scalar multiplication.

THEOREM 3.1. *Let (V, W) be a pair of 2×2 nonsingular matrices which are not parallel to each other. Then $G_{3,4}(V) \cap G_{4,3}(W) = G_{3,3}(V, W)$ if and only if $\bar{W}^{-1}V$ is of the form determined in Lemma 3.1. If (V_1, W_1) and (V_2, W_2) are pairs satisfying these conditions, then $G_{3,3}(V_1, W_1) = G_{3,3}(V_2, W_2)$ if and only if $\bar{W}_1^{-1}V_1 = \bar{W}_2^{-1}V_2$. Especially, we have $G_{3,3}(V, W) = G_{3,3}(\bar{W}^{-1}V, I)$.*

4. MOMENT CURVES ARISING FROM TWO-QUBIT SYSTEM

In this section, we explain how the moment curve arises. To do this, we need to consider the convex cone $\mathbb{S}'_{2\times 2}$ generated by the convex set $\mathbb{S}_{2\times 2}$. This is the convex hull of all positive semidefinite rank one matrices onto a product vector which is not necessarily normalized. We see that

$$\mathbb{S}_{2\times 2} = \{\varrho \in \mathbb{S}'_{2\times 2} : \mathrm{Tr}\,\varrho = 1\}.$$

Faces of the convex cone $\mathbb{S}'_{2\times 2}$ correspond to faces of $\mathbb{S}_{2\times 2}$ in an obvious way. We denote by $G'_{k,\ell}(V, W)$ the face of $\mathbb{S}'_{2\times 2}$ which corresponds to the face $G_{k,\ell}(V, W)$ of $\mathbb{S}_{2\times 2}$.

Now, we suppose that $G_{3,4}(V)\cap G_{4,3}(W)=G_{3,3}(V,W)$. The extreme points in this convex set can be described in two ways, using the unit circle or the real axis, as shown in the proof of Lemma 3.1. We first consider the unit circle. We note that $P_{x\otimes y}$ is an extreme point if and only if y is of the form

$$y_\omega=(a\omega+b,c\omega+d)^{\rm t}\in\mathbb{CP}^1$$

for a complex number ω of modulus one. From the relation $x_\omega\perp\bar{W}y_\omega$ we also see that entries of x_ω must be linear combinations of $\bar\omega$ and 1. Therefore, all entries of $x_\omega\otimes y_\omega$ are linear combinations of $\omega,\bar\omega$ and 1, and all entries of the 4×4 matrix representing the rank one positive semidefinite matrix

$$R_{x_\omega\otimes y_\omega}=(x_\omega\otimes y_\omega)(x_\omega\otimes y_\omega)^*\in G'_{3,3}(V,W)$$

are also linear combinations of $\omega,\bar\omega,\omega^2,\bar\omega^2$, and 1. Therefore, it is now clear that

$$(\omega,\omega^2)\mapsto R_{x_\omega\otimes y_\omega}$$

extends to an affine isomorphism from the convex body $C^4\subset\mathbb{R}^4$ into $G'_{3,3}(V,W)$, which is the convex cone generated by the image of this isomorphism. The map

$$\omega\mapsto(\omega,\omega^2)$$

is nothing but the trigonometric moment curve with $p=2$, as explained in the Introduction.

Now, we consider the face $G_{3,3}(V,W)$ with the specific example

$$V=(1,0,0,-1)=\begin{pmatrix}1&0\\0&-1\end{pmatrix},\qquad W=(0,1,-1,0)=\begin{pmatrix}0&1\\-1&0\end{pmatrix},\tag{4.1}$$

for which there are infinitely many solutions for (3.2), since $\bar{W}^{-1}V=J$. We note that every 4×4 Hermitian matrix ϱ with a kernel vector V must be of the form

$$\varrho=\begin{pmatrix}a&\bar\delta&\alpha&a\\\delta&b&\gamma&\delta\\\bar\alpha&\bar\gamma&c&\bar\alpha\\a&\bar\delta&\alpha&a\end{pmatrix},\qquad\text{with } \varrho^\Gamma=\begin{pmatrix}a&\bar\delta&\bar\alpha&\bar\gamma\\\delta&b&a&\bar\delta\\\alpha&a&c&\bar\alpha\\\gamma&\delta&\alpha&a\end{pmatrix}.\tag{4.2}$$

Since W is a kernel vector of ϱ^Γ, we see that $a=b=c=1/4$ and $\delta=\alpha$. Therefore, ϱ and ϱ^Γ are of the form

$$\varrho(\alpha,\gamma)=\frac14\begin{pmatrix}1&\bar\alpha&\alpha&1\\\alpha&1&\gamma&\alpha\\\bar\alpha&\bar\gamma&1&\bar\alpha\\1&\bar\alpha&\alpha&1\end{pmatrix},\qquad\varrho(\alpha,\gamma)^\Gamma=\frac14\begin{pmatrix}1&\bar\alpha&\bar\alpha&\bar\gamma\\\alpha&1&1&\bar\alpha\\\alpha&1&1&\bar\alpha\\\gamma&\alpha&\alpha&1\end{pmatrix}.\tag{4.3}$$

Considering the determinants of principal submatrices, we finally see that both ϱ and ϱ^Γ are positive semidefinite if and only if

$$|\alpha| \leqslant 1, \qquad |\gamma| \leqslant 1, \qquad 2|\alpha|^2 + |\gamma|^2 - \alpha^2\bar{\gamma} - \bar{\alpha}^2\gamma \leqslant 1. \tag{4.4}$$

Therefore, the face $G_{3,3}(V,W)$ is determined by 4×4 matrices in (4.3) whose entries satisfy the three inequalities in (4.4).

Now, we see that an extreme point $P_{x\otimes y}$ belongs to $G_{3,3}(V,W)$ if and only if

$$x = (1, \bar{\omega}), \qquad y = (1, \omega)$$

for a complex number ω with $|\omega| = 1$. These extreme points are realized by the following 4×4 matrix:

$$P_{x\otimes y} = \frac{1}{4}\begin{pmatrix} 1 & \bar{\omega} & \omega & 1 \\ \omega & 1 & \omega^2 & \omega \\ \bar{\omega} & \bar{\omega}^2 & 1 & \bar{\omega} \\ 1 & \bar{\omega} & \omega & 1 \end{pmatrix} = \varrho(\omega, \omega^2)$$

with $|\omega| = 1$. We note that the map

$$(\alpha, \gamma) \mapsto \varrho(\alpha, \gamma) \tag{4.5}$$

defines an affine isomorphism from $C^4 \subset \mathbb{R}^4$ onto $G_{3,3}(V,W) \subset \mathbb{T}_{2\times 2}$, which sends extreme points (ω, ω^2) of C^4 onto extreme points $P_{x_\omega \otimes y_\omega} = \varrho(\omega, \omega^2)$ of $G_{3,3}(V,W)$. Finally, we note that $(\alpha,\gamma) \in C^4$ if and only if $\varrho(\alpha,\gamma) \in G_{3,3}(V,W)$ if and only if (α,γ) satisfies the relations (4.4). This gives us the description of the convex body C^4 by inequalities.

If the circle is represented by $y_t = (at+b, ct+d)^{\mathrm{t}}$ with $t \in \mathbb{R}$, then all entries of $R_{x_t\otimes y_t}$ are linear combinations of $1, t, t^2, t^3$, and t^4. Therefore, the map

$$(t, t^2, t^3, t^4) \mapsto R_{x_t \otimes y_t}$$

extends to an affine isomorphism from the convex hull of the moment curve into a face of the form $G'_{3,3}$, which is the convex cone generated by the image. For a concrete example, we take $C = I$ in Lemma 3.1, and consider the face $G'_{3,3}(I,I)$. Extreme points are given by

$$R_{(1,-t)\otimes(t,1)} = R_{(t,1,-t^2,-t)} = \begin{pmatrix} t^2 & t & t^3 & -t^2 \\ t & 1 & t^2 & -t \\ t^3 & t & t^4 & -t^3 \\ -t^2 & -t & -t^3 & t^2 \end{pmatrix}, \qquad t \in \mathbb{R}.$$

In this way, we have a concrete realization of the convex body generated by the moment curve.

Now, we pay attention to the face $G_{3,4}(V)$ itself, with V given by (4.1). We see that an extreme point $P_{x\otimes y}$ belongs to the face $G_{3,4}(V)$ if and only if $x \perp V\bar{y}$ if and only if $x\otimes y$ is of the form $(x_1,x_2)\otimes(x_2,x_1)$. Therefore, the extreme point of the face $G_{3,4}(V)$ is determined by $x=(x_1,x_2)\in\mathbb{C}^2$, and the corresponding rank one matrix $\varrho_x = R_{(x_1,x_2)\otimes(x_2,x_1)}$ is of the form

$$\varrho_x = \begin{pmatrix} |x_1x_2|^2 & |x_1|^2\bar{x}_1x_2 & |x_2|^2x_1\bar{x}_2 & |x_1x_2|^2 \\ |x_1|^2x_1\bar{x}_2 & |x_1|^4 & x_1^1\bar{x}_2^2 & |x_1|^2x_1\bar{x}_2 \\ |x_2|^2\bar{x}_1x_2 & \bar{x}_1^1x_2^2 & |x_2|^4 & |x_2|^2\bar{x}_1x_2 \\ |x_1x_2|^2 & |x_1|^2\bar{x}_1x_2 & |x_2|^2x_1\bar{x}_2 & |x_1x_2|^2 \end{pmatrix}.$$

Note that this is of the form determined in (4.2), as expected. If $\|x\|=1$ then ϱ_x is of trace one. Furthermore, if two unit vectors x and z are parallel to each other, then $\varrho_x=\varrho_z$. Therefore, the map

$$x \mapsto \varrho_x$$

gives rise to a homeomorphism from $\mathbb{CP}^1$ into $G_{3,4}(V)$. If we write

$$S(x) = (|x_1|^4, |x_2|^4, |x_1|^2x_1\bar{x}_2, |x_2|^2\bar{x}_1x_2, x_1^2\bar{x}_2^2) \in \mathbb{R}^2\times\mathbb{C}^3 = \mathbb{R}^8,$$

then we see that $S(x)\leftrightarrow\varrho_x$ is an affine isomorphism. If we parameterize $\mathbb{CP}^1$ by the spherical coordinate $x=(\cos\phi,\sin\phi\cos\theta,\sin\phi\sin\theta)$ by $x_1=\cos\phi$ and $x_2=e^{-i\theta}\sin\phi$, then we have the *moment surface* given by

$$\begin{aligned} S(x) = (&\cos^4\phi, \sin^4\phi, \cos^3\phi\sin\phi\cos\theta, \cos^3\phi\sin\phi\sin\theta, \cos\phi\sin^2\phi\cos\theta, \\ &-\cos\phi\sin^2\phi\sin\theta, \cos^2\phi\sin^2\phi\cos 2\theta, \cos^2\phi\sin^2\phi\sin 2\theta) \in \mathbb{R}^8. \end{aligned}$$

The convex body S^8 in $\mathbb{R}^8$ generated by the image of S is affinely isomorphic to the maximal face $G_{3,4}(V)$. A point in the convex body S^8 is an extreme point if and only if it is a point on the surface. The convex combination of any two extreme points is an edge. The image of circles in $\mathbb{CP}^1$ under the map S generates maximal faces of S^8, which are four-dimensional. There is no more nontrivial face of S^8.

5. MOMENT CURVES ARISING FROM QUBIT-QUDIT SYSTEM

In this final section, we construct the trigonometric curve (1.1) from a face of the convex set $\mathbb{S}_{2\times p}$ of all $2\otimes p$ separable states. To do this, we define $2\times p$ matrices V_i and W_i by

(5.1)
$$V_i = e_{1,i}-e_{2,i+1}\in M_{2\times p},\qquad W_i = e_{1,i+1}-e_{2,i}\in M_{2\times p},\qquad i=1,2,\dots,p-1,$$

where $\{e_{i,j}\}$ denotes the standard matrix units of $M_{2\times p}$. Suppose that $x\otimes y$ is a product vector in $\mathbb{C}^2\otimes\mathbb{C}^p$ so that $P_{x\otimes y}$ belongs to the face $\tau(\{V_i\}^\perp,\{W_i\}^\perp)$ of $\mathbb{T}_{2\times p}$. Then we have

(5.2)
$$V_i^*x \perp \bar{y},\qquad x\perp \bar{W}_iy.$$

Note that $V_i^* x = x_1 e_i - x_2 e_{i+1} \in \mathbb{C}^p$ for $i = 1, 2, \dots, p-1$, with the standard orthonormal basis $\{e_i\}$ of $\mathbb{C}^p$. We see that $\{V_i^* x : i = 1, 2, \dots, p-1\}$ is linearly independent for every nonzero $x \in \mathbb{C}^2$, and so y is uniquely determined by x, up to scalar multiplication. We actually have

$$y = x_2^{p-1} e_1 + x_1 x_2^{p-2} e_2 + \dots + x_1^{p-2} x_2 e_{p-1} + x_1^{p-1} e_p \in \mathbb{C}^p.$$

Since $\bar{W}_i y = (x_1^i x_2^{p-(i+1)}, -x_1^{i-1} x_2^{p-i})^{\mathrm{t}} \in \mathbb{C}^2$, we see that $x \perp \bar{W}_i y$ holds if and only if

$$|x_1|^2 x_1^{i-1} x_2^{p-(i+1)} = |x_2|^2 x_1^{i-1} x_2^{p-(i+1)}, \qquad i = 1, 2, \dots, p-1.$$

Hence the solution of the equation (5.2) is given by

$$x_\omega = (1, \bar{\omega})^{\mathrm{t}} \in \mathbb{CP}^1, \qquad y_\omega = (1, \omega, \omega^2, \dots, \omega^{p-1})^{\mathrm{t}} \in \mathbb{CP}^{p-1}, \qquad |\omega| = 1,$$

and the corresponding pure product states are of the following form:

$$P_\omega := \frac{1}{2p} P_{x_\omega \otimes y_\omega} = \frac{1}{2p} \begin{pmatrix} A & B \\ B^* & A \end{pmatrix} \in \mathbb{S}_{2\times p} \subset M_2 \otimes M_p,$$

with

$$A = \begin{pmatrix} 1 & \bar{\omega} & \cdots & \bar{\omega}^{p-1} \\ \omega & 1 & & \bar{\omega}^{p-2} \\ \vdots & & \ddots & \vdots \\ \omega^{p-2} & & & \bar{\omega} \\ \omega^{p-1} & \omega^{p-2} & \cdots & 1 \end{pmatrix}, \quad B = \begin{pmatrix} \omega & 1 & \cdots & \bar{\omega}^{p-2} \\ \omega^2 & \omega & & \bar{\omega}^{p-3} \\ \vdots & & \ddots & \vdots \\ \omega^{p-1} & & & 1 \\ \omega^p & \omega^{p-1} & \cdots & \omega \end{pmatrix}.$$

Therefore, we see that

$$(\omega, \omega^2, \dots, \omega^p) \leftrightarrow P_\omega$$

extends to an affine isomorphism from the convex set C^{2p} onto the convex hull of pure product states P_ω. The homeomorphism

$$\omega \mapsto (\omega, \omega^2, \dots, \omega^p) \in \mathbb{C}^p = \mathbb{R}^{2p}, \qquad |\omega| = 1,$$

is nothing but the trigonometric moment curve given by (1.1).

THEOREM 5.1. *The convex hull of pure product states P_ω coincides with the face $\tau(D, E)$ of the convex set $\mathbb{T}_{2\times p}$.*

P r o o f. We denote by C the convex hull of P_ω; then $C = \tau(D, E) \cap \mathbb{S}_{2\times p}$ is a subset of $\tau(D, E)$. We also denote by $\{\zeta^i : i = 0, 1, \dots p\}$ the $(p+1)$-st root of unity. For any ω with $|\omega| = 1$, we have $\sum_{i=0}^{p} (\omega\zeta^i)^k = \sum_{i=0}^{p} (\zeta^i)^k = 0$ for $k = 1, 2, \dots, p$, and so it follows that

$$\sum_{i=0}^{p} P_{\zeta^i} = \sum_{i=0}^{p} P_{\omega\zeta^i} = P_\omega + \sum_{i=1}^{p} P_{\omega\zeta^i}.$$

Since P_ω is an arbitrary extreme point of C, this means that

$$\varrho_I := \frac{1}{p+1} \sum_{i=0}^{p} P_{\zeta^i} = \frac{1}{2p(p+1)} \begin{pmatrix} I_p & J \\ J^* & I_p \end{pmatrix} \in M_2 \otimes M_p$$

is an interior point of C, where $J = \sum_{i=1}^{p-1} e_{i,i+1} \in M_p$. It is easy to check that the range spaces of ϱ_I and ϱ_I^Γ coincide with D and E, respectively. Therefore, ϱ_I is a common interior point of both C and $\tau(D, E)$, and so we have $\operatorname{int} C \subset \operatorname{int} \tau(D, E)$.

Now, assume that C is a proper subset of $\tau(D, E)$. Then there exists a maximal face F of C such that $\operatorname{int} F \subset \operatorname{int} \tau(D, E)$. Take $\varrho_1 \in \operatorname{int} F$ and an extreme point ϱ_0 of C which is not in F. Then, by Proposition 2.5 in [18], we see that

$$\varrho_t := (1 - t)\varrho_0 + t\varrho_1$$

is an interior point of C for every t with $0 < t < 1$, and so it is an interior point of $\tau(D, E)$. Since $\varrho_1 \in \operatorname{int} F$ is an interior point of $\tau(D, E)$, there exists $a > 1$ such that $\varrho_a \in \tau(D, E)$, which is an entangled state because $\varrho_a \notin C$. Let μ be the maximum so that $\varrho_\mu \in \tau(D, E)$. If $1 < a < \mu$, then ϱ_a is an interior point of $\tau(D, E)$, and so $\operatorname{rank} \varrho_a = \operatorname{rank} \varrho_a^\Gamma = p + 1$. Because ϱ_a is the convex combination of ϱ_0 and ϱ_μ, and ϱ_0 is an extreme point, we conclude that $\operatorname{rank} \varrho_\mu = \operatorname{rank} \varrho_\mu^\Gamma = p$ by Theorem 3 of [5].

Finally, it is easy to see that if $\varrho \in \tau(D, E)$ is supported on $\mathbb{C}^2 \otimes \mathbb{C}^{p-1}$ in the sense of [17], then $\operatorname{rank} \varrho \leqslant p - 1$ and $\operatorname{rank} \varrho^\Gamma \leqslant p - 1$. Therefore, we see that ϱ_μ must be supported on $\mathbb{C}^2 \otimes \mathbb{C}^p$, and so it is separable by [17]. This contradiction completes the proof. ∎

Now, the convex hull C^{2p} of the trigonometric moment curve is affinely isomorphic to the convex hull of the image of the curve

$$\omega \mapsto P_\omega \in \mathbb{S}_{2\times p}, \qquad |\omega| = 1.$$

Therefore, we identify the convex set C^{2p} and the face $\tau(D, E)$ of $\mathbb{T}_{2\times p}$ by Theorem 5.1. We look for proper faces of the convex set C^{2p} or, equivalently, the convex set $\tau(D, E)$. It must be of the form $\tau(D_1, E_1)$ for subspaces D_1 and E_1 of D and E, respectively, at least one of which is proper. Consider a matrix in $D \ominus D_1$ or $E \ominus E_1$. Then we see that if an extreme point P_ω belongs to $\tau(D_1, E_1)$, then ω satisfies an equation given by the matrix, which turns out to be a polynomial of degree p. This means that the cardinality of extreme points of any proper face of C^{2p} is less than or equal to p. Therefore, we conclude that any boundary point of C^{2p} is the convex combination of k extreme points with $k \leqslant p$. For the converse, if we take extreme points whose cardinality is less than $p+1$, then it is clear that the convex hull ϱ of them in $\tau(D,E)$ has the rank less than $p+1$. This means that the range space of ϱ is a proper subspace of D, and so we see that ϱ is a boundary point of C^{2p}. We conclude that

$$(\omega_1, \dots, \omega_p) \mapsto \text{conv}\,\{P_{\omega_1}, \dots, P_{\omega_p}\}$$

is a one-to-one correspondence from the p-dimensional torus onto the lattice of all nontrivial faces of C^{2p}, where the lattice structure on the p-dimensional torus is given by the set inclusion of the entries of the ordered sets $(\omega_1, \dots, \omega_p)$ representing points of the p-dimensional torus. We also see, by [10], that every face is exposed.

If we take distinct $\omega_1, \dots, \omega_k$ with $k \leqslant p$, then we see that $\{x_{\omega_i}\}$ is mutually distinct and $\{y_{\omega_i}\}$ is linearly independent. By the result in [1] and [16], we conclude that the convex hull of $\{P_{\omega_i} : i = 1, 2, \dots, k\}$ is a simplex. Therefore, we see that any proper face of the convex set C^{2p} is a simplex with k extreme points, where $k = 1, 2, \dots, p$. If ϱ is an interior point of $\tau(D,E)$, then rank $\varrho =$ rank $\varrho^\Gamma = p+1$, and so we apply Theorem 3 of [5] to conclude that ϱ is the convex combination of $p+1$ extreme points.

If we take any k distinct complex numbers ω_i of modulus one with $k \leqslant 2p+1$, then the corresponding extreme points P_{ω_i} are linearly independent by Proposition 2.2 of [11]. Thus, their convex hull must be a simplex. The number $2p+1$ is the maximum number of extreme points of C^{2p} whose convex hull is a simplex, because the affine dimension of C^{2p} is $2p$. We summarize as follows:

THEOREM 5.2. *The convex hull C^{2p} of the trigonometric moment curve has the following properties for any $p = 1, 2, \dots$*

(i) *A point of C^{2p} is an extreme point if and only if it is on the trigonometric moment curve.*

(ii) *Any point of C^{2p} is the convex combination of k extreme points with $k \leqslant p+1$.*

(iii) *If we take k distinct extreme points with $k \leqslant 2p+1$, then their convex combination is a simplex. It is a face of C^{2p} if and only if $k \leqslant p$. Every face is exposed, and there are no more nontrivial faces.*

Now, we can express elements of C^{2p} with $2p \times 2p$ matrices as in (4.2) for $p = 2$. These matrices have p complex variables. If we consider the determinants of principal submatrices, then we get the finite set of inequalities as in (4.4), which determines elements of C^{2p}.

We also note that the convex combination ϱ of ℓ distinct extreme points with $\ell \geqslant p+1$ and nonzero coefficients is an interior point by Theorem 5.2. If we take an arbitrary extreme point P_ω of the convex set C^{2p}, then the line segment from P_ω to ϱ can be extended until it meets a boundary point which should be expressed uniquely as the convex combination of k extreme points with $k \leqslant p$. Therefore, the interior point ϱ can be expressed uniquely as the convex combination of P_ω and other k extreme points with $k \leqslant p$. The situation is visible when $p = 1$, with the picture of a circle on the plane.

Finally, we remark that it is also possible to construct trigonometric moment curve in the convex set $\mathbb{S}_{m\times n}$. To do this, we begin with

$$x_\omega = (1, \bar\omega, \bar\omega^2, \dots, \bar\omega^{m-1})^{\rm t} \in \mathbb{CP}^{m-1}, \quad y_\omega = (1, \omega, \omega^2, \dots, \omega^{n-1})^{\rm t} \in \mathbb{CP}^{n-1}$$

for a complex number ω of modulus one, and consider the projection $P_\omega := P_{x_\omega \otimes y_\omega}$ onto the product vector $x_\omega \otimes y_\omega$. Then we see that the correspondence

$$(\omega, \omega^2, \dots, \omega^{m+n-2}) \leftrightarrow P_\omega$$

gives rise to an affine isomorphism from the convex hull $C^{2(m+n-2)}$ of the trigonometric curve onto the convex hull of $\{P_\omega : |\omega| = 1\}$. For any interior point ϱ of this convex hull, we have rank $\varrho =$ rank $\varrho^\Gamma = m + n - 1$, as for the case of C^{2p} arising from $\mathbb{S}_{2\times p}$.

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Received on 12.2.2013;
revised version on 24.9.2013