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Extremal Quantum States in Coupled Systems

K. R. Parthasarathy

Indian Statistical Institute, Delhi Centre
7, SJSS Marg, New Delhi–110 016, India

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by

K. R. Parthasarathy

Indian Statistical Institute, Delhi Centre,

7, S. J. S. Sansanwal Marg,

New Delhi - 110 016, India.

e-mail : krp@isid.ac.in

In memory of Paul André Meyer

Abstract

Let $\mathcal{H}_1$, $\mathcal{H}_2$ be finite dimensional complex Hilbert spaces describing the states of two finite level quantum systems. Suppose ρ_i is a state in $\mathcal{H}_i$, $i = 1, 2$. Let $\mathcal{C}(\rho_1, \rho_2)$ be the convex set of all states ρ in $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ whose marginal states in $\mathcal{H}_1$ and $\mathcal{H}_2$ are ρ_1 and ρ_2 respectively. Here we present a necessary and sufficient criterion for a ρ in $\mathcal{C}(\rho_1, \rho_2)$ to be an extreme point. Such a condition implies, in particular, that for a state ρ to be an extreme point of $\mathcal{C}(\rho_1, \rho_2)$ it is necessary that the rank of ρ does not exceed $\left(d_1^2 + d_2^2 - 1\right)^{\frac{1}{2}}$, where $d_i =$ dim $\mathcal{H}_i$, $i = 1, 2$. When $\mathcal{H}_1$ and $\mathcal{H}_2$ coincide with the 1-qubit Hilbert space $\mathbb{C}^2$ with its standard orthonormal basis $\{|0>, |1>\}$ and $\rho_1 = \rho_2 = \frac{1}{2}I$ it turns out that a state $\rho \in \mathcal{C}(\frac{1}{2}I, \frac{1}{2}I)$ is extremal if and only if ρ is of the form $|\Omega >< \Omega|$ where $|\Omega >= \frac{1}{\sqrt{2}}\left(|0>|\psi_0> + |1>|\psi_1>\right)$, $\{|\psi_0>, |\psi_1>\}$ being an arbitrary orthonormal basis of $\mathbb{C}^2$. In particular, the extremal states are the maximally entangled states.

Key words : Coupled quantum systems, marginal states, extreme points.

1 Introduction

One of the well-known problems of classical probability theory is the determination of the set of all extreme points in the convex set of all probability distributions in a product Borel space $(X \times Y,\ \mathcal{F} \times \mathcal{G})$ with fixed marginal distributions μ and ν on $(X, \mathcal{F})$ and $(Y, \mathcal{G})$ respectively. Denote this convex set by $C(\mu, \nu)$. When $X = Y = \{1, 2, \ldots, n\}$, $\mathcal{F} = \mathcal{G}$ is the field of all subsets of X and $\mu = \nu$ is the uniform distribution then the problem is answered by the famous theorem of Birkhoff [1] that the set of extreme points of the convex set of all doubly stochastic matrices of order n is the set of all permutation matrices of order n. Problems of this kind have a natural analogue in quantum probability. Suppose $\mathcal{H}_1$ and $\mathcal{H}_2$ are finite dimensional complex Hilbert spaces describing the states of two finite level quantum systems S_1 and S_2 respectively. Then the Hilbert space of the coupled system S_{12} is $\mathcal{H}_1 \otimes \mathcal{H}_2$. Suppose ρ_i is a state of S_i in $\mathcal{H}_i$, $i = 1, 2$. Any state ρ in S_{12} yields marginal states $\mathrm{Tr}_{\mathcal{H}_2}\rho$ in $\mathcal{H}_1$ and $\mathrm{Tr}_{\mathcal{H}_1}\rho$ in $\mathcal{H}_2$ where $\mathrm{Tr}_{\mathcal{H}_i}$ is the relative trace over $\mathcal{H}_i$. Denote by $\mathcal{C}(\rho_1, \rho_2)$ the convex set of all states ρ of the coupled system S_{12} whose marginal states in $\mathcal{H}_1$ and $\mathcal{H}_2$ are ρ_1 and ρ_2 respectively. One would like to have a complete description of the set of all extreme points of $\mathcal{C}(\rho_1, \rho_2)$. In this paper we shall present a necessary and sufficient criterion for an element ρ in $\mathcal{C}(\rho_1, \rho_2)$ to be an extreme point. This leads to an interesting (and perhaps surprising) upper bound on the rank of such an extremal state ρ. Indeed, if ρ is an extreme point of $\mathcal{C}(\rho_1, \rho_2)$ then the rank of ρ cannot exceed $\left(d_1^2 + d_2^2 - 1\right)^{\frac{1}{2}}$ where $d_i = \dim \mathcal{H}_i$. Note that the rank of an arbitrary state in $\mathcal{H}_1 \otimes \mathcal{H}_2$ can vary from 1 to $d_1 d_2$. When $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^2$, $\{|0>, |1>\}$ is the standard (computational) basis of $\mathbb{C}^2$ and $\rho_1 = \rho_2 = \frac{1}{2}I$ it turns out that a state ρ in $\mathcal{C}\left(\frac{1}{2}I, \frac{1}{2}I\right)$ is extremal if and only if ρ has the form $|\Omega><\Omega|$ where $|\Omega> = \frac{1}{\sqrt{2}}\left(|0>|\psi_0> + |1>|\psi_1>\right)$, $\{|\psi_0>, |\psi_1>\}$ being any orthonormal basis of $\mathbb{C}^2$. These are the well-known maximally entangled states.

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2 Extreme points of the convex set $\mathcal{C}(\rho_1, \rho_2)$

In the analysis of extreme points in a compact convex set of positive definite matrices the following proposition plays an important role [5]. See also [2-4].

Proposition 2.1 Let ρ be any positive definite matrix of order n and rank $k < n$. Then there exists a permutation matrix σ of order n, a $k \times (n-k)$ matrix A and a strictly positive definite matrix K of order k such that

$$\sigma\rho\sigma^{-1} = \left[\begin{array}{c|c} K & KA \\ \hline A^{\dagger}K & A^{\dagger}KA \end{array}\right] \tag{2.1}$$

If, in addition, $\rho = \frac{1}{2}(\rho' + \rho'')$ where ρ' and ρ'' are also positive definite matrices then there exist positive definite matrices K', K'' of order k such that

$$\sigma\rho^{\#}\sigma^{-1} = \left[\begin{array}{c|c} K^{\#} & K^{\#}A \\ \hline A^{\dagger}K^{\#} & A^{\dagger}K^{\#}A \end{array}\right] \tag{2.2}$$

where $\#$ indicates $'$ and $''$.

Proof: Choose vectors $\boldsymbol{u}_i \in \mathbb{C}^n, \ i = 1, 2, \ldots, n$ such that

$$\rho = (((\boldsymbol{u}_i|\boldsymbol{u}_j))), \ i, j \in \{1, 2, \ldots, n\}.$$

Since rank $\rho = k$, the linear span of all the $\boldsymbol{u}_i$'s has dimension k. Hence modulo a permutation σ of $\{1, 2, \ldots, n\}$ we may assume that $\boldsymbol{u}_1, \boldsymbol{u}_2, \ldots, \boldsymbol{u}_k$ are linearly independent and

$$\boldsymbol{u}_{k+j} = a_{1j}\boldsymbol{u}_1 + a_{2j}\boldsymbol{u}_2 + \cdots + a_{kj}\boldsymbol{u}_k, \ 1 \le j \le n - k. \tag{2.3}$$

Putting

$$\begin{aligned} K &= (((\boldsymbol{u}_i|\boldsymbol{u}_j))), \ i, j \in 1, 2, \ldots, k, \\ A &= ((a_{ij})), \ i = 1, 2, \ldots, k; \ j = 1, 2, \ldots, n - k \end{aligned}$$

and denoting by the same letter σ, the permutation unitary matrix of order n corresponding to σ we obtain the relation (2.1). To prove the second part we express

$$\sigma\rho\sigma^{-1} = \left[\begin{array}{c|c} K & KA \\ \hline A^{\dagger}K & A^{\dagger}KA \end{array}\right] = \frac{1}{2}\left[\begin{array}{c|c} K' & B_1 \\ \hline B_1^{\dagger} & C_1 \end{array}\right] + \frac{1}{2}\left[\begin{array}{c|c} K'' & B_2 \\ \hline B_2^{\dagger} & C_2 \end{array}\right]$$

where the two partitioned matrices on the right hand side are the matrices $\sigma\rho'\sigma^{-1}$ and $\sigma\rho''\sigma^{-1}$. Now construct vectors $\boldsymbol{v}_i$, $\boldsymbol{w}_i$, $i = 1, 2, \ldots, n$ such that

$$\begin{aligned} \sigma\rho'\sigma^{-1} &= (((\boldsymbol{v}_i|\boldsymbol{v}_j))), \ i, j \in \{1, 2, \ldots, n\} \qquad (2.4) \\ \sigma\rho''\sigma^{-1} &= (((\boldsymbol{w}_i|\boldsymbol{w}_j))), \ i, j \in \{1, 2, \ldots, n\}. \qquad (2.5) \end{aligned}$$

Let $|0>, |1>$ be the standard orthonormal basis of $\mathbb{C}^2$. Define

$$|\boldsymbol{\varphi}_i> = \frac{1}{\sqrt{2}}(|\boldsymbol{v}_i> |0> + |\boldsymbol{w}_i> |1>), \ 1 \le i \le n. \tag{2.6}$$

Then we have

$$\begin{aligned} <\boldsymbol{\varphi}_i|\boldsymbol{\varphi}_j> &= \frac{1}{2}(\langle\boldsymbol{v}_i|\boldsymbol{v}_j\rangle + \langle\boldsymbol{w}_i|\boldsymbol{w}_j\rangle) \\ &= \langle\boldsymbol{u}_i|\boldsymbol{u}_j\rangle \quad \text{for all } i, j\{1, 2, \ldots, n\}. \end{aligned}$$

Thus the correspondence $\boldsymbol{u}_i \to \boldsymbol{\varphi}_i$ is an isometry. Hence by (2.3) we have

$$\boldsymbol{\varphi}_{k+j} = a_{1j}\boldsymbol{\varphi}_1 + a_{2j}\boldsymbol{\varphi}_2 + \cdots + a_{kj}\boldsymbol{\varphi}_k, \;\; 1 \leq j \leq n-k.$$

Substituting for the $\boldsymbol{\varphi}_i$'s from (2.6) and using the orthogonality of $|0>$ and $|1>$ we conclude that

$$|\boldsymbol{v}_{k+j}> \;=\; \sum_{i=1}^{k} a_{ij}|\boldsymbol{v}_i>, \tag{2.7}$$

$$|\boldsymbol{w}_{k+j}> \;=\; \sum_{i=1}^{k} a_{ij}|\boldsymbol{w}_i> . \tag{2.8}$$

Putting

$$\begin{aligned} K' &= (((\langle \boldsymbol{v}_i|\boldsymbol{v}_j\rangle)), \quad i,j \in \{1,2,\ldots,k\} \\ K'' &= (((\langle \boldsymbol{w}_i|\boldsymbol{w}_j\rangle)), \quad i,j \in= \{1,2,\ldots,k\} \end{aligned}$$

and substituting (2.7) and (2.8) in (2.4) and (2.5) we obtain $B_1 = K'A$, $C_1 = A^{\dagger}K'A$, $B_2 = K''A$, $C_2 = A^{\dagger}K''A$. Thus we have (2.2). ■

Let $\mathcal{H}_1$, $\mathcal{H}_2$ be two complex Hilbert spaces of finite dimension d_1, d_2 and equipped with orthonormal bases $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_{d_1}\}$, $\{\boldsymbol{f}_1, \boldsymbol{f}_2, \cdots, \boldsymbol{f}_{d_2}\}$ respectively. Consider the tensor product $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ equipped with the orthonormal basis $\boldsymbol{g}_{ij} = \boldsymbol{e}_i \otimes \boldsymbol{f}_j$ with the ordered pairs ij in the lexicographic order. For any operator X on $\mathcal{H}$ we associate its marginal operators X_i in $\mathcal{H}_i$ by putting

$$X_1 = \mathrm{Tr}_{\mathcal{H}_2}X, \quad X_2 = \mathrm{Tr}_{\mathcal{H}_1}X$$

where $\mathrm{Tr}_{\mathcal{H}_i}$ stands for the relative trace over $\mathcal{H}_i$. If ρ is a state on $\mathcal{H}$, i.e., a positive operator of unit trace, then its marginal operators are states in $\mathcal{H}_1$ and $\mathcal{H}_2$. Now we fix two states ρ_1 and ρ_2 in $\mathcal{H}_1$ and $\mathcal{H}_2$ respectively and consider the compact convex set

$$\mathcal{C}(\rho_1, \rho_2) = \{\rho|\rho \text{ a state on } \mathcal{H} \text{ with marginals } \rho_1 \text{ and } \rho_2 \text{ in } \mathcal{H}_1 \text{ and } \mathcal{H}_2 \text{ respectively. }\}$$

in $\mathcal{B}(\mathcal{H})$. Let $\mathcal{E}(\rho_1, \rho_2) \subset \mathcal{C}(\rho_1, \rho_2)$ be the set of all extreme points in $\mathcal{C}(\rho_1, \rho_2)$.

Proposition 2.2 Let $\rho \in \mathcal{E}(\rho_1, \rho_2)$. Then ρ is singular.

Proof: Suppose ρ is nonsingular. Choose nonzero hermitian operators L_i in $\mathcal{H}_i$ with zero trace. Then for all sufficiently small and positive ε, the operators $\rho \pm \varepsilon L_1 \otimes L_2$ are positive definite. Since the marginal operators of $L_1 \otimes L_2$ are 0, both of the operators $\rho \pm \varepsilon L_1 \otimes L_2$ belong to $\mathcal{C}(\rho_1, \rho_2)$ and

$$\rho = \frac{1}{2}\left((\rho + \varepsilon L_1 \otimes L_2) + (\rho - \varepsilon L_1 \otimes L_2)\right)$$

and ρ is not extremal. ■

Proposition 2.3 Let $n = d_1 d_2, \quad \rho \in \mathcal{C}(\rho_1, \rho_2)$, rank $\rho = k < n$ and let σ be a permutation of the ordered basis $\{\boldsymbol{g}_{ij}\}$ of $\mathcal{H}$ such that

$$\sigma\rho\sigma^{-1} = \left[\begin{array}{c|c} K & KA \\ \hline A^\dagger K & A^\dagger K A \end{array}\right], \tag{2.9}$$

where K is a strictly positive definite matrix of order k. Then, in order that $\rho \in \mathcal{E}(\rho_1, \rho_2)$ it is necessary that there exists no nonzero hermitian matrix L of order k such that both the marginal operators of

$$\sigma^{-1} \left[\begin{array}{c|c} L & LA \\ \hline A^\dagger L & A^\dagger L A \end{array}\right] \sigma \tag{2.10}$$

vanish.

Proof: Suppose there exists a nonzero hermitian matrix L of order k such that both the marginals of the operator (2.10) vanish. Since K in (2.9) is nonsingular and positive definite it follows that for all sufficiently small and positive ε, the matrices $K \pm \varepsilon\, L$ are strictly positive definite. Hence

$$\rho = \frac{1}{2}\left\{\sigma^{-1}\left[\begin{array}{c|c} K+\varepsilon L & (K+\varepsilon L)A \\ \hline A^\dagger(K+\varepsilon L) & A^\dagger(K+\varepsilon L)A \end{array}\right]\sigma + \sigma^{-1}\left[\begin{array}{c|c} K-\varepsilon L & (K-\varepsilon L)A \\ \hline A^\dagger(K-\varepsilon L) & A^\dagger(K-\varepsilon L)A \end{array}\right]\sigma\right\}$$

where each summand on the right hand side has the same marginal operators as ρ. Furthermore

$$\left[\begin{array}{c|c} K \pm \varepsilon L & (K \pm \varepsilon L) \\ \hline A^\dagger(K \pm \varepsilon L) & A^\dagger(K \pm \varepsilon L)A \end{array}\right] = \left[\frac{I}{A^\dagger}\right](K \pm \varepsilon L)\,[I|A] \geq 0.$$

Thus ρ is not extremal. ■

Corollary Let $\rho \in \mathcal{E}(\rho_1, \rho_2)$. Then rank $\rho \leq \sqrt{d_1^2 + d_2^2 - 1}$.

Proof: Let rank $\rho = k$. By proposition 2.2, $k < n$. Since ρ is a positive definite matrix in the basis $\{\boldsymbol{g}_{ij}\}$ such that $\sigma\rho\sigma^{-1}$ can be expressed in the form (2.9). The extremality of ρ implies that there exists no nonzero hermitian matrix L of order k such that the matrix (2.10) has both its marginals equal to 0. The vanishing of both the marginals of (2.10) is equivalent to

$$\mathrm{Tr}\,\sigma^{-1}\left[\begin{array}{c|c} L & LA \\ \hline A^\dagger L & A^\dagger L A \end{array}\right]\sigma\left(X_1 \otimes I^{(2)} + I^{(1)} \otimes X_2\right) = 0 \tag{2.11}$$

for all hermitian operators X_i in $\mathcal{H}_i$, $I^{(i)}$ being the identity operator in $\mathcal{H}_i$. Equation (2.11) can be expressed as

$$\mathrm{Tr}\,L\ [I_k|A]\,\sigma\left(X_1 \otimes I^{(2)} + I^{(1)} \otimes X_2\right)\sigma^{-1}\left[\frac{I_k}{A^\dagger}\right] = 0.$$

In other words L is in the orthogonal complement of the real linear space

$$\mathcal{D} = \left\{[I_k|A]\sigma\left(X_1 \otimes I^{(2)} + I^{(1)} \otimes X_2\right)\sigma^{-1}\left[\frac{I_k}{A^t}\right]\middle|\, X_i \text{ hermitian in } \mathcal{H}_i, i = 1, 2\right\},$$

with respect to the scalar product $\langle L|M\rangle = \operatorname{Tr} LM$ between any two hermitian matrices of order k. Thus the extremality of ρ implies that $\mathcal{D}^{\perp} = \{0\}$. The real linear space of all hermitian matrices of order k has dimension k^2. The real linear space of all hermitian operators of the form $X_1 \otimes I^{(2)} + I^{(1)} \otimes X_2$ is $d_1^2 + d_2^2 - 1$. Thus $k^2 = \dim \mathcal{D} \leq d_1^2 + d_2^2 - 1$. ∎

Proposition 2.4 Let $\rho \in \mathcal{C}(\rho_1, \rho_2), k, \sigma, K, A$ be as in Proposition 2.3. Suppose there is no nonzero hermitian matrix L of order k such that both the marginal operators of

$$\sigma^{-1}\left[\begin{array}{c|c} L & LA \\ \hline A^{\dagger}L & A^{\dagger}LA \end{array}\right]\sigma$$

vanish. Then $\rho \in \mathcal{E}(\rho_1, \rho_2)$.

Proof: Suppose $\rho \notin \mathcal{E}(\rho_1, \rho_2)$. Then there exist two distinct states ρ', ρ'' in $\mathcal{C}(\rho_1, \rho_2)$ such that

$$\rho = \frac{1}{2}(\rho' + \rho''), \quad \rho' \neq \rho''.$$

Since rank $\rho = k$ it follows from Proposition 2.1 that there exist positive definite matrices K', K'' of order k such that

$$\sigma\rho^{\#}\sigma^{-1} = \left[\begin{array}{c|c} K^{\#} & K^{\#}A \\ \hline A^{\dagger}K^{\#} & A^{\dagger}K^{\#}A \end{array}\right]$$

where $(\rho^{\#}, K^{\#})$ stands for any of the three pairs (ρ, K), (ρ', K'), (ρ'', K''). Since $\rho' \neq \rho''$ and hence $\sigma\rho'\sigma^{-1} \neq \sigma\rho''\sigma^{-1}$ it follows that $K' \neq K''$. Putting $L = K' - K'' \neq 0$ we obtain a nonzero hermitian matrix L of order k such that both the marginal operators of

$$\sigma^{-1}\left[\begin{array}{c|c} L & LA \\ \hline A^{\dagger}L & A^{\dagger}LA \end{array}\right]\sigma$$

vanish. This is a contradicton. ∎

Combining Proposition 2.3, its Corollary and Proposition 2.4 we have the following theorem.

Theorem 2.5 Let $\mathcal{H}_1$, $\mathcal{H}_2$ be complex finite dimensional Hilbert spaces of dimension d_1, d_2 respectively. Suppose $\mathcal{C}(\rho_1, \rho_2)$ is the convex set of all states ρ in $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ whose marginal states in $\mathcal{H}_1$ and $\mathcal{H}_2$ are ρ_1 and ρ_2 respectively. Let $\{\boldsymbol{e}_i\}$, $\{\boldsymbol{f}_j\}$ be orthonormal bases for $\mathcal{H}_1$, $\mathcal{H}_2$ respectively and let $\boldsymbol{g}_{ij} = \boldsymbol{e}_i \otimes \boldsymbol{f}_j$, $i = 1, 2, \ldots, d_1$; $j = 1, 2, \ldots, d_2$ be the orthonormal basis of $\mathcal{H}$ in the lexicographic ordering of the ordered pairs ij. In order that an element ρ in $\mathcal{C}(\rho_1, \rho_2)$ be an extreme point it is necessary that its rank k does not exceed $\sqrt{d_1^2 + d_2^2 - 1}$. Let σ be a permutation unitary operator in $\mathcal{H}$, permuting the basis $\{\boldsymbol{g}_{ij}\}$ and satisfying

$$\sigma\rho\sigma^{-1} = \left[\begin{array}{c|c} K & KA \\ \hline A^{\dagger}K & A^{\dagger}KA \end{array}\right]$$

where K is a strictly positive definite matrix of order k. Then ρ is an extreme point of the convex set $\mathcal{C}(\rho_1, \rho_2)$ if and only if the real linear space

$$\mathcal{D} = \left\{ [I_k|A]\sigma\left(X_1 \otimes I^{(2)} + I^{(1)} \otimes X_2\right)\sigma^{-1}\left[\frac{I}{A^t}\right] \middle| X_i \text{ hermitian in } \mathcal{H}_i,\ i = 1, 2 \right\}$$

coincides with the space of all hermitian matrices of order k.

Proof: Immediate from Proposition 2.3, its Corollary and Proposition 2.4. ■

3 The case $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^2$

We consider the orthonormal basis

$$|0>= \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1>= \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

in $\mathbb{C}^2$ and write

$$|xy>= |x> \otimes |y> \text{ for all } x, y \in \{0, 1\}.$$

Then $\boldsymbol{e}_1 = |00>$, $\boldsymbol{e}_2 = |01>$, $\boldsymbol{e}_3 = |10>$, $\boldsymbol{e}_4 = |11>$ constitute an ordered orthonormal basis for $\mathbb{C}^2 \otimes \mathbb{C}^2$. For any state ρ in $\mathbb{C}^2 \otimes \mathbb{C}^2$ define

$$K_\rho\left((x,y),(x',y')\right) = \langle xy|\rho|x'y'\rangle \;\; x, y, x', y' \in \{0,1\}. \tag{3.1}$$

If ρ has marginal states ρ_1, ρ_2 then

$$K_\rho\left((x,0),(x',0)\right) \;+\; K_\rho\left((x,1),(x',1)\right) = \langle x|\rho_1|x'\rangle, \tag{3.2}$$

$$K_\rho\left((0,y),(0,y')\right) \;+\; K_\rho\left((1,y),(1,y')\right) = \langle y|\rho_2|y'\rangle \tag{3.3}$$

for all x, y, x', y' in $\{0,1\}$. If ρ is an extreme point of the convex set $\mathcal{C}(\rho_1, \rho_2)$ it follows from Theorem 2.5 that the rank of ρ cannot exceed $\sqrt{7}$. In other words, every extremal state ρ' in $\mathcal{C}(\rho_1, \rho_2)$ has rank 1 or 2. When $\rho_1 = \rho_2 = \frac{1}{2}I$ we have the following theorem :

Theorem 3.1 Let $\mathcal{H}_1 = \mathcal{H}_2 = \mathbb{C}^2$. A state ρ in $\mathcal{C}(\frac{1}{2}I, \frac{1}{2}I)$ is an extreme point if and only if $\rho = |\Omega><\Omega|$ where

$$|\Omega>= \frac{1}{\sqrt{2}}\left(|0>\otimes|\psi_0> + |1>\otimes|\psi_1>\right),$$

$\{|\psi_0>, |\psi_1>\}$ being an orthonormal basis of $\mathbb{C}^2$.

Proof: We shall first show that there is no extremal state ρ of rank 2 in $\mathcal{C}(\frac{1}{2}I, \frac{1}{2}I)$. To this end choose and fix a state ρ of rank 2 in $\mathcal{C}(\frac{1}{2}I, \frac{1}{2}I)$. Then the right hand sides of (3.2) and (3.3) coincide with $\frac{1}{2}\delta_{xx'}$ and $\frac{1}{2}\delta_{yy'}$ respectively and in the ordered basis $\{\boldsymbol{e}_j, 1 \le j \le 4\}$ the positive definite matrix K_ρ of rank 2 in (3.1) assumes the form

$$K_\rho = \begin{bmatrix} \frac{a}{2} & x & y & z \\ \bar{x} & \frac{1-a}{2} & t & -y \\ \bar{y} & \bar{t} & \frac{1-a}{2} & -x \\ \bar{z} & -\bar{y} & -\bar{x} & \frac{a}{2} \end{bmatrix} \tag{3.4}$$

for some $0 \le a \le 1$, $x, y, z, t \in \mathbb{C}$. The fact K_ρ has rank 2 implies that one of the following three cases holds :

(1) $\begin{bmatrix} \frac{a}{2} & x \\ \bar{x} & \frac{1-a}{2} \end{bmatrix}$ is strictly positive definite ;

(2) $\begin{bmatrix} \frac{a}{2} & y \\ \bar{y} & \frac{1-a}{2} \end{bmatrix}$ is strictly positive definite ;

(3) $|x|^2 = |y|^2 = \frac{a(1-a)}{4}$ and one of the matrices $\begin{bmatrix} \frac{a}{2} & z \\ \bar{x} & \frac{a}{2} \end{bmatrix}$, $\begin{bmatrix} \frac{1-a}{2} & t \\ \bar{t} & \frac{1-a}{2} \end{bmatrix}$ is strictly positive definite.

We shall first show that case (3) is vacuous. We assume that

$$|x|^2 = |y|^2 = \frac{a(1-a)}{4}, \; |z|^2 < \frac{a^2}{4}, \quad \text{rank } K_\rho = 2. \tag{3.5}$$

conjugation by the unitary permutation matrix corresponding to the permutation (1)(24)(3) brings (3.4) to the form

$$\left[\begin{array}{cc|cc} \frac{a}{2} & z & y & x \\ \bar{z} & \frac{a}{2} & -\bar{x} & -\bar{y} \\ \hline \bar{y} & -x & \frac{1-a}{2} & \bar{t} \\ \bar{x} & -y & t & \frac{1-a}{2} \end{array}\right] \tag{3.6}$$

with rank 2. By Proposition 2.1 this implies that

$$\begin{bmatrix} \frac{1-a}{2} & \bar{t} \\ t & \frac{1-a}{2} \end{bmatrix} = A^\dagger K A \tag{3.7}$$

where

$$A = K^{-1} \begin{bmatrix} y & x \\ -\bar{x} & -\bar{y} \end{bmatrix}, \quad K = \begin{bmatrix} \frac{a}{2} & z \\ \bar{z} & \frac{a}{2} \end{bmatrix} \tag{3.8}$$

Putting $x = \frac{\sqrt{a(1-a)}}{2} e^{i\theta}$, $y = \frac{\sqrt{a(1-a)}}{2} e^{i\varphi}$, substituting the expressions of (3.8) in (3.7) and equating the 11-entry of the matrices on both sides of (3.7) we get

$$\left| \frac{a}{2} + z\, e^{-i(\theta+\varphi)} \right|^2 = 0$$

and therefore $|z|^2 = \frac{a^2}{4}$, a contradiction.

The case $|t|^2 < \frac{(1-a)^2}{4}$ is dealt with in the same manner.

Now we shall prove that ρ is not extremal. Express (3.4) as

$$K_\rho = \left[\begin{array}{c|c} K & KA \\ \hline A^\dagger K & A^\dagger K A \end{array}\right] \tag{3.9}$$

where

$$K = \begin{bmatrix} \frac{a}{2} & x \\ \bar{x} & \frac{1-a}{2} \end{bmatrix}, \quad A = K^{-1} \begin{bmatrix} y & z \\ t & -y \end{bmatrix} \tag{3.10}$$

$$A^{\dagger}KA = dK^{-1}, \quad d = \frac{a(1-a)}{4} - |x|^2 > 0 \tag{3.11}$$

This implies the existence of a unitary matrix U such that

$$K^{\frac{1}{2}}A = d^{\frac{1}{2}}UK^{-\frac{1}{2}}.$$

From (3.10) we have

$$\begin{bmatrix} y & z \\ t & -y \end{bmatrix} = KA = d^{1/2}K^{1/2}UK^{-1/2}.$$

Hence $\mathrm{Tr}\, U = 0$. Since U is a unitary matrix of zero trace it has the form

$$U = e^{i\theta}\, V$$

where V is a selfadjoint unitary matrix of determinant -1. In particular

$$A = d^{1/2}e^{i\theta}K^{-1/2}VK^{-1/2} \tag{3.12}$$

where V is selfadjoint and unitary. We now examine the linear space

$$\mathcal{D} = \left\{ [I_2|A]\,(X_1 \otimes I_2 + I_2 \otimes X_2)\,[\frac{I_2}{A^t}] \middle| X_i \text{ is hermitian for each } i \right\}. \tag{3.13}$$

In the ordered basis $\{\boldsymbol{e}_j,\ j = 1,2,3,4\}$ it is easily verified that $X_1 \otimes I_2 + I_2 \otimes X_2$ in $\mathcal{D}$ varies over all matrices of the form

$$\left\{ \left[\begin{array}{c|c} X + pI_2 & rI_2 \\ \hline \bar{r}I_2 & X + qI_2 \end{array} \right] \middle| X \text{ hermitian}, p, q \in \mathbb{R}, r \in \mathbb{C} \right\}.$$

Thus

$$\mathcal{D} = \left\{ X + AXA^{\dagger} + rA^{\dagger} + \bar{r}A + qAA^{\dagger} + pI \middle| X \text{ hermitian}, p, q\varepsilon\mathbb{R}, r \in \mathbb{C} \right\}.$$

We now search for a hermitian matrix L of order 2 in $\mathcal{D}^{\perp}$ with respect to the scalar product $\langle X_1|X_2\rangle = \mathrm{Tr}\, X_1X_2$ for any two hermitian matrices of order 2. In other words we search for a hermitian L satisfying

$$\left.\begin{array}{l} \mathrm{Tr}\ L = 0,\ \mathrm{Tr}\ L\,K^{-1/2}V\,K^{1/2} = 0 \\ \mathrm{Tr}\ L\left(X + dK^{-1/2}VK^{-1/2}XK^{-1/2}VK^{-1/2}\right) = 0 \end{array}\right\} \tag{3.14}$$

for all hermitian X. (Here we have substituted for A from (3.12)).

Note that $\sqrt{d}K^{-1/2}VK^{-1/2} = B$ is a hermitian matrix of determinant -1. Thus (3.14) reduces to

$$\mathrm{Tr}\ L = 0, \quad \mathrm{Tr}\ LB = 0, \quad L + BLB = 0. \tag{3.15}$$

The matrix B can be expressed as

$$B = WDW^t$$

where W is unitary and

$$D = \begin{bmatrix} \alpha & 0 \\ 0 & -\alpha^{-1} \end{bmatrix}, \quad \alpha > 0.$$

Then for any $\xi \in \mathbb{C}$ the hermitian matrix

$$L = W^t \begin{bmatrix} 0 & \xi \\ \bar{\xi} & 0 \end{bmatrix} W$$

satisfies (3.15). In other words $\mathcal{D}^\perp \neq \{0\}$ and therefore the linear space $\mathcal{D}$ in (3.13) is not the space of all hermitian matrices of order 2. Hence by Theorem 2.5, the state ρ is not extremal.

Thus every extremal state ρ in $\mathcal{C}(\frac{1}{2}I, \frac{1}{2}I)$ is of rank 1. Such an extremal state ρ has the form

$$\rho = |\Omega><\Omega|$$

where

$$|\Omega> \; = \sum_{x,y \in \{0,1\}} a_{xy}|xy>,$$
$$\sum_{x,y} |a_{xy}|^2 = 1.$$

The fact that $|\Omega><\Omega|$ has its marginal operators equal to $\frac{1}{2}I$ implies that $((a_{xy})) = \frac{1}{\sqrt{2}}((u_{xy}))$ where $((u_{xy}))$ is a unitary matrix of order 2. Putting

$$\sum_{y=0}^{1} u_{xy}|y> = |\psi_x>$$

we see that

$$|\Omega> = \frac{1}{\sqrt{2}}(|0>|\psi_0> + |1>|\psi_1>) \tag{3.16}$$

where $\{|0>, |1>\}$ is the canonical orthonormal basis in $\mathbb{C}^2$ and $\{|\psi_0>, |\psi_1>\}$ is another orthonormal basis in $\mathbb{C}^2$ (which may coincide with $\{|0>, |1>\}$). Varying the orthonormal basis $\{|\psi_0>, |\psi_1>\}$ of $\mathbb{C}^2$ in (3.16) we get all the extremal states of $\mathcal{C}(\frac{1}{2}I, \frac{1}{2}I)$ as $|\Omega><\Omega|$. ■

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