# Extremal Quantum States in Coupled Systems


by

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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 $\rho_i$ is a state in $\mathcal{H}_i$, $i = 1, 2$. Let $\mathcal{C}(\rho_1, \rho_2)$ be the convex set of all states $\rho$ in $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ whose marginal states in $\mathcal{H}_1$ and $\mathcal{H}_2$ are $\rho_1$ and $\rho_2$ respectively. Here we present a necessary and sufficient criterion for a $\rho$ in $\mathcal{C}(\rho_1, \rho_2)$ to be an extreme point. Such a condition implies, in particular, that for a state $\rho$ to be an extreme point of $\mathcal{C}(\rho_1, \rho_2)$ it is necessary that the rank of $\rho$ 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 $\rho$ is of the form $|\Omega><\Omega|$ where $|\Omega> = \frac{1}{\sqrt{2}}(|0>|\psi_0> + |1>|\psi_1>)$, $\{|\psi_0>, |\psi_1>\}$ being an arbitrary orthonormal basis of $\mathbb{C}^2$. In particular, the extremal states are the maximally entangled states. Using the Weyl commutation relations in the space $L^2(A)$ of a finite abelian group we exhibit a mixed extremal state in $\mathcal{C}\left(\frac{1}{n}I_n, \frac{1}{n^2}I_{n^2}\right)$.



Key words : Coupled quantum systems, marginal states, extreme points, doubly stochastic matrices, separable and nonseparable states.

# 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 $\mu$ and $\nu$ 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 and von Neumann [1], [2] 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 $\rho_i$ is a state of $S_i$ in $\mathcal{H}_i,\ \ i = 1, 2$. Any state $\rho$ 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 $\mathcal{C}\left(\rho_1, \rho_2\right)$ the convex set of all states $\rho$ of the coupled system $S_{12}$ whose marginal states in $\mathcal{H}_1$ and $\mathcal{H}_2$ are $\rho_1$ and $\rho_2$ respectively. One would like to have a complete description of the set of all extreme points of $\mathcal{C}\left(\rho_1, \rho_2\right)$. In this paper we shall present a necessary and sufficient criterion for an element $\rho$ in $\mathcal{C}\left(\rho_1, \rho_2\right)$ to be an extreme point. This leads to an interesting (and perhaps surprising) upper bound on the rank of such an extremal state $\rho$. Indeed, if $\rho$ is an extreme point of $\mathcal{C}\left(\rho_1, \rho_2\right)$ then the rank of $\rho$ cannot exceed $(d_1^2 + d_2^2 - 1)^{\frac{1}{2}}$ 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 $\rho$ in $\mathcal{C}\left(\frac{1}{2}I, \frac{1}{2}I\right)$ is extremal if and only if $\rho$ 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 [7]. See also [3], [4] and [6].

**Proposition 2.1** Let $\rho$ be any positive definite matrix of order $n$ and rank $k < n$. Then there exists a permutation matrix $\sigma$ 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 $\rho'$ and $\rho''$ 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

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

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

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

Putting

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

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

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

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

$$\sigma\rho'\sigma^{-1} = ((\langle \boldsymbol{v}_i | \boldsymbol{v}_j \rangle)), \;\; i,j \in \{1,2,\ldots,n\} \tag{2.4}$$

$$\sigma\rho''\sigma^{-1} = ((\langle \boldsymbol{w}_i | \boldsymbol{w}_j \rangle)), \;\; i,j \in \{1,2,\ldots,n\}. \tag{2.5}$$

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

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

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

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

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 $\{\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_{d_1}\}$, $\{\boldsymbol{f}_1, \boldsymbol{f}_2, \ldots, \boldsymbol{f}_{d_2}\}$ 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 $\rho$ 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 $\rho_1$ and $\rho_2$ 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 $\rho$ is singular.

**Proof:** Suppose $\rho$ is nonsingular. Choose nonzero hermitian operators $L_i$ in $\mathcal{H}_i$ with zero trace. Then for all sufficiently small and positive $\varepsilon$, 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 $\rho$ is not extremal. ■

**Proposition 2.3** Let $n = d_1 d_2$, $\rho \in \mathcal{C}(\rho_1, \rho_2)$, rank $\rho = k < n$ and let $\sigma$ 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

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

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 $\varepsilon$, 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 $\rho$. Furthermore

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

Thus $\rho$ 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 $\rho$ 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 $\rho$ 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

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

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 $\langle L|M\rangle = \mathrm{Tr}\, LM$ between any two hermitian matrices of order $k$. Thus the extremality of $\rho$ 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 $\rho \in \mathcal{C}\left(\rho_1, \rho_2\right), k, \sigma, K, A$ be as in Proposition 2.3. Suppose there is no nonzero hermitian matrix $L$ of order $k$ such that both the marginal operators of

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

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 $\rho', \rho''$ 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 $\left(\rho^{\#}, K^{\#}\right)$ stands for any of the three pairs $(\rho, K)$, $(\rho', K')$, $(\rho'', K'')$. 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 $\rho$ in $\mathcal{H}=\mathcal{H}_1\otimes\mathcal{H}_2$ whose marginal states in $\mathcal{H}_1$ and $\mathcal{H}_2$ are $\rho_1$ and $\rho_2$ 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 $\rho$ 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 $\sigma$ 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 $\rho$ 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 $\rho$ 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 $\rho$ has marginal states $\rho_1$, $\rho_2$ 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 $\rho$ is an extreme point of the convex set $\mathcal{C}(\rho_1,\rho_2)$ it follows from Theorem 2.5 that the rank of $\rho$ cannot exceed $\sqrt{7}$. In other words, every extremal state $\rho'$ 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 $\rho$ 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 $\rho$ of rank 2 in $\mathcal{C}(\frac{1}{2}I,\frac{1}{2}I)$. To this end choose and fix a state $\rho$ 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 $K_\rho$ 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 $K_\rho$ 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 $\begin{bmatrix} \frac{a}{2} & z \\ \bar{z} & \frac{a}{2} \end{bmatrix}$, $\begin{bmatrix} \frac{1-a}{2} & t \\ \bar{t} & \frac{1-a}{2} \end{bmatrix}$ 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 $\rho$ is not extremal. Express (3.4) as

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

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 $\langle X_1|X_2\rangle = \text{Tr}\, X_1X_2$ for any two hermitian matrices of order 2. In other words we search for a hermitian $L$ satisfying

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

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

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

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 $\rho$ is not extremal.

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

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

where

$$\begin{aligned} |\Omega> \quad &= \sum_{x,y\in\{0,1\}} a_{xy}|xy>, \\ & \sum_{x,y} |a_{xy}|^2 = 1. \end{aligned}$$

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

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

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 $|\Omega><\Omega|$. ∎

# 4 An example of a mixed extremal state in $\mathcal{C}\left(\frac{1}{n}I_n, \frac{1}{n^2}I_{n^2}\right)$ which is also nonseparable

Let $A$ be a finite additive abelian group of cardinality $n$, addition operation $+$ and null element 0. Choose and fix a symmetric bicharacter $\langle .,. \rangle$ on $A \times A$ satisfying

$$\begin{aligned} \langle a, b \rangle &= \langle b, a \rangle, \quad |\langle a, b \rangle| = 1, \\ \langle a, \ b + c \rangle &= \langle a, b \rangle \langle a, c \rangle \end{aligned}$$

for all $a, b, \ c \in A$. Denote by $\mathcal{H}$ the Hilbert space $L^2(A)$ with respect to the counting measure in $A$ and consider the orthonormal basis :

$$|a> = \ 1_{\{a\}}, \quad a \in A,$$

where the right hand side denotes the indicator function of the singleton $\{a\}$ in $A$. Define the unitary operators $U_a$, $V_b$ in $\mathcal{H}$ by

$$\begin{aligned} U_a \ |c> &= |a + c>, \\ V_b \ |c> &= \langle b, c \rangle \ |c> \end{aligned}$$

for all $a, b, c$ in $A$. Then we have the Weyl commutation relations

$$U_a U_b = U_{a+b}, V_a V_b = V_{a+b}, V_b U_a = \langle a, b \rangle U_a V_b \text{ for all } a, \; b \in A.$$

Put

$$W_x = U_a V_b, \quad x = (a, b) \in A \times A.$$

Then the family $\{W_x\}$ is irreducible and

$$\text{Tr } W_x^\dagger W_y = n\delta_{xy}.$$

In particular $\left\{\frac{1}{\sqrt{n}} W_x, \; x \in A \times A\right\}$ is an orthonormal basis in the Hilbert space $\mathcal{B}(\mathcal{H})$ of all operators on $\mathcal{H}$ with the scalar product

$$\langle X|Y\rangle = \text{ Tr}\, X^\dagger Y, \; X, Y \in \mathcal{B}(\mathcal{H}).$$

Define the operator matrix

$$P = \frac{1}{n^2}\left[W_x^\dagger W_y\right], \quad x, y \in A \times A \tag{4.1}$$

of order $n^2$ with entries from $\mathcal{B}(\mathcal{H})$. Then $P = P^\dagger = P^2$ and Tr $P = n$, when $P$ is considered as an operator in $\mathcal{H} \otimes \mathcal{K}$ where $\mathcal{K} = L^2\left(A \times A\right)$. Thus $P$ is a projection of rank $n$ in an $n^3$-dimensional Hilbert space. Define the state

$$\rho_0 = \frac{1}{n} P \tag{4.2}$$

**Theorem 4.1** $\rho_0$ is an extremal state in the convex set $\mathcal{C}\left(\frac{1}{n} I_{\mathcal{H}}, \frac{1}{n^2} I_{\mathcal{K}}\right)$ where $I_{\mathcal{H}}$ and $I_{\mathcal{K}}$ are the identity operators in $\mathcal{H}$ and $\mathcal{K}$ respectively. Furthermore, in the range of $\rho_0$ there does not exist a nonzero product vector of the form $u \otimes f$, $u \in \mathcal{H}$, $f \in \mathcal{K}$.

**Proof :** Observe that $\rho_0$ can be expressed in the block form

$$\rho_0 = \frac{1}{n^3}\left[\begin{array}{c|c} I_{\mathcal{H}} & B \\ \hline B^\dagger & B^\dagger B \end{array}\right]$$

where $B = [W_x, \; x \in A \times A, \; x \neq 0]$ and rank $\rho_0 =$ rank $I_{\mathcal{H}} = n$. Now consider a hermitian operator $L$ in $\mathcal{H}$ and put

$$\alpha_L = \left[ \begin{array}{c|c} L & LB \\ \hline B^\dagger L & B^\dagger LB \end{array} \right].$$

Suppose that the relative traces of $\alpha_L$ in $\mathcal{H}$ and $\mathcal{K}$ vanish. This would, in particular, imply

$$\mathrm{Tr}\, L\, W_x = 0 \quad \text{for all } x \in A \otimes A.$$

Since the family $\left\{ \frac{1}{\sqrt{n}} W_x, x \in A \times A \right\}$ is an orthonormal basis in $\mathcal{B}(\mathcal{H})$ it follows that $L = 0$. In other words $\rho_0$ satisfies the conditions of Proposition 2.3 and therefore $\rho_0$ is an extreme point of the convex set $\mathcal{C}\left(\frac{1}{n} I_{\mathcal{H}}, \frac{1}{n^2} I_{\mathcal{K}}\right)$.

To prove the second part, suppose that there exists a nonzero product vector $u \otimes f$ in the range of $\rho_0$. It follows from (4.1) and (4.2) that

$$P\, u \otimes f = u \otimes f$$

or equivalently

$$\frac{1}{n^2} \sum_{y \in A \times A} f(y) W_y u = f(x) W_x u \quad \text{for all } x \in A \times A.$$

Thus the right hand side is independent of $x$ and therefore

$$f(x) W_x u = f(0,0) u.$$

Since $u \otimes f \neq 0$ it follows that $f(0,0) \neq 0$ and therefore $f(x) \neq 0$ for every $x \in A \times A$. Thus $\mathbb{C}u$ is a 1 - dimensional invariant subspace for the irreducible family $\{W_x, x \in A \times A\}$. This is a contradiction. ■

**Remark** The last part of Theorem 4.1 implies that the state $\rho_0$ is not separable in the sense that $\rho_0$ cannot be expressed as $\sum_i p_i \alpha_i \otimes \beta_i$, where $i$ runs over a finite index set $S$, $\{p_i\}$ is a probability distribution on $S$, $\{\alpha_i\}$ and $\{\beta_i\}$ are families of states in $\mathcal{H}$ and $\mathcal{K}$ respectively (See [5] ).

**Theorem 4.2** Let $\mathcal{H}$, $\mathcal{K}$ be Hilbert spaces of dimension $m$, $n$ respectively and let $\rho$ be a state in $\mathcal{H} \otimes \mathcal{K}$ such that $\rho \in \mathcal{C}\left(\frac{1}{m} I_{\mathcal{H}}, \frac{1}{n} I_{\mathcal{K}}\right)$. Then

$$S(\rho) \geq |\log_2 m - \log_2 n|$$

where $S(\rho)$ denotes the von Neumann entropy of $\rho$. In particular,

$$\text{rank } \rho \geq \frac{\max(m,n)}{\min(m,n)}$$

**Proof.** Consider a spectral decomposition of $\rho$ in the form

$$\rho = \sum_{j=1}^{k} p_j |\Omega_j >< \Omega_j|$$

where $\{|\Omega_j >, 1 \leq j \leq k\}$ is an orthonormal set and $\{p_j, 1 \leq j \leq k\}$ is a probability distribution with $p_j > 0$ for every $j$. In particular, rank $(\rho) = k$. Let $\{|e_r >, 1 \leq r \leq m\}$, $\{|f_s >, 1 \leq s \leq n\}$ be orthonormal bases in $\mathcal{H}$, $\mathcal{K}$ respectively. Define

$$P(j,r,s) = p_j |\langle e_r \otimes f_s | \Omega_j \rangle|^2.$$

Then $P(.,.,.)$ can be viewed as a joint probability distribution of three random variables $X, Y, Z$ assuming values in the sets $\{1,2,\ldots,k\}$, $\{1,2,\ldots,m\}$, $\{1,2,\ldots,n\}$ respectively. Using the symbol $H$ for the Shannon entropy as well as conditional entropy for random variables assuming a finite number of values we have

$$H(XYZ) = H(Y) + H(XZ|Y) = H(Z) + H(XY|Z).$$

By the hypothesis on $\rho$ we conclude that $Y$ and $Z$ are uniformly distributed in $\{1,2,\ldots,m\}$ and $\{1,2,\ldots,n\}$ respectively. Thus we get

$$\begin{aligned} \log_2 m - \log_2 n &= H(Y) - H(Z) \\ &= H(XY|Z) - H(XZ|Y) \\ &\leq H(XY|Z) \\ &\leq H(X|Z) \\ &\leq H(X) \\ &= S(\rho). \end{aligned}$$

Interchanging $Y$ and $Z$ in this argument and combining the two inequalities we get

$$S(\rho) \geq |\log_2 m - \log_2 n|.$$

This completes the proof of the first part. We have

$$S(\rho) = -\sum_{j=1}^{k} p_j \log_2 p_j \leq \log_2 k$$

which yields the second part. ∎

**Remark** It is interesting to note that, in view of Theorem 4.2, the extremal state $\rho_0$ constructed in Theorem 4.1 is, indeed, of minimal rank.

We conclude with an example which is of some interest, particularly, in the context of Theorem 3.1 and Theorem 4.1 with $n = 2$ which cover the cases $\mathbb{C}^2 \otimes \mathbb{C}^2$ and $\mathbb{C}^2 \otimes \mathbb{C}^4$.

**Example 4.3** Let $\mathcal{H} = \mathbb{C}^2$, $\mathcal{K} = \mathbb{C}^3$ with labeled orthonormal bases $\{|0>, |1>\}$, $\{|0>, |1>, |2>\}$ respectively. Suppose $\rho_0 = \frac{1}{2}P$ whre $P$ is the 2-dimensional projection in $\mathcal{H} \otimes \mathcal{K}$ onto the span of $\{|00> + |11> + i|12>, \quad |10> + |01> - i|02>\}$. Using the ordered orthonormal basis $\{|00>, |10>, |01>, |11>, |02>, |12>\}$ in $\mathcal{H} \otimes \mathcal{K}$ and looking upon $\mathcal{H} \otimes \mathcal{K}$ as $\mathbb{C}^2 \oplus \mathbb{C}^2 \oplus \mathbb{C}^2$, $P$ can be expressed as a block matrix :

$$P = \frac{1}{3}\left[\begin{array}{c|c|c} I_2 & \sigma_1 & \sigma_2 \\ \hline \sigma_1 & I_2 & i\sigma_3 \\ \hline \sigma_2 & -i\sigma_3 & I_2 \end{array}\right]$$

where $\sigma_i$, $i = 1, 2, 3$ are the $2 \times 2$ Pauli matrices. Since the trace of any Pauli matrix is 0 it follows that $\rho_0 \in \mathcal{C}\left(\frac{1}{2}I_2, \frac{1}{3}I_3\right)$. It is straightforward to verify that there is no product vector in the range of $P$. Thus $\rho_0$ is a mixed entangled state with both the marginals having maximum entropy. If $L$ is a $2 \times 2$ hermitian matrix such that the marginals of the operator

$$T_L = \left[\begin{array}{c|c|c} L & L\sigma_1 & L\sigma_2 \\ \hline \sigma_1 L & \sigma_1 L \sigma_1 & \sigma_1 L \sigma_2 \\ \hline \sigma_2 L & \sigma_2 L \sigma_1 & \sigma_2 L \sigma_2 \end{array}\right]$$

in $\mathcal{H}$ and $\mathcal{K}$ are 0 then it follows that Tr $L =$ Tr $L\sigma_1 =$ Tr $L\sigma_2 =$ Tr $L\sigma_3 = 0$ and therefore $L = 0$. By Proposition 2.4 it follows that $\rho_0$ is an extremal state in $\mathcal{C}\left(\frac{1}{2}I_2, \frac{1}{3}I_3\right)$. By Theorem 4.2, $\rho_0$ has minimal rank.

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