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RANKS AND EIGENVALUES OF STATES WITH PRESCRIBED REDUCED STATES[*]

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Abstract. For a quantum state represented as an $n \times n$ density matrix $\sigma \in M_n$, let $\mathcal{S}(\sigma)$ be the compact convex set of quantum states $\rho = (\rho_{ij}) \in M_{m \cdot n}$ with the first partial trace equal to σ, i.e., $\mathrm{tr}_1(\rho) = \rho_{11} + \cdots + \rho_{mm} = \sigma$. It is known that if $m \geq n$ then there is a rank one matrix $\rho \in \mathcal{S}(\sigma)$ satisfying $\mathrm{tr}_1(\rho) = \sigma$. If $m < n$, there may not be any rank one matrix in $\mathcal{S}(\sigma)$. In this paper, we determine the ranks of the elements and ranks of the extreme points of the set $\mathcal{S}$. We also determine $\rho^* \in \mathcal{S}(\sigma)$ with rank bounded by k such that $\|\mathrm{tr}_1(\rho^*) - \sigma\|$ is minimum for a given unitary similarity invariant norm $\| \cdot \|$. Furthermore, the relation between the eigenvalues of σ and those of $\rho \in \mathcal{S}(\sigma)$ is analyzed. Extension of the results and open problems will be mentioned.

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1. Introduction. In quantum information science, quantum states are used to store, process, and transmit information. Mathematically, quantum states are represented by density matrices, i.e., positive semidefinite matrices of trace 1; see [8, 12] for example. Let M_n (H_n) be the set of $n \times n$ complex (Hermitian) matrices, and let $D(n)$ be the set of density matrices in M_n. Suppose $\sigma_1 \in D(m)$ and $\sigma_2 \in D(n)$ are two quantum states. Their product state is $\sigma_1 \otimes \sigma_2$. The combined system is known as the bipartite system, and a general quantum state is represented by a density matrix $\rho \in D(m \cdot n)$. Two basic quantum operations used to extract information of the subsystems from a quantum state of the bipartite system are the partial traces, which are linear maps satisfying

$$\mathrm{tr}_1(\sigma_1 \otimes \sigma_2) = \sigma_2 \quad \text{and} \quad \mathrm{tr}_2(\sigma_1 \otimes \sigma_2) = \sigma_1$$

on tensor states $\sigma_1 \otimes \sigma_2 \in D(m \cdot n)$. Then for a general state $\rho = (\rho_{ij})_{1 \leq i, j \leq m} \in D(m \cdot n)$ such that $\rho_{ij} \in M_n$, we have

$$\mathrm{tr}_1(\rho) = \rho_{11} + \cdots + \rho_{mm} \in M_n \quad \text{and} \quad \mathrm{tr}_2(\rho) = (\mathrm{tr}\rho_{ij})_{1 \leq i, j \leq m} \in M_m.$$

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It is well known that for every $\sigma \in D(n)$ there is a pure state $\rho \in D(n \cdot n)$ such that $\mathrm{tr}_1(\rho) = \sigma$. This is known as the *purification process*, which is useful in the study of quantum computation; for example see [12]. In fact, it is easy to show that for every $\sigma \in D(n)$ of rank r, there is a pure state $\rho \in D(r \cdot n)$ satisfying $\mathrm{tr}_1(\rho) = \sigma$. However, one may not be able to find a purification if the dimension of the first system is bounded, say, due to limitation of resource or restriction on the physical system. In such a case, two questions naturally arise:

PROBLEM 1.1. Can we find a pure state $\rho \in D(m \cdot n)$ such that $\mathrm{tr}_1(\rho)$ is nearest to σ, say, with respect to a certain norm $\|\cdot\|$ on H_n?

PROBLEM 1.2. Can we find $\rho \in D(m \cdot n)$ with rank as low as possible so that $\mathrm{tr}_1(\rho) = \sigma$?

In Section 2, we will give complete answers to these problems. In particular, for a given $\sigma \in D(n)$ and a given positive integers k and m, we determine

$$\min\{\|\mathrm{tr}_1(\rho) - \sigma\| : \rho \in D(m \cdot n) \text{ has rank at most } k\}$$

for any *unitary similarity invariant norm* $\|\cdot\|$ on H_n, i.e., norm $\|\cdot\|$ such that $\|UAU^*\| = \|A\|$ for any $A \in H_n$ and unitary $U \in M_n$. In fact, using the notion of *majorization*, we obtain a general result on the existence of $\rho \in D(m \cdot n)$ with low rank such that $\mathrm{tr}_1(\rho) - \sigma$ satisfies many nice properties.

To better understand quantum states with a prescribed reduced state, we consider the compact convex set

$$\mathcal{S}(\sigma) = \{\rho \in D(m \cdot n) : \mathrm{tr}_1(\rho) = \sigma\}.$$

In Sections 3, we determine the ranks of elements and the ranks of extreme points in $\mathcal{S}(\sigma)$. In Section 4, we analyze the relationship between the eigenvalues of σ and those of the elements in $\mathcal{S}(\sigma)$. We obtain a necessary and sufficient condition relating the eigenvalues of ρ and σ when $m \geq n$, and also in some low dimension cases. The general problem for the case when $m < n$ remains open. In Section 5, we discuss the extensions and difficulties of the study to multi-partite systems.

Researchers have used advanced techniques in representation theory (see [2, 7] and their references) to give a complete description of the relationship between the eigenvalues of the reduced states $\mathrm{tr}_1(\rho), \mathrm{tr}_2(\rho)$, and those of the "parent" state ρ. However, it is not easy to generate (and store) all the inequalities even for a moderate size problem (see [7]). Moreover, it is not easy to use the numerous set of inequalities to answer basic questions. For example, for $(m, n) = (2, 3)$, there is a density matrix $\rho \in M_{2 \cdot 3}$ and reduced states $\mathrm{tr}_2(\rho), \mathrm{tr}_1(\rho)$ with eigenvalues $a_1 \geq \cdots \geq a_6$, $b_1 \geq b_2$, and $c_1 \geq c_2 \geq c_3$ respectively if and only if 41 inequalities are satisfied [7]. However,

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it is not easy to use the result to answer Problems 1 and 2, and other simple problems such as:

1. Characterize the eigenvalues $a_1 \geq \cdots \geq a_6$ of a density matrix $\rho \in M_{2 \cdot 3}$ such that the (first) partial trace is a maximally entangled state, i.e., $\mathrm{tr}_1(\rho) = I_3/3$.
2. Determine all possible ranks of matrices in the convex set

$$\mathcal{S}(I_3/3) = \{\rho \in D(2 \cdot 3) : \mathrm{tr}_1(\rho) = I_3/3\}.$$

3. Determine the ranks of the extreme points of the convex set $\mathcal{S}$ above.

Nevertheless, one can readily answer the above problems using our results in Sections 3 and 4. (See Section 5.)

We conclude this section by fixing some notations. We will use X^t and X^* to denote the transpose and conjugate transpose of a matrix or vector X.

Let $\{e_1^{(m)}, \ldots, e_m^{(m)}\}$ and $\{e_1^{(n)}, \ldots, e_n^{(n)}\}$ be the standard bases for $\mathbb{C}^m$ and $\mathbb{C}^n$, respectively. Then, clearly, $\{e_1^{(m)} \otimes e_1^{(n)}, e_1^{(m)} \otimes e_2^{(n)}, \ldots, e_m^{(m)} \otimes e_n^{(n)}\}$ is the standard basis for $\mathbb{C}^m \otimes \mathbb{C}^n \equiv \mathbb{C}^{mn}$. For $\ell = m, n$ and $1 \leq i, j \leq \ell$, let $E_{ij}^{(\ell)} = e_i^{(\ell)}(e_j^{(\ell)})^t$. Then $\{E_{ij}^{(\ell)} : 1 \leq i, j \leq \ell\}$ is the standard basis for M_ℓ. For simplicity, we use the notation e_i for $e_i^{(m)}$ or $e_i^{(n)}$ and E_{ij} for $E_{ij}^{(\ell)}$, if the dimension is clear in the context. Also, we use $e_i \otimes e_j$ instead of $e_i^{(m)} \otimes e_j^{(n)}$.

Furthermore, we use $PSD(n)$ and $\mathcal{R}_k(n)$ to denote the sets of matrices in M_n which are positive semidefinite and have rank at most k, respectively.

Two linear maps

$$[\,\cdot\,] : \mathbb{C}^{mn} \to M_{n,m} \quad \text{and} \quad \mathrm{vec} : M_{n,m} \to \mathbb{C}^{mn}$$

will be used frequently in our discussion. Here, for $w = (w_1, \ldots, w_{mn})^t \in \mathbb{C}^{mn}$ $W = [w]$ is the $n \times m$ matrix such that the jth column equals $(w_{(j-1)n+1}, \ldots, w_{jn})^t$ for $j = 1, \ldots, m$; and vec is the inverse map which converts an $n \times m$ matrix W to $w = \mathrm{vec}(W) \in \mathbb{C}^{mn}$ so that $W = [w]$. Note that

$$\mathrm{tr}_1(ww^*) = WW^* \quad \text{and} \quad \mathrm{tr}_2(ww^*) = W^t(W^t)^*.$$

2. Approximation by reduced states of low rank states. To state and prove our results, we need the following definitions and notation.

Recall that for $x, y \in \mathbb{R}^n$, x is *majorized* by y, denoted by $x \prec y$, if the sum of entries of the vectors are the same, and the sum of the k largest entries of x is not larger than that of y for $k = 1, \ldots, n-1$. A scalar function $f : \mathbb{R}^n \to \mathbb{R}$ is *Schur convex* provided $f(x) \leq f(y)$ whenever $x \prec y$.

We can extend the definition of majorization and Schur convex function to Hermitian matrix as follows. For every $A \in H_n$, let $\lambda(A) \in \mathbb{R}^n$ be the vector of eigenvalues of A with entries arranged in descending order. For $A, B \in H_n$, we write $A \prec B$ if $\lambda(A) \prec \lambda(B)$. A function $f : \mathbb{R}^n \to \mathbb{R}$ can be extended to $\tilde{f} : H_n \to \mathbb{R}$ by setting $\tilde{f}(A) = f(\lambda(A))$. On the other hand, some scalar functions on H_n or $D(n)$ can be viewed as an extension of $f : \mathbb{R}^n \to \mathbb{R}$. For example, the determinant function $A \mapsto \det(A)$ on H_n corresponds to $f(x_1, \ldots, x_n) = \prod_{j=1}^n x_j$; the von Neumann entropy $\rho \mapsto -\text{tr}\rho(\log \rho)$ on $D(n)$ corresponds to $f(x) = -\sum_{j=1}^n x_j \log x_j$ with the convention that $x_j \log x_j = 0$ if $x_j = 0$. Moreover, every unitary similarity invariant norm $\| \cdot \|$ corresponds to a Schur convex norm function $f : \mathbb{R}^n \to \mathbb{R}$; see [10]. For example, for $1 \leq p \leq \infty$ the Schatten p-norm defined by

$$\|A\|_p = \{\text{tr}|A|^p\}^{1/p}$$

is a unitary similarity invariant norm, where $|A|$ is the unique positive semi-definite matrix such that $|A|^2 = A^*A$. Here, we take the limit $p \to \infty$, and set $\|A\|_\infty = \max\{|\mu| : \mu$ is an eigenvalue of $|A|\}$. Clearly, the Schatten p-norm corresponds to the ℓ_p norm on $\mathbb{R}^n$ defined by $\ell_p(x_1, \ldots, x_n) = (\sum_{j=1}^n |x_j|^p)^{1/p}$.

We have the following result.

THEOREM 2.1. *Let n, m, k be positive integers such that $k \leq m$. Suppose $\sigma \in D(n)$ has rank r and has spectral decomposition $\sum_{j=1}^r \lambda_j x_j x_j^*$ with $\lambda_1 \geq \cdots \geq \lambda_r > 0$. Then there is $\rho \in D(m \cdot n)$ with rank at most k such that $\text{tr}_1(\rho) = \sigma$ if and only if $r \leq mk$.*

If $mk < r$, then there is $\rho \in D(m \cdot n)$ with rank k such that

$$\text{tr}_1(\rho) = \sum_{j=1}^{mk} (\lambda_j + \mu) x_j x_j^*,$$

where $\mu = (\sum_{j=mk+1}^r \lambda_j)/(mk)$, so that

$$(2.1) \quad \lambda(\sigma - \text{tr}_1(\rho)) = (\lambda_{mk+1}, \ldots, \lambda_r, \underbrace{0, \ldots, 0}_{n-r \text{ terms}}, \underbrace{-\mu, \ldots, -\mu}_{mk \text{ terms}}) \prec \lambda(\sigma - \text{tr}_1(\tilde{\rho}))$$

for all $\tilde{\rho} \in D(m \cdot n)$ with rank at most k.

By the properties of Schur convex functions and unitary similarity invariant norm (see [11] and [10]), we immediately have the following.

COROLLARY 2.2. *Suppose σ and ρ satisfy the hypothesis and conclusion of Theorem 2.1. Then for every Schur convex function $f : \mathbb{R}^n \to \mathbb{R}$, we have*

$$f(\lambda(\sigma - \text{tr}_1(\rho))) \leq f(\lambda(\sigma - \text{tr}_1(\tilde{\rho}))) \quad \text{for all } \tilde{\rho} \in D(m \cdot n) \text{ of rank at most } k.$$

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Furthermore, for every unitary similarity invariant norm $\|\cdot\|$ on H_n, we have

$$\|\sigma - \mathrm{tr}_1(\rho)\| \leq \|\sigma - \mathrm{tr}_1(\tilde{\rho})\| \quad \textit{for all } \tilde{\rho} \in D(m \cdot n) \textit{ of rank at most } k.$$

Proof of Theorem 2.1. If $r \leq mk$, then we can write $\sigma = \sigma_1 + \cdots + \sigma_k$, where each σ_i has rank at most m and has a purification $\rho_i \in D(m \cdot n)$. Then $\rho = \rho_1 + \cdots + \rho_k \in D(m \cdot n)$ has rank at most k such that $\mathrm{tr}_1(\rho) = \sigma$.

Conversely, if $\rho \in D(m \cdot n)$ has rank at most k so that it is the sum of at most k rank one matrices $\rho_1, \ldots, \rho_k$. Then $\mathrm{tr}_1(\rho_i)$ has rank at most m, and $\mathrm{tr}_1(\rho)$ has rank at most mk.

Suppose $mk < r$. Let $\hat{\sigma} = \sum_{j=1}^{mk}(\lambda_j + \mu)x_j x_j^* \in H_n$. Then $\hat{\sigma} = \hat{\rho}_1 + \cdots + \hat{\rho}_k$ such that each $\hat{\rho}_j$ has rank m, and admits a purification $\rho_j \in D(m \cdot n)$. Let $\rho = \rho_1 + \cdots + \rho_k$. Then ρ has rank at most k and $\mathrm{tr}_1(\rho) = \hat{\sigma}$.

To prove (2.1), suppose $r > mk$. Let

$$(c_1, c_2 \ldots, c_n) = \lambda(\sigma - \mathrm{tr}_1(\rho)) = (\lambda_{mk+1}, \ldots, \lambda_r, \underbrace{0, \ldots, 0}_{n-r \text{ terms}}, \underbrace{-\mu, \ldots, -\mu}_{mk \text{ terms}}),$$

where $\mu = (\sum_{j=mk+1}^{r} \lambda_j)/(mr)$.

Suppose $\tilde{\rho}$ has rank at most k. Then $\mathrm{tr}_1(\tilde{\rho})$ has rank at most mk. Let

$$\lambda(\mathrm{tr}_1(\tilde{\rho})) = (b_1, \ldots, b_n).$$

Then we have $b_i = 0$ for $mk < i \leq n$.

Suppose $\lambda(\sigma - \mathrm{tr}_1(\tilde{\rho})) = (a_1, \ldots, a_n)$. We will prove that

(2.2) $$(c_1, c_2 \ldots, c_n) \prec (a_1, a_2 \ldots, a_n).$$

Clearly, we have $\sum_{i=1}^{mn} c_i = 0 = \sum_{i=1}^{mn} a_i$. Since $\sigma = (\sigma - \mathrm{tr}_1(\tilde{\rho})) + \mathrm{tr}_1(\tilde{\rho})$, by Wielandt's inequalities [11, Theorem 9.G.1a], for $1 \leq s \leq n - mk$, we have

$$\sum_{i=1}^{s} a_i = \sum_{i=1}^{s} a_i + \sum_{i=1}^{s} b_{mk+i} \geq \sum_{i=1}^{s} \lambda_{mk+i} = \sum_{i=1}^{s} c_i.$$

Let $\tilde{\mu} = (\sum_{j=1}^{n-mk} a_j)/(mk) = -(\sum_{j=n-mk+1}^{n} a_j)/(mk)$. Then we have

$$(c_1, c_2 \ldots, c_n) \prec (a_1, a_2 \ldots, a_{n-mk}, \underbrace{-\tilde{\mu}, \ldots, -\tilde{\mu}}_{mk \text{ terms}}) \prec (a_1, a_2 \ldots, a_n). \quad \square$$

3. Ranks of elements in $\mathcal{S}(\sigma)$. In this section, for $\sigma \in D(n)$, we consider the compact convex set

$$\mathcal{S}(\sigma) = \{\rho \in D(m \cdot n) : \mathrm{tr}_1(\rho) = \sigma\}.$$

We will completely determine the ranks attainable by its elements and by its extreme points. The following lemma is useful in our discussion.

LEMMA 3.1. *Let $\sigma \in D(n)$ and $U \in M_n$ be unitary. Then*

$$\mathcal{S}(U\sigma U^*) = (I_m \otimes U)\mathcal{S}(\sigma)(I_m \otimes U)^* = \{(I_m \otimes U)\rho(I_m \otimes U)^* : \rho \in \mathcal{S}(\sigma)\}.$$

Recall that $\sigma \in D(n)$ is a pure state if $\mathrm{rank}\,(\sigma) = 1$. It is well known that the extreme points of $D(n)$ are pure states. For a pure state $\sigma \in D(n)$, we have the following complete description of $\mathcal{S}(\sigma)$. In particular, all states in the set $\mathcal{S}(\sigma)$ are tensor states.

PROPOSITION 3.2. *Let $\sigma \in D(n)$ be a pure state. Then*

$$\mathcal{S}(\sigma) = \{\xi \otimes \sigma : \xi \in D(m)\}.$$

Consequently, there is $\rho \in \mathcal{S}(\sigma)$ with rank k if and only if $1 \le k \le m$. Moreover, ρ is an extreme point of $\mathcal{S}(\sigma)$ if and only if $\rho = \xi \otimes \sigma$ for a rank one $\xi \in D(m)$.

Proof. By Lemma 3.1, we may assume that $\sigma = E_{11} \in M_n$. Then $\rho = (\rho_{ij})_{1 \le i,j \le m} \in D(m \cdot n)$ with $\rho_{ij} \in M_n$ if and only if $\rho_{11} + \rho_{22} + \cdots + \rho_{mm} = E_{11}$. Since ρ is positive semidefinite, we see that $\rho_{ii} = \xi_i E_{11}$, where $\xi_i \ge 0$ for $i = 1, \ldots,\ m$ and $\sum_{i=1}^{m} \xi_i = 1$. Thus, $\rho_{ij} = \xi_{ij} E_{11}$ for some ξ_{ij}, $i,\ j = 1, \ldots,\ m$, with $\xi_{ii} = \xi_i$. Hence, $\rho = \xi \otimes \sigma$ with $\xi = (\xi_{ij}) = \mathrm{tr}_2(\rho) \in D(m)$.

Clearly, $\mathrm{rank}\,(\rho) = \mathrm{rank}\,(\xi) \in \{1, \ldots,\ m\}$. Also, it is well known that $D(m)$ is a compact convex set with the pure states as the set of extreme points. The last statement follows. $\square$

For a general state $\sigma \in D(n)$, it is not so easy to give a complete description for the set $\mathcal{S}(\sigma)$. In the following, we consider general states $\sigma \in D(n)$ and determine the ranks and extreme points of matrices in $\mathcal{S}(\sigma)$.

THEOREM 3.3. *Let $\sigma \in D(n)$ have rank r. There is $\rho \in \mathcal{S}(\sigma) \subseteq D(m \cdot n)$ with rank k if and only if*

$$\lceil r/m \rceil \le k \le rm.$$

In particular, if there are matrices in $\mathcal{S}(\sigma)$ of rank r_1, r_2 with $r_1 < r_2$, then there are matrices in $\mathcal{S}(\sigma)$ of rank $r_1 + 1, \ldots, r_2 - 1$.

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Proof. By Lemma 3.1, we may assume that $\sigma = \mathrm{diag}(d_1, \ldots, d_r, 0, \ldots, 0)$ with $d_1 \geq \cdots \geq d_r > 0$.

Suppose $\rho = ZZ^* \in \mathcal{S}(\sigma)$ such that Z is $mn \times k$, where k is the rank of ρ and Z has columns $z_1, \ldots, z_k \in \mathbb{C}^{mn}$. Set $Z_j = [z_j]$ for $j = 1, \ldots, k$. Then $\sigma = \mathrm{tr}_1(\rho) = \sum_{j=1}^{k} Z_j Z_j^*$ has rank at most mk because every $Z_j Z_j^*$ has rank at most m. Hence, $r/m \leq k$.

Next, we consider the upper bound for k. Suppose $\rho = (\rho_{ij}) \in \mathcal{S}(\sigma)$ with $\rho_{ij} \in M_n$. Since

$$\sigma = \mathrm{diag}(d_1, \ldots, d_r, 0, \ldots, 0) = \rho_{11} + \rho_{22} + \cdots + \rho_{mm},$$

we have $\rho_{ij} \in \mathrm{span}\,\{E_{pq} : 1 \leq p,\ q \leq r\}$ for all $1 \leq i,\ j \leq m$. Hence, $\rho = (\rho_{ij})$ has rank at most rm.

Finally, we show that for every k between the lower and upper bound, there exists $\rho \in \mathcal{S}(\sigma)$ with rank k. Suppose $r/m \leq k \leq rm$. Then ρ can be constructed as follows.

Case 1. Suppose $r < k \leq rm$ and denote $k = qr + s$ with $0 < q < m$ and $0 < s \leq r$. Let

$$\rho = \sum_{i=1}^{q+1} \sum_{j=1}^{s} \frac{d_j}{q+1} E_{ii}^{(m)} \otimes E_{jj}^{(n)} + \sum_{i=1}^{q} \sum_{j=s+1}^{r} \frac{d_j}{q} E_{ii}^{(m)} \otimes E_{jj}^{(n)}.$$

Then rank $\rho = (q+1)s + q(r-s) = qr + s = k$ and

$$\mathrm{tr}_1(\rho) = \sum_{i=1}^{q+1} \sum_{j=1}^{s} \frac{d_j}{q+1} E_{jj}^{(n)} + \sum_{i=1}^{q} \sum_{j=s+1}^{r} \frac{d_j}{q} E_{jj}^{(n)} = \sum_{j=1}^{r} d_j E_{jj}^{(n)} = \sigma.$$

Case 2. Suppose $r/m \leq k \leq r \leq n$, and $r = k\hat{q} + \hat{s}$ with $0 \leq \hat{q} < m$ and $1 \leq \hat{s} \leq k$. Let $f_j = \sqrt{d_j} e_j^{(n)}$ for $1 \leq j \leq n$, and

$$\rho = \sum_{j=1}^{s} \left(\sum_{i=1}^{\hat{q}+1} e_i^{(m)} \otimes f_{(i-1)k+j} \right) \left(\sum_{i=1}^{\hat{q}+1} e_i^{(m)} \otimes f_{(i-1)k+j} \right)^*$$

$$+ \sum_{j=\hat{s}+1}^{k} \left(\sum_{i=1}^{\hat{q}} e_i^{(m)} \otimes f_{(i-1)k+j} \right) \left(\sum_{i=1}^{\hat{q}} e_i^{(m)} \otimes f_{(i-1)k+j} \right)^*.$$

Then, rank $\rho = \hat{s} + (k - \hat{s}) = k$ and

$$\mathrm{tr}_1(\rho) = \sum_{j=1}^{\hat{s}} \sum_{i=1}^{\hat{q}+1} d_{(i-1)k+j} E_{(i-1)k+j\ \ (i-1)k+j}^{(n)} + \sum_{j=\hat{s}+1}^{k} \sum_{i=1}^{\hat{q}} d_{(i-1)k+j} E_{(i-1)k+j\ \ (i-1)k+j}^{(n)}$$

$$= \sum_{\ell=1}^{r} d_\ell E_{\ell\,\ell}^{(n)} = \sigma. \quad \square$$

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By Theorem 3.3, we have the following corollary, which is part of Theorem 2.1.

COROLLARY 3.4. *Suppose* $\sigma \in D(n)$ *has rank* r. *Then there is* $\rho \in D(m \cdot n)$ *with rank not larger than* k *such that* $\mathrm{tr}_1(\rho) = \sigma$ *if and only if* $km \geq r$. *In particular,* σ *has a purification* $\rho \in D(m \cdot n)$ *if and only if* $m \geq r$.

Next, we consider the extreme points of the set $\mathcal{S}(\sigma)$. We begin with some general observations.

LEMMA 3.5. *Let* $\sigma \in D(n)$ *and let* $\rho \in \mathcal{S}(\sigma) \subseteq D(m \cdot n)$. *Then* ρ *is not an extreme point if and only if there exists a nonzero* $\xi \in H_{mn}$ *such that* $\rho \pm \xi \in PSD(m \cdot n)$ *and* $\mathrm{tr}_1(\xi) = O_n$. *In such a case, there are* $\rho_1, \rho_2 \in \mathcal{S}(\sigma)$ *with* $\mathrm{rank}(\rho_1) < \mathrm{rank}(\rho)$ *such that* $\rho = (\rho_1 + \rho_2)/2$.

Proof. If $\rho \in \mathcal{S}(\sigma)$ is not extreme, then there are two different elements $\rho_1, \rho_2 \in \mathcal{S}(\sigma)$ such that $\rho = (\rho_1 + \rho_2)/2$. Let $\xi = (\rho_1 - \rho_2)/2 \neq 0$. Then $\rho \pm \xi \in \mathcal{S}(\sigma)$ so that $\rho \pm \xi \in PSD(m \cdot n)$ and $\mathrm{tr}_1(\xi) = \mathrm{tr}_1(\rho_1 - \rho_2)/2 = (\sigma - \sigma)/2 = O_n$. Conversely, if $\xi \in H_{mn}$ satisfies $\rho \pm \xi \in D(m \cdot n)$ and $\mathrm{tr}_1(\xi) = O_n$, then we can set $\rho_\pm = \rho \pm \xi$ so that $\rho_+, \rho_- \in \mathcal{S}(\sigma)$ and $\rho = (\rho_+ + \rho_-)/2$.

Now, if $\rho \in \mathcal{S}(\sigma)$ has rank r and is not an extreme point. Then we can choose an orthonormal set $\{z_1, \ldots, z_r\}$ in $\mathbb{C}^{mn}$ such that $\rho = \sum_{j=1}^r \lambda_j z_j z_j^*$. Suppose a nonzero $\xi \in H_{mn}$ is such that $\rho \pm \xi \in PSD(m \cdot n)$ and $\mathrm{tr}_1(\xi) = O_m$. Then $\xi = \sum_{1 \leq i,j \leq r} h_{ij} z_i z_j^*$ for some non-zero $(h_{ij}) \in H_r$. Thus, there exists $t > 0$ such that

1) $\rho \pm t\xi \in PSD(m \cdot n)$,
2) either $\rho_1 = \rho + t\xi$ or $\rho_2 = \rho - t\xi$ has rank $< r$, and
3) $\rho = (\rho_1 + \rho_2)/2$, with $\rho_1, \rho_2 \in \mathcal{S}(\sigma)$.

The last assertion follows. ☐

THEOREM 3.6. *Suppose* $\rho \in \mathcal{S}(\sigma)$ *for a given* $\sigma \in D(n)$ *such that* ρ *has rank* r *and* $\rho = ZZ^* \in D(m \cdot n)$, *where* Z *has columns* $z_1, \ldots, z_r \in \mathbb{C}^{mn}$. *Then* ρ *is an extreme points of* $\mathcal{S}(\sigma)$ *if and only if the set* $T(z_1, \ldots, z_r) = \{[z_i][z_j]^* : 1 \leq i, j \leq r\}$ *is linearly independent.*

Proof. Suppose $T(z_1, \ldots, z_r)$ is linearly dependent. Then there is $H = (h_{ij}) \in M_r$ such that

$$\sum_{i,j} h_{ij} [z_i][z_j]^* = 0.$$

Let $[z_j] = Z_j$ for $j = 1, \ldots, r$. Then $[Z_1 \cdots Z_r](H \otimes I_m)[Z_1 \cdots Z_r]^* = 0$. We may replace H by $e^{it}H + e^{-it}H^*$ for a suitable $t \in [0, 2\pi)$ and assume that $0 \neq H = H^*$. Then for $t > 0$ such that $\|tH\| < 1$, $\rho_\pm = \rho \pm tZHZ^* = Z(I_r \pm tH)Z^*$ is positive

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semidefinite. Moreover,

$$\mathrm{tr}_1(\rho_\pm) = \sum_{j=1}^r Z_j Z_j^* \pm t \sum_{1 \le i,j \le r} h_{ij} Z_i Z_j^* = \sigma$$

and $\mathrm{tr}(\rho_\pm) = \mathrm{tr}(\sigma) = 1$. Thus, $\rho_\pm \in \mathcal{S}(\sigma)$ are two different elements such that $\rho = (\rho_+ + \rho_-)/2$. Hence, ρ is not an extreme points.

Conversely, if ρ is not an extreme point of $\mathcal{S}(\sigma)$, then $\rho = (\rho_+ + \rho_-)/2$ for two different elements ρ_+, ρ_- in $\mathcal{S}(\sigma)$. Then $\rho_+ - \rho = \rho - \rho_- = \tilde{H} \ne 0$ so that $\rho_+ = \rho + \tilde{H} = ZZ^* + \tilde{H} \in \mathcal{S}(\sigma)$ and $\rho_- = \rho - \tilde{H} = ZZ^* - \tilde{H} \in \mathcal{S}(\sigma)$. Thus, the range space of $\tilde{H}$ is a subspace of the range space of ρ, which is the column space of Z. Thus, $\tilde{H}$ has the form ZHZ^* for some $0 \ne (h_{ij}) = H = H^* \in M_r$ so that $I_r \pm H$ are positive semidefinite. Moreover,

$$\mathrm{tr}_1(\rho_\pm) = \mathrm{tr}_1(\rho \pm \tilde{H}) = \mathrm{tr}_1(\rho) = \sigma.$$

It follows that $0 = \mathrm{tr}_1(\tilde{H}) = \sum_{ij} h_{ij} Z_i Z_j^*$. Hence, $T(z_1, \ldots, z_r)$ is linearly dependent. ▯

Next, we determine all possible ranks of the extreme points of $\mathcal{S}(\sigma)$.

THEOREM 3.7. *Suppose* $\sigma \in D(n)$ *and* $\mathrm{rank}\,(\sigma) = r$. *There is an extreme point* $\rho \in \mathcal{S}(\sigma) \subseteq D(m \cdot n)$ *with rank* k *if and only if*

$$\lceil r/m \rceil \le k \le r.$$

Moreover, every $\rho \in \mathcal{S}(\sigma)$ *with rank equal to* $\lceil r/m \rceil$ *is an extreme point. For* $\lceil r/m \rceil < k \le r$, *there exists* $\rho \in \mathcal{S}(\sigma)$ *which is not an extreme point.*

Proof. By Lemma 3.1, we may assume that $\sigma = \mathrm{diag}(d_1, \ldots, d_r, 0, \ldots, 0)$ with $d_1 \ge \cdots \ge d_r > 0$.

(1) We show that any $\rho \in \mathcal{S}(\sigma)$ with $\mathrm{rank}\,(\rho) = k > r$ is not an extreme point.

Suppose $\rho = z_1 z_1^* + \cdots + z_k z_k^*$. Let $Z_i = [z_i]$ for $i = 1, \ldots, k$. Then $\sum_{j=1}^k Z_j Z_j^* = \sigma$. It follows that the last $n - r$ rows of Z_i are zero for $i = 1, \ldots, k$. Thus, $Z_i Z_j^* = C_{ij} \oplus O_{n-r}$ for some $C_{ij} \in M_r$. Thus, $\{Z_i Z_j^* : 1 \le i, j \le k\}$ is linearly dependent as $k^2 > r^2$. By Theorem 3.6, ρ is not an extreme point.

(2) Suppose $r/m \le k \le r$. We show that there is an extreme point $\rho \in \mathcal{S}(\sigma)$ with $\mathrm{rank}\,(\rho) = k$.

Because $r/m \le k \le r$, we can let $r = k\hat{q} + \hat{s}$, and use the construction in Case 2 in the proof of Theorem 3.3 to obtain $\rho = \sum_{j=1}^k z_j z_j^*$. Note that for $1 \le i, j \le k$, $[z_i][z_j]^*$ has the form $\sqrt{\lambda_i \lambda_j} E_{ij}(k) \oplus Y_{ij}$. Thus, $\{[z_i][z_j]^* : 1 \le i, j \le k\}$ is linearly independent, and ρ is an extreme point.

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(3) Suppose $\lceil r/m \rceil < k \leq r$. We show that there is $\rho \in \mathcal{S}(\sigma)$ with rank $(\rho) = k$ such that ρ is not an extreme point.

Because $\lceil r/m \rceil < k \leq r \leq n$, we may use the the construction in Case 2 in the proof of Theorem 3.3, with k replaced by $k-1$ to get $\tilde{\rho} = \sum_{j=1}^{k-1} z_j z_j^*$ such that $\mathrm{tr}_1(\tilde{\rho}) = \sigma$. Since $k-1 < r$, $Z_1 = [z_1]$ has two nonzero columns. Replace z_1 by $\tilde{z}_1 = z_1/\sqrt{2}$ and construct z_k so that $Z_k = [z_k]$ is obtained from $[\tilde{z}_1]$ by multiplying its first column by -1. Then $\rho = \tilde{z}_1 \tilde{z}_1^* + \sum_{j=2}^{k} z_j z_j^* \in \mathcal{S}(\sigma)$ has rank k. Note that $[\tilde{z}_1][\tilde{z}_1]^* = [z_k][z_k]^*$ so that $T(\tilde{z}_1, z_2, \ldots, z_k)$ is linearly dependent. So, ρ is not extreme.

(4) We show that if $\rho \in \mathcal{S}(\sigma)$ has rank $k = \lceil r/m \rceil$, then ρ is an extreme point.

If ρ is not an extreme point, then by Lemma 3.5 $\rho_1, \rho_2 \in \mathcal{S}(\sigma)$ with rank $(\rho_1) <$ rank (ρ) such that $\rho = (\rho_1 + \rho_2)/2$, which is a contradiction. $\square$

COROLLARY 3.8. *Suppose $\sigma \in D(n)$ and $\rho \in \mathcal{S}(\sigma) \subseteq D(m \cdot n)$.*

(a) *If ρ has rank one, then ρ is an extreme point of $\mathcal{S}(\sigma)$.*
(b) *If ρ has rank $k > n$, then ρ is not an extreme point.*

Proof. (a) If $\rho = zz^*$, then $\{[z][z]^*\}$ is linearly independent. So, ρ is an extreme point.

(b) If $\rho = ZZ^*$, where Z has linearly independent columns $z_1, \ldots, z_k$, then $T(z_1, \ldots, z_k) \subseteq M_{n^2}$ has k^2 elements with $k^2 > n^2$, and hence is a linearly dependent set in M_{n^2}. So, ρ is not an extreme point. $\square$

4. Eigenvalues. As mentioned in the introduction, even though we know the inequalities governing the eigenvalues of $\rho \in D(m \cdot n)$ and those of $\sigma_2 = \mathrm{tr}_1(\rho)$ and $\sigma_1 = \mathrm{tr}_2(\rho)$, it is not easy to use them to determine the relations between the eigenvalues of ρ and $\mathrm{tr}_1(\rho)$ (without specifying those of $\mathrm{tr}_2(\rho)$). We have the following result.

THEOREM 4.1. *Suppose $m, n \geq 2$, $\lambda_1 \geq \cdots \geq \lambda_n \geq 0$ and $\mu_1 \geq \cdots \geq \mu_{mn} \geq 0$ satisfy $\sum_{j=1}^{n} \lambda_j = 1 = \sum_{j=1}^{mn} \mu_j$.*

(a) *If there exist $\sigma \in D(n)$ with eigenvalues $\lambda_1, \ldots, \lambda_n$ and $\rho \in S(\sigma) \subseteq D(m \cdot n)$ with eigenvalues $\mu_1, \ldots, \mu_{mn}$, then*

$$(4.1) \qquad \left(\frac{\lambda_1}{m}, \ldots, \frac{\lambda_1}{m}, \frac{\lambda_2}{m}, \ldots, \frac{\lambda_2}{m}, \ldots, \frac{\lambda_n}{m}, \right) \prec (\mu_1, \mu_2, \ldots, \mu_{nm}),$$

so that

$$(4.2) \qquad (\lambda_1, \ldots, \lambda_n) \prec \left(\sum_{j=1}^{m} \mu_j, \sum_{j=1}^{m} \mu_{m+j}, \ldots, \sum_{j=1}^{m} \mu_{(n-1)m+j} \right),$$

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and setting $\lambda_j = 0$ for $j > n$, we have

$$(4.3) \qquad (\mu_1, \ldots, \mu_{mn}) \prec \left(\sum_{j=1}^m \lambda_j, \sum_{j=1}^m \lambda_{m+j}, \ldots, \sum_{j=1}^m \lambda_{m^2n-m+j} \right).$$

(b) *If $m \geq n$ and condition (4.2) holds, then there exist $\sigma \in D(n)$ with eigenvalues $\lambda_1, \ldots, \lambda_n$ and $\rho \in \mathcal{S}(\sigma)$ with eigenvalues $\mu_1, \ldots, \mu_{mn}$.*

Proof. (a) Suppose $\rho = (\rho_{ij})_{1 \leq i,j \leq m} \in S(\sigma)$ has eigenvalues $\mu_1 \geq \cdots \geq \mu_{mn}$. We may assume that $\rho_{11} + \rho_{22} + \cdots + \rho_{mm} = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. Then there is a permutation matrix $P \in M_{mn}$ such that $P\rho P^t = (\tilde{\rho}_{ij})_{1 \leq i,j \leq n}$ such that $\tilde{\rho}_{ij} \in M_m$ such that $\mathrm{tr}\tilde{\rho}_{jj} = \lambda_j$ for $j = 1, \ldots, n$. There are unitary matrices $U_1, \ldots, U_n \in M_m$ such that all the diagonal entries of $U_j \tilde{\rho}_{jj} U_j^*$ equals $\mathrm{tr}(\rho_{jj})/m = \lambda_j/m$. Let $U = U_1 \oplus \cdots \oplus U_n$. Then the vector of diagonal entries of the matrix $UP\rho P^t U^*$ is majorized by the vector of eigenvalues; see [6] and [11, Chapter 5] for example. We get (4.1), and (4.2).

To prove (4.3), suppose that ρ has spectral decomposition $\rho = \mu_1 z_1 z_1^* + \cdots + \mu_{mn} z_{mn} z_{mn}^*$. Then,

$$\sum_{j=1}^k \mu_j = \mathrm{tr}\left(\sum_{j=1}^k \mu_j z_j z_j^* \right) = \mathrm{tr}\left(\mathrm{tr}_1 \left(\sum_{j=1}^k \mu_j z_j z_j^* \right) \right).$$

Because $\mathrm{tr}_1(\sum_{j=1}^k \mu_j z_j z_j^*)$ has rank at most mk and $\mathrm{tr}_1(\rho) - \mathrm{tr}_1(\sum_{j=1}^k \mu_j z_j z_j^*)$ is positive semi-definite, $\mathrm{tr}(\mathrm{tr}_1(\sum_{j=1}^k \mu_j z_j z_j^*))$ is bounded by the sum of the mk largest eigenvalues of $\mathrm{tr}_1(\rho)$, i.e., $\sum_{j=1}^{km} \lambda_j$.

(b) Suppose $m \geq n$ and the majorization holds. Let $w_k = \sum_{j=1}^m \mu_{(k-1)m+j}$ for $k = 1, \ldots, n$. By the result of Horn [6], there exist unitary matrices $U_1, \ldots, U_n \in M_m$ such that

$$A_k = U_k^* \mathrm{diag}(\mu_{(k-1)m+1}, \mu_{(k-1)m+2}, \ldots, \mu_{km}) U_k$$

has constant diagonal $\dfrac{1}{m}(w_k, \ldots, w_k)$. Then the matrix $A = \sum_{k=1}^n A_k \otimes E_{kk}^{(n)}$ has eigenvalues $\mu_1, \ldots, \mu_{mn}$ and has the form $A = (A_{ij})_{i,j=1}^m$, where

$$A_{ii} = \frac{1}{m} \mathrm{diag}(w_1, \ldots, w_n) \in M_n.$$

Let U be a unitary such that $U^* \mathrm{diag}(w_1, \ldots, w_n) U$ has diagonal entries $\lambda_1, \ldots, \lambda_n$. Let $\omega = e^{\frac{2\pi i}{m}}$ and $D = \oplus_{k=0}^{m-1} \mathrm{diag}(\omega^k, \omega^{2k}, \ldots, \omega^{nk})$. Then

$$\rho = D^* (I_m \otimes U)^* A (I_m \otimes U) D$$

will have reduced state $\mathrm{tr}_1(\rho) = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. ☐

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The following corollaries are clear.

COROLLARY 4.2. *Suppose $m = n = 2$, and $\sigma \in D(2)$ has eigenvalues $\lambda_1 \geq \lambda_2 \geq 0$. There exists $\rho \in D(2 \cdot 2)$ with eigenvalues $\mu_1 \geq \cdots \geq \mu_4$ satisfying $\mathrm{tr}_1(\rho) = \sigma$ if and only if $\mu_1 + \mu_2 \geq \lambda_1$*

COROLLARY 4.3. *Suppose $m \geq n$.*

(a) *For any $\sigma \in D(n)$ there is a pure state $\rho \in D(m \cdot n)$ such that $\mathrm{tr}_1(\rho) = \sigma$.*
(b) *If $\sigma \in D(n)$ is a pure state and $\rho \in \mathcal{S}(\sigma)$, then ρ has rank at most m.*

It is interesting to note that if $m \geq n$, the simple majorization condition (4.3) governs the relations between the eigenvalues of ρ and σ with $\rho \in \mathcal{S}(\sigma)$. For $m < n$, the majorization condition is not good enough as shown in the following.

EXAMPLE 4.4. Suppose $m = 2$ and $n = 3$. Let $\sigma = I_3/3$, and $\rho = uu^*$ for a unit vector. Then $\mathrm{tr}_1(\rho)$ has rank at most two and cannot be σ. Note that the rank is not the only obstacle. Suppose $\rho = U^*\mathrm{diag}(1 - 5d, d, d, d, d, d)U = (\rho_{ij})_{1 \leq i,j \leq 2}$ for $d = 0.1$, and $\mathrm{tr}_1(\rho) = \sigma$. Since $\rho_{11} + \rho_{22} = I_3/3$, they commute and we may assume that they are in diagonal form: $\rho_{11} = \mathrm{diag}(d_1, d_2, d_3)$, and $\rho_{22} = I_3/3 - \rho_{11}$. If ρ_{11} has eigenvalues $d_1 \geq d_2 \geq d_3$, then by the generalized interlacing inequality [3], $d \geq d_2 \geq d \Rightarrow d_2 = d$. Similarly, the second largest eigenvalue of ρ_{22} also equals d. But then $d + d = 2d \neq 1/3$.

THEOREM 4.5. *There exist density matrices $\sigma \in M_3$ with eigenvalues $\lambda_1 \geq \lambda_2 \geq \lambda_3$ and $\rho \in M_6$ with eigenvalues $\mu_1 \geq \cdots \geq \mu_6$ such that $\mathrm{tr}_1(\rho) = \sigma$ if and only if $\mu_4 + \mu_5 \leq \lambda_1 \leq \mu_1 + \mu_2$ and $\mu_5 + \mu_6 \leq \lambda_3 \leq \mu_2 + \mu_3$.*

Proof. Suppose $\rho = \begin{bmatrix} \rho_{11} & \rho_{12} \\ \rho_{21} & \rho_{22} \end{bmatrix}$ has eigenvalues $\mu_1 \geq \cdots \geq \mu_6$ such that $\mathrm{tr}_1(\rho) = \sigma$. Then we may assume that $\rho_{11} + \rho_{22} = \mathrm{diag}(\lambda_1, \lambda_2, \lambda_3)$. As in the proof of Theorem 4.1, we have $(\lambda_1, \lambda_2, \lambda_3) \prec (\mu_1 + \mu_2, \mu_3 + \mu_4, \mu_5 + \mu_6)$. Therefore, we have $\lambda_1 \leq \mu_1 + \mu_2$ and $\mu_5 + \mu_6 \leq \lambda_3$. Suppose ρ_{11} and ρ_{22} have eigenvalues $a_1 \geq a_2 \geq a_3$ and $b_1 \geq b_2 \geq b_3$ respectively. Then applying Horn inequalities [4, 5] for the triple $((1, 3), (1, 3), (2, 3))$, we have $a_1 + a_3 + b_1 + b_3 \geq \lambda_2 + \lambda_3 \Rightarrow \lambda_1 \geq a_2 + b_2$. Let $a_i = b_i = 0$ for $i = 4, 5, 6$. By a result in [9], there exist A, $B \in H_6$ with eigenvalues $a_1 \geq \cdots \geq a_6$ and $b_1 \geq \cdots \geq b_6$ respectively, such that $A + B$ has eigenvalues $\mu_1, \ldots, \mu_6$. Applying Horn inequalities for the triple $((2, 4), (2, 4), (4, 5))$, we have

$$\lambda_1 \geq a_2 + b_2 = a_2 + a_4 + b_2 + b_4 \geq \mu_4 + \mu_5.$$

The inequality $\lambda_3 \leq \mu_2 + \mu_3$ follows from symmetry.

Conversely, suppose $\mu_4 + \mu_5 \leq \lambda_1 \leq \mu_1 + \mu_2$ and $\mu_5 + \mu_6 \leq \lambda_3 \leq \mu_2 + \mu_3$. Then λ_1 lies in (at least) one of the following intervals:

(4.4) $[\mu_5 + \mu_4, \mu_5 + \mu_3], [\mu_5 + \mu_3, \mu_5 + \mu_2], [\mu_5 + \mu_2, \mu_4 + \mu_2], [\mu_4 + \mu_2, \mu_3 + \mu_2], [\mu_3 + \mu_2, \mu_1 + \mu_2].$

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Suppose $\mu_i + \mu_j \leq \lambda_1 \leq \mu_i + \mu_k$. Then we can choose $\mu_j \leq \hat{\mu}_j$, $\hat{\mu}_k \leq \mu_k$ such that $\mu_i + \hat{\mu}_j = \lambda_1$ and $\mu_j + \mu_k = \hat{\mu}_j + \hat{\mu}_k$. Let $a = \sqrt{\hat{\mu}_j \hat{\mu}_k - \mu_j \mu_k}$. Then $\begin{bmatrix} \hat{\mu}_j & a \\ a & \hat{\mu}_k \end{bmatrix}$ has eigenvalues μ_j, μ_k.

Let the remaining 3 eigenvalues of ρ be $\{\mu_i, \ \mu_j, \ \mu_k\}^c = \{\mu_{i_1}, \ \mu_{i_2}, \ \mu_{i_3}\}$.

Claim. For some $\ell = 2$ or 3, λ_ℓ satisfies i) $\mu_{i_1} + \mu_{i_2} \leq \lambda_\ell \leq \mu_{i_1} + \mu_{i_3}$ or ii) $\hat{\mu}_k + \mu_{i_2} \leq \lambda_\ell \leq \hat{\mu}_k + \mu_{i_3}$.

Suppose i) in the claim holds. Then we can choose $\mu_{i_2} \leq \hat{\mu}_{i_2}$, $\hat{\mu}_{i_3} \leq \mu_{i_3}$ such that $\mu_{i_1} + \hat{\mu}_{i_2} = \lambda_\ell$ and $\mu_{i_2} + \mu_{i_3} = \hat{\mu}_{i_2} + \hat{\mu}_{i_3}$. Let $b = \sqrt{\hat{\mu}_{i_2} \hat{\mu}_{i_3} - \mu_{i_2} \mu_{i_3}}$. Then $\begin{bmatrix} \hat{\mu}_{i_2} & b \\ b & \hat{\mu}_{i_3} \end{bmatrix}$ has eigenvalues μ_{i_2}, μ_{i_3}. Hence, the matrix

$$
\rho = \left[\begin{array}{ccc|ccc}
\mu_i & 0 & 0 & 0 & 0 & 0 \\
0 & \hat{\mu}_k & 0 & a & 0 & 0 \\
0 & 0 & \hat{\mu}_{i_2} & 0 & b & 0 \\
\hline
0 & a & 0 & \hat{\mu}_j & 0 & 0 \\
0 & 0 & b & 0 & \hat{\mu}_{i_3} & 0 \\
0 & 0 & 0 & 0 & 0 & \mu_{i_1}
\end{array} \right]
$$

has eigenvalues $\mu_1, \ldots, \mu_6$ and $\mathrm{tr}_1(\rho)$ has eigenvalues λ_1, λ_2 and λ_3.

The proof for the case ii) is similar.

We are going to show that the claim holds in each of the cases in (4.4).

1. $\mu_5 + \mu_4 \leq \lambda_1 \leq \mu_5 + \mu_3$: Then the remaining 3 eigenvalues are μ_1, μ_2 and μ_6. We have $\lambda_2 \leq \lambda_1 \leq \mu_5 + \mu_3 \leq \mu_2 + \mu_1$ and

$$
\lambda_2 \geq \sum_{i=1}^{6} \mu_i - 2\lambda_1 \geq \sum_{i=1}^{6} \mu_i - 2(\mu_5 + \mu_3) \geq \mu_2 + \mu_6.
$$

2. $\mu_5 + \mu_3 \leq \lambda_1 \leq \mu_5 + \mu_2$: Then the remaining 3 eigenvalues are μ_1, μ_4 and μ_6. We have $\lambda_2 \leq \lambda_1 \leq \mu_2 + \mu_5 \leq \mu_1 + \mu_4$ and

$$
\lambda_2 \geq \left(\sum_{i=1}^{6} \mu_i - \lambda_1 \right) / 2 \geq \left(\sum_{i=1}^{6} \mu_i - (\mu_5 + \mu_2) \right) / 2 \geq \mu_4 + \mu_6.
$$

3. $\mu_5 + \mu_2 \leq \lambda_1 \leq \mu_4 + \mu_2$: Then the remaining 3 eigenvalues are μ_1, μ_3 and μ_6. We have $\lambda_2 \leq \lambda_1 \leq \mu_2 + \mu_4 \leq \mu_1 + \mu_3$ and

$$
\lambda_2 \geq \left(\sum_{i=1}^{6} \mu_i - \lambda_1 \right) / 2 \geq \left(\sum_{i=1}^{6} \mu_i - (\mu_4 + \mu_2) \right) / 2 \geq \mu_3 + \mu_6.
$$

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4. $\mu_4 + \mu_2 \leq \lambda_1 \leq \mu_3 + \mu_2$: Then the remaining 3 eigenvalues are μ_1, μ_5 and μ_6. We have $\lambda_3 \geq \mu_5 + \mu_6$ and

$$\lambda_3 \leq \left(\sum_{i=1}^{6} \mu_i - \lambda_1 \right) /2 \leq \left(\sum_{i=1}^{6} \mu_i - (\mu_4 + \mu_2) \right) /2 \leq \mu_1 + \mu_5.$$

5. $\mu_3 + \mu_2 \leq \lambda_1 \leq \mu_1 + \mu_2$: Since $\mu_5 + \mu_6 \leq \lambda_3 \leq \mu_2 + \mu_3$, consider the following cases:
   (a) If $\mu_5 + \mu_6 \leq \lambda_3 \leq \mu_5 + \mu_4$, then we are done.
   (b) If $\mu_5 + \mu_4 \leq \lambda_3 \leq \mu_3 + \mu_4$, then we use $\mu_6 + \mu_2 \leq \lambda_1 \leq \mu_1 + \mu_2$ and we are done.
   (c) If $\mu_3 + \mu_4 \leq \lambda_3 \leq \mu_3 + \mu_2$, then we have

$$\lambda_1 + \lambda_2 \geq \mu_3 + \mu_2 + \mu_3 + \mu_4 \geq \mu_2 + \mu_3 + \mu_4 + \mu_6 \Rightarrow \lambda_2 \leq \mu_1 + \mu_5.$$

So we can use $\mu_6 + \mu_5 \leq \lambda_2 \leq \mu_1 + \mu_5$ and we are done. □

5. Final remarks and further research. First, let us give the solutions of the simple questions mentioned in Section 1 using the results in Section 3 and 4. (Theorems 4.5, 3.3, and 3.6).

1. There exists a density matrix $\rho \in M_{2 \cdot 3}$ with eigenvalues $a_1 \geq \cdots \geq a_6$ such that $\mathrm{tr}_1(\rho) = I_3/3$ if and only if

$$a_2 + a_3 \geq 1/3 \geq a_4 + a_5.$$

2. There exists a density matrix in $\mathcal{S}(I_3/3)$ with rank k if and only if $2 \leq k \leq 6$.
3. There exists an extreme point of $\mathcal{S}(I_3/3)$ with rank k if and only if $2 \leq k \leq 3$.

One may consider extending the results in the previous sections to the compact convex set

$$\mathcal{S}(\sigma_1, \sigma_2) = \{ \rho \in D(m \cdot n) : \mathrm{tr}_1(\rho) = \sigma_2, \mathrm{tr}_2(\rho) = \sigma_1 \}$$

for given $\sigma_1 \in D(m), \sigma_2 \in D(n)$. As mentioned in the introduction, Klyachko [7] has studied the relationship between the eigenvalues of $\rho \in \mathcal{S}(\sigma_1, \sigma_2)$ and those of σ_1, σ_2. The answers depend on numerous linear inequalities that are difficult to handle. As mentioned in the introduction, it is not easy to generate and store all the inequalities and it is hard to use them to deduce answers for simple problems such as:

PROBLEM 5.1. Determine the ranks of the elements in $\mathcal{S}(\sigma_1, \sigma_2)$.

PROBLEM 5.2. Determine the ranks of the extreme points of the set $\mathcal{S}(\sigma_1, \sigma_2)$.

Note also that unlike the case of $\mathcal{S}(\sigma)$, the ranks of the elements in $\mathcal{S}(\sigma_1, \sigma_2)$ cannot be determined only by the ranks of σ_1 and σ_2. For example, suppose σ_1 and

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σ_2 have the same rank. If σ_1, σ_2 have the same set of non-zero eigenvalues, then there is a rank one matrix in $\mathcal{S}(\sigma_1, \sigma_2)$. Otherwise, there is no rank one matrix in $\mathcal{S}(\sigma_1, \sigma_2)$. While it is difficult to determine the minimum rank of the matrices in $\mathcal{S}(\sigma_1, \sigma_2)$, it is easy to show that the largest rank of the matrices in $\mathcal{S}(\sigma_1, \sigma_2)$ equal rank (σ_1)rank (σ_2). Also, it is not hard to show that a matrix in $\mathcal{S}(\sigma_1, \sigma_2)$ with minimum rank is an extreme point. However, it is not easy to determine the ranks of extreme points in general. In [13], it was shown that the rank of an extreme point in $\mathcal{S}(\sigma_1, \sigma_2)$ cannot exceed $(m^2 + n^2 - 1)^{1/2}$. In fact, one can show that if σ_i has rank r_i for $i = 1, 2$, then the rank of an extreme point of $\mathcal{S}(\sigma_1, \sigma_2)$ cannot exceed $(r_1^2 + r_2^2 - 1)^{1/2}$ based on the following extension of Lemma 3.5.

LEMMA 5.3. *Let $\sigma_1 \in D(m)$, $\sigma_2 \in D(n)$ and $\rho \in \mathcal{S}(\sigma_1, \sigma_2) \subseteq D(m \cdot n)$. Then ρ is not an extreme point if and only if there exists a nonzero $\xi \in H_{mn}$ such that $\rho \pm \xi \in PSD(m \cdot n)$, $\mathrm{tr}_1(\xi) = O_n$ and $\mathrm{tr}_2(\xi) = O_m$. In such a case, there are $\rho_1, \rho_2 \in \mathcal{S}(\sigma_1, \sigma_2)$ with rank $(\rho_1) <$ rank (ρ) such that $\rho = (\rho_1 + \rho_2)/2$.*

Of course, similar questions can be asked for the set

$$\mathcal{S}(\sigma_1, \dots, \sigma_k) = \{\rho \in D(n_1 \cdots n_k) : \mathrm{tr}_{j'}(\rho) = \sigma_j\},$$

where $\mathrm{tr}_{j'}(\rho)$ is the reduced state of ρ in the jth system, for given $\sigma_j \in D(n_j)$ with $j = 1, \dots, k$. Even more challenging problems will be the study of ρ and reduced states in subsystems that have overlaps.

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