SEPARABILITY OF MULTI-QUBIT STATES IN TERMS OF
DIAGONAL AND ANTI-DIAGONAL ENTRIES

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Abstract. We give separability criteria for general multi-qubit states in terms of
diagonal and anti-diagonal entries. We define two numbers which are obtained from
diagonal and anti-diagonal entries, respectively, and compare them to get criteria.
They give rise to characterizations of separability when all the entries are zero except
for diagonal and anti-diagonal, like Greenberger-Horne-Zeilinger diagonal states. The
criteria is strong enough to detect nonzero volume of entanglement with positive
partial transposes.

1. Introduction

Entanglement is one of the key resources in the current quantum information and
computation theory, and it is very important to distinguish entanglement among sepa-
rability. Positivity of partial transposes is one of the earlier separability criteria: Every
separable state is of PPT [1, 2]. The converse is true for $2 \otimes 2$ and $2 \otimes 3$ systems [3, 4, 5],
and so we may confirm the separability in those systems without a decomposition into
the sums of pure product states, which is just the definition of (full) separability. A
non-separable state is called entangled.

In this paper, we propose a separability criterion for multi-qubit systems by an
inequality between two numbers arising from the diagonal and anti-diagonal entries,
respectively. This criterion is also sufficient for separability when states have nonzero
entries only for diagonal and anti-diagonal parts. This is one of very few criteria in the
literature with which we can confirm the separability without decomposition.

A state is called an $X$-shaped state, or an $X$-state if all the entries are zero except for
diagonal and anti-diagonal entries. Multi-qubit $X$-states appear in various contexts in
quantum information theory [6, 7, 8, 9, 10, 11]. Greenberger-Horne-Zeilinger diagonal
states [12, 13, 14] are typical examples of multi-qubit $X$-states which have real anti-
diagonals. Our criterion characterizes the separability of GHZ diagonal state.

Following the earlier work [15, 16, 17] on the separability of three qubit GHZ di-
agonal states, the second and the third authors [18] characterized separability of three
qubit GHZ diagonal states. After they [19] noticed that the phases, the angular parts,
of anti-diagonal entries play important roles, a complete characterization \[20\] of separability of three qubit X-states has been obtained. In this paper, we explore analogues for general multi-qubit systems. The main tool will be the duality \[21\] between separability of multi-partite states and positivity of multi-linear maps. In the next section, we fix the notations we use and summarize the results in this paper.

The first and the second authors are grateful to Sanbeot community for their hospitality during their stay at the community hall.

2. Notations and Summary of the results

A function from the set \([n] = \{1, 2, \ldots, n\}\) into \(\{0, 1\}\) will be called an \(n\)-bit index, just an \(n\)-index or index which will be denoted by a string of 0, 1. The set of all \(n\)-bit indices will be denoted by \(I_{[n]}\). For example, we have \(I_{[1]} = \{0, 1\}\), \(I_{[2]} = \{00, 01, 10, 11\}\) and \(I_{[3]} = \{000, 001, 010, 011, 100, 101, 110, 111\}\). For a subset \(S \subset \{1, 2, \ldots, n\}\) and an index \(i \in I_{[n]}\), we define the index \(\overline{i}_S \in I_{[n]}\) by

\[
\overline{i}_S(k) = \begin{cases} 
    i(k) + 1 \mod 2, & k \in S, \\
    i(k), & k \notin S.
\end{cases}
\]

In short, \(\overline{i}_S\) is obtained by switching the \(k\)-th digit for \(k \in S\). When \(S = \{1, \ldots, n\}\) is the whole set, the index \(\overline{i}^{(1, \ldots, n)}\) will be denoted by just \(\overline{i}\).

We denote by \(\mathcal{V}_n^\mathbb{R}\) (respectively \(\mathcal{V}_n^+\)) the set of all real valued (respectively nonnegative) functions on the set \(I_{[n]}\), and by \(\mathcal{V}_n^{sa}\) the set of all complex functions \(u : i \mapsto u_i\) on \(I_{[n]}\) satisfying the relation \(u_i = \overline{u}_i\) for each \(i \in I_{[n]}\). We note that both \(\mathcal{V}_n^\mathbb{R}\) and \(\mathcal{V}_n^{sa}\) are real vector spaces of dimension \(2^n\). For \(s \in \mathcal{V}_n^\mathbb{R}\) and \(u \in \mathcal{V}_n^{sa}\), we denote by \(X(s, u)\) the \(n\)-qubit self-adjoint matrix in the \(n\)-fold tensor product \(M_2^\otimes n\) with the entries \([w_{i,j}]\) given by

\[
w_{i,j} = \begin{cases} 
    s_i, & j = i, \\
    u_i, & j = \overline{i}, \\
    0, & \text{otherwise}.
\end{cases}
\]

If we endow \(I_{[n]}\) with the lexicographic order then \(X(s, u)\) can be considered as a usual matrix as follows:

\[
X(s, u) = \begin{pmatrix}
    s_{00\ldots0} & \cdots & \cdots & \cdots & \cdots & s_{0\ldots0} \\
    \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
    \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
    \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
    \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\
    u_{1\ldots1} & \cdots & \cdots & \cdots & \cdots & u_{0\ldots0}
\end{pmatrix}.
\]
We first determine pairs \((s, u) \in \mathcal{V}_n^+ \times \mathcal{V}_n^{sa}\) for which \(W = X(s, u)\) is an entanglement witness. To do this, we introduce the notation:

\[
\delta_i = \prod_{k=1}^{n} z_k^{1-2i(k)},
\]

for \(i \in I_n\) and \(z = (z_1, z_2, \ldots, z_n) \in \mathbb{C}^n\) with \(z_k \neq 0\) for \(k = 1, 2, \ldots, n\). We have \((e^{i\theta_1}, e^{i\theta_2}, e^{i\theta_3})^{001} = e^{i\theta_1}e^{i\theta_2}e^{-i\theta_3}\), for example. With this notation, we define the following two numbers:

\[
\delta_n(s) = \inf_{r \in \mathbb{R}_+^n} \sum_{i \in I_n} s_i r^i, \quad \|u\|_{X_n} = \sup_{\alpha \in \mathbb{T}^n} \sum_{i \in I_n} u_i \alpha^i,
\]

for \(s \in \mathcal{V}_n^+\) and \(u \in \mathcal{V}_n^{sa}\), where \(\mathbb{R}_+ = (0, \infty)\) and \(\mathbb{T}\) is the unit circle on the complex plane. Note that \(u \mapsto \|u\|_{X_n}\) defines a norm on the real vector space \(\mathcal{V}_n^{sa}\), because the set \(\{\sum_{i \in I_n} u_i \alpha^i\}\) of real numbers is symmetric with respect to the origin. As for \(\delta_n(s)\), we have the relation \(\delta_n(\lambda s) = \lambda \delta_n(s)\) for \(\lambda \geq 0\).

We show in Theorem 3.2 that a non-positive matrix \(W = X(s, u) \in M_2^\otimes n\) is an entanglement witness if and only if the inequality

\[
\delta_n(s) \geq \|u\|_{X_n}
\]

holds. In order to characterize the separability of an \(n\)-qubit state \(\varrho = X(a, c)\), we also introduce in Section 4 the numbers

\[
\Delta_n(a) = \inf \{ \langle s, a \rangle : s \in \mathcal{V}_n^+, \ \delta_n(s) = 1\},
\]

\[
\|c\|'_{X_n} = \sup \{ \langle u, c \rangle : u \in \mathcal{V}_n^{sa}, \ \|u\|_{X_n} = 1\},
\]

for \(a \in \mathcal{V}_n^+\) and \(c \in \mathcal{V}_n^{sa}\), where \(\langle s, a \rangle = \sum_{i \in I_n} s_i a_i\) is the usual bi-linear pairing. Note that \(\| \cdot \|'_{X_n}\) is nothing but the dual norm of \(\| \cdot \|_{X_n}\). The main result in this paper, Theorem 4.3, tells us that the state \(\varrho = X(a, c)\) is separable if and only if the inequality

\[
\Delta_n(a) \geq \|c\|'_{X_n}
\]

holds. We show that the \(X\)-part of a separable multi-qubit state is again separable, and so the above inequality gives rise to a separability criterion for general \(n\)-qubit states in terms of diagonal and anti-diagonal entries.

In the remainder of this paper, we estimate the numbers \(\Delta_n(a)\) and \(\|c\|'_{X_n}\) to get separability criteria for multi-qubit states. Recall that a multiset is a collection which allows repetition of elements, unlike a set. A multiset \(T\) of \(n\)-indices will be said to be balanced if \(r \mapsto \prod_{i \in T} r^i\) is the constant function 1 on \(\mathbb{R}_+^n\). This happens if and only if the number of indices \(i\) in \(T\) with \(i(k) = 0\) coincides with the number of indices \(i \in T\) with \(i(k) = 1\) for every \(k = 1, 2, \ldots, n\). The cardinality of \(T\) will be called the order of \(T\) and denoted by \(#T\). The order of a balanced multiset must be even. If \(#T = 2\) then \(\{i, j\}\) is a balanced multiset if and only if \(j = i\). We show in Section 5 that the inequality \((\prod_{i \in T} a_i)^{1/\#(T)} \geq \Delta_n(a)\) holds for every balanced multiset \(T\). We say that a balanced multiset is irreducible when it cannot be partitioned into balanced multisets.
It is easily seen that the set $G_n$ of all irreducible balanced multisets of $n$-indices is finite. We get in Section 5 the following upper bound

$$
\tilde{\Delta}_n(a) := \min \left\{ \left( \prod_{i \in T} a_1 \right)^{1/\#(T)} : T \in G_n \right\} \geq \Delta_n(a)
$$

for $\Delta_n(a)$. The number $\tilde{\Delta}_3(a)$ for the three qubit case appears in Gühne’s separability criterion [15]. We show that the equality $\Delta_3(a) = \tilde{\Delta}_3(a)$ holds for three qubit case, which recovers the main result in [20]. The notion of multisets is also useful to deal with the anti-diagonal part, and will be used to characterize separability of half rank states $X(a,c)$ in Theorem 5.3. Especially, we show that $\prod_{i \in T} c_i$ is constant for every irreducible balanced multiset $T$ of order four. The number of irreducible balanced multisets of order four increases very rapidly as the number of qubits increases.

For a given $c \in \mathcal{V}_n^{sa}$ with the polar decompositions $c_1 = |c_1|e^{i\theta_1}$, the function $\theta \in \mathcal{V}_n^{p}$ is called the phase part of $c \in \mathcal{V}_n^{sa}$. Note that the phase part of a vector in $\mathcal{V}_n^{sa}$ belongs to the subspace $\mathcal{V}_n^{ph}$ of $\mathcal{V}_n^{p}$ consisting of all $\theta \in \mathcal{V}_n^{p}$ satisfying the relation $\theta_1 = -\theta_i$ for each $i \in I_{[n]}$. Note that $\mathcal{V}_n^{ph}$ is of $2^{n-1}$ dimension. Section 6 will be devoted to analyze the phase parts of the anti-diagonal entries of separable states. The main tool is the linear map $\Theta_n : \mathbb{R}^n \rightarrow \mathcal{V}_n^{p}$ defined by

$$
[\Theta_n(e_k)]_{i} = \begin{cases} 
+1, & \text{if } i(k) = 0, \\
-1, & \text{if } i(k) = 1,
\end{cases}
$$

for each $k = 1, 2, \ldots, n$, where $\{e_k\}$ is the usual orthonormal basis of $\mathbb{R}^n$. We say that $\theta \in \mathcal{V}_n^{ph}$ satisfies the phase identities when it belongs to the image of $\Theta_n$. We construct a basis of the orthogonal complement $\mathcal{V}_n^{ph} \ominus \text{Im} \Theta_n$ arising from irreducible balanced multisets, to express phase identities. In a circumstance, we will see that parts of the identities are required for separability.

The phase difference of $\theta \in \mathcal{V}_n^{ph}$ is defined as the coset in the quotient $\mathcal{V}_n^{ph} / \text{Im} \Theta_n$ to which $\theta$ belongs. In Section 7 we will show that the dual norm $\|c\|_{\mathcal{V}_n}^\prime$ depends only on the phase difference of the phase part as well as the magnitudes. We also show that $\|c\|_{\mathcal{V}_n}^\prime$ is strictly greater than $\|c\|_{\mathcal{V}_n}^\infty$ whenever $c \in \mathcal{V}_n^{sa}$ shares a common magnitude of entries and has a nontrivial phase difference. From this, we may construct boundary separable $n$-qubit states with full ranks for each $n \geq 3$. This also tells us that our criterion is strong enough to detect PPT entanglement of nonzero volume.

3. Multi-qubit $X$-shaped entanglement witnesses

We say that an $n$-qubit self-adjoint matrix $W$ in $\bigotimes_{k=1}^n M_2$ is block-positive when $\langle \varrho, W \rangle \geq 0$ for every separable state $\varrho$. Note that a non-positive self-adjoint $W$ is an entanglement witness if and only if it is block-positive. For a given partition $[n] = S \sqcup T$, we defined in [22] the linear map $\phi_{W}^{S,T}$ from $\bigotimes_{k \in S} M_2$ into $\bigotimes_{k \in T} M_2$, which is very useful
to characterize the bi-separability of multi-partite states. For a given \((n+1)\)-qubit self-adjoint matrix \(W = [w_{ij}]_{i,j \in I_{n+1}}\), we consider the partition \([n+1] = \{n+1\} \cup [n]\) to get the map

\[
\phi := \phi_{W^{\otimes n+1}}^{\{n+1\},[n]} : M_2 \to M_2^{\otimes n}.
\]

Following the construction in [22], the map \(\phi\) sends \(|i\rangle\langle j| \in M_2\) to \([w_{ij}]_{i,j \in I_{[n]}} \in M_2^{\otimes n}\), and so \(\langle \phi(|i\rangle\langle j|), |i\rangle\langle j|\rangle = w_{ij,ij}\) for every \(i,j \in I_{[n]}\) and \(i,j = 0,1\). Therefore, we have

\[
\langle W, |i\rangle\langle j|\langle j|\langle i| \rangle = \langle W, |ii\rangle\langle jj| \rangle = w_{ii,jj} = \langle \phi(|i\rangle\langle j|), |i\rangle\langle j|\rangle,
\]

which implies the following identity

\[
\langle \phi(a_{n+1}), a_1 \otimes \cdots \otimes a_n \rangle = \langle W, a_1 \otimes \cdots \otimes a_n \otimes a_{n+1} \rangle,
\]

for every \(2 \times 2\) matrices \(a_1, \ldots, a_{n+1}\). Hence, we have the following:

**Lemma 3.1.** An \((n+1)\)-qubit self-adjoint matrix \(W \in M_2^{\otimes (n+1)}\) is block-positive if and only if \(\phi(P) \in M_2^{\otimes n}\) is block-positive for every positive \(P \in M_2\).

If \(W\) is an \(X\)-shaped \((n+1)\)-qubit self-adjoint matrix with entries \(\{w_{ij} : i,j \in I_{[n+1]}\}\), then \(\phi(|0\rangle\langle 0|)\) and \(\phi(|1\rangle\langle 1|)\) are diagonal matrices with diagonal entries \(\{w_{10,10} : i \in I_{[n]}\}\) and \(\{w_{11,11} : i \in I_{[n]}\}\), respectively. We also note that \(\phi(|0\rangle\langle 1|)\) and \(\phi(|1\rangle\langle 0|)\) are anti-diagonal matrix with the anti-diagonal entries \(\{w_{10,11} : i \in I_{[n]}\}\) and \(\{w_{11,10} : i \in I_{[n]}\}\), respectively. We write \(P_{r,\alpha} = \begin{pmatrix} r & \alpha \\ \bar{\alpha} & r^{-1} \end{pmatrix}\). Then sums of nonnegative scalar multiples of \(P_{r,\alpha}\) with \(r \in \mathbb{R}_+\) and \(\alpha \in \mathbb{T}\) make a dense subset for \(2 \times 2\) positive matrices. Now, we are ready to prove the main result in this section. Recall the definitions of \(\delta_n(s)\) and \(\|u\|_{X_n}\) in [1] for \(s \in \mathcal{V}_n^+\) and \(u \in \mathcal{V}_n^{\alpha}\).

**Theorem 3.2.** An \(n\)-qubit \(X\)-shaped self-adjoint matrix \(W = X(s,u)\) is block-positive if and only if the inequality \(\delta_n(s) \geq \|u\|_{X_n}\) holds.

**Proof.** When \(n = 1\) with \(I_{[1]} = \{0,1\}\), we have

\[
\delta_1(s) = \inf_{r_1 \in \mathbb{R}_+} (s_0 r_1 + s_1 r_1^{-1}) = 2\sqrt{s_0 s_1},
\]

\[
\|u\|_{X_1} = \sup_{\alpha_1 \in \mathbb{T}} (u_0 \alpha_1 + u_1 \alpha_1^{-1}) = \sup_{\alpha_1 \in \mathbb{T}} (u_0 \alpha_1 + \bar{u}_0 \bar{\alpha}_1) = 2|u_0| = \|u\|_1,
\]

which show that the inequality \(\delta_1(s) \geq \|u\|_{X_1}\) holds if and only if \(W\) is positive.

In order to use finite induction, suppose that the statement holds for the \(n\)-qubit case. For an \((n+1)\)-qubit \(X\)-shaped self-adjoint matrix \(W\), we see that the map \(\phi\) in (5) sends \(P_{r_{n+1},\alpha_{n+1}}\) to the \(n\)-qubit \(X\)-shaped matrix whose \(i\)-th diagonal and anti-diagonal entries are given by

\[
r_{n+1}s_{i0} + r_{n+1}^{-1}s_{i1} \quad \text{and} \quad \alpha_{n+1}u_{i0} + \alpha_{n+1}^{-1}u_{i1},
\]
respectively. Furthermore, we have
\[
\inf_{r_{n+1} \in \mathbb{R}_+} \inf_{r \in \mathbb{R}_+^n} \sum_{i \in I_{[n]}} (r_{n+1} s_{i0} + r_{n+1}^{-1} s_{i1}) r_i^j = \inf_{r_{n+1} \in \mathbb{R}_+} \inf_{r \in \mathbb{R}_+^n} \sum_{i \in I_{[n]}} (s_{j0} r_{n+1}^j + s_{j1} r_{n+1}^{-1})
\]
\[
= \inf_{r \in \mathbb{R}_+^n} \sum_{j \in I_{[n+1]}} s_j r^j = \delta_{n+1}(s),
\]
and
\[
\sup_{\alpha_{n+1} \in \mathbb{T}} \sup_{\alpha \in \mathbb{T}^n} \sum_{i \in I_{[n]}} (\alpha_{n+1} u_{i0} + \alpha_{n+1}^{-1} u_{i1}) \alpha_i = \|u\|_{X_{n+1}},
\]
similarly. Therefore, we see that \(W\) is block-positive if and only if \(\phi(P_{r_{n+1}, \alpha_{n+1}}) \in M_2^\otimes n\) is block-positive for every \(r_{n+1} \in \mathbb{R}_+\) and \(\alpha_{n+1} \in \mathbb{T}\) by Lemma 3.1 if and only if \(\delta_{n+1}(s) \geq \|u\|_{X_{n+1}}\) by the induction hypothesis. \(\Box\)

In the case of \(n = 2\), we have
\[
\delta_2(s) = \inf_{r_1, r_2 \in \mathbb{R}_+} (s_{00} r_1 r_2 + s_{01} r_1 r_2^{-1} + s_{10} r_1^{-1} r_2 + s_{11} r_1^{-1} r_2^{-1})
\]
\[
= \inf_{r_2 \in \mathbb{R}_+} \left[ \inf_{r_1 \in \mathbb{R}_+} [(s_{00} r_2 + s_{01} r_2^{-1}) r_1 + (s_{10} r_2 + s_{11} r_2^{-1}) r_1^{-1}] \right]
\]
\[
= \inf_{r_2 \in \mathbb{R}_+} 2 \sqrt{(s_{00} r_2 + s_{01} r_2^{-1})(s_{10} r_2 + s_{11} r_2^{-1})}
\]
\[
= \inf_{r_2 \in \mathbb{R}_+} 2 \sqrt{s_{00} s_{10} r_2^2 + s_{01} s_{11} r_2^{-2} + s_{00} s_{11} + s_{01} s_{10}}
\]
\[
= 2 \sqrt{2 s_{00} s_{10} r_2^2 + s_{01} s_{11} + s_{00} s_{11} + s_{01} s_{10} = 2(\sqrt{s_{00} s_{10}} + \sqrt{s_{01} s_{10}})},
\]
and
\[
\|u\|_{X_2} = \sup_{\alpha_1, \alpha_2 \in \mathbb{T}} \left( u_{00} \alpha_1 \alpha_2 + u_{01} \alpha_1 \bar{\alpha}_2 + u_{10} \bar{\alpha}_1 \alpha_2 + u_{11} \bar{\alpha}_1 \bar{\alpha}_2 \right)
\]
\[
= \sup_{\alpha_1, \alpha_2 \in \mathbb{T}} \left( u_{00} \alpha_1 \alpha_2 + u_{01} \alpha_1 \bar{\alpha}_2 + \bar{u}_{00} \bar{\alpha}_1 \alpha_2 + \bar{u}_{01} \bar{\alpha}_1 \bar{\alpha}_2 \right)
\]
\[
= 2 \sup_{\alpha_1, \alpha_2 \in \mathbb{T}} (\text{Re} (u_{00} \alpha_1 \alpha_2 + u_{01} \alpha_1 \bar{\alpha}_2)) = 2(|u_{00}| + |u_{01}|) = \|u\|_1,
\]
because we can take \(\alpha_1, \alpha_2 \in \mathbb{T}\) so that the last equality holds. Alternatively, we have
\[
\|u\|_{X_2} = 2 \sup_{\alpha_2 \in \mathbb{T}} \left( \sup_{\alpha_1 \in \mathbb{T}} (\text{Re} (u_{00} \alpha_2 + u_{01} \bar{\alpha}_2) \alpha_1) \right)
\]
\[
= 2 \sup_{\alpha_2 \in \mathbb{T}} |u_{00} \alpha_2 + u_{01} \bar{\alpha}_2| = 2(|u_{00}| + |u_{01}|) = \|u\|_1.
\]

We proceed to find inductive formulae for \(\delta_n(s)\) and \(\|u\|_{X_n}\). For a function \(s \in \mathcal{V}_{n+1}^\mathbb{R}\) defined on \(I_{[n+1]} = I_{[n]} \times \{0, 1\}\) and a real number \(r \in \mathbb{R}_+\), we define \(s[r] \in \mathcal{V}_n^\mathbb{R}\) by
\[
s[r]_{[i]} = s_{i0} r + s_{i1} r^{-1}, \quad i \in I_{[n]}.
\]
By the relation
\[
\sum_{i \in I_{[n+1]}} s_1 \cdot (r_1, \ldots, r_n, r_{n+1})^j = \sum_{j \in I_{[n]}} (s_{j0} r_{n+1} + s_{j1} r_{n+1}^{-1}) \cdot (r_1, \ldots, r_n)^j
\]
\[
= \sum_{j \in I_{[n]}} s[r_{n+1}]^j \cdot (r_1, \ldots, r_n)^j,
\]
we have

\begin{equation}
\delta_{n+1}(s) = \inf_{r_{n+1} \in \mathbb{R}_+} \left[ \inf_{(r_1, \ldots, r_n) \in \mathbb{R}_+^n} \sum_{i \in I_n} s[r_{n+1}] \cdot (r_1, \ldots, r_n) \right] = \inf_{r \in \mathbb{R}_+} \delta_n(s[r]).
\end{equation}

In the case of \( n = 3 \), we have

\[ \delta_3(s) = \inf_{r \in \mathbb{R}_+} \delta_2(s[r]) \]
\[ = 2 \inf_{r \in \mathbb{R}_+} \left[ \sqrt{s[r][00]s[r][11]} + \sqrt{s[r][01]s[r][10]} \right] \]
\[ = 2 \inf_{r \in \mathbb{R}_+} \left[ \sqrt{(s_{000}r + s_{001}r^{-1})(s_{110}r + s_{111}r^{-1})} \right. \]
\[ + \left. \sqrt{(s_{010}r + s_{011}r^{-1})(s_{100}r + s_{101}r^{-1})} \right] \]
\[ = 2 \inf_{r \in \mathbb{R}_+} \left[ \sqrt{(s_{000}r + s_{010}r^{-1})(s_{101}r + s_{111}r^{-1})} + \sqrt{(s_{001}r + s_{011}r^{-1})(s_{100}r + s_{110}r^{-1})} \right] \]
\[ = 2 \inf_{r \in \mathbb{R}_+} \left[ \sqrt{(s_{000}r + s_{100}r^{-1})(s_{011}r + s_{111}r^{-1})} + \sqrt{(s_{001}r + s_{101}r^{-1})(s_{100}r + s_{110}r^{-1})} \right]. \]

The last one has been considered in \([23, 18]\) to characterize three qubit block-positivity up to the scalar multiplication by 2.

For given \( u \in \mathcal{V}_{n+1}^{sa} \) and \( \alpha \in \mathbb{T} \), we define \( u[\alpha] \in \mathcal{V}_n^{sa} \) by \( u[\alpha]_i = u_{i0} \alpha + u_{ii} \overline{\alpha} \) for \( i \in I_n \). Then we have

\[ \|u\|_{x_{n+1}} = \sup_{\alpha \in \mathbb{T}} \|u[\alpha]\|_{x_n} \]

by the same reasoning. We also have

\[ \|u\|_{x_3} = 2 \sup_{\alpha \in \mathbb{T}} \left( |u_{000} \alpha + u_{001} \overline{\alpha}| + |u_{010} \alpha + u_{011} \overline{\alpha}| \right) \]
\[ = 2 \sup_{\alpha \in \mathbb{T}} \left( |u_{000} \alpha + u_{001}| + |u_{010} \alpha + u_{011}| \right), \]

and the identities

\[ \|u\|_{x_3} = 2 \sup_{\alpha \in \mathbb{T}} \left( |u_{000} \alpha + u_{010}| + |u_{001} \alpha + u_{011}| \right) \]
\[ = 2 \sup_{\alpha \in \mathbb{T}} \left( |u_{000} \alpha + u_{100}| + |u_{001} \alpha + u_{101}| \right). \]

Motivated by the characterization of block-positivity of three qubit \( X \)-shaped matrices in \([23]\), the half of the last number was taken as the definition of \( B(u) \) in \([18]\), and has been calculated \([20, 18]\) in terms of entries \( u_i \) in several cases.

**Proposition 3.3.** We have \( 2\|u\|_\infty \leq \|u\|_{x_n} \leq \|u\|_1 \) for every \( u \in \mathcal{V}_n^{sa} \).

**Proof.** The inequality \( \|u\|_{x_n} \leq \|u\|_1 \) follows from

\begin{equation}
\|u\|_{x_n} = \max_{\alpha \in \mathbb{T}^n} \sum_{i \in I_n} u_i \alpha^i \leq \max_{\alpha \in \mathbb{T}^n} \sum_{i \in I_n} |u_i \alpha^i| = \sum_{i \in I_n} |u_i| = \|u\|_1.
\end{equation}
We will use finite induction to prove the other inequality. Given $i \in I_{[n]}$, we take $\alpha \in \mathbb{T}$ such that $|u_{i0}\alpha + u_{i1}\bar{\alpha}| = |u_{i0}| + |u_{i1}|$. Then we have
\[ \|u\|_{X_{n+1}} \geq \|u[\alpha]\|_{X_n} \geq 2|u[\alpha]|_1 \geq 2\max\{|u_{i0}|, |u_{i1}|\}. \]
We used the induction hypothesis in the second inequality. This shows $\|u\|_{X_{n+1}} \geq 2|u_j|$ for every $j \in I_{[n+1]}$. □

4. Separability of X-shaped multi-qubit states

In this section, we characterize the separability of multi-qubit $X$-states $\rho = X(a, c)$. We begin with the following observation whose three qubit version appears in [18].

**Proposition 4.1.** The $X$-part of a multi-qubit separable state is again separable.

*Proof.* It suffices to prove that the $X$-part of an $n$-qubit pure product state is separable. For a given $|x\rangle = (x_0, x_1)^t \in \mathbb{C}^2$, we write $|x_{\pm}\rangle = (x_0, \pm x_1)^t$. When $n = 2$ and $\rho = |x\rangle \langle x| \otimes |y\rangle \langle y|$, the $X$-part $\rho_X$ of $\rho$ is given by
\[ \rho_X = \frac{1}{2} (|x_+\rangle \langle x_+| \otimes |y_+\rangle \langle y_+| + |x_-\rangle \langle x_-| \otimes |y_-\rangle \langle y_-|). \]
We will proceed by induction. Let $\omega$ be an $(n - 1)$-qubit pure product state and $\rho = \omega \otimes |x\rangle \langle x|$. By the induction hypothesis, the $X$-part $\omega_X$ of $\omega$ is separable. Let $\omega_X^-$ be a separable state obtained by multiplying the anti-diagonal part of $\omega_X$ by $-1$. This is obtained by the local unitary operation with $\text{diag}(1, -1) \otimes (1, 1) \otimes \cdots \otimes (1, 1)$.

Then, $\omega_X \otimes |x\rangle \langle x|$ is a block $X$-state whose blocks are $2 \times 2$ matrices, and its diagonal and the anti-diagonal blocks are given by
\[ \omega_{11} \left( \begin{array}{cc} |x_0|^2 & x_0\bar{x}_1 \\ \bar{x}_0x_1 & |x_1|^2 \end{array} \right) \quad \text{and} \quad \omega_{11} \left( \begin{array}{cc} |x_0|^2 & x_0\bar{x}_1 \\ \bar{x}_0x_1 & |x_1|^2 \end{array} \right), \]
respectively. Similarly, $\omega_X^- \otimes |x_-\rangle \langle x_-|$ is also a block $X$-state whose diagonal and the anti-diagonal blocks are given by
\[ \omega_{11} \left( \begin{array}{cc} |x_0|^2 & -x_0\bar{x}_1 \\ -\bar{x}_0x_1 & |x_1|^2 \end{array} \right) \quad \text{and} \quad -\omega_{11} \left( \begin{array}{cc} |x_0|^2 & -x_0\bar{x}_1 \\ -\bar{x}_0x_1 & |x_1|^2 \end{array} \right) = \omega_{11} \left( \begin{array}{cc} -|x_0|^2 & x_0\bar{x}_1 \\ \bar{x}_0x_1 & -|x_1|^2 \end{array} \right), \]
respectively. Therefore, we have
\[ \rho_X = \frac{1}{2} (\omega_X \otimes |x\rangle \langle x| + \omega_X^- \otimes |x_-\rangle \langle x_-|), \]
which is separable. □

By the exactly same argument as in Proposition 3.1 of [18], we have the following:

**Corollary 4.2.** The $X$-part of a multi-qubit block-positive matrix is again block-positive.

**Proposition 4.3.** For an $n$-qubit state $\rho = X(a, c)$ with $a \in V_n^+$ and $c \in V_n^{sa}$, the following are equivalent:

(i) $\rho$ is separable;
(ii) $\langle W, \rho \rangle \geq 0$ for every $X$-shaped block-positive $n$-qubit matrix $W = X(s, u)$;
(iii) \( \delta_n(s) \geq \| u \|_{X_n} \) with \( s \in \mathcal{V}_n^+ \) and \( u \in \mathcal{V}_n^{sa} \) implies \( \langle a, s \rangle + \langle c, u \rangle \geq 0 \);
(iv) \( \delta_n(s) \geq \| u \|_{X_n} \) with \( s \in \mathcal{V}_n^+ \) and \( u \in \mathcal{V}_n^{sa} \) implies \( \langle a, s \rangle \geq \langle c, u \rangle \);
(v) \( \delta_n(s) = \| u \|_{X_n} \) with \( s \in \mathcal{V}_n^+ \) and \( u \in \mathcal{V}_n^{sa} \) implies \( \langle a, s \rangle \geq \langle c, u \rangle \);
(vi) \( \inf_{s \in \mathcal{V}_n^+} \frac{\delta_n(s)}{\| u \|} \geq \sup_{u \in \mathcal{V}_n^{sa}} \frac{\langle a, s \rangle}{\| u \|_{X_n}} \).

Proof. The equivalence (i) \( \iff \) (ii) follows from the duality and Corollary 4.1.2. On the other hand, Theorem 3.2 tells us that (ii) and (iii) are equivalent to each other, because \( \langle a, X(s,u) \rangle = \langle a, s \rangle + \langle c, u \rangle \). We also get (iii) \( \iff \) (iv) by replacing \( u \) by \( -u \), and the direction (iv) \( \implies \) (v) is clear. Now, we prove the direction (v) \( \implies \) (iv). If \( \delta_n(s) > \| u \|_{X_n} \), then we take \( \lambda = \| u \|_{X_n} / \delta_n(s) \in [0,1) \) to get \( \delta_n(\lambda s) = \| u \|_{X_n} \). Therefore, we have \( \langle a, s \rangle \geq \langle a, \lambda s \rangle \geq \langle c, u \rangle \). The remaining implications (v) \( \iff \) (vi) follows from \( \delta_n(s/\delta_n(s)) = \| u / \| u \|_{X_n} \| X_n \| = 1 \). \( \square \)

Recall the definitions of \( \Delta_n(a) \) and \( \| c \|_{X_n} \) in (2). Then the inequality in Proposition 4.3 (vi) is nothing but the following main result in this paper:

**Theorem 4.4.** An \( X \)-shaped \( n \)-qubit state \( \varrho = X(a,c) \) is separable if and only if the inequality \( \Delta_n(a) \geq \| c \|_{X_n} \) holds.

By Proposition 4.1, we have the following criterion for general multi-qubit states.

**Theorem 4.5.** Let \( \varrho \) be a multi-qubit state with the \( X \)-part \( X(a,c) \). If \( \varrho \) is separable then the inequality \( \Delta_n(a) \geq \| c \|_{X_n} \) holds.

By Proposition 3.3 and the duality, we have

\[
(9) \quad \| c \|_\infty \leq \| c \|_{X_n} \leq \frac{1}{2} \| c \|_1,
\]

for every \( c \in \mathcal{V}_n^{sa} \). We also have

\[
\| c \|_{X_1} = \| c \|_\infty, \quad \| c \|_{X_2} = \| c \|_\infty,
\]

because \( \| u \|_{X_1} = \| u \|_1 \) and \( \| u \|_{X_2} = \| u \|_1 \).

In order to estimate \( \Delta_n(a) \) for \( a \in \mathcal{V}_n^+ \), we consider \( s_\lambda \in \mathcal{V}_n^+ \) defined by

\[
s_\lambda = \frac{1}{2} (\lambda e_i + \lambda^{-1} e_i) \in \mathcal{V}_n^+
\]

for each \( \lambda > 0 \), where \( e_i \in \mathcal{V}_n^\mathbb{R} \) is given by \( (e_i)_j = 1 \) for \( i = j \) and \( (e_i)_j = 0 \) for \( i \neq j \). Then it is easy to see that \( \delta_n(s_\lambda) = 1 \). We also have

\[
\inf_{\lambda > 0} \langle a, s_\lambda \rangle = \inf_{\lambda > 0} \frac{1}{2} (\lambda a_i + \lambda^{-1} a_i) = \sqrt{a_i a_i}.
\]

Therefore, we see that \( \Delta_n(a) \leq \sqrt{a_i a_i} \) for each \( i \in I_{[n]} \), and we have

\[
(10) \quad \Delta_n(a) \leq \min \{ \sqrt{a_i a_i} : i \in I_{[n]} \}, \quad a \in \mathcal{V}_n^+, \ n = 1, 2, \ldots
\]

When \( n = 1 \), we have

\[
a_0 s_0 + a_1 s_1 \geq \sqrt{a_0 a_1} \cdot 2 \sqrt{s_0 s_1} = \sqrt{a_0 a_1} \delta_1(s),
\]
because $\delta_1(s) = 2\sqrt{s_0s_1}$. In the case of $n = 2$, we also have

\[
s_{00}a_{00} + s_{01}a_{01} + s_{10}a_{10} + s_{11}a_{11} \\
\geq 2\sqrt{s_{00}s_{11}a_{00}a_{11}} + 2\sqrt{s_{01}s_{10}a_{01}a_{10}} \\
\geq \min\{\sqrt{a_{00}a_{11}}, \sqrt{a_{01}a_{10}}\} \cdot 2(\sqrt{s_{00}s_{11}} + \sqrt{s_{01}s_{10}}) \\
= \min\{\sqrt{a_{00}a_{11}}, \sqrt{a_{01}a_{10}}\} \cdot \delta_2(s)
\]

because $\delta_2(s) = 2(\sqrt{s_0s_{11}} + \sqrt{s_{01}s_{10}})$. Therefore, we have the following:

\[
\Delta_1(a) = \sqrt{a_{0}a_{1}}, \quad \Delta_2(a) = \min\{\sqrt{a_{00}a_{11}}, \sqrt{a_{01}a_{10}}\},
\]

and the inequality $\Delta_2(a) \geq \|c\|_{X_n}$ says that the 2-qubit state $\rho = X(a, c)$ is of PPT, which is equivalent to the separability in this case.

By the relation $\delta_n(s) \leq \|s\|_1$, we have $\min\{a_i\} \delta_n(s) \leq \langle s, a \rangle$, which implies

\[
\min\{a_i : i \in I_{[n]}\} \leq \Delta_n(a), \quad a \in V_n^+.
\]

If $a_i = a_i$ for every index $i \in I_{[n]}$, then we have $\Delta_n(a) = \min\{a_i : i \in I_{[n]}\}$ by (10). Hence, we have the following:

**Corollary 4.6.** Suppose that the diagonal entries of an $n$-qubit state $\rho = X(a, c)$ satisfies $a_i = a_i$ for each $i \in I_{[n]}$. Then $\rho$ is separable if and only if $\min a_i \geq \|c\|_{X_n}$.

GHZ diagonal states are typical examples of $n$-qubit states satisfying the condition of Corollary 4.6. These are states which are diagonal in the $n$-qubit orthonormal GHZ-basis [12, 14] consisting of $2^n$ vectors given by

\[
|\xi_i\rangle = \frac{1}{\sqrt{2}}(|i\rangle + (-1)^{i_1}|\bar{i}\rangle), \quad i = i_1i_2\ldots i_n.
\]

So, every $n$-qubit GHZ diagonal state is of the form $X(a, c)$ with $a_i = a_i \geq 0$ and $c_i = c_i \in \mathbb{R}$ for each $i \in I_n$. In the case of 3-qubit GHZ diagonal states, the dual norm $\|c\|_{X_3}$ has been calculated in terms of anti-diagonal entries [18], which are real numbers.

### 5. Separability and multiset of indices

In order to improve the inequality (10), we consider multisets of indices. Recall that a multiset of $n$-indices is called balanced if the following

\[
\#\{i \in T : i(k) = 0\} = \#\{i \in T : i(k) = 1\}
\]

holds for every $k = 1, 2, \ldots, n$.

**Proposition 5.1.** For every $a \in V_n^+$, the inequality

\[
\left(\prod_{i \in T} a_i\right)^{1/\ell} \geq \Delta_n(a)
\]

holds for every balanced multiset $T$ of length $\ell$. 


Proof. If \( a_i = 0 \) for some \( i \in I_n \) then we have \( \Delta_n(a) = 0 \) by (10). We consider the case when \( a_i > 0 \) for every \( i \in I_n \). For a given \( a \in V^+_n \) and a balanced multiset \( T \) with \( \#T = \ell \), we define

\[
s = \frac{1}{\ell} \left( \prod_{i \in T} a_i \right)^{1/\ell} \sum_{i \in T} \frac{1}{a_i} \in V^+_n.
\]

Then we have

\[
\delta_n(s) = \frac{1}{\ell} \left( \prod_{i \in T} a_i \right)^{1/\ell} \inf_{r \in \mathbb{R}^+_n} \left( \sum_{i \in T} \frac{1}{a_i} r_i \right) \geq \frac{1}{\ell} \left( \prod_{i \in T} a_i \right)^{1/\ell} \left( \prod_{i \in T} \frac{1}{a_i} \right)^{1/\ell} = 1,
\]

and so, it follows that

\[
\Delta_n(a) \leq \left\langle a, \frac{s}{\delta_n(s)} \right\rangle = \frac{1}{\delta_n(s)} \langle a, s \rangle \leq \langle a, s \rangle = \left( \prod_{i \in T} a_i \right)^{1/\ell},
\]

as it was desired. \( \Box \)

Proposition 5.1 gives us nontrivial restrictions on the \( X \)-parts \( X(a, c) \) of separable multi-qubit states. Especially, we have the restriction on the diagonal parts

\[
\left( \prod_{i \in T} a_i \right)^{1/\ell} \geq \|c\|_\infty
\]

by Theorem 4.4 and (9), whenever \( T \) is a balanced multiset of order \( \ell \).

Suppose that a balanced multiset \( T \) can be partitioned into the multiset union of balanced multisets \( T_1 \) and \( T_2 \). Then we have the inequality

\[
\min \left\{ \left( \prod_{i \in T_1} a_i \right)^{1/\#T_1}, \left( \prod_{i \in T_2} a_i \right)^{1/\#T_2} \right\} \leq \left( \prod_{i \in T} a_i \right)^{1/\#T},
\]

by taking logarithms. Therefore, we may consider only irreducible balanced multisets when we estimate the number \( \Delta_n(a) \) using Proposition 5.1. Furthermore, there exist only finitely many irreducible balanced multisets of \( n \)-indices. In fact, the maximum possible order of an irreducible balanced multiset is \( 2^n - 1 \), because if the order of a balanced multiset \( T \) exceeds \( 2^n - 1 \) then there exists \( i \in I_n \) such that both \( i \) and \( \bar{i} \) belong to \( T \). Therefore, we can define the number \( \tilde{\Delta}_n(a) \) for \( a \in V^+_n \) by (3), and get the following:

**Theorem 5.2.** For every \( a \in V^+_n \), we have \( \tilde{\Delta}_n(a) \geq \Delta_n(a) \).

The notion of balanced multisets is also useful to get separability criteria regarding anti-diagonal entries. To see this, we consider the separability of \( n \)-qubit states whose \( X \)-part is of rank \( 2^n - 1 \). For \( r \in \mathbb{R}^n_+ \) and \( \alpha \in \mathbb{T}^n \), we define \( \tilde{r} \in V^+_n \) and \( \tilde{\alpha} \in V^+_n \) by

\[
\tilde{r}_i = r^i \quad \text{and} \quad \tilde{\alpha}_i = \alpha^i, \quad i \in I_n,
\]
respectively. If \( \delta_n(s) \geq \|u\|_{X_n} \), then we have
\[
\langle \tilde{r}, s \rangle = \sum_{i \in I_\mathcal{N}} r^i s_i \geq \delta_n(s) \geq \|u\|_{X_n} \geq \sum_{i \in I_\mathcal{N}} \alpha^i u_i = \langle \tilde{\alpha}, u \rangle,
\]
so the \( X \)-state \( \varrho = X(\tilde{r},\tilde{\alpha}) \) is separable by Proposition 4.3. Furthermore, it is of half rank \( 2^{n-1} \). We show that every separable \( X \)-state of half rank is in this form up to positive scalar multiples. Suppose that \( \varrho = X(a,c) \) is separable. Then we have \( a_i a_i \geq |c_i|^2 \) for every \( i,j \in I_\mathcal{N} \) by the PPT condition in [22]. If a separable state \( \varrho = X(a,c) \) is of half rank \( 2^{n-1} \) then the identity \( a_i a_i = |c_i|^2 \) holds for every \( i,j \in I_\mathcal{N} \). Without loss of generality, we may assume that \( a_i a_i = |c_i|^2 = 1 \) for every index \( i \), to characterize the separability for multi qubit \( X \)-states with half rank.

**Theorem 5.3.** Let \( \varrho = X(a,c) \) be an \( n \)-qubit \( X \)-state with \( a_i a_i = |c_i|^2 = 1 \) for every index \( i \). Then the following are equivalent:

1. \( \varrho \) is separable;
2. there exist \( r \in \mathbb{R}_+^n \) and \( \alpha \in \mathbb{T}^n \) such that \( a = \tilde{r} \) and \( c = \tilde{\alpha} \);
3. there exists a product vector \( |\xi\rangle \) such that \( \varrho \) is the \( X \)-part of \( |\xi\rangle \langle \xi| \);
4. \( \prod_{i \in T} a_i = \prod_{i \in T} c_i = 1 \) for every balanced multiset \( T \);
5. \( \prod_{i \in T} a_i = \prod_{i \in T} c_i = 1 \) for every irreducible balanced multiset \( T \);
6. \( \prod_{i \in T} a_i = \prod_{i \in T} c_i = 1 \) for every irreducible balanced multiset \( T \) of order four.

**Proof.** We first note that the separability of \( \varrho \) implies
\[
1 = \|c\|_{\infty} \leq \|c\|_{X_n} = \Delta_n(a) \leq \min\{\sqrt{a_i a_i} : i \in I_\mathcal{N} \} = 1,
\]
by (4), and so we have \( \Delta_n(a) = \|c\|_{X_n} = 1 \). Taking \( s = \sum_{i \in I_\mathcal{N}} a_i e_i \in \mathcal{V}_n^+ \), we have
\[
2^n = \langle a, s \rangle \geq \Delta_n(a) \delta_n(s) = \delta_n(s) = \inf_{r \in \mathbb{R}_+^n} \sum_{i \in I_\mathcal{N}} a_i r^i = \frac{1}{2} \inf_{r \in \mathbb{R}_+^n} \sum_{i \in I_\mathcal{N}} (r^i|^a_i|^2 + a_i r^i) \geq 2^n,
\]
since \( a_i = a_i^{-1} \) and \( r^i = (r^i)^{-1} \). Therefore, we see that the equality holds in the above inequality, and so there exists \( r \in \mathbb{R}_+^n \) such that \( a_i r^i = a_i r^i \), that is, \( a_i = r^i \) for each \( i \in I_\mathcal{N} \). This tells us that \( a = \tilde{r} \). On the other hand, we take \( u = \sum_{i \in I_\mathcal{N}} \tilde{c}_i e_i \in \mathcal{V}_n^+ \) to get
\[
2^n = \langle c, u \rangle \leq \|c\|_{X_n} \|u\|_{X_n} = \|u\|_{X_n} = \sup_{\alpha \in \mathbb{T}^n} \sum_{i \in I_\mathcal{N}} \tilde{c}_i |\alpha|^i \leq 2^n.
\]
This shows that there exists \( \alpha \in \mathbb{T}^n \) such that \( c = \tilde{\alpha} \) by the same argument, and we have the equivalence (i) \( \iff \) (ii).

For \( z \in \mathbb{C}^n \), we denote by \( z^2 \) the vector in \( \mathbb{C}^n \) whose \( k \)-th entry is given by \( z^2_k \). For the direction (ii) \( \implies \) (iii), we take \( s \in \mathbb{R}_+^n \) and \( \beta \in \mathbb{T}^n \) such that \( s^2 = r \) and \( \beta^2 = \alpha \), and consider the vector
\[
|\xi\rangle = (s_1 \beta_1, s_1^{-1} \bar{\beta}_1)^t \otimes \cdots \otimes (s_n \beta_n, s_n^{-1} \bar{\beta}_n)^t.
\]
We note that the \( i \)-th entry of \( |\xi\rangle \) is \( s^i \beta^i \), and so we see that the \( X \)-part of \( |\xi\rangle \langle \xi| \) is just \( X(\tilde{r},\tilde{\alpha}) \). For the direction (iii) \( \implies \) (ii), we note that every product vector \( |\xi\rangle \) with
nonzero entries can be expressed by (11) up to scalar multiplications. The implication (ii) ⇒ (iv) follows from the definition of balanced multisets, and the implications (iv) ⇒ (v) ⇒ (vi) are trivial.

It remains to show the direction (vi) ⇒ (ii). To do this, we first show that the system

\[(12) \quad r^i = a_i, \quad i \in I_n\]

of equations with unknowns \(r_1, r_2, \ldots, r_n\) can be solved. If we choose \(i \in I_n\) and \(k \in [n]\) and we multiply two equations \(r^i = a_i\) and \(r^i = a_i\), then all but \(r_k\) are canceled. So, we get a candidate for the solution as

\[r_k = \begin{cases} \sqrt{a_i a_{i(k)}}, & i(k) = 0, \\ 1/\sqrt{a_i a_{i(k)}}, & i(k) = 1. \end{cases}\]

We show that \(r = (r_1, \ldots, r_n)\) is independent of the choice of \(i \in I_n\). Let \(i, j \in I_n\). If \(i(k) = j(k)\), then the multiset \(\{i, i(k)^c, j, j(k)^c\}\) is balanced, so we have \(a_i a_{i(k)} = a_j a_{j(k)}\) by (vi). If \(i(k) \neq j(k)\), then the multiset \(\{i, i(k)^c, j, j(k)^c\}\) is balanced, so we also have \(a_i a_{i(k)} = 1/a_j a_{j(k)}\). It remains to show that \(r = (r_1, \ldots, r_n)\) is a solution of (12). For a given index \(i = i_1 i_2 \cdots i_n\), we consider indices

\[i_k = \bar{i}_1 \bar{i}_2 \cdots \bar{i}_{k-1} i_k \cdots i_n, \quad j_k = i_1 i_2 \cdots i_k i_{k+1} \cdots \bar{i}_n.\]

Then, they satisfy \(i_k(k) = i_k, j_k(k) = j_k\), \(j_{k-1} = i_k\) and \(i_1 = i = j_n\). It follows that

\[(r^i)^2 = (r_1^2)^{1-2i_1} (r_2^2)^{1-2i_2} \cdots (r_n^2)^{1-2i_n} = (a_i a_{i_1}) (a_{i_2} a_{j_2}) \cdots (a_{i_n} a_{j_n}) = a_i a_{i_1} \cdots a_{i_{n-1}} a_n = (a_i)^2,\]

as it was required. The equation \(a_i^2 = c_i\) can be solved similarly. □

The argument above shows that the system (12) of equations with unknowns \(r_k\)'s has a unique solution whenever the condition in (vi) is satisfied. In the three qubit case, it is easy to see that there are only two irreducible balanced multisets of order greater than or equal to 4: \(\{000, 011, 101, 110\}\) and \(\{111, 100, 010, 001\}\). Therefore, a three qubit \(X\)-state \(\varrho = X(a, c)\) of rank four with \(a_i a_i = |c_i|^2 = 1\) \((i \in I_3)\) is separable if and only if the identities

\[a_{000} a_{011} a_{101} a_{110} = 1, \quad c_{000} c_{011} c_{101} c_{110} = 1\]

hold. This recovers a result in [19]. We also have

\[\tilde{\Delta}_3(a) = \min\{\sqrt{a_{000} a_{111}}, \sqrt{a_{000} a_{111}}, \sqrt{a_{000} a_{111}}, \sqrt{a_{010} a_{101}}, \sqrt{a_{010} a_{101}}, \sqrt{a_{010} a_{101}}, \sqrt{a_{010} a_{101}}\}.\]

This number appears in the Gühne’s separability criterion [15]. We show that the equality \(\Delta_3(a) = \tilde{\Delta}_3(a)\) holds for the three qubit case, from which we recover the main result in [20]. It would be nice to know if the identity \(\Delta_n(a) = \tilde{\Delta}_n(a)\) holds for \(n \geq 4\).

**Proposition 5.4.** We have the identity \(\Delta_3(a) = \tilde{\Delta}_3(a)\) for every \(a \in V_3^+\).
Proof. In order to prove $\tilde{\Delta}_3(a) \leq \Delta_3(a)$, it suffices to show that $\tilde{\Delta}_3(a) = 1$ implies $\Delta_3(a) \geq 1$. Note that $\tilde{\Delta}_3(a) = 1$ implies

$$\max\{a_{000}^{-1}, a_{110}^{-1}, a_{101}^{-1}, a_{100}^{-1}\} \leq \min\{a_{111}a_{001}a_{010}, a_{011}\}.$$ 

Take $b_{011}$ between these two numbers. Because all the three intervals $[a_{000}^{-1}, a_{111}]$, $[a_{110}^{-1}, a_{001}]$ and $[a_{101}^{-1}, a_{010}]$ are nonempty, we can take $b_{000}, b_{001}, b_{100}$ so that

$$b_{000}^{-1}b_{001}b_{100} = b_{011},$$

$$a_{000}^{-1} \leq b_{000}^{-1} \leq a_{111}, \quad a_{110}^{-1} \leq b_{001} \leq a_{001}, \quad a_{101}^{-1} \leq b_{100} \leq a_{010}.$$ 

Take $b \in V_3^+$ so that $b_i b_{\bar{i}} = 1$ for each $i \in I_3^\star$. Then we see that $X(a, 1)$ is the sum of $X(b, 1)$ and a diagonal state, with $1 = (1, 1, \ldots, 1)$. By Theorem 5.3, we see that $X(b, 1)$ is separable, and so is $X(a, 1)$. Since $\|1\|_{X_3} = 1$, we have $\Delta_3(a) \geq 1$ by Theorem 4.4. □

Now, we look for balanced multisets. To do this, we first note that the following are equivalent:

- The multiset $\{i_1, \ldots, i_m, j_1, \ldots, j_m\}$ is balanced,
- its conjugate $\{\bar{i}_1, \ldots, \bar{i}_m, \bar{j}_1, \ldots, \bar{j}_m\}$ is balanced,
- $i_1(k) + i_2(k) + \cdots + i_m(k) = j_1(k) + j_2(k) + \cdots + j_m(k)$ for every $k = 1, 2, \ldots, n$.

We use the notation

$$i_1 + i_2 + \cdots + i_m \equiv j_1 + j_2 + \cdots + j_m$$

whenever the last condition holds. If we identify an index $i = i_1i_2\ldots i_n$ with the natural number $i = \sum_{k=1}^n i_k 2^{n-k}$ using binary expansion, then we see that the relation \[13\] implies the identity $i_1 + i_2 + \cdots + i_m = j_1 + j_2 + \cdots + j_m$ as natural numbers. Note that the converse does not hold. In the three qubit case, the relation $000 + 011 = 001 + 010$, or equivalently $0 + 3 \equiv 1 + 2$ represents two balanced multisets $\{000, 011, 110, 101\}$ and $\{111, 100, 001, 010\}$. It is easily checked that they are irreducible, and there is no more irreducible balanced multiset of order four. Note that we may assume that all the indices $i_k$ and $j_k$ begin with 0, when we look for multisets of the form $\{i_1, \ldots, i_m, j_1, \ldots, j_m\}$.

Irreducible balanced multisets of order four in the four qubit system can be expressed by the identities

$$0 + 7 \equiv 1 + 6 \equiv 2 + 5 \equiv 3 + 4,$$

$$0 + 3 \equiv 1 + 2, \quad 4 + 7 \equiv 5 + 6,$$

$$0 + 5 \equiv 1 + 4, \quad 2 + 7 \equiv 3 + 6,$$

$$0 + 6 \equiv 2 + 4, \quad 1 + 7 \equiv 3 + 5.$$ 

One may check that these are all possible identities, and so we have $(6 + 6) \times 2 = 24$ irreducible balanced multisets of order four. By a simple combinatorial method, one may also check that there are $8 \times 2 = 16$ irreducible balanced multisets of order six,
which can be expressed by the identities
\[ 0 + 0 + 7 \equiv 1 + 2 + 4, \quad 1 + 1 + 6 \equiv 0 + 3 + 5, \]
\[ 2 + 2 + 5 \equiv 0 + 3 + 6, \quad 3 + 3 + 4 \equiv 1 + 2 + 7, \]
\[ 3 + 4 + 4 \equiv 0 + 5 + 6, \quad 2 + 5 + 5 \equiv 1 + 4 + 7, \]
\[ 1 + 6 + 6 \equiv 2 + 4 + 7, \quad 0 + 7 + 7 \equiv 3 + 5 + 6. \]
The relation \( 0 + 0 + 7 \equiv 1 + 2 + 4 \), or equivalently \( 0000 + 0000 + 0111 \equiv 0001 + 0010 + 0100 \) represents two irreducible balanced multisets
\[ \{0000, 0000, 0111, 1110, 1101, 1011\}, \quad \{1111, 1111, 1000, 0001, 0010, 0100\}. \]
It is not difficult to show that there is no irreducible balanced multiset of order eight. Consequently, we found all the irreducible balanced multisets in the four qubit case, which gives rise to the number \( \tilde{\Delta}_4(a) \) for \( a \in \mathcal{V}_4^+ \). This number is given by the minimum of \( 8 + 24 + 16 = 48 \) numbers.

In general, we can find all irreducible balanced multisets of order four in the \( n \)-qubit system, in a recursive way. For an index \( \mathbf{i} = i_1i_2 \ldots i_{n+1} \in I_{[n+1]} \), we define the index \( \tilde{i} = i_2 \ldots i_{n+1} \in I_{[n]} \) by deleting the leftmost bit of \( \mathbf{i} \), and denote \( T_{n,m} \) be the family of all irreducible balanced multisets of order \( m \) in the \( n \)-qubit system. If \( T = \{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3, \mathbf{i}_4\} \) is in \( T_{n+1,4} \), then the balanced multiset \( \{\tilde{i}_1, \tilde{i}_2, \tilde{i}_3, \tilde{i}_4\} \) in \( n \)-qubit system is one of the following:

- an irreducible balanced multiset of order four,
- a disjoint union of two irreducible balanced multisets of order 2.

Now, we consider the reverse direction. For a given multiset \( \{\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3, \mathbf{i}_4\} \) in \( T_{n,4} \), we can construct the following six multisets in \( T_{n+1,4} \):
\[
\{0\mathbf{i}_1, 0\mathbf{i}_2, 1\mathbf{i}_3, 1\mathbf{i}_4\}, \quad \{0\mathbf{i}_1, 1\mathbf{i}_2, 0\mathbf{i}_3, 1\mathbf{i}_4\}, \quad \{0\mathbf{i}_1, 1\mathbf{i}_2, 1\mathbf{i}_3, 0\mathbf{i}_4\},
\{1\mathbf{i}_1, 1\mathbf{i}_2, 0\mathbf{i}_3, 0\mathbf{i}_4\}, \quad \{1\mathbf{i}_1, 0\mathbf{i}_2, 1\mathbf{i}_3, 0\mathbf{i}_4\}, \quad \{1\mathbf{i}_1, 0\mathbf{i}_2, 0\mathbf{i}_3, 1\mathbf{i}_4\}.
\]
For any given two disjoint multisets \( \{\mathbf{i}, \tilde{\mathbf{i}}\} \) and \( \{\mathbf{j}, \tilde{\mathbf{j}}\} \) in \( T_{n,2} \), we also obtain two multisets
\[
\{0\mathbf{i}, 0\tilde{\mathbf{i}}, 1\mathbf{j}, 1\tilde{\mathbf{j}}\}, \quad \{1\mathbf{i}, 1\tilde{\mathbf{i}}, 0\mathbf{j}, 0\tilde{\mathbf{j}}\}
\]
in \( T_{n+1,4} \). So, we can construct \( 2 \cdot \binom{2^{n-1}}{2} = 2^{n-1}(2^{n-1} - 1) \) multisets in \( T_{n+1,4} \) from \( 2^{n-1} \) multisets in \( T_{n,2} \). Consequently, \( T_{n+1,4} \) can be obtained inductively from \( T_{n,4} \) and \( T_{n,2} \), with the following recursion formula:
\[
\#T_{3,4} = 2, \quad \#T_{n+1,4} = 6(\#T_{n,4}) + 2^{n-1}(2^{n-1} - 1), \quad n = 3, 4, \ldots.
\]
For example, we have \( \#T_{4,4} = 24, \#T_{5,4} = 200 \) and \( \#T_{6,4} = 1440 \).

6. Phase identities

We take logarithm on the system (12) of equations with \( n \) unknowns and \( 2^n \) equations, and write \( R_k = \log r_k \) for \( k = 1, 2, \ldots, n \), and \( A_i = \log a_i \) for \( \mathbf{i} \in I_n \). Then we have the equation \( \Theta_n R = A \) with the linear map \( \Theta_n : \mathbb{R}^n \rightarrow \mathcal{V}_n^\mathbb{R} \) defined in (1). Therefore, the equation (12) has a solution if and only if \( A = \log a \in \text{Im} \Theta_n \). This
is also the case for the phase part of anti-diagonal $c \in \mathcal{V}_n^{sa}$: The equation $\tilde{\alpha} = c$ in Theorem 5.3 (ii) has a solution if and only if the phase part $\theta \in \mathcal{V}_n^{ph}$ of $c \in \mathcal{V}_n^{sa}$ belongs to the range of $\Theta_n$.

We take the orthonormal basis $\{e_i : i \in I_n\}$ of $\mathcal{V}_n^{sa}$, then the associated matrices with $\Theta_n$ with respect to these bases are given by

$$
\Theta_1 = \begin{pmatrix} + \\ - \end{pmatrix}, \quad \Theta_2 = \begin{pmatrix} + & + \\ + & - \\ - & + \\ - & - \end{pmatrix}, \quad \Theta_3 = \begin{pmatrix} + & + & + \\ + & - & - \\ - & + & - \\ - & - & + \end{pmatrix},
$$

for $n = 1, 2, 3$, where $+$ and $-$ represent $+1$ and $-1$, respectively. We recall that a vector $\theta \in \mathcal{V}_n^{ph}$ satisfies the phase identities when $\theta \in \text{Im} \Theta_n$. We rephrase the condition (ii) in Theorem 5.3 to get the following:

**Proposition 6.1.** Let $\varrho = X(a,c)$ be an $n$-qubit $X$-state with $a_i a_i = |c_i|^2 = 1$ for every index $i$. Then $\varrho$ is separable if and only if both $\log a \in \mathcal{V}_n^{ph}$ and the phase part $\theta \in \mathcal{V}_n^{ph}$ of $c$ satisfy the phase identities.

In order to check if $\theta$ satisfies the phase identities, we have to consider the orthogonal complement $\mathcal{V}_n^{ph} \ominus \text{Im} \Theta_n$, which is a real vector space of dimension $\lambda(n) := 2^{n-1} - n$. For a given multiset $T$ of $n$ indices, we define the vector

$$
\xi_T = \frac{1}{2} \sum_{i \in T} (e_i - e_i) \in \mathcal{V}_n^{ph}.
$$

Then, the multiset $T$ is balanced if and only if the vector $\xi_T$ belongs to $\mathcal{V}_n^{ph} \ominus \text{Im} \Theta_n$ because we have the identity:

$$
\langle \xi_T, \Theta(e_k) \rangle = \frac{1}{2} \sum_{i \in T} (e_i - e_i), \Theta(e_k) = \frac{1}{2} \left( \sum_{i \in T} \Theta(e_k)_i - \Theta(e_k)_{\overline{i}} \right) = \# \{ i \in T : i(k) = 0 \} - \# \{ i \in T : i(k) = 1 \}.
$$

We say that a family $\mathcal{T}$ of irreducible balanced multisets is basic when $\{\xi_T : T \in \mathcal{T}\}$ is a basis of $\mathcal{V}_n^{ph} \ominus \text{Im} \Theta_n$. We note that $\langle \theta, \xi_T \rangle = \sum_{i \in T} \theta_i$, which implies the following:

**Proposition 6.2.** Let $\mathcal{T}$ be a basic family of irreducible balanced multisets. For $\theta \in \mathcal{V}_n^{ph}$, the following are equivalent:

(i) $\theta$ satisfies the phase identities;

(ii) $\sum_{i \in T} \theta_i = 0$ for every $T \in \mathcal{T}$;

(iii) $\sum_{i \in T} \theta_i = 0$ for every balanced multiset $T$. 

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In the three qubit case, any basic family consists of a single multiset \{000, 011, 101, 110\} or its conjugate \{111, 100, 010, 001\}. Therefore, \(\theta \in \mathcal{V}_3^{\text{ph}}\) satisfies the phase identities if and only if the identity \(\theta_{000} + \theta_{011} + \theta_{101} + \theta_{110} = 0\), or equivalently
\[
\theta_{000} + \theta_{011} = \theta_{001} + \theta_{010}
\]
holds, which arises from the relation \(000 + 011 \equiv 001 + 010\). This is exactly the phase identity considered in [19].

The condition (vi) of Theorem 5.3 suggests that there exists a basic family consisting of irreducible balanced multisets of order four. To get a basic family of such kind, we take an index which begins with 0 and in which 1 appears at least two times. We call that a non-elementary index. They correspond natural numbers which are not of the form \(2^\ell\). We decompose such number \(i\) as the sum of the smallest number of the form \(2^\ell\) with the same position of 1 as \(i\) and the other. In the three qubit case, we have only one non-elementary index with the decomposition as follows:

\[
0 + 3 = 000 + 011 \equiv 001 + 010 = 1 + 2
\]

In the four qubit case, we have four non-elementary indices: One of them appears in the three qubit case, and the other three cases are listed as follows:

\[
0 + 5 = 0000 + 0101 \equiv 0001 + 0100 = 1 + 4
\]

\[
0 + 6 = 0000 + 0110 \equiv 0010 + 0100 = 2 + 4
\]

\[
0 + 7 = 0000 + 0111 \equiv 0001 + 0110 = 1 + 6
\]

There are \(\lambda(5) = 11\) non-elementary indices for the five qubit case. Four of them appear in the three and four qubit cases, and we list up the other seven cases:

\[
0 + 9 \equiv 1 + 8, \quad 0 + 10 \equiv 2 + 8, \quad 0 + 11 \equiv 1 + 10, \quad 0 + 12 \equiv 4 + 8,
\]

\[
0 + 13 \equiv 1 + 12, \quad 0 + 14 \equiv 2 + 12, \quad 0 + 15 \equiv 1 + 14.
\]

Formally, for a non-elementary index \(i = i_1 i_2 \ldots i_n\), we take the biggest \(k\) such that \(i_k = 1\). Define \(i_{\min} \in I_n\) by \(i_{\min}(k) = 1\) and \(i_{\min}(\ell) = 0\) for \(\ell \neq k\). Put \(i_{\res} = i - i_{\min}\). Since \(0 + i \equiv i_{\min} + i_{\res}\), we see that

\[
T_i = \{0, i, i_{\min}, i_{\res}\}
\]

is an irreducible balanced multiset of order four, where \(0 = 00 \ldots 0\). We note that the number of non-elementary indices is exactly \(2^{n-1} - n\), which coincides with the dimension of \(\mathcal{V}_n^{\text{ph}} \ominus \text{Im } \Theta_n\). One may also verify that \(\xi_{T_i}\) with non-elementary indices \(i\)'s are linearly independent, so \(\{T_i\}\) with non-elementary indices \(i\)'s is basic. Therefore, \(\theta \in \mathcal{V}_4^{\text{ph}}\) satisfies the phase identity if and only if the following four identities

\[
\begin{align*}
\theta_{0000} + \theta_{0011} &= \theta_{0001} + \theta_{0010} \\
\theta_{0000} + \theta_{0101} &= \theta_{0001} + \theta_{0100} \\
\theta_{0000} + \theta_{0110} &= \theta_{0010} + \theta_{0100} \\
\theta_{0000} + \theta_{0111} &= \theta_{0001} + \theta_{0110}
\end{align*}
\]
Suppose that there exist two indices \( i_1, i_2 \) with \( i_1 \neq i_2 \) and \( i_1 \neq \bar{i}_2 \) satisfying the relation
\[ \sqrt{a_i a_i} = |c_i| = \|c\|_\infty, \quad i = i_1, i_2. \]

Therefore, we have
\[ \theta_{i_1} + \theta_{i_2} = \theta_{\bar{i}_1} + \theta_{\bar{i}_2} \mod 2\pi, \]
whenever \( \{i_1, i_2, \bar{j}_1, \bar{j}_2\} \) is an irreducible balanced multiset.

**Proof.** We write \( \varrho = \sum_k \lambda_k \omega_k \) with \( \lambda_k > 0 \), \( \sum_k \lambda_k = 1 \) and pure product states \( \omega_k \), whose \( X \)-parts are given by \( X(a^k, c^k) \) with \( a^k \in \mathcal{V}_n^+ \) and \( c^k \in \mathcal{V}_n^{sa} \). By the Cauchy-Schwartz inequality, we have
\[ |c_1| = |\sum_k \lambda_k c^k| \leq \sum_k |\lambda_k c^k| \leq \sum_k \lambda_k \sqrt{a_i a_i^k} \leq \left( \sum_k \lambda_k a_i^k \right)^{1/2} \left( \sum_k \lambda_k a_i^k \right)^{1/2} = \sqrt{a_i a_i}, \]
which become identities for \( i = i_1, i_2 \). By the first identity \( |\sum_k \lambda_k c^k| = \sum_k |\lambda_k c^k| \) with \( i = i_1, i_2 \), we have \( \theta_i = \arg c^k \) for \( i = i_1, i_2 \). Since the \( X \)-part of a pure state is diagonal or non-diagonal of rank \( 2^{n-1} \), we have \( \sqrt{a_i a_i^k} = |c_j^k| \) for every \( i, j \in I_{[n]} \), whenever \( c^k \neq 0 \) by the PPT condition. This number will be denoted by \( r_k \). It follows that
\[ c^k_i = r_k e^{i\theta_i} \quad (i = i_1, i_2) \quad \text{and} \quad \|c\|_\infty = |c_{i_1}| = |c_{i_2}| = \sum_k \lambda_k r_k. \]

Therefore, we have
\[ |c_{j_1}|^2 = c_{j_1} \bar{c}_{j_1} = \left( \sum_k \lambda_k r_k e^{i\theta_k} \right) \left( \sum_l \lambda_l r_l e^{-i\theta_l} \right) = \sum_{k,l} \lambda_k \lambda_l r_k r_l e^{i(\theta_k - \theta_l)} \]
with \( \theta^k_i = \arg c^k_i \) for \( c^k \neq 0 \). Now, suppose that \( \{i_1, i_2, \bar{j}_1, \bar{j}_2\} \) is an irreducible balanced multiset. Then we have
\[ \theta^k_{j_1} + \theta^k_{j_2} = \theta^k_{i_1} + \theta^k_{i_2} = \theta^\ell_{i_1} + \theta^\ell_{i_2} = \theta^\ell_{j_1} + \theta^\ell_{j_2}, \mod 2\pi \]
by Theorem 5.3. Therefore, \( \theta^k_{j_1} - \theta^\ell_{j_2} \) may be replaced by \( \theta^\ell_{j_2} - \theta^k_{j_2} \) in (20), and so we have the identity \( |c_{j_1}| = |c_{j_2}|. \)
We also have
\[ c_3c_2 = \left( \sum_{k} \lambda_k r_k e^{i \theta_{j1}} \right) \left( \sum_{\ell} \lambda_\ell r_\ell e^{i \theta_{j2}} \right) \]
\[ = \sum_{k, \ell} \lambda_k \lambda_\ell r_k r_\ell e^{i (\theta_{j1} + \theta_{j2})} \]
\[ = \frac{1}{2} \sum_{k, \ell} \lambda_k \lambda_\ell r_k r_\ell e^{i (\theta_{j1} + \theta_{j2})} + \lambda_\ell \lambda_k r_k r_\ell e^{i (\theta_{j1} + \theta_{j2})} \]
\[ = \frac{1}{2} \sum_{k, \ell} \lambda_k \lambda_\ell r_k r_\ell \left( e^{i (\theta_{j1} + \theta_{j2})} e^{i (\theta_{j1} - \theta_{j2})} + e^{i (\theta_{j1} + \theta_{j2})} e^{i (\theta_{j1} - \theta_{j2})} \right). \]

Applying the identity (21), we have
\[ c_3c_2 = e^{i (\theta_{i1} + \theta_{i2})} \sum_{k, \ell} \lambda_k \lambda_\ell r_k r_\ell \cos(\theta_{j2}^k - \theta_{j1}^k). \]

We see that the phase part of \( c_3c_2 \) is given by \( \theta_{i1} + \theta_{i2} \), because
\[ \sum_{k, \ell} \lambda_k \lambda_\ell r_k r_\ell \cos(\theta_{j2}^k - \theta_{j1}^k) = \sum_{k, \ell} \lambda_k \lambda_\ell r_k r_\ell (\cos \theta_{j2}^k \cos \theta_{j1}^k + \sin \theta_{j2}^k \sin \theta_{j1}^k) \]
\[ = \left( \sum_k \lambda_k r_k \cos \theta_{j1}^k \right)^2 + \left( \sum_k \lambda_k r_k \sin \theta_{j1}^k \right)^2 \geq 0. \]

This implies the required identity \( \theta_{i1} + \theta_{i2} = \theta_{i3} + \theta_{i4} \). \( \square \)

Note that Theorem 6.3 may be applied whenever a separable \( X \)-state \( \varphi \) has corank \( \geq 2 \). In the three qubit case, we apply Theorem 6.3 for \( \{i_1, i_2\} = \{000, 110\} \). In this case, we see that \( \{i_1, i_2, j_1, j_2\} \) is an irreducible balanced multiset if and only if \( \{j_1, j_2\} = \{101, 011\} \), which implies the separability criteria \( |c_{010}| = |c_{100}| \) and \( \theta_{000} + \theta_{110} = \theta_{010} + \theta_{100} \), or equivalently \( |c_{010}| = |c_{011}| \) and \( \theta_{000} + \theta_{011} = \theta_{001} + \theta_{010} \). In this way, we see that if a three qubit \( X \)-state \( \varphi = X(a, c) \) of rank six is separable then there exists a partition \( \{i_1, i_2\} \cup \{j_1, j_2\} \) of indices beginning 0 such that
\[ |c_{i1}| = |c_{i2}|, \quad |c_{j1}| = |c_{j2}|, \quad \theta_{000} + \theta_{011} = \theta_{001} + \theta_{010}. \]

Note that the phase identity \( \theta_{000} + \theta_{011} = \theta_{001} + \theta_{010} \) must be retained regardless of partition. Theorem 5.1 of [19] tells us that this is essentially a characterization of separability of a three qubit \( X \)-state of rank six.

7. Phase Differences

The phases also play important roles to investigate properties of the numbers \( \|u\|_{X_n} \) and \( \|c\|_{X_n} \) in the characterization of block-positivity and separability. Suppose that \( u \in \mathcal{V}_n^{ss} \) has the phase part \( \phi \in \mathcal{V}_n^{ph} \). We write \( \alpha_k = e^{i \theta_k} \) for each \( k = 1, 2, \ldots, n \). Then we have
\[ \alpha^i = \prod_{k=1}^n e^{i ((1-2i(k)) \theta_k} = e^{i \sum_{k=1}^n (1-2i(k)) \theta_k} = e^{i \Theta_n(\theta)_i} \]
for each \( i \in I_{[n]} \), and so it follows that
\[
\sum_{i \in I_{[n]}} u_i \alpha^i = \sum_{i \in I_{[n]}} |u_i| e^{i(\phi_i + \Theta_n(\theta))} = \langle |u|, e^{i(\phi + \Theta_n(\theta))} \rangle.
\]
Therefore, we see that the range of the function \( \alpha \mapsto \sum_{i \in I_{n}} u_i \alpha^i \in \mathbb{R} \) defined on \( \mathbb{R}^n \) is determined the modulus vector \( |u| \) and the coset \( \phi + \text{Im} \Theta_n \) in the quotient space \( \mathcal{V}^\text{ph}_n / \text{Im} \Theta_n \). The phase difference of \( u \in \mathcal{V}^\text{sa}_n \) with nonzero entries is defined by the coset to which its phase part \( \phi \) belongs. It is also called the phase difference of \( \phi \in \mathcal{V}^\text{ph}_n \). The phase differences of \( \phi, \psi \in \mathcal{V}^\text{ph}_n \) coincide if and only if \( \phi - \psi \) satisfies the phase identities. The phase difference is uniquely expressed by a vector in the space \( \mathcal{V}^\text{ph}_n \), which will be denoted by \( \Phi_n(u) \). We see that \( u \in \mathcal{V}^\text{sa}_n \) satisfies the phase identities if and only if it has the trivial phase difference. We summarize our discussion as follows:

**Proposition 7.1.** If \( u, v \in \mathcal{V}^\text{sa}_n \) satisfy \( \Phi_n(u) = \Phi_n(v) \) and \( |u_i| = |v_i| \) for each \( i \in I_{[n]} \), then we have \( \|u\|_{\mathcal{X}_n} = \|v\|_{\mathcal{X}_n} \).

In the three qubit case, we note that \( \mathcal{V}^\text{ph}_3 \cap \text{Im} \Theta_3 \) is of dimension \( \lambda(3) = 1 \) and it is spanned by the vector \( \xi_T \) with the balanced multiset \( T = \{000, 011, 101, 110\} \). In this case, the phase difference can be expressed by the scalar
\[
\theta_{000} - \theta_{001} - \theta_{010} + \theta_{011} = \langle \Phi_n(c), \xi_T \rangle.
\]
This is exactly the phase difference of a three qubit state introduced in [19]. The following theorem tells us that the separability of an X-shaped multi-qubit states depends only on the phase differences of the anti-diagonal parts, as well as magnitudes of diagonal and anti-diagonal parts.

**Theorem 7.2.** Suppose that \( c, d \in \mathcal{V}^\text{sa}_n \) satisfy \( \Phi_n(c) = \Phi_n(d) \) and \( |c_i| = |d_i| \) for each \( i \in I_{[n]} \). Then we have \( \|c\|_{\mathcal{X}_n} = \|d\|_{\mathcal{X}_n} \).

**Proof.** For a given \( z \in \mathcal{V}^\text{sa}_n \) with \( \|z\|_{\mathcal{X}_n} = 1 \), we define \( w \in \mathcal{V}^\text{sa}_n \) by
\[
w_i = |z_i| e^{i(\arg z_i + \arg c_i - \arg d_i)}, \quad i \in I_{[n]}.
\]
Since \( \arg c - \arg d \in \text{Im} \Theta_n \) by \( \Phi_n(c) = \Phi_n(d) \), we have
\[
\arg w + \text{Im} \Theta_n = \arg z + \arg c - \arg d + \text{Im} \Theta_n = \arg z + \text{Im} \Theta_n,
\]
and so we have \( \|z\|_{\mathcal{X}_n} = \|w\|_{\mathcal{X}_n} \) by Proposition 7.1. We also have
\[
\langle c, z \rangle = \sum_{i \in I_{[n]}} |c_i||z_i| e^{i(\arg c_i + \arg z_i)} = \sum_{i \in I_{[n]}} |d_i||w_i| e^{i(\arg d_i + \arg w_i)} = \langle d, w \rangle.
\]
We have shown that for every \( z \in \mathcal{V}^\text{sa}_n \) with \( \|z\|_{\mathcal{X}_n} = 1 \) there exists \( w \in \mathcal{V}^\text{sa}_n \) such that \( \|w\|_{\mathcal{X}_n} = 1 \) and \( \langle c, z \rangle = \langle d, w \rangle \). This implies that \( \|c\|_{\mathcal{X}_n} \leq \|d\|_{\mathcal{X}_n} \). The reverse inequality holds by the same argument. \( \square \)

Recall the inequality \( \|c\|_{\mathcal{X}_n} \geq \|c\|_{\infty} \) in [19]. Now, we proceed to get another lower bound of the dual norm \( \|c\|_{\mathcal{X}_n} \) for \( c \in \mathcal{V}^\text{sa}_n \) in terms of the norms \( \|\cdot\|_{\mathcal{X}_n} \) of some elements.
in $\mathcal{V}^n_{\text{sa}}$. To do this, we take $\phi \in \mathcal{V}^n_{\text{ph}}$ to get
\[
\|c\|_{X_n} \geq \frac{\langle c, \hat{\alpha} \circ e^{i\phi} \rangle}{\|\hat{\alpha} \circ e^{i\phi}\|_{X_n}}
\]
for every $\alpha \in \mathbb{T}^n$, where $a \circ b$ is define by $(a \circ b)_i = a_ib_i$. Now, we have
\[
\langle c, \hat{\alpha} \circ e^{i\phi} \rangle = \langle c \circ e^{i\phi} \circ \hat{\alpha} \rangle, \quad \|\hat{\alpha} \circ e^{i\phi}\|_{X_n} = \|e^{i\phi}\|_{X_n}
\]
by (11) or Proposition 7.1, because $\Phi_n(\hat{\alpha}) = 0$. Therefore, we have the inequality
\[
(22) \quad \|c\|_{X_n} \geq \max_{\phi \in \mathcal{V}^n_{\text{ph}}} \frac{\|c \circ e^{i\phi}\|_{X_n}}{\|e^{i\phi}\|_{X_n}}.
\]
for every $c \in \mathcal{V}^n_{\text{sa}}$. In the three qubit case of $n = 3$, this is exactly Proposition 5.6 of [20]. The number $\|u\|_{X_n}$ has a natural upper bounds $\|u\|_1$ by Proposition 3.3. If all the entries of $u$ is nonnegative then it is clear that $\|u\|_{X_n} = \|u\|_1$ by taking $\alpha = 1$ in (11). We investigate when the strict inequalities hold in $\|u\|_{X_n} \leq \|u\|_1$ and $\|c\|_{X_n} \geq \|c\|_\infty$.

**Theorem 7.3.** For $u, c \in \mathcal{V}^n_{\text{sa}}$, we have the following:

(i) $\|u\|_{X_n} = \|u\|_1$ holds if and only if $u$ has the trivial phase difference;

(ii) Suppose that $|c_i| = |c_j|$ for every $i, j \in I_{[n]}$. Then $\|c\|_{X_n} = \|c\|_\infty$ if and only if $c$ has the trivial phase difference.

**Proof.** If the phase part of $u$ is $0 \in \mathcal{V}^n_{\text{ph}}$, then we have $\|u\|_{X_n} = \|u\|_1$. This is also the case whenever $\Phi_n(u) = 0$ by Proposition 7.1. We note that
\[
u_i \alpha^1 + u_i \alpha^1 \leq |u_i \alpha^1 + u_i \alpha^1| \leq |u_i| + |u_i|
\]
for each $i \in I_{[n]}$. If $\|u\|_{X_n} = \|u\|_1$ then there exists $\alpha \in \mathbb{T}^n$ such that $u_i \alpha^1 = |u_i|$ for every $i \in I_{[n]}$ in (8). Therefore, the phase part of $u$ is given by $\theta$ with $\theta_1 = - \arg \alpha^1$, which belongs to $\text{Im} \Theta_n$. This proves the statement (i).

To prove (ii), we may assume that $|c_i| = 1$ for every $i \in I_{[n]}$. If $\|u\|_{X_n} = 1$ then we have $\langle u, 1 \rangle = \sum_{i\in I_{[n]}} u_i \leq \|u\|_{X_n} = 1$, which implies that $\|1\|_{X_n} \leq 1$. Therefore, we have $\|1\|_{X_n} = 1$ by (9), and $\|c\|_{X_n} = 1$ whenever $c$ has a trivial phase difference by Theorem 7.2. For the converse, suppose that $\|c\|_{X_n} = 1$. Then we have $\|e^{i\phi}\|_{X_n} = \|c \circ e^{i\phi}\|_{X_n}$ for every $\phi \in \mathcal{V}^n_{\text{ph}}$ by (22). Take $\phi = -\theta$ with the phase part $\theta$ of $c \in \mathcal{V}^n_{\text{sa}}$. Then we have
\[
\|e^{-i\theta}\|_{X_n} \geq \|c \circ e^{-i\theta}\|_{X_n} = \|1\|_{X_n} = \|1\|_1 = \|e^{i(-\theta)}\|_1.
\]
This implies that $e^{i(-\theta)}$ has the trivial phase difference by (i), and completes the proof. \(\Box\)

Finally, we show that our criterion, Theorem 4.5, detects nonzero volume of PPT entanglement with respect to the affine space of all self-adjoint matrices with trace one. To do this, we consider the general situations to compare two convex sets. Let $C$ be a convex set in a finite dimensional real vector space. Recall that a point $p \in C$ is called an interior point when it is a topological interior point of $C$ with respect to the affine manifold generated by $C$, and a boundary point if it is not an interior point.
We denote by \( \text{int} C \) and \( \partial C \) the sets of all interior points and the boundary points of \( C \), respectively. If two convex sets \( C_1 \) and \( C_2 \) generate the common affine manifold \( M \), then we may use all the topological notions, like interior, closure, boundary, with respect \( M \).

**Proposition 7.4.** Let \( C_1 \subset C_2 \) be a finite dimensional convex sets which generate a common affine manifold. Then the following are equivalent:

(i) \( C_2 \setminus C_1 \) has the nonempty interior;

(ii) \( \overline{\partial C_1} \cap \text{int} C_2 \) is nonempty.

**Proof.** The assumption implies that \( \text{int} C_1 \subset \text{int} C_2 \). We fix a common interior point \( p_0 \) of \( C_1 \) and \( C_2 \). For the direction (i) \( \implies \) (ii), take an interior point \( p_1 \) of \( C_2 \setminus C_1 \), and consider the line segment \( p_t = (1-t)p_0 + tp_1 \). Put \( t_0 = \sup \{ t : p_t \in \overline{C_1} \} \). Then \( t_0 > 0 \) since \( p_0 \) is an interior point of \( C_1 \). We also have \( t_0 < 1 \), because \( p_1 \) is an interior point of \( C_2 \setminus C_1 \). Therefore, we see that \( p_{t_0} \) belongs to \( \overline{\partial C_1} \cap \text{int} C_2 \).

For (ii) \( \implies \) (i), take \( p_1 \in \overline{\partial C_1} \cap \text{int} C_2 \) and put \( t_0 = \sup \{ t : p_t \in C_2 \} \). Since \( p_1 \) is an interior point of \( C_2 \), we have \( t_0 > 1 \). Then \( p_t \) with \( 1 < t < t_0 \) is an interior point of \( C_2 \). Because \( \overline{C_1} \) is convex, we conclude that \( p_t \) is an interior point of \( C_2 \setminus C_1 \). \( \square \)

Proposition 7.4 has been used implicitly in [24, 21], to see that an entanglement witness \( W \) detects nonzero volume of PPT entanglement if and only if every partial transpose of \( W \) has the full rank. We denote by \( \mathcal{C} \) the set of all states satisfying the criterion in Theorem 4.5. We show that \( \mathcal{C} \) is convex and closed.

**Proposition 7.5.** The set \( \mathcal{C} \) is convex and closed.

**Proof.** For given \( a,b \in \mathcal{V}_n^+ \) and \( c,d \in \mathcal{V}_n^{sa} \), we have the inequalities

\[
\Delta_n(a+b) \geq \Delta_n(a) + \Delta_n(b), \quad \|c\|_{X_n} + \|d\|_{X_n} \geq \|c+d\|_{X_n}.
\]

Therefore, we see that \( \mathcal{C} \) is a convex set. To show that \( \mathcal{C} \) is closed, take a sequence \( \{ \varrho^m \} \) in \( \mathcal{C} \) with the \( X \)-parts \( X(a^m,c^m) \) which converges to \( \varrho \) with the \( X \)-part \( X(a,c) \). Take \( s \in \mathcal{V}_n^+ \) with \( \delta_n(s) = 1 \) such that \( \langle a, s \rangle \leq 1 \Delta_n(a) + \varepsilon \). Put \( \alpha = \varepsilon/\|s\|_1 \). Then, for every \( m \) with \( \|a^m - a\|_\infty < \alpha \), we have

\[
\|c^m\|_{X_n} \leq \Delta_n(a^m) \leq \Delta_n(a + \alpha 1) \leq \langle a + \alpha 1, s \rangle \leq \langle a, s \rangle + \alpha \|s\|_1 \leq \Delta_n(a) + 2\varepsilon.
\]

Therefore, we see that \( \|c\|_{X_n} \leq \Delta_n(a) + 2\varepsilon \). Because \( \varepsilon > 0 \) was arbitrary, we conclude that \( \varrho \) belongs to \( \mathcal{C} \). \( \square \)

It seems to be well known among specialists that every self-adjoint matrix in the tensor product can be expressed as a linear combination of tensor products of self-adjoint matrices. See [25] for example. Indeed, every self-adjoint element \( z = \sum_{k=1}^n v_k \otimes w_k \in (V \otimes W)_{sa} \) in the tensor product \( V \otimes W \) of *-vector spaces \( V \) and \( W \) can be written
by

\[ z = \frac{1}{2} \sum_{k=1}^{n} v_k \otimes w_k + \frac{1}{2} \sum_{k=1}^{n} v_k^* \otimes w_k^* \]

\[ = \sum_{k=1}^{n} \left( \frac{v_k + v_k^*}{2} \right) \otimes \left( \frac{w_k + w_k^*}{2} \right) - \sum_{k=1}^{n} \left( \frac{v_k - v_k^*}{2i} \right) \otimes \left( \frac{w_k - w_k^*}{2i} \right), \]

which belongs to tensor product \( V_{sa} \otimes W_{sa} \) of self-adjoint parts. Now, we denote by \( D, T \) and \( S \) the convex sets of all states, PPT states and separable states, respectively. Then the above decomposition shows that both \( S \) and \( D \) generate the affine manifold consisting of all self-adjoint matrices with trace one. Therefore, we can apply Proposition 7.4 for two convex sets \( C \cap T \) and \( T \), since \( S \subset C \cap T \subset T \subset D \).

Take \( c \in V_{sa}^n \) so that \(|c_i| = 1\) for each \( i \in I_n\), and consider the following \( n \)-qubit self-adjoint matrix

\[ \varrho_t = 2^{-n} X(1, tc) \]

for \( t \geq 0\). We have the following:

- \( \varrho_t \in D \iff \varrho_t \in T \iff t \leq 1; \)
- \( \varrho_t \in S \iff \varrho_t \in C \cap T \iff \Delta_n(a) \geq \|tc\|_{X_n} \iff t \leq 1/\|c\|_{X_n}. \)

Take \( t_0 = 1/\|c\|_{X_n} \). We have \( t_0 < 1 \) by Theorem 7.3 whenever we take \( c \in V_{sa}^n \) with \(|c_i| = 1\) and nontrivial phase difference. Then we see that \( \varrho_{t_0} \) is a boundary point of \( C \cap T \) and an interior point of \( T \). Therefore, we conclude that \( T \setminus C \cap T \) has the nonempty interior. This tells us that Theorem 4.5 detects nonzero volume of PPT entanglement.

We also see that \( \varrho_{t_0} \) belongs to \( \partial S \cap \text{int } T \). Therefore, \( \varrho_{t_0} \) is an \( n \)-qubit boundary separable state with full ranks in the sense of [26], because \( \varrho \in \text{int } T \) if and only if all the partial transposes of \( \varrho \) have the full ranks. Such states have been constructed in \( 3 \otimes 3 \) system [27], \( 2 \otimes 4 \) system [28] and three qubit system [21, 29]. We recall that a nontrivial phase difference occurs only when \( n \geq 3 \), because dimension of \( V_{ph}^n \ominus \text{Im } \Theta_n \) is \( 2^{n-1} - n = 0 \) for \( n = 1, 2 \).

8. Conclusion

In this paper, we have defined two numbers \( \Delta_n(a) \) and \( \|c\|_{X_n}^\prime \) arising from the diagonal part \( a \in V_n^+ \) and the anti-diagonal part \( c \in V_{sa}^n \) of an \( n \)-qubit X-state \( X(a, c) \), and showed that \( \varrho = X(a, c) \) is separable if and only if the inequality

\[ \Delta_n(a) \geq \|c\|_{X_n}^\prime \]

holds. Since the X-part of a separable \( n \)-qubit state is again separable, this inequality gives rise to a necessary criterion for separability, which detects PPT entanglement of nonzero volume. Two numbers \( \Delta_n(a) \) and \( \|c\|_{X_n}^\prime \) in the above inequality have natural
upper and lower bounds
\[
\min_{i \in I(n)} \{ \sqrt{a_i a_i^*} \} \geq \Delta_n(a), \quad \|c\|_{X_n}^\prime \geq \|c\|_\infty,
\]
respectively, by (10) and (9). Note that \( \varrho = X(a, c) \) is of PPT if and only if the inequality \( \min\{ \sqrt{a_i a_i^*} \} \geq \|c\|_\infty \) holds, and so the strict inequalities in (24) reflect the existence of PPT entanglement.

In order to estimate the above two numbers \( \Delta_n(a) \) and \( \|c\|_{X_n}^\prime \) more precisely, we have introduced the notion of irreducible balanced multisets of indices, and defined the number \( \tilde{\Delta}_n(a) \) which is an upper bound for \( \Delta_n(a) \). The number \( \tilde{\Delta}_n(a) \) can be easily evaluated with the entries of \( a \), and actually coincides with \( \Delta_n(a) \) for \( n = 1, 2, 3 \). It seems to be very difficult to evaluate the number \( \delta_n(s) \) in terms of the entries, even for the case of \( n = 3 \). In this regard, it is remarkable that its ‘dual’ object \( \Delta_3(a) \) can be evaluated by the identity \( \Delta_3(a) = \tilde{\Delta}_3(a) \). It would be very interesting to know if the identity \( \Delta_n(a) = \tilde{\Delta}_n(a) \) holds for \( n \geq 4 \).

The norm \( \|u\|_{X_n} \) and its dual norm \( \|c\|_{X_n}^\prime \) depend on the phase parts of \( u \in \mathcal{V}_n^{sa} \) and \( c \in \mathcal{V}_n^{sa} \) as well as the magnitude parts. We have introduced the notions of phase identities and phase differences to explain these phenomena. Nontrivial phase differences appear only when \( n \geq 3 \), and this reflects the fact that there exists no PPT entanglement in the two qubit system. We gave a lower bound for the dual norm \( \|c\|_{X_n}^\prime \) to see that our criteria detects nonzero volume of PPT entanglement whenever \( n \geq 3 \).

Evaluation of \( \|c\|_{X_n}^\prime \) in terms of entries seems to be very difficult, even though it was possible in several cases of the three qubit system [20, 18, 19]. It would be nice to evaluate \( \|c\|_{X_n}^\prime \) when the entries of \( c \in \mathcal{V}_n^{sa} \) share a common magnitude. See [20, 19] for the formula in the three qubit case.

Note that there are other notions for separability like bi-separability and full bi-separability, according to bi-partitions of local systems. Such notions of separability have been already characterized for X-states in [30, 16, 22, 31, 32]. In these characterization, the phase part of anti-diagonal plays no role.

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