Polytope structures for Greenberger–Horne–Zeilinger diagonal states

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Abstract
We explore the polytope structures for genuine entanglement, biseparability, full biseparability and Bell inequality of multi-qubit GHZ diagonal states. We first show that biseparable GHZ diagonal states make hypersimplices inside the simplices consisting of all GHZ diagonal states. Next, we consider full biseparability which is equivalent to positive partial transpose for GHZ diagonal states, and show that they make the convex hulls of simplices and cubes. We also visualize which part of the simplex violates multipartite Bell inequality. Finally, we compute precise volumes for genuine entanglement, biseparability, full biseparability and states violating Bell inequality among all GHZ diagonal states.

Keywords: Greenberger–Horne–Zeilinger diagonal state, polytope, bi-separable, fully bi-separable, Mermin inequality, volume

1. Introduction

The notion of entanglement arising from quantum mechanics is now recognized as one of the most important resources in the current quantum information and computation theory. The Greenberger–Horne–Zeilinger states [1, 2] are key examples of genuine entanglement in multi-qubit systems, and have many applications in various fields of quantum information theory. See survey articles [3, 4]. They also play important roles in the classification of entanglement in multi-qubit systems [5–7].

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A mixed state is called separable if it is a mixture of product states, and entangled if it is not separable. In the multi-partite systems, the notion of entanglement depends on partitions of systems. A multi-partite state is called biseparable if it is a mixture of separable states with respect to bipartitions of systems, and called genuinely entangled if it is not biseparable. On the other hand, a state is called fully biseparable if it is biseparable with respect to any bipartitions of systems.

The GHZ diagonal states are mixtures of GHZ states [5, 8]. The mixture with the uniform distribution gives rise to the maximally mixed states, that is, the scalar multiples of the identity. By the results in [9–12], we have now complete criteria for biseparability and full biseparability of GHZ diagonal states. We first note that those criteria are given by finitely many linear inequalities, and so the resulting convex sets are polytopes. We recall that a convex set in a finite dimensional space is called a polytope if it has finitely many extreme points. It is well known that this is equivalent to the condition that it has finitely many facets, that is, maximal faces given by hyperplanes. See [13–16] for examples.

The main purpose of this note is to explore the polytope structures for biseparable and fully biseparable GHZ diagonal states. We recall [12] that a GHZ diagonal state is fully biseparable if and only if it is of PPT. We also visualize which GHZ diagonal states violate Bell type inequalities. We first note that the convex set $G_n$ of all $n$-qubit GHZ diagonal states is the regular simplex of dimension $d - 1$ with the side length $\sqrt{2}$, where we retain the notation $d = 2^n$ throughout this note. The GHZ states correspond to vertices and the maximally mixed state is located at the center of the simplex. We show that the convex set $B_n$ consisting of all biseparable GHZ diagonal states is a truncation polytope [13], that is, a polytope obtained from a simplex by successive truncations of vertices. Genuine entanglement among GHZ diagonal states are located in the truncated parts which consist of $d$ pieces of $(d - 1)$ regular simplices with the side length $\frac{1}{\sqrt{2}}$. The remaining polytope $S_n$ is the convex hull of midpoints of edges of $G_n$, which is the half sized hypersimplex $\Delta_{d-1}(2)$ [15, 16]. On the other hand, the convex set $F_n$ of all fully biseparable GHZ diagonal states is the convex hull of the $\frac{d}{4}$ regular simplex and the $\frac{d}{4}$ regular cube which locate in the perpendicular position and share only the maximally mixed state. We note that $B_2 = F_2$ holds for the two qubit case, and their polytope structures are already known in [17]. We consider Mermin inequality as a multipartite Bell inequality, and see that the part of $G_n$ satisfying the inequality is also a truncation polytope by a single truncation.

With this information, we compute precise values of volumes, relative volumes and relative volume radii for genuine entanglement, biseparability, full biseparability and violation of Mermin inequality among all GHZ diagonal states. We also find the largest balls inside the polytopes $G_n$, $B_n$ and $F_n$. It is interesting to note that all of them coincide.

2. Polytopes

Throughout this note, we denote by $I_n$ the set of all $n$-bit indices which are, by definition, functions from $\{1, 2, \ldots, n\}$ into $\{0, 1\}$. Therefore, they are $\{0, 1\}$ strings of length $n$. For examples, we have $I_2 = \{00, 01, 10, 11\}$, $I_3 = \{000, 001, 010, 011, 100, 101, 110, 111\}$, and so, $I_n$ may be considered as the set of natural numbers from $0$ to $2^n - 1$ with the binary expression. For a given index $i \in I_n$, the index $\bar{i} \in I_n$ is defined by $\bar{i}(k) = i(k) + 1 \mod 2$. For an example, we have $0101 = 101$. 

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2.1. GHZ diagonal states

For each index \( i \in I_n \), the GHZ state is given by
\[
|\text{GHZ}_i\rangle = \frac{1}{\sqrt{2}} (|i\rangle + (-1)^k |\bar{i}\rangle).
\]

For example, we have \( |\text{GHZ}_{00}\rangle = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle) \) and \( |\text{GHZ}_{101}\rangle = \frac{1}{\sqrt{2}} (|101\rangle - |010\rangle) \). An \( n \)-qubit state is called GHZ diagonal if it is a convex combination of the above states. We remind the readers of our convention \( d = 2^n \). Because the above states are orthonormal, we see that the convex set \( G_n \) of all \( n \)-qubit GHZ diagonal states is the regular \((d-1)\) simplex with \( d \) vertices
\[
v_i := |\text{GHZ}_i\rangle (|\text{GHZ}_i\rangle^*), \quad i \in I_n,
\]
and every GHZ diagonal state is uniquely written by
\[
\rho_p := \sum_{i \in I_n} p_i v_i
\]
with a probability distribution \( p \) over \( I_n \). For a given fixed index \( i \), we note that the convex hull
\[
G^i_n := \text{conv} \{ v_j : j \neq i \} = \{ \rho_p \in G_n : p_i = 0 \}
\]
is a facet of \( G_n \) which is given by the hyperplane \( p_i = 0 \), and every facet of \( G_n \) arises in this way. If we endow the index set \( I_n \) with the lexicographic order, then the GHZ diagonal state \( \rho_p \) may be expressed by the following \( d \times d \) matrix
\[
X(a, z) := \begin{pmatrix}
 a_{00...0} & a_i & z_{01...0} \\
 a_i & \ddots & \ddots \\
 z_{11...1} & \ddots & a_i \\
 & \ddots & \ddots \\
 & & a_{11...1}
\end{pmatrix},
\]
with \( a_i = \frac{1}{2} (p_i + p_{\bar{i}}) \) and \( z_i = \frac{(-1)^k}{2} (p_i - p_{\bar{i}}) \).

With the uniform distribution, we have the center point \( c := \frac{1}{d} \sum v_i = \frac{1}{d} I_d \) of the simplex \( G_n \), which is the maximally mixed state. The center of the facet \( G^i_n \) is given by \( c^i := \frac{1}{d-1} \sum_{j \neq i} v_j \). We note that the three points \( v_i, c \) and \( c^i \) are collinear. We also see that the ‘height’ of the simplex \( G_n \) is the distance between \( v_i \) and \( c^i \), which is given by \( \sqrt{d/(d-1)} \) with respect to the Hilbert–Schmidt norm. The center point \( c \) divides the height by the ratio \( 1 - \frac{1}{d} \), and so it approaches \( c^i \) as the number of qubit increases. See figure 1.

2.2. Biseparable states

It is known [9] that the GHZ diagonal state \( \rho_p \) of (1) is biseparable if and only if the inequality
\[
|z_i| \leq \frac{1}{2} \sum_{j \neq i} a_j
\]
holds for every \( i \in I_n \). The inequality can be written as \( |p_i - p_{\bar{i}}| \leq \sum_{j \neq i} p_j \),
Figure 1. The triangle and its base represent the simplex $G_n$ and the facet $G^i_n$, respectively. The center $c$ of the simplex approaches the center $c^i$ of the facet $G^i_n$ as the dimension increases.

of which the right-hand side is equal to $1 - p_i - p_{\bar{i}}$. Hence, $\varrho_p$ is biseparable if and only if

$$p_i \leq \frac{1}{2}, \text{ for every } i \in I_n.$$  \hfill (2)

In other words, a GHZ diagonal state $\varrho_p$ is genuinely entangled if and only if $p_i > \frac{1}{2}$ for some $i \in I_n$. From this, we see that genuine entanglement is detected by the hyperplanes $p_i = \frac{1}{2}$, which also determine facets

$$B^i_n := \{ \varrho_p \in G_n : p_i = \frac{1}{2} \}$$

of the convex set $B_n$ consisting of all $n$-qubit biseparable GHZ diagonal states. Especially, we see that $B_n$ is a polytope; it has finitely many facets. For each $i \in I_n$, the region $\{ \varrho_p \in G_n : p_i > \frac{1}{2} \}$ contains only one vertex $v_i$, and so $B_n$ is a truncation polytope. Genuine entanglement consists of such regions through indices $i \in I_n$. We note that an algebraic formula for genuinely multipartite concurrence for GHZ diagonal states in [11] is given by

$$C_{GM}(\varrho_p) = \max \{0, 2(\max_{i} p_i) - 1 \}.$$  \hfill (3)

Therefore, we see that a level set of $C_{GM}(\varrho)$ is parallel to a facet $B^i_n$ of the convex set $B_n$, and $C_{GM}(\varrho)$ takes the maximum at vertices of $G_n$.

In order to understand the polytope structures of $B_n$, we proceed to search for all extreme points. First of all, we consider the case when $\varrho_p$ satisfies $p_i = 0$ or $p_i = \frac{1}{2}$ for each $i$. In this case, there exist exactly two indices $i, j$ such that $p_i = p_j = \frac{1}{2}$, and so we see that the resulting state

$$\varrho_p = \frac{1}{2}(v_i + v_j) := m_{ij}$$

is the midpoint of the edge of $G_n$ connecting two vertices $v_i$ and $v_j$. It is also clear that $m_{ij}$ is an extreme point of $B_n$ since it is the unique point of $B_n$ on this edge by (2). Note that $m_{ij}$ is a diagonal state with two nonzero diagonal entries. Conversely, suppose that $\varrho_p \in B_n$ satisfies $0 < p_i < \frac{1}{2}$ for some $i$. Then we take the largest $p_i$ and the second largest $p_{\bar{i}}$, and consider the line segment $\varrho = (1 - t)m_{i\bar{i}} + t\varrho_p$. Since $p_{i\bar{i}}, p_{\bar{i}} > 0$ and $p_i < \frac{1}{2}$ for $i \neq i_1, i_2$, we see that $\varrho_{i+\varepsilon}$ satisfies (2) for small $\varepsilon > 0$, and so $\varrho_p$ is not an extreme point of $B_n$. Therefore, we conclude that the polytope $B_n$ is the convex hull of mid points of edges, as they are listed in
Figure 2. The polytope $G_2$ has four vertices $v_{00}, v_{01}, v_{10}$ and $v_{11}$ which make the regular three simplex. The polytope $B_2$ of biseparable states has six vertices which are midpoints of edges of $G_2$. In this picture, we have the vertex $v_{00}$ on the top level, the facet $B^{00}_2$ of $B_2$ on the middle level and the facet $G^{00}_2 \cap B_2$ on the bottom level. The facet $B^{00}_2$ is the regular two simplex, and $G^{00}_2 \cap B_2$ is the half sized hypersimplex $\Delta_d(2)$ sitting in the two simplex $G^{00}_2$.

(3). This also tells us that $B_n$ is obtained by maximal truncations of all vertices with the same size. The polytope $B_n$ can be considered as the half sized hypersimplex $\Delta_{d-1}(2)$, whose vertex coordinates consist of 0 and 1, where the numbers of 0 and 1 are $(d-2)$ and 2, respectively.

Note that the vertex coordinates of $G_n$ also consists of $(d-1)$ number of 0’s and one 1.

We will bipartition extreme points into two groups. To do this, we fix an index $i$. We note that an extreme point $m_{i,j}$ belongs to the facet $B^i_n$ for every $j$ different from $i$. If $j, k \neq i$, then $m_{i,k}$ belongs to the another facet

$$G^i_n \cap B_n = \{ \sigma_p \in B_n : p_i = 0 \}$$

of $B_n$ which is determined by the hyperplane $p_i = 0$. Therefore, we see that extreme points of $B_n$ are bipartitioned into two groups, one group in the facet $B^i_n$ and other group in the facet $G^i_n \cap B_n$. Therefore, we conclude that $B_n$ is the convex hull of two parallel facets $B^i_n$ and $G^i_n \cap B_n$. We note that $B^i_n$ is the $(d-2)$ simplex. On the other hand, $G^i_n \cap B_n$ is the half sized hypersimplex $\Delta_{d-2}(2)$ sitting in $G^i_n$. Every index $i$ corresponds to such a bipartition of extreme points, and corresponding two facets. Therefore, the number of facets is given by $2d$. See figure 2 for two-qubit case. We finally note that every extreme point $m_{i,j}$ is contained in exactly $d$ facets; $B^i_n, B^j_n$ and $G^k_n \cap B_n$ for $k \neq i,j$.

Our geometric approach also gives rise to a simple proof for the characterization [9] of biseparability among GHZ diagonal states. For the nontrivial part to prove that the condition (2) implies biseparability, it is enough to show that extreme points $m_{i,j}$ are biseparable. To do this, let $S$ and $T$ be the set of natural numbers $k = 1, 2, \ldots, n$ such that $i(k) = j(k)$ and $i(k) \neq j(k)$, respectively. Then it is easily seen that $m_{i,j}$ is separable with respect to the bipartition $S \cup T$ of systems, as in the two qubit case.

2.3. Fully biseparable states

Now, we turn our attention to full biseparability. It was shown in [12] that a GHZ diagonal state is fully biseparable if and only if it is of PPT with respect to any bi-partition of parties. Therefore, a GHZ diagonal state $\rho_p$ of (1) is fully biseparable if and only if the following

$$|z_j| \leq a_i, \quad \text{for every } i, j \in I_n$$

(4)
holds. Note that the above inequalities are combinations of linear inequalities, and so the convex set $F_n$ of all fully biseparable GHZ diagonal states is also a polytope.

For a given $\varrho_p \in F_n$ in (1), we denote by $\lambda = \max |z_i|$. Then we see that $\varrho_p$ is the sum of the diagonal unnormalized state $\sum_i (a_i - \lambda) |\bar{i}\rangle |\bar{i}\rangle$ and another unnormalized state $X(\lambda, z)$ with the notation in (1), where $I_1 = 1$ for each $i \in I_n$. Since $a_i = a_\bar{i}$ and $m_{ij} = \frac{1}{d} (|i\rangle |j\rangle + |j\rangle |i\rangle)$, we have

$$\varrho_p = \sum_{i \in I_n} (a_i - \lambda) m_{ij} + \lambda d X \left( \frac{1}{d} I, w \right)$$

with $w = \frac{\lambda}{d}$ satisfying $-\frac{1}{d} \leq w \leq \frac{1}{d}$ and $w_1 = w_1$ for each index $i \in I_n$. Therefore, we see that $F_n$ is the convex hull of the following two polytopes

$$F_n^\triangle := \text{conv} \{ m_{ij} : i \in I_n \},$$

$$F_n^{\square} := \left\{ X \left( \frac{1}{d} I, w \right) : -\frac{1}{d} \leq w_1 \leq \frac{1}{d}, w_1 = w_1 \right\}.$$

We note that $F_n^{\triangle}$ consisting of diagonal states is the regular $(\frac{d}{2} - 1)$ simplex with the unit side length since $\{ m_{ij} \}$ is an orthogonal family with the uniform norm $1/\sqrt{d}$. It is clear that $F_n^{\triangle}$ is the regular $\frac{d}{2}$ cube with the side length $2\sqrt{d}/d$.

Suppose that $\sigma$ is a collection of $2^{n-1}$ indices which has exactly one index among $i$ and $\bar{i}$. In case of two qubit, we have four such choices; $\{00, 01\}$, $\{00, 10\}$, $\{11, 01\}$ and $\{11, 10\}$. In general, we have $2^d/2$ choices for the $n$-qubit case. We denote by $v_\sigma^{\sqcup}$ the GHZ diagonal state with the uniform distribution over $\sigma$, that is, we define

$$v_\sigma^{\sqcup} := \frac{2}{d} \sum_{i \in \sigma} v_i = X \left( \frac{1}{d} I, w \right),$$

where $w_1 = w_1 = (-1)^{k \bar{i}} \frac{1}{d}$ for $i \in \sigma$. These states $v_\sigma^{\sqcup}$s are vertices of the cube $F_n^{\sqcup}$. In fact, $v_\sigma^{\sqcup}$ is an extreme point of $F_n$ since it is the only one point of $F_n$ in the face $G_\sigma^\nu$ of $G_n$ generated by $v_i$ with $i \in \sigma$ by the PPT condition. Therefore, there are exactly $\frac{d}{2} + 2d/2$ extreme points of $F_n$. Note that extreme points of $F_1$, together with $B_1$, have been found in [18, 19].

In conclusion, the polytope $F_n$ of all fully biseparable GHZ diagonal states is the convex hull of the regular $(\frac{d}{2} - 1)$ simplex $F_n^\triangle$ and the regular $\frac{d}{2}$ cube $F_n^{\sqcup}$. Two polytopes $F_n^\triangle$ and $F_n^{\square}$ are perpendicular, and share only one point which is the maximally mixed state. We see by [20, proposition 3.1] that every face of $F_n$ is the convex hull of a (possibly empty) face of $F_n^\triangle$ and a (possibly empty) face of $F_n^{\square}$. Because both $F_n^\triangle$ and $F_n^{\square}$ contain the maximally mixed state which is an interior point of $F_n$, we see that every facet of $F_n$ is given by the convex hull of proper faces of $F_n^\triangle$ and $F_n^{\square}$. On the other hand, facets of $F_n^\triangle$ and $F_n^{\square}$ are given by

$$\text{conv} \{ m_{ik} : k \neq i, \bar{i} \} \quad \text{and} \quad \left\{ X \left( \frac{1}{d} I, w \right) \in F_n^{\sqcup} : w_1 = (-1)^{k \bar{i}} \frac{1}{d} \right\},$$

for choices of indices $i$ and $j$, respectively, and their convex hull is the collection of $X(a, w) \in F_n$ satisfying $a_i = (-1)^{k \bar{i}} w_1$ determined by the identity in (4). Therefore, we conclude that the convex hull of facets of $F_n^{\triangle}$ and $F_n^{\square}$ is a facet of $F_n$, and every facet of $F_n$ arises in this way. We note that facets of $F_n^\triangle$ and $F_n^{\square}$ are determined by choices of $\{i, \bar{i}\}$ and $j$, respectively. They
give rise to the facet \( F_{ij} \) of the polytope \( F_n \), which is the convex hull of two convex sets in (6). This facet is also given by the equation

\[
F_{ij} = \{ \varrho_p \in F_n : p_i + \bar{p}_i = p_j - \bar{p}_j \}
\]

in terms of probability distribution by (4). We also note that the number of facets of the polytope \( F_n \) is given by \( \frac{d^2}{2} \). See figure 3 for the two qubit case.

Using the geometry, we may also give a simple proof of the equivalence between PPT and full biseparability for GHZ diagonal states. For the nontrivial part to show every GHZ diagonal state of PPT is fully biseparable, it suffices to consider an extreme point \( v_\sigma \) of \( F_n \). We fix a bipartition \( S \cup T \), and denote by \( \bar{S} \) the index obtained by changing \( k \)th symbols for \( k \in S \), and similarly for \( \bar{T} \). Then, for each \( i \in \sigma \), either \( \bar{S} \in \sigma \) or \( \bar{T} \in \sigma \) holds. Thus, \( v_\sigma \) is the average of states of the form \( m_i, \bar{S} \) or \( m_i, \bar{T} \) by (5). For example, if \( \sigma = \{000, 001, 011, 101\} \) and the bipartition is \( A-BC \), then \( v_\sigma \) is the average of \( m_{000,001} \) and \( m_{001,101} \) which are \( A-BC \) separable as in the two qubit case.

### 2.4. Bell inequalities

In this subsection, we consider multipartite Bell inequalities and figure out which parts violate the inequalities. See [21] for a survey on Bell inequalities. We begin with the Mermin inequality [22], which considers two settings on each side. Following [3], we put

\[
M_n := \sum_{i} X_i X_2 X_3 X_4 X_5 \cdots X_n - \sum_{i} Y_1 Y_2 X_3 X_4 X_5 \cdots X_n + \sum_{i} Y_1 Y_2 Y_3 Y_4 X_5 \cdots X_n - \cdots,
\]

where \( X_i \) and \( Y_i \) represent the Pauli matrices \( \sigma_x, \sigma_y \) on the \( i \)th qubit, and \( \sum_{i} \) represents the sum of all possible permutations of the qubits that give distinct terms. Then the Mermin inequality is given by

\[
\langle M_n \rangle_\varrho := \text{Tr}(M_n \varrho) \leq \mu_n := \begin{cases} 
2^{n/2}, & n \text{ even}, \\
2^{(n-1)/2}, & n \text{ odd}.
\end{cases}
\]
Recall the notation $\mathbf{1}$ given by $\mathbf{1}_i = 1$ for each $i \in I_n$. We also use the notation $\mathbf{0}$ given by $\mathbf{0}_i = 0$ for each $i \in I_n$. We have

$$M_n|\mathbf{0}\rangle = |\mathbf{1}\rangle - \sum_\pi i^\pi |\mathbf{1}\rangle + \sum_\pi i^\pi |\mathbf{1}\rangle - \sum_\pi i^\pi |\mathbf{1}\rangle + \cdots = (a C_0 + a C_2 + a C_4 + \cdots) |\mathbf{1}\rangle = 2^{n-1} |\mathbf{1}\rangle$$

and $M_n|\mathbf{1}\rangle = 2^{n-1} |\mathbf{0}\rangle$ similarly. Since $\{\frac{1}{\sqrt{2}} \sigma_x, \frac{1}{\sqrt{2}} \sigma_y\}$ is orthonormal, we have

$$\|M_n\|_2^2 = 2^n \left(\frac{1}{\sqrt{2}}\right)^n M_n |\mathbf{1}\rangle = 2^n (a C_0 + a C_2 + a C_4 + \cdots) = 2^{2n-1}.$$}

On the other hand, we also have

$$|\langle 0|M_n|\mathbf{1}\rangle|^2 + |\langle 1|M_n|\mathbf{0}\rangle|^2 = 2^{2n-1} = \|M_n\|_2^2,$$

which implies $\langle i|M_n|j\rangle = 0$ whenever $\{i, j\} \neq \{0, 1\}$. Therefore, we have

$$\langle i|M_n|j\rangle = \begin{cases} 2^{n-1}, & (i, j) = (0, 1), (1, 0), \\ 0, & \text{otherwise} \end{cases}$$

and so it follows that

$$\langle M_n \rangle_{\varphi} = 2^{n-1} (p_0 - p_1),$$

for a GHZ diagonal state $\varphi_p$.

Now, we conclude that a GHZ diagonal state $\varphi_p$ violates the Mermin inequality if and only if

$$p_0 - p_1 > \nu_n := \begin{cases} 2/\sqrt{d}, & n \text{ even} \\ \sqrt{2}/\sqrt{d}, & n \text{ odd} \end{cases}$$

and the GHZ state $\varphi_0$ violates the inequality maximally. The hyperplane

$$H_M := \{ \varphi_p \in G_n : p_0 - p_1 = \nu_n \}$$

is perpendicular to the edge $\overline{w_1w_2}$ of the simplex $G_n$ of all GHZ diagonal states, and meets the edges $\overline{w_1w_i}$ for $i \neq 0$ at the points

$$w_1 := \left(\frac{1}{2} + \frac{1}{2} \nu_0\right)v_0 + \left(\frac{1}{2} - \frac{1}{2} \nu_0\right)v_1, \quad w_i := \nu_i v_0 + (1 - \nu_i)v_i, \quad i \neq 0, 1. \quad (8)$$

We note that $\nu_n = \frac{1}{2}$ for $n = 3, 4$ and $\nu_n < \frac{1}{2}$ for $n \geq 5$. This means that the hyperplane $H_M$ is tangent to the facet $B_3$ of the convex set $B_n$ for $n = 3, 4$. Therefore, we see that three or four qubit biseparable GHZ diagonal states never violate the Mermin inequality. On the other hand, there exists $n$ qubit biseparable GHZ diagonal states which violate the inequality for $n \geq 5$. See figure 4.

As for fully biseparable states or equivalently PPT states, we see that $\langle M_n \rangle_{\varphi} = 0$ and $\langle M_n \rangle_{\varphi} = \pm 1$ for extreme points of $F_n$. Therefore, we see that no GHZ diagonal state of PPT
violates the Mermin inequality. Using the Lagrange method, the distance from the hyperplane $H_M$ to the convex set $F_n$ is calculated by
\[
\text{dist}(H_M, F_n) = \frac{1}{\sqrt{2}} \left( \nu_n - \frac{2}{d} \right).
\]

We also consider the Ardehali inequality [23], which is another multi-partite Bell inequality. The exactly same argument may be applied for Ardehali inequality in [3], to see that the hyperplane determining the violation of Ardehali inequality is a translation of $H_M$. In this case, we also see that this hyperplane meets the interior of $B_n$ when and only when $n \geq 4$.

3. Volume

We note that the whole $n$-qubit GHZ diagonal states are trisected by the following three parts:
- $G_n \setminus B_n$: genuine entanglement,
- $B_n \setminus F_n$: biseparable but not fully biseparable states,
- $F_n$: fully biseparable states.

We first compute precise volumes for the above parts with respect to the Hilbert Schmidt norm. We note that there are lots of estimates for the volumes of separable states in various situations in the literature. See [24–30] for examples.

When two convex sets $C_1$ and $C_2$ with a common point are perpendicular to each other, we denote by $C_1 \oplus C_2$ the convex hull of them. Since they are perpendicular, the common point is unique. When $\Delta_p$ is the regular $p$ simplex with the side length $\ell$ and $C$ is a $q$-dimensional convex body with volume $V_0$, we will compute the volume $V_p$ of the convex set $\Delta_p \oplus C$.

When $p = 1$, the volume $V_1$ of $\Delta_1 \oplus C$ is given by $V_1 = \frac{1}{1+q} \cdot \ell \cdot V_0$. We also note that $\Delta_p = [h_p \Delta_1] \oplus \Delta_{p-1}$, where $h_p = \frac{1}{\sqrt{2}} \sqrt{\frac{p+1}{p}}$ is the ‘height’ of the $p$ simplex with the unit side length. We translate $C$ so that it meets $\Delta_{p-1}$. Since $\Delta_p$ and $C$ are perpendicular, the volume $V_p$ does not change. Therefore, we have the following inductive formula

\[
V_p = \text{vol} \left( [h_p \Delta_1] \oplus (\Delta_{p-1} \oplus C) \right) = \frac{1}{p+q} \cdot h_p \cdot \ell \cdot V_{p-1},
\]
from which we have

$$\text{vol} (\Delta_p \Theta C') = \frac{q! \sqrt{p+1}}{(p+q)!} \cdot \left( \frac{\ell}{\sqrt{2}} \right)^p \cdot \text{vol} (C').$$

With this formula, we have the following volumes:

$$\text{vol} (G_n) = \frac{\sqrt{d}}{(d-1)!},$$

$$\text{vol} (F_n) = \text{vol} (F^d_n \Theta F^c_n) = \frac{(d/2)! \sqrt{d}}{(d-1)!} \left( \frac{2}{d} \right)^{d/2}.$$

Because $G_n \setminus B_n$ consists of $d$ pieces of simplices with the side length $1/ \sqrt{2}$, we also have

$$\text{vol} (G_n \setminus B_n) = d \cdot \left( \frac{1}{2} \right)^{d-1} \cdot \text{vol} (G_n) = \frac{(d/2)!}{(d/2)^{d/2}}.$$

Therefore, we have the following relative volumes with respect to the whole simplex $G_n$:

$$\frac{\text{vol} (G_n \setminus B_n)}{\text{vol} (G_n)} = \frac{d \cdot (1/2)^{d-1}}{(d-1)!}, \quad \frac{\text{vol} (F_n)}{\text{vol} (G_n)} = \frac{(d/2)!}{(d/2)^{d/2}}.$$

Both of them tend to zero, as the number of qubits tends to infinity.

The volume radius of a set $X$ is given by the radius of a Euclidean ball whose volume is same as that of $X$, as it was introduced in [25]. For subsets $X = G_n \setminus B_n, B_n \setminus F_n$ and $F_n$ of $G_n$, we will consider the relative volume radius $r_{vr}(X) := \left( \frac{\text{vol} (X)}{\text{vol} (G_n)} \right)_{\text{min}}$ with respect to the whole simplex $G_n$. We have

$$r_{vr}(G_n \setminus B_n) = \frac{1}{2} d^{1/(d-1)},$$

$$r_{vr}(B_n \setminus F_n) = \left( 1 - \frac{d}{2^{d-1}} - \frac{(d/2)!}{(d/2)^{d/2}} \right)^{1/(d-1)},$$

$$r_{vr}(F_n) = \left( \frac{(d/2)!}{(d/2)^{d/2}} \right)^{1/(d-1)},$$

and they approach $\frac{1}{2}, \frac{1}{\sqrt{2}}, \frac{1}{\sqrt{d}}$, respectively, as $n \to \infty$. The last follows from

$$\frac{1}{d-1} \log \frac{(d/2)!}{(d/2)^{d/2}} = \frac{1}{d-1} \sum_{k=1}^{d/2} \log \frac{k}{d/2} \to \frac{1}{2} \int_0^1 \log x \, dx = -\frac{1}{2}.$$

Now, we also consider the largest balls inside the polytopes $G_n, B_n$ and $F_n$. The largest ball inside density matrices, separable states and biseparable states have been considered by several authors [31–37]. For a given fixed state $\varrho_p$ in $G_n$, the radius $r_p$ of the largest ball inside $G_n$ around $\varrho_p$ is given by the minimum distance from $\varrho_p$ to facets. The distance from $\varrho_p$ to the facet $G^i_n$ can be obtained by the distance to the linear manifold given by $\sum_j p_j = 1$ and $p_i = 0$. Using the Lagrange method, the distance is given by $p_i \sqrt{d/(d-1)}$ whose minimum over $i \in I_n$ is just $r_p$. Therefore, the maximum of $r_p$ occurs when $p$ is the uniform distribution, and so we conclude that the largest ball inside $G_n$ is centered at the maximally mixed state.
and the radius is given by $\sqrt{1/d(d-1)}$ which is the distance between $c$ and $c^i$ in figure 1. This number was shown in [31] to be the radius of the largest ball in the density matrices. Our result shows that the maximum radius also occurs within GHZ diagonal states. The exactly same argument shows that the largest ball inside the polytope $B_n$ coincides with the largest ball inside $G_n$. In order to find the largest ball inside the polytope $F_n$, we first compute the distance from a state $\psi_p$ to the facet $F_{i,j}^n$, the linear manifold given by $\sum_k \rho_k = 1$ and (7). If $j \in \{i, \bar{i}\}$ then the distance is given by $\sqrt{d/(d-1)}$ as before. Otherwise, we use the Lagrange method again to get the distance $\frac{1}{2}|\psi_i + \psi_j - \psi_1|\sqrt{d/(d-1)}$. From this, we conclude that the largest ball inside $F_n$ coincides again with the largest ball inside the whole simplex $G_n$.

Finally, we consider the convex set $M_n$ of all $n$-qubit GHZ diagonal states which violate the Mermin inequality. Because the hyperplane $H_M$ meet edges at the points in (8), we see that the volume of $M_n$ is given by

$$\text{vol}(M_n) = \text{vol}(G_n) \times \left(1 - \nu_n\right)^{d-2} \times \frac{(1 - \nu_n)^{d-1} \sqrt{d}}{2(d-1)!}.$$ 

Note that the relative volume

$$\frac{\text{vol}(M_n)}{\text{vol}(G_n)} = \frac{(1 - \nu_n)^{d-1}}{2}$$

converges to zero, even though the vertices $w_i$ of $M_n$ converge to $v_i$ for $i \neq 0, 1$ and to $m_{0,1}$ for $i = 1$. We see that the relative volume radius $\text{rvr}(M_n) = \frac{1}{2}(1 - \nu_n)$ converges to 1 as $n \to \infty$.

4. Conclusion

In this paper, we have explored polytope structures for genuine entanglement, biseparability, full biseparability and Bell inequality of multi-qubit GHZ diagonal states. Through the discussion, we may visualize which parts of the simplices of all GHZ diagonal states represent genuine entanglement, PPT states and those violating multipartite Bell inequality, respectively. With these pictures, we have computed precise volume related values and their asymptotic behaviors for genuine entanglement, biseparability, full biseparability or equivalently PPT, and violating Bell inequality. All of them look reasonable, but we could not explain why $\lim_{n \to \infty} \text{rvr}(F_n)$ is given by the number $\sqrt{2}$. We also have seen that the largest balls inside three polytopes coincide. This means that the largest balls do not explain the relative volumes in case of GHZ diagonal states. It would be nice to compute the precise volume of the convex set consisting of fully separable GHZ diagonal states. But this job must be much more involved, because fully separable GHZ diagonal states do not make a polytope anymore. See [38, 39].

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Data availability statement

No new data were created or analysed in this study.

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