A hierarchy of entanglement criteria for four-qubit symmetric Greenberger–Horne–Zeilinger diagonal states

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Abstract
With a two-step method of optimizing entanglement witness, we propose a set of necessary and sufficient entanglement criteria for four-qubit symmetric Greenberger–Horne–Zeilinger (GHZ) diagonal states. The criterion set contains four criteria. Two of them are linear with density matrix elements. The other two criteria are nonlinear with density matrix elements. The criterion set has a nest structure. A proper subset of the criteria is necessary and sufficient for entanglement of the corresponding subset of states. We illustrate the nest structure of criterion set with highly symmetric GHZ diagonal state set, its subset the general Werner state set and its superset the symmetric GHZ diagonal state set.

Keywords GHZ diagonal state · Entanglement criterion · Entanglement witness

1 Introduction
Entanglement plays a central role in quantum computation, quantum simulation and multipartite quantum communication. However, determining whether a given quantum state is entangled or not is by no means easy in both theory and experiment. Many criteria had been developed to detect entanglement [1–8]; see Ref. [9] and [10] for overviews. A solution to the entanglement detection problem, known as entanglement witnessing, relies on the geometry of the set of all separable quantum states [2,10]. The method of entanglement witness (EW) can easily be extended to multipartite cases [11]. Recent developments of the entanglement witness-based criteria are entanglement witness for continuous variable system [12], ultrafine entanglement witness [13], entanglement witness game [14] and separability eigenvalue equation [15]. In principle, there exists extremal EW [15] such that entanglement criteria are
necessary and sufficient. Practically, finding a solution to the separability eigenvalue equation is still very difficult in multipartite scenario. Hence the aim of optimal detecting entanglement in a multipartite system is not easily reached in general. The proper starting point for such an aim is to investigate the states that are diagonal in GHZ basis [16]. GHZ diagonal states as special multipartite quantum states arise frequently in quantum information processing. GHZ diagonal states are tractable in many theoretical problems such as quantum channel capacity [17]. Most of multipartite entangled states prepared in experiments are GHZ states. Recently, there are experiments on four-qubit GHZ states: Long-lived four-qubit GHZ states are realized [18], and test of irreducible four-qubit GHZ paradox has been produced [19]. When imperfections in the preparation and decays are considered, the states prepared are usually GHZ diagonal states. The relationship of positive partial transpose (PPT) criterion and full separability of GHZ diagonal states had been studied [16] and a simple condition had been given. When the condition is not fulfilled, the border of full separability and entanglement may not be uncovered by PPT criterion. Then a complicated EW would be devised to detect the border. For three-qubit GHZ diagonal states, the EW has been found [20–22]; hence, the necessary and sufficient criterion of full separability has been known. For the four-qubit GHZ diagonal states, the tripartite separability has been investigated [23], and the full separability criterion had known for GHZ state mixed with white noise [24,25] (also known as generalized Werner state [26]). We may put the criterion in a criterion set $C_1$. Let the set of all the generalized Werner states to be the state set $S_1$. Then the criterion set $C_1$ is necessary and sufficient for the full separability of the state set $S_1$.

To detect the (multipartite) entanglement of multi-qubit systems (state set $S_N$), we should consider a hierarchy of state sets. The sets can be graph diagonal state set $S_5$, GHZ diagonal state set $S_4$, symmetric GHZ diagonal state set $S_3$, highly symmetric GHZ diagonal state set $S_2$ and generalized Werner state set $S_1$. For a four-qubit system, we will build the criterion set $C_3$ which is necessary and sufficient for state set $S_3$ and it is a pretty good necessary criterion set for larger state set $S_j$ with $j \geq 4$. We will show that $C_1 \subset C_2 \subset C_3$ for the state set inclusion relations $S_1 \subset S_2 \subset S_3$.

We use a two-step procedure of finding the proper EW for a given four-qubit GHZ state. The first step is to make the EW optimal in order to obtain necessary criterion of full separability; we will illustrate it in Sect. 2. The second step is to match the optimal EW with the state under investigation in order to obtain sufficient criterion of full separability; we will illustrate it in Sect. 3. Sections 4 and 5 are devoted to state sets $S_2$, $S_3$ and their necessary and sufficient criterion sets $C_2$, $C_3$, respectively. We discuss the relationship of PPT criterion and our criteria in Sect. 6 and conclude in Sect. 7.

**2 Optimal entanglement witness**

Suppose there is a composed Hilbert space $\mathcal{H} = \mathcal{H}_1 \otimes \cdots \otimes \mathcal{H}_n$. A quantum state $\sigma$ is called fully separable (hereafter abbreviated as ‘separable’ sometimes), if it can be written as a probability mixture of product states [27]:

\[ \sigma = \sum_i p_i \rho_i, \]

where $\rho_i$ are product states.
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\[ \sigma = \sum_i q_i |\psi_1^{(i)}\rangle \langle \psi_1^{(i)}| \otimes \cdots \otimes |\psi_n^{(i)}\rangle \langle \psi_n^{(i)}|, \]  
(1)

with \( q_i \) being a probability distribution and \( |\psi_j^{(i)}\rangle \) being a pure state in the Hilbert space \( \mathcal{H}_j \). A quantum state is entangled if it can be written as (1).

A four-qubit GHZ diagonal state takes the form

\[ \rho = \sum_{j=1}^{16} p_j |\text{GHZ}_j\rangle \langle \text{GHZ}_j|, \]  
(2)

where \( p_j \) is a probability distribution. The GHZ state basis consists of sixteen vectors \( |\text{GHZ}_j\rangle = \frac{1}{\sqrt{2}}(|0x_2x_3x_4\rangle \pm |1\overline{x}_2\overline{x}_3\overline{x}_4\rangle) \), with \( x_i, \overline{x}_i \in \{0, 1\} \) and \( x_i \neq \overline{x}_i \). In the binary notation, \( j - 1 = 0x_2x_3x_4 \) for the ‘+’ states and \( j - 1 = 1\overline{x}_2\overline{x}_3\overline{x}_4 \) for the ‘-’ states.

A four-qubit symmetric GHZ diagonal state takes the form

\[ \rho = p_1 |\text{GHZ}_1\rangle \langle \text{GHZ}_1| + p_2 \sum_{j=2,3,5,8} |\text{GHZ}_j\rangle \langle \text{GHZ}_j| + p_{16} |\text{GHZ}_{16}\rangle \langle \text{GHZ}_{16}| + p_{15} \sum_{j=9,12,14,15} |\text{GHZ}_j\rangle \langle \text{GHZ}_j| 
+ p_4 \sum_{j=4,6,7} |\text{GHZ}_j\rangle \langle \text{GHZ}_j| + p_{13} \sum_{j=10,11,13} |\text{GHZ}_j\rangle \langle \text{GHZ}_j|, \]

with \( p_i \geq 0 \) and normalization

\[ p_1 + p_{16} + 4(p_2 + p_{15}) + 3(p_4 + p_{13}) = 1. \]  
(3)

A four-qubit highly symmetric GHZ diagonal state investigated in this paper takes the form

\[ \rho = p_1 |\text{GHZ}_1\rangle \langle \text{GHZ}_1| + p_{16} |\text{GHZ}_{16}\rangle \langle \text{GHZ}_{16}| 
+ p_2 \sum_{j=2}^{8} |\text{GHZ}_j\rangle \langle \text{GHZ}_j| + p_{15} \sum_{j=9}^{15} |\text{GHZ}_j\rangle \langle \text{GHZ}_j| \]  
(4)

is a special symmetric GHZ diagonal state with \( p_i \geq 0 \) and normalization

\[ p_1 + p_{16} + 7(p_2 + p_{15}) = 1. \]  
(5)

A generalized Werner state [26]

\[ \rho_W = p |\text{GHZ}\rangle \langle \text{GHZ}| + \frac{1-p}{16} \mathbb{I} \]  
(6)
Fig. 1 Regions in \(xy\) plane for the maximal mean \(\tilde{g}\) in \(xy\) plane, here \(x = \frac{M_8}{M_9}, y = \frac{M_{15}}{M_9}\). \(\Delta\) is bounded by two straight-line sections and two curve sections. The two line sections are 
\[x = 3, y \in [-3, 3] \text{ and } \]
\[y = 3, x \in [-3, 3], \text{ respectively.} \]
The two curve sections are 
\[y = 3 + \frac{1}{2} \left( \frac{9}{2} x \right), x \in [-3, -1] \]
\[\text{and } x = 3 + \frac{1}{2} \left( \frac{9}{2} y \right), \]
y \(\in [-3, -1], \text{ respectively.} \)

is a special highly symmetric GHZ diagonal state, with \(|\text{GHZ}\rangle = |\text{GHZ}_1\rangle\) and \(I\) being the identity matrix.

EW is a Hermitian operator \(\hat{\omega}\) such that \(Tr \rho_3 \hat{\omega} \geq 0\) for all separable state \(\rho_3\) and \(Tr \rho \hat{\omega} < 0\) for at least one entangled state \(\rho\). We may assume \(\hat{\omega} = \Lambda I - \hat{M}\), where 
\[
\Lambda = \max_{\rho_3} Tr \rho_3 \hat{M} \text{ such that } \hat{\omega} \text{ is an optimal EW}. \]
(The equality in \(Tr \rho_3 \hat{\omega} \geq 0\) can be reached.) We may express the multi-qubit state and the EW with their characteristic functions. Correspondingly, the operator \(\hat{M}\) is characterized by real parameters \(M_i\) \((i = 1, \ldots, 2^n - 1)\) in detecting the entanglement of a \(n\)-qubit state. Here the number of parameters \(M_i\) is equal to the number of free real parameters for describing the density matrix. One of the widely used numeric methods of finding a proper EW resorts to semi-definite programming. The procedure of analytically finding a precise EW is divided into two steps. The first step is to find \(\Lambda\) for the given \(M_i\). Notice that any operator \(\hat{M}\) corresponds to a valid EW if \(\Lambda\) is obtained. Hence the first step gives a valid necessary criterion of separability. The second step is to adjust the parameters \(M_i\) such that the EW detects all the entanglement. The parameters \(M_i\) should match to the state under consideration, so the second step gives the sufficient criterion of separability.

The two steps of finding entanglement criterion are just the two kinds of optimizations. The first step is the maximization to obtain \(\Lambda\) (thus optimal EW) for a given set of parameters \(M_i\). The second step is to optimize with respect to \(M_i\) such that the criterion is tight.

Let \(\hat{M}\) be a Hermitian operator which is a linear combination of the tensor products of Pauli operators appearing in the four-qubit GHZ diagonal states, namely

\[
\hat{M} = M_1 IZZ + M_2 IIZ + M_3 IZZ + M_4 ZIZ
+ M_5 ZIZ + M_6 ZII + M_7 ZZZ
+ M_8 XXZ + M_9 XYY + M_{10} YYX
+ M_{11} YYYY + M_{12} XYY + M_{13} YXY
+ M_{14} YYX + M_{15} YYY,
\] (7)
where $X, Y$ and $Z$ are Pauli matrices, $I$ is the $2 \times 2$ identity matrix and $M_i$ are parameters mentioned above.

The mean of the operator $\hat{M}$ on the pure product state $|\psi\rangle = |\psi_1\rangle|\psi_2\rangle|\psi_3\rangle|\psi_4\rangle$ is $\langle \psi | \hat{M} | \psi \rangle$. Where $|\psi_j\rangle$ is a pure state of the $jth$ qubit, we parameterize it with angles $\theta_j, \varphi_j$, namely $|\psi_j\rangle = \cos \frac{\theta_j}{2}|0\rangle + \sin \frac{\theta_j}{2}e^{i\varphi_j}|1\rangle$. We may alternatively denote the mean as $\langle \psi | \hat{M} | \psi \rangle = f(\theta, \varphi)$, where

$$f(\theta, \varphi) = M_1z_3z_4 + M_2z_2z_4 + M_3z_2z_3 + M_4z_1z_4$$
$$M_5z_1z_3 + M_6z_1z_2 + M_7z_1z_2z_3z_4 + g(\varphi)t_1t_2t_3t_4$$

with $z_j = \cos \theta_j, t_j = \sin \theta_j$ and $\theta = (\theta_1, \theta_2, \theta_3, \theta_4), \varphi = (\varphi_1, \varphi_2, \varphi_3, \varphi_4)$. The function $g(\varphi)$ is defined as

$$g(\varphi) = M_{8c_1c_2c_3c_4} + M_{9c_1c_2s_3s_4} + M_{10c_1s_2c_3s_4}$$
$$+ M_{11c_1s_2s_3s_4} + M_{12s_1c_2s_3s_4} + M_{13s_1c_2s_3s_4}$$
$$+ M_{14s_1s_2c_3s_4} + M_{15s_1s_2s_3s_4}$$

with $c_j = \cos \varphi_j, s_j = \sin \varphi_j$. The maximization of the mean of operator $\hat{M}$ with respect to product states is transformed to the maximization of function $f(\theta, \varphi)$ with respect to the angles $\theta_j, \varphi_j (j = 1, \ldots, 4)$. We can see that the maximization on $\varphi_j$ is independent of the maximization on $\theta_j$. The structure of the density matrix of GHZ diagonal states is ‘$X$’ type. The density matrix contains diagonal and anti-diagonal entries, and all the other entries are zeros. In computational basis, the operator $\hat{M}$ can also be expressed as a matrix containing diagonal and anti-diagonal entries and all the other entries are zeros. The function $g(\varphi)$ is responsible for the property of anti-diagonal part of $\hat{M}$.

Denote $\tilde{g} = \max_{\varphi} g(\varphi)$. Two of the angles can be removed by obvious optimization of triangle function. After some algebra, we have $\tilde{g} = \max_{\varphi_+, \varphi_-} g_1(\varphi_+, \varphi_-)$, with $\varphi_\pm = \varphi_1 \pm \varphi_2$, and

$$g_1(\varphi_+, \varphi_-) = \sqrt{(A_1c_+ + A_3c_-)^2 + (A_5s_+ - A_7s_-)^2}$$
$$+ \sqrt{(A_2c_+ + A_4c_-)^2 + (A_6s_+ - A_8s_-)^2}$$

with $(A_1, A_2, A_3, A_4) = \frac{1}{2}(M_8, -M_9, -M_{14}, M_{15})H$, $(A_5, A_6, A_7, A_8) = \frac{1}{2}(M_{10}, M_{11}, M_{12}, M_{13})H$, $c_\pm = \cos \varphi_\pm, s_\pm = \sin \varphi_\pm$, where $H$ is the $4 \times 4$ Hadamard matrix.

For general parameters $M_i (i = 8, \ldots, 15)$, it is not obvious how to remove $\varphi_j$ from (10) by maximization. Based on the symmetric consideration, we assume

$$M_9 = M_{10} = M_{11} = M_{12} = M_{13} = M_{14}.$$  \hfill (11)

Although the assumption may limit the entanglement detecting power of the optimal EW derived from operator $\hat{M}$, it greatly simplifies the analysis. Assumption (11) on the parameters $M_i$ simplifies $g_1(\varphi_+, \varphi_-)$ to...
\[ g_1 = \sqrt{(A_1c_+ + A_2c_-)^2 + (A_5s_+)^2 + |A_2c_+ + A_4c_-|}. \]

It is not difficult to show that the second derivative of \( g_1 \) with respect to \( c_- \) is always nonnegative. Hence we have

\[
    g_2(\varphi_+) = \max_{c_-} g_1(\varphi_+, \varphi_-) = \max\{g_1|_{c_-=+1}, g_1|_{c_-=-1}\} \\
    = \sqrt{(A_1c_+ + A_2)^2 + (A_5s_+)^2 + |A_2c_+ + A_4|}. \tag{12}
\]

In the last equality, we have merged the \( c_- = \pm 1 \) cases into the sign of \( c_+ \). Thus \( \tilde{g} = \max_{\varphi_+} g_2(\varphi_+) \). The maximization over \( \varphi_+ \) can be carried out and we at last have

\[
    \tilde{g} = \begin{cases} 
    \text{sign}(M_9) \frac{9M_9^2-M_8M_15}{6M_9-M_8-M_15}, & \text{if } \left( \frac{M_8}{M_9}, \frac{M_15}{M_9} \right) \in \Delta; \\
    \max \left\{ \frac{1}{2}(|M_8+M_9|+|M_8-M_9|), \frac{1}{2}(|M_15+M_9|+|M_15-M_9|) \right\}, & \text{otherwise}
    \end{cases}
\tag{13}
\]

where \( \Delta \) is a region shown in Fig. 1.

Denote \( f_1(\theta) = \max_{\varphi} f(\theta, \varphi) \). By optimizing on \( \theta_4 \) and denoting \( f_2(\theta_1, \theta_2, \theta_3) = \max_{\theta_4} f_1(\theta) \), we then have

\[
    f_2(\theta_1, \theta_2, \theta_3) = M_6z_1z_2 + M_5z_1z_3 + M_3z_2z_3 \\
    + \sqrt{[M_4z_1 + M_2z_2 + M_1z_3 + M_7z_1z_2z_3]^2 + (\tilde{g}t_1t_2t_3)^2}. \tag{14}
\]

The maximal mean of the operator \( \hat{M} \) over all product states is denoted as

\[
    \Lambda = \max_{\psi}(\psi|\hat{M}||\psi) = \max_{\theta, \varphi} f(\theta, \varphi) = \max_{\theta_1, \theta_2, \theta_3} f_2(\theta_1, \theta_2, \theta_3). \tag{15}
\]

**Proof** For each point \( P_i \), a direct calculation shows that \( \Lambda(P_i) = \tilde{g} \). Notice that \( f_1 \) is linear with respect to the parameters \( M_i, (i = 1, \ldots, 7) \). So inside the polyhedron \( (P_1, P_2, P_3, P_4, P_5, P_6, P_7, P_8) \), we have \( f_1(M_1, M_2, M_3, M_4, M_5, M_6, M_7) = \sum_{i=1}^8 p_i f_1(P_i) \) with some probability distribution \( \{p_i\} \). Then we have \( \Lambda(M_1, M_2, M_3, M_4, M_5, M_6, M_7) \leq \sum_{i=1}^8 p_i \Lambda(P_i) = \tilde{g} \) due to the fact that each \( \Lambda(P_i) \) may be achieved at its own special \( \theta_j \) variables. On the other hand, we get the lower bound of \( \Lambda(M_1, M_2, M_3, M_4, M_5, M_6, M_7) \) by noticing that \( f_2(\theta_1 = \pm \frac{\pi}{2}, \theta_2 = \pm \frac{\pi}{2}, \theta_3 = \pm \frac{\pi}{2}) = \tilde{g} \), so that \( \Lambda(M_1, M_2, M_3, M_4, M_5, M_6, M_7) \geq \tilde{g} \). Thus (15) follows. \( \square \)
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3 Matched entanglement witness and separable criterion

A four-qubit GHZ diagonal state can be written as

\[ \rho = \frac{1}{16} (IIII + R_1 IIZZ + R_2 IZZI + R_3 IZZI + R_4 ZIIZ + R_5 ZIZI + R_6 ZZII + R_7 ZZZZ + R_8 XXXX + R_9 XYYX + R_{10} YXYX + R_{11} YXXX + R_{12} YYYY + R_{13} YXXY + R_{14} YYXX + R_{15} YYYY). \]  

(16)

Then \( \text{Tr} \rho \hat{M} = \sum_{i=1}^{15} M_i R_i \). Let

\[ L = \frac{\Lambda}{\sum_{i=1}^{15} M_i R_i}. \]  

(17)

With the convention of \( \sum_{i=1}^{15} M_i R_i > 0 \), we say the entanglement of \( \rho \) is detected if \( L < 1 \). For all possible optimal EWs, we want to find an EW with the smallest \( L \). We will call it matched EW with respect to the given state \( \rho \). Hence the problem is to minimize \( L \) with respect to \( \hat{M} \).

\[ L_{\text{min}} = \min_{\hat{M}} L. \]  

(18)

3.1 Matching anti-diagonal elements of states

In order to minimize \( L \) with respect to \( M_i \) (i = 1,…,15), we first consider \( \tilde{R} = \max \sum_{i=8,...,15} M_i R_i / \tilde{g} \). Here the anti-diagonal part of state \( \rho \) in (16) is described by \( R_i \) (i = 8,…,15). With assumption (11) and notations \( x = \frac{M_8}{M_9}, y = \frac{M_{15}}{M_9} \), we have \( \tilde{R} = \max_{x,y} \frac{1}{L_g} \), where

\[ L_g = \frac{\tilde{g}}{M_9 (x R_8 + y R_{15} + R'_9)}, \]  

(19)

with \( R'_9 = \sum_{i=9}^{14} R_i \). Suppose \( R'_9 > 0 \) without loss of generality, we may choose \( M_9 > 0 \) to match with the sign of \( R'_9 \). If \( R_8 < 0 \), we consider the region in the left side of Fig. 1 specified by its boundary lines \( A' A'' \), \( D' D'' \) and curve \( A' D' \). In this region, we have \( \tilde{g} = |M_8| = -x |M_9| \), then

\[ L_{g}^{-1} = -R_8 + \frac{y}{|x|} R_{15} + \frac{1}{|x|} R'_9. \]  

(20)

For a given \( y \), the maximum of \( L_{g}^{-1} \) achieves at the region boundary lines \( A' A'' \), \( D' D'' \) and curve \( A' D' \). \( L_{g}^{-1} \) monotonically increases with the decrease of \( |x| \) since
\[ R_9' + yR_{15} > 0. \] (We may choose the sign of \( y \) to be the sign of \( R_{15} \). We omit the case \( R_9' + yR_{15} < 0 \) which gives rise to a local maximum \(-R_8\) for \( \mathcal{L}_g^{-1} \) when \( x \to -\infty \).)

Along with the lines \( A'A'' \) and \( D'D'' \), \( \mathcal{L}_g^{-1} \) monotonically increases with the decrease of \(|x|\). So, we only need to consider the maximization of \( \mathcal{L}_g^{-1} \) on curve \( A'D' \). Similar analyses can be applied to the other regions in Fig. 1 except region \( \Delta_1 \). Thus the region for maximization of \( \mathcal{L}_g^{-1} \) can be reduced to \( \Delta_1 \) including its boundary. In region \( \Delta \), we have

\[
\mathcal{L}_g^{-1} = \frac{(6-x-y)(xR_8 + yR_{15} + R_9')}{9 - xy}. \tag{21}
\]

We consider the change of \( \mathcal{L}_g^{-1} \) on the straight-line connecting point \( C' \) and some point in curve \( A'D' \) or curve \( A'B' \). The equation for such a straight line is \( y = kx + 3(1-k) \). On the line, we have \( \frac{(6-x-y)}{9-xy} = \frac{1+k}{3+kx} \); thus,

\[
\mathcal{L}_g^{-1} = (1+k) \left( \frac{R_8}{k} + R_{15} \right) + \frac{3(1+k)}{3+kx} \left( \frac{R_9'}{k} - \frac{R_8}{k} - kR_{15} \right). \tag{22}
\]

Notice that \( k \geq 0 \) and in the domain \( \Delta \) we can verify that \( 3+kx > 0 \). Hence \( \mathcal{L}_g^{-1} \) maximizes at point \( C' \) when

\[
\frac{R_8}{k} + kR_{15} > \frac{R_9'}{3} \tag{23}
\]

and maximizes at curve \( B'A'D' \) otherwise. A tighter alternative of (23) is

\[
\frac{R_8 R_{15}}{R_9'^2} > \frac{1}{36}. \tag{24}
\]

We further consider the maximization of \( \mathcal{L}_g^{-1} \) on curve \( A'D' \). We have the equation of curve \( A'D' \) to be \( \frac{(6-x-y)}{9-xy} = -\frac{1}{x} \) from (13); hence,

\[
\mathcal{L}_g^{-1} = -R_8 + \frac{1}{2}R_{15} - (3R_{15} + R_9') \frac{1}{x} - \frac{9R_{15}}{2} \frac{1}{x^2}. \tag{25}
\]

So \( \mathcal{L}_g^{-1} \) achieves its maximum in curve \( A'D' \) with \( x = -\frac{9R_{15}}{3R_{15} + R_9'} \) when

\[
\frac{R_{15}}{R_9'} > \frac{1}{6}. \tag{26}
\]

It achieves its maximum at point \( A' \) otherwise. Similarly, \( \mathcal{L}_g^{-1} \) achieves its maximum in curve \( A'B' \) with \( y = -\frac{9R_8}{3R_8 + R_9'} \) when

\[
\frac{R_8}{R_9'} > \frac{1}{6}. \tag{27}
\]
It achieves its maximum at point \( A' \) otherwise. The explicit formula for \( \tilde{R} \) (regardless of the sign of \( R_0' \)) is

\[
\tilde{R} = \begin{cases} 
|R'_0 - R_8 - R_{15}|, & \text{if } \frac{R_8}{R_9} \leq \frac{1}{6}, \frac{R_{15}}{R_9} \leq \frac{1}{6}; \\
\frac{1}{3} R'_9 + R_8 + R_{15}, & \text{if } \frac{R_8 R_{15}}{R_9^2} \geq \frac{1}{36}, \frac{R_8}{R_9} > 0; \frac{R_{15}}{R_9} > 0; \\
|R_{15} - R_8 + \frac{1}{3} R'_9 + \frac{R_9^2}{18 R_8}|, & \text{if } \frac{R_{15}}{R_9} > \frac{1}{6}, \frac{R_8 R_{15}}{R_9^2} < \frac{1}{36}; \\
|R_8 - R_{15} + \frac{1}{3} R'_9 + \frac{R_9^2}{18 R_8}|, & \text{if } \frac{R_8}{R_9} > \frac{1}{6}, \frac{R_8 R_{15}}{R_9^2} < \frac{1}{36}. 
\end{cases}
\] (28)

3.2 Matching diagonal elements of state

The quantity \( \mathcal{L}_{\text{min}} \) defined in (18) is

\[
\mathcal{L}_{\text{min}} = \min_{M_m, m=1,...,7} \frac{\Lambda}{\sum_{m=1}^7 M_m R_m + \tilde{g} \tilde{R}}.
\] (29)

The parameter space \((M_1, M_2, M_3, M_4, M_5, M_6, M_7)/\tilde{g}\) is divided into two parts: One is the outside of polyhedron \((P_1, P_2, P_3, P_4, P_5, P_6, P_7, P_8)\), and the other is the inside of the polyhedron (including the boundary). Suppose the point \((N_1, N_2, N_3, N_4, N_5, N_6, N_7)/\tilde{g}\) be on the boundary of the polyhedron, then

\[
\mathcal{L}_{\text{boundary}} = \left[ \left( \sum_{m=1}^7 N_m R_m \right)/\tilde{g} + \tilde{R} \right]^{-1}.
\] (30)

Notice that the origin is inside the polyhedron since it is the geometrical center of the points \( P_1, \ldots, P_8 \). Let \( \delta > 0 \), then \((M_1, M_2, M_3, M_4, M_5, M_6, M_7)/\tilde{g}^{-1} = (1 + \delta)(N_1, N_2, N_3, N_4, N_5, N_6, N_7)/\tilde{g}^{-1}\) be a point outside the polyhedron in the parameter space, we have \( \Lambda = (1 + \delta)\tilde{g}, \mathcal{L} = \left[ (\sum_{m=1}^7 N_m R_m)/\tilde{g} + \tilde{R} (1 + \delta) \right]^{-1} > \mathcal{L}_{\text{boundary}}. \)

Hence the minimal \( \mathcal{L} \) can only be achieved inside the polyhedron.

Let \((M_1, M_2, M_3, M_4, M_5, M_6, M_7)/\tilde{g}^{-1} = (1 + \delta)(N_1, N_2, N_3, N_4, N_5, N_6, N_7)/\tilde{g}^{-1}\) \((1 \geq \delta \geq 0)\) be a point inside the polyhedron in the parameter space, we have \( \Lambda = \tilde{g} \); thus, \( \mathcal{L} = \left[ (\sum_{m=1}^7 N_m R_m)/\tilde{g} + \tilde{R} \right]^{-1} > \mathcal{L}_{\text{boundary}} \) as far as \( \sum_{m=1}^7 N_m R_m \) is positive. If \( \sum_{m=1}^7 N_m R_m \) is negative, we have \( \mathcal{L} = \tilde{R}^{-1} = \mathcal{L}_{\text{origin}}. \)

Thus the minimal \( \mathcal{L} \) is achieved either on the boundary or on the original point of the parameter space. Notice that \( \mathcal{L}^{-1}_{\text{boundary}} \) is linear with respect to the parameter \((N_1, N_2, N_3, N_4, N_5, N_6, N_7)/\tilde{g}^{-1}\); hence, the maximal of \( \mathcal{L}^{-1}_{\text{boundary}} \) is achieved on one of the extremal points \( P_i, i = 1, \ldots, 8 \). The original point is excluded since a point with nonnegative \( \sum_{m=1}^7 N_m R_m \) always exists on the boundary. In fact, the values of \( \sum_{m=1}^7 N_m R_m \) for points \( P_i, (i = 1, \ldots, 8) \) are \( 1 - 8(\rho_{i,i} + \rho_{17-i,17-i})(i = 1, \ldots, 8) \),
respectively. Then we choose the maximum of $1 - 8(\rho_{i,i} + \rho_{17-i,17-i})$ to minimize $\mathcal{L}_{\text{boundary}}$. Thus

$$\mathcal{L}_{\text{min}} = [1 - 8 \min_i (\rho_{i,i} + \rho_{17-i,17-i}) + \tilde{R}]^{-1}. \quad (31)$$

### 3.3 Separable criteria

The separable criterion is $\mathcal{L}_{\text{min}} \geq 1$. Namely, we have a theorem:

**Theorem 1** The necessary criterion of full separability for a four-qubit state is

$$\min_i (\rho_{i,i} + \rho_{17-i,17-i}) \geq \frac{1}{8} \tilde{R}. \quad (32)$$

Violation of it implies entanglement.

The separable criteria have an operational meaning of comparing the anti-diagonal part of the density matrix (represented by $\tilde{R}$) and the diagonal part of the density matrix (represented the minimal $\rho_{i,i} + \rho_{17-i,17-i}$). A state is necessarily separable when its diagonal part is larger than its anti-diagonal part and it is entangled otherwise.

The simplest separable criterion comes from the first line of (28) and (32). It is

**Criterion I**:

$$|\rho_{1,16}| \leq \frac{1}{2} \min_i (\rho_{i,i} + \rho_{17-i,17-i}); \quad (33)$$

Criterion I is just the criterion for the generalized Werner states. In fact, it is just the positive partial transpose fully separable criterion for four-qubit GHZ diagonal states. We may substitute the second lines of (28) and into (32) to obtain the following criterion.

**Criterion II**:

$$\left| \frac{1}{3} |\rho_{4,13} + \rho_{6,11} + \rho_{7,10}| \right| \leq \Omega, \quad (34)$$

where

$$\Omega = \frac{1}{2} \min_i (\rho_{i,i} + \rho_{17-i,17-i}).$$

The other criteria are

**Criterion III**:

$$|R_{15} - R_8 + \frac{1}{3} R_9' + \frac{R_9^2}{18 R_{15}}| \leq 16 \Omega, \quad (35)$$

and

**Criterion IV**:

$$|R_8 - R_{15} + \frac{1}{3} R_9' + \frac{R_9^2}{18 R_8}| \leq 16 \Omega. \quad (36)$$
Fig. 2 Numeric calculated boundaries of fully separable state set of four-qubit highly symmetric GHZ diagonal states with \( p_{16} = 0 \) (GJHG) and \( p_{16} = 0.3 \) (KLMNK) specified by dots. Theoretical results for the boundaries are displayed with solid lines. The dashed lines are for the theoretical results of \( p_{16} = 0.0625 \).

We have classified the separable criteria into four types for the full separability of four-qubit GHZ diagonal states. We will show that two of them are necessary and sufficient for the full separability of four-qubit (highly) symmetric GHZ diagonal states.

4 Application to highly symmetric GHZ diagonal states

A four-qubit highly symmetric GHZ diagonal state \( \rho \) is the mixture of GHZ basis states with the probabilities: \( \{ p_i, i = 1, \ldots, 16 \} \) and \( p_2 = p_3 = \cdots = p_8; p_9 = p_{10} = \cdots = p_{15} \). The state is symmetric under interchange of any pair of qubits. Hence we get four positive parameters \( p_1, p_2, p_{15}, p_{16} \) with normalization

\[
p_1 + p_{16} + 7(p_2 + p_{15}) = 1. \tag{37}
\]

The nonzero entries of \( \rho \) are

\[
\rho_{1,1} = \rho_{16,16} = \frac{1}{2}(p_1 + p_{16}); \quad \rho_{1,16} = \rho_{16,1} = \frac{1}{2}(p_1 - p_{16}); \quad \rho_{2,2} = \rho_{3,3} = \cdots = \rho_{15,15} = \frac{1}{2}(p_2 + p_{15}); \quad \rho_{2,15} = \rho_{3,14} = \cdots = \rho_{15,2} = \frac{1}{2}(p_2 - p_{15}).
\]

We have numerically calculated the boundaries of separable state sets for above states in the cases of \( p_{16} = 0 \) and \( p_{16} = 0.3 \). We choose \( p_2 \) and \( p_{15} \) as free parameters, and \( p_1 \) is determined by the normalization (37). The boundaries are shown in Fig. 2. The numeric calculation has rounds of three steps: (i) to choose \( M_i \) randomly (ii) to calculate \( \Lambda \) (iii) to record the minimal \( L \).

For the convenience of later uses, we list the relevant \( R_j \) below

\[
R_7 = R_1 = 1 - 8(p_2 + p_{15}), \\
R_8 = 1 - 2p_{16} - 14p_{15}, \\
R_{15} = -R_9 = 1 - 2p_{16} - 8p_2 - 6p_{15},
\]
$R'_9 = 6R_9$, $R'_1 = 6R_1$. We alternatively use parameters $u$, $v$, $\alpha$ for convenience, with $u = 1 - 2p_{16}$, $(p_{15}, p_2) = (\frac{vu}{\alpha}, \frac{(1-v)u}{\alpha})$, $v \in [0, 1]$. Hence

\begin{align*}
R_8 &= u \left(1 - \frac{14v}{\alpha}\right), \\
R_{15} &= u \left(1 - \frac{8 - 2v}{\alpha}\right).
\end{align*}

(38) (39)

### 4.1 Necessary criteria

For our four-qubit highly symmetric GHZ diagonal state $\rho$, we have

$$\Omega = \min(\rho_{1,1}, \rho_{2,2}).$$

Criterion I turns out to be

$$|p_1 - p_{16}| \leq (p_2 + p_{15})$$

(40)

when $p_1 + p_{16} \geq (p_2 + p_{15})$. When $p_1 > p_{16}$, the criterion gives the upper bound of $\alpha$ corresponding to straight-line boundaries $GH$, $PQ$ and $KL$ in Fig. 2, with $\alpha = 8$. We have denoted the intersections of the criteria by points $G$, $H$... in Fig. 2. When $p_1 < p_{16}$, the criterion gives the lower bound of $\alpha$ corresponding to straight-line boundary $MN$ in Fig. 2, with $\alpha = 6$.

Criterion II now is

$$|p_2 - p_{15}| \leq p_1 + p_{16}.$$  

(41)

It is

$$\alpha \geq u(8 - 2v) \quad \text{for} \quad v \leq \frac{1}{2},$$

(42)

$$\alpha \geq u(6 + 2v) \quad \text{for} \quad v \geq \frac{1}{2}.$$  

(43)

Condition (42) accounts for the line boundary $GJ$ in Fig. 2.

Criterion III turns out to be $|p_2 - p_{15}| \leq p_1 + p_{16}$ too.

When $p_1 + p_{16} \geq p_2 + p_{15}$, Criterion IV leads to

$$v \geq \frac{1}{36}[18 - \alpha - \sqrt{(\alpha + 42)(\alpha - 6)}],$$

(44)

$$v \leq \frac{1}{36}[32 - \alpha + \sqrt{(56 - \alpha)(8 - \alpha)}],$$

(45)

with $\alpha \in [6, 8]$. Inequality (44) gives rise to boundary curve $K N$ in Fig. 2, with

$$v_K = 0; \quad \text{for} \quad \alpha = 8; \quad v_N = \frac{1}{3}; \quad \text{for} \quad \alpha = 6.$$  

(46)
Inequality (45) gives rise to boundary curve $LM$ in Fig. 2, with

$$v_M = 1; \quad \alpha = 6; \quad v_L = \frac{2}{3} \quad \text{for} \quad \alpha = 8. \quad (47)$$

The straight line $KL$ then is limited to $v \in [v_K, v_L]$ and the straight line $MN$ is limited to $v \in [v_M, v_L]$. When $p_1 + p_{16} \leq p_2 + p_{15}$, Criterion IV leads to

$$\alpha \geq a_1 + \sqrt{a_1^2 + b_1} \quad \text{for} \quad v \in [v_1, v_2], \quad (48)$$

$$\alpha \geq a_2 - \sqrt{a_2^2 - b_2} \quad \text{for} \quad v \in [v_3, v_4], \quad (49)$$

where $a_1 = 3u + (7 + u)v$, $b_1 = 4u(4 - 37v + 9v^2)$, $a_2 = 4u + (7 - u)v$, $b_2 = 4u(3v + 2)^2$. Here $v_1 = \frac{1}{18}(9 - 4u - \sqrt{(4u + 21)(4u - 3)})$ and $v_4 = \frac{7}{6}(4 - u - \sqrt{(7 - u)(1 - u)})$ are determined by condition $p_1 + p_{16} = p_2 + p_{15}$ (namely $\alpha = 8u$) and the equality in (44) and (45), respectively. $v_2 = \frac{5u + 2}{3(1 + u)}$ and $v_3 = \frac{4 - 3u}{1 + u}$ come from physical boundary condition $p_{16} + p_2 + p_{15} = 1$ (namely $\alpha = \frac{14u}{1 + u}$) and the equality in (48) and (49), respectively.

It happens that the straight line $\alpha = u(6 + 2v)$ and the curve $\alpha = a_2 - \sqrt{a_2^2 - b_2}$ intersect at $(v = v_3, \alpha = \frac{14u}{1 + u})$. We can verify that $a_2 - \sqrt{a_2^2 - b_2} > u(6 + 2v)$ when $v > v_3$. Thus inequality (49) is better than inequality (43) as a separable criterion. We can also show that $a_1 + \sqrt{a_1^2 + b_1} > u(8 - 2v)$; thus, inequality (48) is better than inequality (42) as a separable criterion. We conclude that Criterion II and Criterion III are not useful in determining the separable boundary of four-qubit highly symmetric GHZ diagonal state set. Criterion I and Criterion IV suffice as necessary criterion set for full separability.

When $p_{16} = 0$, inequality (48) turns out to be (42) and inequality (49) leads to

$$\alpha = 4 + 6v, \quad \text{for} \quad v \in \left[\frac{1}{2}, \frac{2}{3}\right]. \quad (50)$$

Equation (50) is just the straight-line boundary $HJ$ in Fig. 2. As a criterion, it is better than inequality (43). The states inside the triangle $GHJ$ are separable due to the convexity of separable state set.

We have shown the boundaries of fully separable states for $p_{16} = 0$ and $p_{16} = 0.3$ in Fig. 2, respectively. The figure for the case of $p_{16} \in (0, \frac{1}{8})$ is quite different. As shown in Fig. 2 for $p_{16} = 0.0625$, the fully separable set has boundary $PQSTUVP$.

Straight line $PQ$ is specified by $\alpha = 8$, $v \in [0, \frac{3}{5}]$. Curve $PV$ ($QS$) is determined by the equality in (44)/(45) until it reaches $\alpha = 8u$ with $v = v_1(v_3)$. Curve $VU$ ($ST$) is determined by the equality in (48)/(49) until it reaches $\alpha = \frac{14u}{1 + u}$ with $v = v_2(v_3)$. Finally the straight-line section $UT$ represents the physical boundary $p_1 = 0$.  

\[ \text{Equation (50) is just the straight-line boundary $HJ$ in Fig. 2. As a criterion, it is better than inequality (43). The states inside the triangle $GHJ$ are separable due to the convexity of separable state set.} \]
4.2 Sufficient criteria

The sufficient condition of separability relies on the ability of decomposing the state into probability mixture of product states. Usually, it is rather technical to write down the decomposition. For the known operator $\hat{M}$, we will find the product state corresponding to its largest mean $\Lambda_1$ and use it to construct the explicit decomposition of a state $\rho$ at the boundary of fully separable state set.

4.2.1 Sufficiency of Criterion I

In the case of Criterion I, we start by setting $M_1 = M_2 = \cdots = M_6 = 0$, $M_7 = 1$, $M_8 = M_{15} = -M_9 = \pm 1$. We thus have the operator $\hat{M} = \sum_{i=1}^4 \pm (XXX - XXYY - XYXY - YXXY - XYYX - YYXX + YYYY).$ The EW is $\mathbb{I} - \hat{M}$. The maximal mean of $\hat{M}$ over product state $|\psi\rangle = \bigotimes_{i=1}^4 |\psi_i\rangle$ is

$$\Lambda = \max_{\Theta, \Phi} \left[ \prod_{i=1}^4 z_i \pm \prod_{i=1}^4 t_i \cos \left( \sum_{j=1}^4 \varphi_j \right) \right].$$

The maximum is known to be 1 which is achieved when (i) $\prod_{i=1}^4 z_i = 1$ or (ii) $\prod_{i=1}^4 t_i = \pm 1$ and $\sum_{j=1}^4 \varphi_j = 0$. Case (i) corresponds to separable states $|0000\rangle, |0011\rangle, |0101\rangle, |1001\rangle, |0110\rangle, |1010\rangle, |1100\rangle, |1111\rangle$. Case (ii) is realized by separable state

$$|\psi(\varphi_1, \varphi_2, \varphi_3)\rangle = \frac{1}{4} \left[ \bigotimes_{j=1}^3 (|0\rangle + e^{i\varphi_j} |1\rangle) \right] \left( |0\rangle \pm e^{-i\sum_{j=1}^3 \varphi_j} |1\rangle \right).$$

In order to construct the GHZ diagonal states, we may expand the product state $|\psi(\varphi_1, \varphi_2, \varphi_3)\rangle$ with products of Pauli matrices. Then we will eliminate the unnecessary terms by the following procedure. Denote $\varrho_1(\varphi_1, \varphi_2, \varphi_3) = |\psi(\varphi_1, \varphi_2, \varphi_3)\rangle\langle \psi(\varphi_1, \varphi_2, \varphi_3)|$. Let $k = (k_1, k_2, k_3) \in \{0, 1\}^3$, denote

$$\varrho_2(\varphi_1, \varphi_2, \varphi_3) = \frac{1}{8} \sum_k \varrho_1(\varphi_1 + k_1\pi, \varphi_2 + k_2\pi, \varphi_3 + k_3\pi)$$

$$\varrho_3(\varphi) = \frac{1}{2} [\varrho_2(\varphi, \varphi, \varphi) + \varrho_2^* (\varphi, \varphi, \varphi)].$$

The density matrix $\varrho_2(\varphi_1, \varphi_2, \varphi_3)$ is already in ‘X’ shape, and all its entries are nullified except diagonal and anti-diagonal entries. The real density matrix $\varrho_3(\varphi)$ is

$$\frac{1}{16} \sum_{\varphi} \left[ \cos 3\varphi \cos^3 \varphi XXX - \sin 3\varphi \sin^3 \varphi YYYY \right.$$  
$$+ \cos 3\varphi \cos \varphi \sin^2 \varphi (XYYX + YYXY + YXXY)$$  
$$- \sin 3\varphi \sin \varphi \cos^2 \varphi (XXYY + XYXY + YXXX) \right].$$
The permutational symmetry of the state requires \( \cos 3\varphi \cos \varphi \sin^2 \varphi = -\sin 3\varphi \sin \varphi \cos^2 \varphi \). It leads to \( \varphi = \frac{i\pi}{4} \), with \( i = 0, \ldots, 7 \). We obtain independent separable states \( \varrho_3(0), \varrho_3(\frac{\pi}{4}), \varrho_3(\frac{\pi}{2}) \). A mixture of these states will give rise to

\[
\varrho_4 = (1 - q_1 - q_2)\varrho_3(0) + q_1\varrho_3\left(\frac{\pi}{4}\right) + q_2\varrho_3\left(\frac{\pi}{2}\right),
\]

where \( 0 \leq q_1, q_2 \leq 1; q_1 + q_2 \leq 1 \). Then a state on line sections \( GH, KL PQ \) in Fig. 2 can be written as

\[
\rho = u\varrho_4 + p_{16}(|0000\rangle\langle0000| + |1111\rangle\langle1111|),
\]

where ‘+’ is chosen from ‘±’ in \( \varrho_3 \) for state \( \varrho_4 \). We then have

\[
R_8 = u\left(1 - \frac{5}{4}q_1 - q_2\right), \quad R_9 = u\left(-\frac{1}{4}q_1\right), \quad R_{15} = u\left(q_2 - \frac{1}{4}q_1\right).
\]

Notice that \( R_{15} = -R_9 \), so \( q_2 = \frac{1}{2}q_1 \). Hence \( q_1 \leq \frac{2}{3} \). Comparing \( R_i \) with their expressions of parameters \((\alpha = 8, v)\), we have \( v = q_1 \),

\[
0 \leq v \leq \frac{2}{3},
\]

for the states on the line sections \( GH \) and \( KL \).

A state on line section \( MN \) in Fig. 2 can be written as

\[
\rho = (1 - 2p_1)\varrho_4 + p_1(|0000\rangle\langle0000| + |1111\rangle\langle1111|),
\]

where ‘−’ is chosen from ‘±’ in \( \varrho_3 \) for state \( \varrho_4 \). We compare \( R_i \) obtained from (55) with their expressions of parameters \((\alpha = 6, v)\). We have \( v = 1 - q_1 \),

\[
\frac{1}{3} \leq v \leq 1,
\]

for the states on the line section \( MN \).

The sufficient conditions for the full separability of the states on straight-line sections \( KL, MN, GH \) are proved. The sufficient conditions of Criterion I coincide with the necessary conditions. So Criterion I is necessary and sufficient for the full separability of states on straight-line sections \( KL, MN, GH \).

The general Werner state is a special highly symmetric GHZ diagonal state, with \( p_2 = \cdots = p_{15} = p_{16} \) and \( p = p_1 - p_2 > 0 \). Criterion I reads \( p \leq \frac{1}{5} \). It is the necessary and sufficient criterion of full separability for the general Werner states [21,25]. Thus the criterion set \( C_1 = \{\text{Criterion I}\} \) is necessary and sufficient for the full separability of the states in the general Werner state set \( \mathcal{S}_1 \).
4.2.2 Sufficiency of Criterion IV

The solutions to the maximization of (12) are $s_+ = 0$ and $c_+ = \frac{A_2}{1-A_1} = \frac{M_8-M_{15}}{6M_9-M_8-M_{15}}$. The latter leads to the first line of (13) for $\tilde{g}$. The corresponding separable state can be written as

$$|\psi(\varphi, m)\rangle = \frac{1}{4} \bigotimes_{j=1}^{4} (|0\rangle + e^{i\varphi_j}|1\rangle),$$

where $m = (m_1, m_2, m_3, m_4) \in \{0, 1\}^{\otimes 4}, \varphi_j = \varphi + m_j \pi$. Let $l = \text{mod} (\sum_j m_j, 2)$ be the parity of $m$. Define $\varrho_{+(-)}(\varphi) = \sum_{m|l=0(1)} |\psi(\varphi, m)\rangle\langle\psi(\varphi, m)|$. Then we have

$$\varrho_{\pm}(\varphi) = \frac{1}{16} [I_{III} \pm (\cos^4 \varphi XX + \sin^4 \varphi YY)
+ \cos^2 \varphi \sin^2 \varphi (XXY + XYX + XYX + YXX)]. \quad (57)$$

Denote

$$\varrho_5^\pm = \frac{1}{1+\sin^2 \varphi} \left( \varrho_{\pm}(\varphi) + \sin^2 \varphi \varrho_{\mp} \left( \frac{\pi}{2} \right) \right).$$

The separable states in the curves $LM$ and $KN$ in Fig. 2 can be expressed as

$$\rho = (1 - R_7)\varrho_5^\mp + \frac{R_7}{2} (|0000\rangle\langle0000| + |1111\rangle\langle1111|), \quad (58)$$

respectively. Hence $R_8 = \mp K \cos^4 \varphi, R_{15} = \pm K \cos^2 \varphi \sin^2 \varphi$ with $K = \frac{1-|R_7|}{1+\sin^2 \varphi} = \frac{8a}{\alpha(1+\sin^2 \varphi)}$. Compare them with Eqs.(38) and (39), we have

$$v = \frac{1}{1+\sin^2 \varphi}, \quad \alpha = \frac{14 - 8 \cos^4 \varphi}{1+\sin^2 \varphi} \quad (59)$$

for curve $LM$ in Fig. 2;

$$v = \frac{\sin^2 \varphi}{1+\sin^2 \varphi}, \quad \alpha = \frac{14 \sin^2 \varphi + 8 \cos^4 \varphi}{1+\sin^2 \varphi} \quad (60)$$

for curve $KN$ in Fig. 2. Here $\sin^2 \varphi = \frac{1}{2}(1 - c_+) = \frac{3M_9-M_8}{6M_9-M_8-M_{15}}$. Notice that Criterion IV is derived along with the curve $A'B'$ in Fig. 1. In curve $A'B'$, we have $\sin^2 \varphi \in [0, \frac{1}{2}]$. The maximal value $\sin^2 \varphi = \frac{1}{2}$ gives rise to the end points $L, N$ of the curves. The minimal value $\sin^2 \varphi = 0$ gives rise to the end points $K, M$ of the curves.
For the situation of \( R_7 < 0 \) (namely \( \alpha < 8u \)) described by \( STUVS \) in Fig. 2, we should have

\[
\rho = (1 + R_1' + R_7)\rho_{5\mp} + \frac{-R_1' - R_7}{2}((|0\rangle \langle 0|)^\otimes 4 + (|1\rangle \langle 1|)^\otimes 4).
\]

(61)

Hence \( R_8 = \mp K \cos^4 \varphi \), \( R_{15} = \pm K \cos^2 \varphi \sin^2 \varphi \) with \( K = \frac{1+6R_1+R_7}{1+\sin^2 \varphi} \). With Eq. (38) and (39), we have the solution pair \( \alpha, v \) as functions of \( K, \varphi \); hence,

\[
\begin{align*}
\alpha &= \frac{7u[1 + \sin^2 \varphi \mp \cos^2 \varphi(8 \sin^2 \varphi - 1)]}{(1 + \sin^2 \varphi)u \mp \cos^2 \varphi(8 \sin^2 \varphi - 1)}, \\
\alpha &= 8 - 2v + 8(2v - 1) \sin^2 \varphi,
\end{align*}
\]

(62)

(63)

where we have used the fact that \( 1 + 6R_1 + R_7 = 1 + 7R_7 = 8(1 - \frac{7u}{\alpha}) \). Instead of expressing \( v \) as a function of \( K, \varphi \), we use \( R_8/R_{15} \) to obtain Eq. (63). For the case of \( p_{16} = 0 \), we have \( u = 1 \) so that \( \alpha \neq 7 \) can only occur when \( 1 + \sin^2 \varphi \mp \cos^2 \varphi(8 \sin^2 \varphi - 1) = 0 \). The solutions are \( \sin^2 \varphi = 0, \frac{1}{2} \), respectively. The equations of line sections \( GJ \) and \( HJ \) in Fig. 2 are obtained from (63) with \( \sin^2 \varphi = 0, \frac{1}{2} \). Hence Criterion IV is also sufficient for states on \( GJ \) and \( HJ \).

For the states in between \( \alpha = 8u \) and the physical limitation \( p_1 = 0(\alpha = \frac{14u}{1+u}) \), the corresponding \( \sin^2 \varphi = \frac{1}{8}(4u - 1 - \sqrt{(4u + 21)(4u - 3)}), \frac{1}{2}, 0, \frac{1}{2}(2 - u - \sqrt{(1 - u)(7 - u)}) \) can be derived for \( v_1, v_2, v_3, v_4 \). Thus Criterion IV is also sufficient condition for the full separability of the states in the curves.

Hence, for the four-qubit highly symmetric GHZ diagonal state set \( S_2 \), the necessary and sufficient criterion set is \( C_2 = \{ \text{Criterion I, Criterion IV} \} \).

### 5 Application to four-qubit symmetric GHZ diagonal states

A GHZ diagonal state is called a symmetric GHZ diagonal state if it is invariant under any qubit permutation. From (16), we have \( R_1 = R_2 = R_3 = R_4 = R_5 = R_6 \), \( R_9 = R_{10} = R_{11} = R_{12} = R_{13} = R_{14} \) for a four-qubit symmetric GHZ diagonal state. Thus the state is specified by \( R_1, R_7, R_8, R_9, R_{15} \). Alternatively, we may use density matrix elements \( \rho_{1,1}, \rho_{1,6}, \rho_{2,2}, \rho_{2,15}, \rho_{4,4}, \rho_{4,13} \) to characterize the state with \( \rho_{i,i} = \rho_{17-i,17-i}, \rho_{i,17-i} = \rho_{17-i,i} \) and

\[
\begin{align*}
\rho_{1,1} &= \frac{1}{16}(1 + 6R_1 + R_7), \\
\rho_{1,6} &= \frac{1}{16}(R_8 - 6R_9 + R_{15}), \\
\rho_{2,2} &= \rho_{3,3} = \rho_{5,5} = \rho_{8,8} = \frac{1}{16}(1 - R_7), \\
\rho_{2,15} &= \rho_{3,14} = \rho_{5,12} = \rho_{8,9} = \frac{1}{16}(R_8 - R_{15}), \\
\rho_{4,4} &= \rho_{6,6} = \rho_{7,7} = \frac{1}{16}(1 - 2R_1 + R_7),
\end{align*}
\]

\( \odot \) Springer
Curved surfaces and the other plane surfaces are the boundaries of fully separable state set. We show the positive $\rho_{2,15}$ in the figure with $\Omega = \frac{1}{16}$. The mirror reflection of the figure with respect to $\rho_{1,16} - \rho_{4,13}$ plane is not shown.

The normalization condition is $\rho_{1,1} + 4 \rho_{2,2} + 3 \rho_{4,4} = \frac{1}{2}$.

Due to Criterion III and Criterion IV, the equations of the curved surfaces detecting entangled states (outside the surfaces, the states are entangled) are

$$\frac{|\rho_{2,15}|}{\Omega} = \frac{1}{2} \left( 1 - \frac{\rho_{4,13}}{\Omega} + \sqrt{\left( 1 + \frac{\rho_{4,13}}{\Omega} \right) \left( 1 + \frac{\rho_{1,16}}{\Omega} \right)} \right)$$  \hspace{1cm} (64)

for $\rho_{1,16} \geq \rho_{4,13}$ and

$$\frac{|\rho_{2,15}|}{\Omega} = \frac{1}{2} \left( 1 + \frac{\rho_{4,13}}{\Omega} + \sqrt{\left( 1 - \frac{\rho_{4,13}}{\Omega} \right) \left( 1 - \frac{\rho_{1,16}}{\Omega} \right)} \right)$$  \hspace{1cm} (65)

for $\rho_{1,16} < \rho_{4,13}$, respectively. $\Omega$ defined previously can be explained as the minimal diagonal element. We show the surfaces in Fig. 3 with $\Omega = \frac{1}{16}$.

If Eqs. (64) and (65) can be achieved by fully separable states, then the sufficiencies of Criterion III and Criterion IV are proved for the four-qubit symmetric GHZ diagonal states. Without loss of generality, we set $\Omega = \frac{1}{16}$. We may construct the fully separable state from (57). Let

$$\rho = \frac{1}{1+\mu} \left[ \rho_+(\varphi) + \mu \rho_-(\frac{\pi}{2}) \right],$$  \hspace{1cm} (66)

with $\mu \geq 0$ and $\cos(2\varphi) \geq 0$. Then $\rho_{1,16} = \frac{1}{16(1+\mu)} [\cos(4\varphi) - \mu]$, $\rho_{2,15} = \frac{1}{16(1+\mu)} [\cos(2\varphi) + \mu]$, $\rho_{4,13} = \frac{1}{16(1+\mu)} (1 - \mu)$. It can be easily checked that Eq. (64) satisfies. Alternatively, if we choose
\[
\rho = \frac{1}{1 + \mu} [\varrho_+ (\varphi) + \mu \varrho_-(0)],
\]
with \(\cos(2\varphi) \leq 0\). We have \(\rho_{1,16} = \frac{1}{16(1+\mu)} [\cos(4\varphi) - \mu]\), \(\rho_{2,15} = \frac{1}{16(1+\mu)} [\cos(2\varphi) - \mu]\), \(\rho_{4,13} = \frac{1}{16(1+\mu)} (1 - \mu)\). Then Eq. (65) satisfies. Similarly, Eq. (64) (or (65)) satisfies by setting \(\rho\) to be the mixture of \(\varrho_-(\varphi)\) and \(\varrho_+ (\frac{\pi}{2})\) (or \(\varrho_+(0)\)). Hence Criterion III and Criterion IV are necessary and sufficient for the full separability of symmetric GHZ diagonal states.

The states in the plane surfaces of Fig. 3 can be composed with fully separable states in the following way. Criterion I gives rise to Eq. (52). It follows the elements of density matrix:

\[
\rho_{1,16} = \Omega; \quad \rho_{4,13} = (1 - 2q_1)\Omega; \quad \rho_{2,15} = (1 - q_1 - 2q_2)\Omega,
\]
with \(\Omega = \frac{4}{15}\). The probability distribution \((q_1, q_2, 1 - q_1 - q_2)\) limits us with \(0 \leq q_2 \leq 1 - q_1\); thus, in the plane \(\rho_{1,16} = \Omega\) we have two straight-line sections \(\rho_{2,15} = \frac{1}{2}(\Omega + \rho_{4,13})\) when \(q_2\) is set to 0 (its lower bound) and \(\rho_{2,15} = -\frac{1}{2}(\Omega + \rho_{4,13})\) when \(q_2\) is set to \(1 - q_1\) (its upper bound). Hence all the states enclosed by the line sections in the plane are separable sufficiently. More precisely, the states in the triangle with vertices \((\Omega, -\Omega, 0), (\Omega, \Omega, \Omega), (\Omega, -\Omega, -\Omega)\) in the three-dimensional coordinate system \((\rho_{1,16}, \rho_{4,13}, \rho_{2,15})\) are separable sufficiently. A state inside the triangle should meet the requirements of \(\rho_{2,15} \leq \frac{1}{2}(\Omega + \rho_{4,13})\) and \(\rho_{2,15} \geq -\frac{1}{2}(\Omega + \rho_{4,13})\), and they are just the conditions \(R_{5/6} \leq 1, R_{15/16} \leq 1\) in (28) for Criterion I. Similarly, the states in the triangle with vertices \((-\Omega, \Omega, 0), (-\Omega, -\Omega, -\Omega), (-\Omega, -\Omega, \Omega)\) in the coordinate system are separable sufficiently. Hence Criterion I is necessary and sufficient for the full separability of symmetric GHZ diagonal states.

The intersection of the curved surface (64) and the plane \(\rho_{4,13} = \Omega\) is a parabola

\[
\frac{\rho_{2,15}}{\Omega} = \sqrt{\frac{1}{2} (1 + \frac{\rho_{1,16}}{\Omega})},
\]
with \(\Omega \geq \rho_{1,16} \geq -\Omega\). The states enclosed by the parabola should meet the requirement of \(\frac{\rho_{2,15}}{\Omega} \leq \sqrt{\frac{1}{2} (1 + \frac{\rho_{1,16}}{\Omega})}\), and it is just the condition \(R_3 R_{15} R_3 \geq 1\) in (28) for Criterion II. In the plane of \(\rho_{3,14} = \Omega\), the states enclosed by parabola (69) can be decomposed as probability mixture of the states on the parabola; thus, they are fully separable due to the full separability of the states on the parabola. Hence Criterion II is necessary and sufficient for the states enclosed by parabola (69) on the plane \(\rho_{3,14} = \Omega\). Similarly we can show that Criterion II is necessary and sufficient for the states enclosed by parabola \(\frac{\rho_{2,15}}{\Omega} = \sqrt{\frac{1}{2} (1 - \frac{\rho_{1,16}}{\Omega})}\) on the plane \(\rho_{3,14} = -\Omega\).

All the boundaries determined by the necessary criteria for the four-qubit symmetric GHZ diagonal states are proved to be also sufficient, since the states on boundaries are proved to be fully separable. Outside the boundaries, the states are entangled.

Hence, for the four-qubit symmetric GHZ diagonal state set \(S_3\), the necessary and sufficient criterion set is \(C_3 = \{\text{Criterion I, Criterion II, Criterion III, Criterion IV}\}\).
6 Discussion

The PPT criterion of separability for the four-qubit GHZ diagonal states is

$$\max_i |\rho_{i,17-i}| \leq \min_j \rho_{j,j},$$  \hspace{1cm} (70)

and the maximal absolute anti-diagonal element does not exceed the minimal diagonal element. This criterion can also be obtained with proper $M_i$ subjecting to $|M_i| = 1$. More explicitly, from (9) we have

$$g(\phi) = \cos(\phi_1 + \phi_2 + \phi_3 + \phi_4) \leq 1,$$  \hspace{1cm} (71)

by setting $M_8 = M_{15} = 1, M_9 = \cdots = M_{14} = -1$. Thus $\tilde{g} = 1$. Notice that $\sum_{i=8}^{15} M_i R_i = 16\rho_{1,16}$. Changing the sign of $\phi_j$ ($j = 1,2,3,4$) leads to different assignment of signs for $M_i$ ($i = 8,\ldots,15$) while keeping $\tilde{g} = 1$. The maximal $\sum_{i=8}^{15} M_i R_i$ is $16 \max |\rho_{i,17-i}|$ ($i = 1,\ldots,16$).

For the four-qubit symmetric GHZ diagonal states, the PPT criterion (70) defines a cube. The surface of cube coincides with the some parts of border surface between separable and entangled states.

For GHZ diagonal states, there is a sufficient condition for the coincidence of the PPT criterion and the full separability criterion [16]. The condition can be written as

$$R_9 R_{15} \leq 0 \text{ and } R_9 R_8 \leq 0.$$  \hspace{1cm} (72)

The border states in the planes $\rho_{4,13} = -\Omega$ and $\rho_{4,13} = \Omega$ do not satisfy the condition (72). On plane surfaces $\rho_{1,16} = \pm \Omega$, the border states form two triangles. Only some of these states satisfy the condition (72), and they form two less size triangles.

7 Conclusion

We have found that the set of necessary and sufficient criteria of separability has a subset structure. The smallest criterion set $C_1$ has one criterion (Criterion I), and it can detect the full separability of the generalized Werner state (GHZ state mixed with white noise or identity) set $S_1$ necessarily and sufficiently. The state set $S_2$ is the set of four-qubit highly symmetric GHZ diagonal states. It includes $S_1$ as its subset. We have found the criterion set $C_2$ with two criteria (Criterion I and Criterion IV) which can detect the full separability of states in $S_2$. The criterion set $C_1$ is a subset of $C_2$. Criterion set $C_3$ has four criteria: Criterion I, Criterion II, Criterion III and Criterion IV. Criterion set $C_3$ is necessary and sufficient for the state set $S_3$ of four-qubit symmetric GHZ diagonal states. We have necessary and sufficient criterion set $C_i$ for state set $S_i$ for $i = 1, 2, 3$, with $C_2$ being the subset of $C_3$ and the superset of $C_1$, $S_2$ being the subset of $S_3$ and the superset of $S_1$. The nest structure of the criterion set suggests us a way of developing criterion set for large state set from some seed state set.

We have used the two-step optimizations to analytically obtain $C_3$ when the state is a four-qubit symmetric GHZ diagonal state. We proved the sufficiency of $C_3$ for these
symmetric states by explicitly constructing these states with fully separable states. All boundaries of the fully separable state set of four-qubit symmetric GHZ diagonal states have been found by the criteria.

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