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Separability criteria for genuine multiparticle entanglement

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Abstract. We present a method to derive separability criteria for different classes of multiparticle entanglement, especially genuine multiparticle entanglement. The resulting criteria are necessary and sufficient for certain families of states. This, for example, completely solves the problem of classifying $N$-qubit Greenberger–Horne–Zeilinger states mixed with white noise according to their separability and entanglement properties. Further, the criteria are superior to all known entanglement criteria for many other families; also they allow the detection of bound entanglement. We next demonstrate that they are easily implementable in experiments and discuss applications to the decoherence of multiparticle entangled states.
1. Introduction

Entanglement is relevant for many effects in quantum optics or condensed matter physics and its characterization is of eminent importance for studies in quantum information processing [1, 2]. Concerning entanglement between two particles, many questions are still open, but there exist at least various criteria that can be used to test whether a given quantum state is entangled or separable. For more than two particles, however, the situation is significantly more complicated, as several inequivalent classes of multiparticle entanglement exist and it is difficult to decide to which class a given state belongs. Entanglement witnesses and Bell inequalities can sometimes distinguish between the different classes [2, 3]. However, it would be desirable to have useful criteria that allow us to detect the different classes of multiparticle entanglement directly from a given density matrix; a general method to derive such criteria is missing [4].

In this paper, we present such a systematic way to develop multiparticle entanglement criteria. The resulting criteria solve the separability problem for certain families of states (notably the well-studied N-qubit Greenberger–Horne–Zeilinger (GHZ) states mixed with white noise) and improve known results in many other cases. Also, they allow us to detect bound entangled states that are separable under each partition, but not fully separable. Moreover, our criteria can easily be used in today’s experiments and they improve the understanding of decoherence in multiparticle quantum systems.

Let us recall the main definitions for multipartite entanglement. For three particles, a pure state is fully separable if it is of the form \(|\psi^{fs}\rangle = |a\rangle|b\rangle|c\rangle\) and a mixed state is fully separable if it can be written as a convex combination of fully separable pure states

\[
\rho^{fs} = \sum_k p_k |\psi_k^{fs}\rangle \langle \psi_k^{fs}| ,
\]

where the \(p_k\) forms a probability distribution. A pure state is called biseparable if it is separable under some bipartition. An example is \(|\psi^{bs}\rangle = |a\rangle|\phi^{bc}\rangle\), where \(|\phi^{bc}\rangle\) is a possibly entangled state on particles \(B\) and \(C\). This state is biseparable under the \(A|BC\)-partition; other bipartitions are the \(B|AC\)- or \(C|AB\)-partition. A mixed state is biseparable if it can be written as \(\rho^{bs} = \sum_k p_k |\psi_k^{bs}\rangle \langle \psi_k^{bs}|\), where \(|\psi_k^{bs}\rangle\) might be biseparable under different partitions. Finally, a state is genuinely multipartite entangled if it is not biseparable. This class of entanglement one usually aims to generate and verify in experiments\(^5\) and we mainly consider entanglement criteria for

\(^5\) For a justification, see section 3.2.2 in [2].
this type of entanglement. Note that generalizations and further classifications can be found, e.g., in [2], [5]–[7].

2. Three qubits

We explain our main ideas using three qubits; the generalization to more particles (or higher dimensions) is straightforward and will be discussed later. For a three-qubit density matrix \( \rho \) we denote its entries by \( \rho_{i,j} \), where \( 1 \leq i, j \leq 8 \); here and in the following, we always use the standard product basis \([|000\rangle, |001\rangle, \ldots, |111\rangle]\). Then we have:

**Observation 1.** Let \( \rho \) be a biseparable three-qubit state. Then its matrix entries fulfill

\[
|\rho_{1,8}| \leq \sqrt{|\rho_{2,2}\rho_{7,7}|} + \sqrt{|\rho_{3,3}\rho_{6,6}|} + \sqrt{|\rho_{4,4}\rho_{5,5}|}
\]

and violation implies genuine three-qubit entanglement.

**Proof.** First, note that for two positive linear functions \( f(x) \) and \( g(x) \) the function \( h = \sqrt{fg} \) is concave, that is, \( h(rx_1 + (1-r)x_2) \geq rh(x_1) + (1-r)h(x_2) \) for any mixing ratio \( r \).\(^6\)

Consequently, the function \( \sqrt{|\rho_{2,2}\rho_{7,7}|} + \sqrt{|\rho_{3,3}\rho_{6,6}|} + \sqrt{|\rho_{4,4}\rho_{5,5}|} - |\rho_{1,8}| \) is concave in the state, because it is a sum of concave functions of the matrix entries (the absolute value is convex). So it suffices to prove its positivity for pure biseparable states; then mixtures of these will inherit the bound. Let \( |\psi\rangle = (a_0|0\rangle + a_1|1\rangle) \otimes (b_0|0\rangle + b_1|1\rangle) \) be a pure state, which is biseparable under the \( A|BC \) partition. For that, one can directly see that \( |\rho_{1,8}| = \sqrt{|\rho_{4,4}\rho_{5,5}|} \). For the other two bipartitions one finds \( |\rho_{1,8}| = \sqrt{|\rho_{3,3}\rho_{6,6}|} \) and \( |\rho_{1,8}| = \sqrt{|\rho_{2,2}\rho_{7,7}|} \); hence, equation (2) is valid for any pure biseparable state, which proves the claim. \( \square \)

This criterion has also been derived in the context of quadratic Bell inequalities [5]; however, our proof is considerably shorter and, most importantly, it can be generalized to derive other characterizations of the different entanglement classes. Note that equation (2) is independent of the normalization of the state, simplifying many calculations below. Equation (2) is maximally violated by the GHZ state, \( |GHZ_3\rangle = (|000\rangle + |111\rangle)/\sqrt{2} \). For other states, one may first change the local basis (leading, e.g., to the criterion \( |\rho_{2,7}| \leq \sqrt{|\rho_{1,1}\rho_{8,8}|} + \sqrt{|\rho_{3,3}\rho_{6,6}|} + \sqrt{|\rho_{4,4}\rho_{5,5}|} \), but these will not be considered as independent criteria.

To discuss the strength of observation 1, we consider states that are diagonal in the GHZ basis. This basis consists of the eight states \( |\psi_i\rangle = (|x_1x_2x_3\rangle \pm |\bar{x}_1\bar{x}_2\bar{x}_3\rangle)/\sqrt{2} \), where \( x_j, \bar{x}_j \in \{0, 1\} \) and \( x_j \neq \bar{x}_j \). States that are diagonal in this basis are of the form

\[
\rho^{(dia)} = \frac{1}{N} \begin{bmatrix}
\lambda_1 & 0 & 0 & 0 & 0 & 0 & \mu_1 \\
0 & \lambda_2 & 0 & 0 & 0 & \mu_2 & 0 \\
0 & 0 & \lambda_3 & 0 & 0 & \mu_3 & 0 \\
0 & 0 & 0 & \lambda_4 & \mu_4 & 0 & 0 \\
0 & 0 & 0 & \mu_4 & \lambda_5 & 0 & 0 \\
0 & 0 & \mu_3 & 0 & 0 & \lambda_6 & 0 \\
\mu_2 & 0 & 0 & 0 & 0 & \lambda_7 & 0 \\
\mu_1 & 0 & 0 & 0 & 0 & 0 & \lambda_8 \\
\end{bmatrix},
\]

\(^6\) More generally, one has that if \( f_1, \ldots, f_n \) are positive concave functions, then \( g = (\prod_{i=1}^n f_i)^{1/n} \) is also concave. This can be seen as follows: first, as the function \( h(x) = (x)^{1/n} \) is monotonically increasing, it suffices to prove the claim for linear \( f_i \). Then, one can directly calculate that the second derivative of \( g \) is not positive. See also page 87 in [8].
Fully separable

biseparable, yet inseparable under bipartitions

genuine multipartite entangled

Figure 1. The entanglement properties of $N$-qubit GHZ states mixed with white noise, $\rho^{(ghzN)} = (1 - p)|GHZ_N\rangle\langle GHZ_N| + p\mathbb{I}/2^N$. It was known before [6] that these are fully separable iff $1/[1 + 2^{1-N}] \leq p \leq 1$, while for smaller $p$ they are inseparable under any partition. Our results show that iff $0 \leq p < 1/[2(1 - 2^{-N})]$ the states are genuinely multipartite entangled. Consequently, in the region in between the two bounds, the states $\rho^{(ghzN)}$ are biseparable yet inseparable under any fixed bipartition.

with real $\lambda_i$ and $\mu_i$, fulfilling $\lambda_i = \lambda_{9-i}$ for $i = 1, \ldots, 4$, and $N$ denotes a normalization. We can state:

**Observation 2.** For GHZ-diagonal states, the criterion from observation 1 constitutes a necessary and sufficient criterion for genuine multipartite entanglement.

**Proof.** The proof is given in the appendix.

This shows that the criterion of observation 1 is a strong criterion in the vicinity of GHZ states; indeed its later generalization solves the problem of classifying $N$-qubit GHZ states mixed with white noise (see figure 1).

It remains to investigate what happens for other states, such as the W state, $|W_3\rangle = (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$. First, one can apply local unitary operations before testing equation (2). This indeed works for the pure W state, but one can also derive stronger criteria:

**Observation 3.** Any biseparable three-qubit state fulfills

$$|\varrho_{2,3}| + |\varrho_{2,5}| + |\varrho_{3,5}| \leq \sqrt{\varrho_{1,1}\varrho_{4,4}} + \sqrt{\varrho_{1,1}\varrho_{6,6}} + \sqrt{\varrho_{1,1}\varrho_{7,7}} + \frac{1}{2}(\varrho_{2,2} + \varrho_{3,3} + \varrho_{5,5}).$$

(4)

**Proof.** Again, it suffices to consider pure states. Then, for a state that is $A|BC$-biseparable, one sees that $|\varrho_{2,5}| = \sqrt{\varrho_{1,1}\varrho_{6,6}}$ and $|\varrho_{3,5}| = \sqrt{\varrho_{1,1}\varrho_{7,7}}$. Furthermore, one has $|\varrho_{2,3}| \leq (\varrho_{2,2} + \varrho_{3,3})/2$, which follows already from the positivity of the density matrix. Therefore, equation (4) holds for the $A|BC$ partition, and similarly one can prove it holds for the other two bipartitions.

This observation deserves two comments. Firstly, this criterion is quite strong. It detects W states mixed with white noise, i.e. $\varrho^{(w3)}(p) = (1 - p)|W_3\rangle\langle W_3| + p\mathbb{I}/8$, for $p < 8/17 \approx 0.471$ as genuine tripartite entangled, whereas the best known entanglement witness detects it only for $p < 8/19 \approx 0.421$.\footnote{For three qubits, this witness is $\mathcal{W} = (2/3) \cdot (|111\rangle\langle111|) - |W_3\rangle\langle W_3|$; see also section 6.8.2 in [2].}

Secondly, it should be noted that observation 3 is independent of...
observation 1: the states $\varrho^{(w3)}(p)$ for $p \in (0.413; 0.471)$ are directly detected by observation 3. They are, however, not detected by equation (2), even if local filter operations $\varrho \mapsto \varrho = F_1 \otimes F_2 \otimes F_3 \otimes F_4 \otimes F_5 \otimes F_6$ are applied with arbitrary matrices $F_i$, as can be checked numerically.

So far, we have only considered criteria for biseparable states. Our approach also allows us to derive criteria for other entanglement classes:

Observation 4. (i) For fully separable three-qubit states, the following inequalities hold:

$$|\varrho_{1,8}| \leq (\varrho_{1,1} \cdot \varrho_{4,4} \cdot \varrho_{5,5} \cdot \varrho_{6,6} \cdot \varrho_{7,7})^{1/2}$$

$$|\varrho_{1,8}| \leq (\varrho_{1,1} \cdot \varrho_{4,4} \cdot \varrho_{5,5} \cdot \varrho_{6,6} \cdot \varrho_{7,7})^{1/8}$$

(ii) Equations (5) and (6) are connected via the substitution $\varrho_{2,2} \varrho_{3,3} = \varrho_{1,1} \varrho_{4,4}$. Similarly, one obtains new separability criteria from equation (5) by making the substitutions $\varrho_{6,6} \varrho_{7,7} = \varrho_{5,5} \varrho_{8,8}$, $\varrho_{2,2} \varrho_{5,5} = \varrho_{1,1} \varrho_{6,6}$, $\varrho_{3,3} \varrho_{7,7} = \varrho_{1,1} \varrho_{4,4}$ and $\varrho_{4,4} \varrho_{6,6} = \varrho_{2,2} \varrho_{8,8}$. Combining such substitutions, one also obtains new separability criteria, e.g. $|\varrho_{1,8}| \leq (\varrho_{2,2} \cdot \varrho_{3,3} \cdot \varrho_{5,5} \cdot \varrho_{8,8})^{1/4}$.

(iii) A condition for full separability that is violated in the vicinity of a $W$ state is

$$|\varrho_{2,3}| + |\varrho_{2,5}| + |\varrho_{3,5}| \leq \sqrt{|\varrho_{1,1} \varrho_{4,4}| + \sqrt{|\varrho_{1,1} \varrho_{5,5}| + \sqrt{|\varrho_{1,1} \varrho_{7,7}|}}.$$  

(iv) Equation (5) is a necessary and sufficient criterion for full separability for GHZ states mixed with white noise.

Proof. The proof is essentially the same as before, using the concavity of more generalized functions [8]. The inequalities (5) and (7) are equalities for pure fully separable states. The substitutions as in equation (6) can be made, since $\varrho_{2,2} \varrho_{3,3} = \varrho_{1,1} \varrho_{4,4}$, etc hold for any pure fully separable state. Concerning (iv), note that equation (5) detects noisy GHZ states for $p < 4/5$, and this value is known to mark the border of the fully separable states [6]. □

Surprisingly, substitutions as in equation (6) do indeed improve the criterion in some cases. For example, consider the family of bound entangled states of [7]. These are states as in equation (3) with $\lambda_1 = \lambda_8 = \mu_1 = 1$ and $\lambda_2 = 1/\lambda_7$, $\lambda_3 = 1/\lambda_6$, $\lambda_4 = 1/\lambda_5$ and $\mu_2 = \mu_3 = \mu_4 = 0$. For $\lambda_2$, $\lambda_3 \neq \lambda_4$ these states are separable under each bipartition, but not fully separable. Their entanglement is detected by equation (6) or other substitutions. Moreover, as one can directly check, for the special case $\lambda_2 = \lambda_3 = \lambda_5$ the inequality in (ii) tolerates significantly more noise than the best known witness [9] and gives more significant results for recent experiments 8.

3. Many qubits

Let us start with introducing a compact notation. Firstly, we label the diagonal elements of $\varrho$ by the corresponding product vector in the standard basis. That is, if $I = (i_1, i_2, \ldots, i_N)$ is a tuple consisting of $N$ indices $i_k \in \{0, 1\}$ then $\varrho_I = \varrho_{(i_1, i_2, \ldots, i_N)}$ is the diagonal entry corresponding to $|i_1, i_2, \ldots, i_N\rangle \langle i_1, i_2, \ldots, i_N|$. For example, for three qubits $\varrho_{(000)} = \varrho_{1,1}$ and $\varrho_{(001)} = \varrho_{2,2}$, etc. For a given $I$, one can define $I$ as the tuple arising from $I$ if zeroes and ones are exchanged, e.g. $(001) = (110)$. Furthermore, let $|I|$ denote the number of $i_k = 1$ in $I$, then $\sum_{|I| = n}$ denotes a sum over all $I$ with $|I| = n$.

8 In [10], this state has been experimentally prepared, and its entanglement has been confirmed with 2.9 standard deviations. Our new criterion detects it with a significance of 4.5 standard deviations.
Secondly, let $\sigma = |\psi\rangle \langle \psi|$ be a target state and $\varrho$ be a different state. We abbreviate with $\Sigma^{(\psi)}(\varrho)$ the sum of the absolute values of the off-diagonal elements of $\varrho$ in the upper triangle, which correspond to matrix entries where $\sigma$ does not vanish. For instance, for the three-qubit GHZ state, we have $\Sigma^{(\text{GHZ})}_{(1,2)}(\varrho) = |\varrho_{1,8}|$ and equation (4) can now be conveniently rewritten as $\Sigma^{(\text{W})}_{(1)}(\varrho) \leq \sum_{|I|=2} \sqrt{\varrho_{(000)I}^*} + \frac{1}{2} \sum_{|I|=1} \varrho_{I}^*$.

The idea behind this notation is to estimate all off-diagonal elements similarly as in observation 1. Explicitly, we have for four qubits:

**Observation 5.** (i) *From the four-qubit GHZ state,* $|\text{GHZ}_4\rangle = (|0000\rangle + |1111\rangle)/\sqrt{2}$, a necessary condition for biseparability of a general state $\varrho$ is

$$\Sigma^{(\text{GHZ}_4)}(\varrho) \leq \frac{1}{2} \sum_{|I|=|1,2,3|} \sqrt{\varrho_{I}^* \varrho_{I}}. \tag{8}$$

This condition is necessary and sufficient for biseparability of GHZ-diagonal states in the sense of observation 2.

(ii) *From the four-qubit W state,* $|\text{W}_4\rangle = (|0001\rangle + |0010\rangle + |0100\rangle + |1000\rangle)/2$, a criterion is derived as

$$\Sigma^{(\text{W}_4)}(\varrho) \leq \sum_{|I|=2} \sqrt{\varrho_{(0000)I}^*} + \sum_{|I|=1} \varrho_{I}. \tag{9}$$

(iii) *From the four-qubit Dicke state,* $|\text{D}_4\rangle = (|0011\rangle + |0101\rangle + |1001\rangle + |0110\rangle + |1010\rangle + |1100\rangle)/\sqrt{6}$, a criterion is derived as

$$\Sigma^{(\text{D}_4)}(\varrho) \leq \sqrt{\varrho_{(0000)(1111)}} + \sum_{|I|=1} \sum_{|J|=3} \sqrt{\varrho_{I}^* \varrho_{J}} + \frac{3}{2} \sum_{|I|=2} \varrho_{I}. \tag{10}$$

**Proof.** (i) is proved as in observations 1 and 2. The factor $1/2$ takes into account that each possible term occurs twice in the sum. (ii) and (iii) follow as in observation 3. Here, estimating an off-diagonal element can be simplified by the following rule: if the off-diagonal element $\eta$ corresponds to $|i_1i_2i_3i_4\rangle \langle j_1j_2j_3j_4|$ and the state is separable under the $A|BCD$-bipartition, one has $\eta \leq \sqrt{\varrho_{(i_1i_2j_1j_2)(i_3i_4j_3j_4)}}$, while one has $\eta \leq \sqrt{\varrho_{(i_1i_2j_1j_2)(i_3i_4j_3j_4)}}$ for the $AB|CD$-bipartition, etc. Further, one needs that for a positive $n \times n$ matrix $P$, the bound $\sum_{i<j} |P_{ij}| \leq ((n-1)/2)\text{Tr}(P)$ holds.\(^9\)

Again, these criteria improve known conditions: for the four-qubit W state mixed with white noise, equation (9) detects genuine multipartite entanglement for $p < 4/9 \approx 0.444$, while the fidelity-based witness detects it only for $p < 4/15 \approx 0.267$ and the improved witness (see footnote 7) for $p < 8/21 \approx 0.381$, whereas the best known witness detects it for $p > 16/45 \approx 0.356$.\(^{10}\)

For arbitrary states, similar entanglement criteria can be derived as follows. In a given basis and for a fixed partition, any off-diagonal element can be estimated as in the proof of observation 5. Then, all these estimates can be summarized to an estimate of the sum of all

\[^9\] This generalizes the estimate $|\varrho_{23}| \leq (\varrho_{22} + \varrho_{33})/2$ from observation 3 and can be seen as follows: one has for any $|x\rangle$ that $\langle x|P|x\rangle \geq 0$, and taking $|x\rangle$ of the type $|x\rangle = (1, e^{i\theta}, 0, \ldots, 0)$ and summing over all possible permutations thereof gives the bound.

\[^{10}\] The best known witness is $W = (2/3) \cdot I - |D_4\rangle \langle D_4|$, see [11].
off-diagonal elements. This might be further improved by considering a weighted sum. For instance, for \( N \)-qubit GHZ states, the criterion reads \( \mathcal{S}^{(GHZ_N)}(\varrho) \leq \frac{1}{3} \sum_{i=1}^{N-1} \sqrt{\varrho_{ii} \varrho_{ii}} \) and is again necessary and sufficient for GHZ diagonal states as the proof of observation 2 can directly be generalized (see figure 1). Further criteria for cluster states or the four-qubit singlet state will be presented elsewhere.

4. Experimental consequences

Obviously, these criteria can be applied to experiments where the full density matrix has been determined [12]. However, often this cannot be done. Still, our results may be directly applied. For example, let us consider equation (4) for the detection of entanglement around the three-qubit W state. Using the fidelity \( F = \text{Tr}(\varrho |W_3\rangle \langle W_3|) \) one may rewrite equation (4) as

\[
F \leq \frac{2}{3} (\sqrt{\varrho_{1,1} \varrho_{4,4}} + \sqrt{\varrho_{1,1} \varrho_{6,6}} + \sqrt{\varrho_{1,1} \varrho_{7,7}} + \varrho_{2,2} + \varrho_{3,3} + \varrho_{5,5}).
\]

The fidelity of the W state can be measured experimentally with five local measurements [13] and the diagonal elements can also be determined from measurement of \( \sigma_x \otimes \sigma_x \otimes \sigma_z \), which is already included in the measurements needed for the fidelity. This shows that equation (4) (and similarly all other criteria presented) is experimentally easily testable. For the usual error models in photon experiments, one can also check that criterion (4) detects entanglement with a higher statistical significance than the witness, unless the fidelity is close to one and the significance of both methods is high.

5. Decoherence

Finally, our results also shed light on the decoherence of multipartite entanglement. Consider an \( N \)-qubit GHZ state, influenced by relaxation—the noise that is dominant in ion traps [14]. On a single qubit, this changes the density matrix according to \( |0\rangle \langle 0| \rightarrow |0\rangle \langle 0| + (1 - x)|1\rangle \langle 1| + x(1 - x)|0\rangle \langle 0| \) and \( (|0\rangle \langle 1| + \text{h.c.}) \rightarrow x^{1/2}|0\rangle \langle 0| + \text{h.c.} \) (with \( x = e^{-\gamma t} \)) and corresponds to a coupling to a bath with zero temperature. The total density matrix can directly be computed [15], resulting in \( \varrho_{1,2} = x^{N/2} \) for the off-diagonal element and \( \varrho_{ii} = [\delta_{ii} + x^{1/2}(1 - x)^{N-1}]/2 \) for the diagonal elements. Here, we have used the same notation as in observation 5.

This state is not diagonal in the GHZ basis, but applying on each qubit a filter \( \varrho \mapsto \mathcal{F}_\varrho \mathcal{F} \) with \( \mathcal{F} = \alpha|0\rangle \langle 0| + (1/\alpha)|1\rangle \langle 1| \) and \( \alpha^4 = x/(1 - x) \) maps it to a state that differs from a GHZ diagonal state only in the element \( \varrho_{1,1} \). This filtering keeps all entanglement properties, but finally observations 1 and 2 can be used. From this one can conclude that GHZ states coupled to a bath with zero temperature are genuine multipartite entangled, if and only if \( t < -\ln[1 - (2N-1)^{-2/N}] / \gamma \).

6. Conclusion

We present a method to derive separability criteria for different classes of multipartite entanglement directly in terms of density matrix elements. The resulting criteria are strong and can be used in experiments, as well as for the investigation of decoherence. It would be interesting to use our approach to discriminate between more special entanglement classes (such as the W and GHZ class for three qubits [7]) and to connect it to the quantification of entanglement with entanglement measures.

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Appendix

Here, we prove observation 2. Since $\mathcal{Q}(\text{dia}) \geq 0$, we have $|\mu_i| \leq \lambda_i$ and we can assume that $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ as one can achieve that by a local change of the basis. Then, equation (2) reads $|\mu_1| \leq \lambda_2 + \lambda_3 + \lambda_4$, and we will show that if this holds, a decomposition into biseparable states can be found. Note that due to the ordering of the $\lambda_i$ other conditions for biseparability (e.g. $|\mu_2| \leq \lambda_1 + \lambda_3 + \lambda_4$) can then never be violated.

Let us define the unnormalized state $\mathcal{Q}(12)(\lambda)$ with $\lambda_1 = \mu_1 = \lambda_2 = \mu_2 = \lambda$, while all other matrix entries vanish. This state is $AB|C$-biseparable, since it can be written as

$$\mathcal{Q}(12)(\lambda) = 2\lambda (|\chi\rangle \langle \chi| \otimes |\eta\rangle \langle \eta|)_{AB} + |\chi\rangle \langle \chi| \otimes |\eta\rangle \langle \eta|)_{C}$$

(A.1)

with $|\chi\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}$ and $|\eta\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$. Analogously, one can consider states $\mathcal{Q}(kl)$ for any $k, l = 1, \ldots, 4$ with $k \neq l$ and find that they are also biseparable, as one only has to permute or flip some qubits.

1. Firstly, we consider the extremal case when $\mu_i = \lambda_i$ for all $i$ and by assumption the separability condition implies that we have $\mu_i = \sum_{k \neq i} \lambda_k$, where for the index $1 \leq k \leq 4$. If $\lambda_1 = \lambda_2 + \lambda_3 + \lambda_4$ we can directly write $\mathcal{Q}(\text{dia}) = \sum_{k=2,3,4} \mathcal{Q}(1k)(\lambda_k)$; hence $\mathcal{Q}(\text{dia})$ is biseparable. Otherwise, the idea is to write

$$\mathcal{Q}(\text{dia}) = \sum_{k=2,3,4} \mathcal{Q}(1k)(\lambda_k) + \mathcal{Q}(r)$$

(A.2)

for some parameters $\chi_k$ such that the rest $\mathcal{Q}(r)$ (which is then characterized by parameters $\lambda_k^{(r)}$) fulfills two conditions. Its first and last column and row should vanish ($\mathcal{Q}(1,1) = \lambda_1^{(r)} = 0$) and it should still fulfill all biseparability conditions (e.g. $\lambda_2^{(r)} \leq \lambda_3^{(r)} + \lambda_4^{(r)}$). Then, $\mathcal{Q}(r)$ can be iteratively further decomposed and finally a decomposition of $\mathcal{Q}(\text{dia})$ into biseparable states can be found.

The idea is to choose the $\lambda_k^{(r)}$, $k = 2, 3$ and 4, as equal as possible (they have to fulfill $\lambda_k^{(r)} \leq \lambda_k$, but monotonically decreasing. For that, we define $\alpha_4 := \lambda_2 + \lambda_3 + \lambda_4 - \lambda_1 = \lambda_2^{(r)} + \lambda_3^{(r)} + \lambda_4^{(r)} > 0$ and then recursively $\lambda_4^{(r)} = \min\{\lambda_4, \alpha_4/3\}$, then $\alpha_3 = \alpha_4 - \lambda_4^{(r)}$ and then $\lambda_3^{(r)} = \min\{\lambda_3, \alpha_3/2\}$ and finally $\alpha_2 = \alpha_3 - \lambda_3^{(r)}$ and $\lambda_2^{(r)} = \min\{\lambda_2, \alpha_2\}$. Then $\mathcal{Q}(\text{dia}) = \sum_{k=2,3,4} \mathcal{Q}(1k)(\lambda_k - \lambda_k^{(r)}) + \mathcal{Q}(r)$ with $\lambda_2^{(r)} \geq \lambda_3^{(r)} > \lambda_4^{(r)}$. Then we cannot have that both $\lambda_4^{(r)} = \lambda_4$ and $\lambda_3^{(r)} = \lambda_3$, because if these were true, then from the definition of $\alpha_4$ it would follow that $\lambda_2^{(r)} = \lambda_2 - \lambda_1 \leq 0$. So we have $\lambda_3^{(r)} = \alpha_3/2$ ($\lambda_4^{(r)} = \alpha_4/3$ also implies $\lambda_3^{(r)} = \alpha_3/2$), which due to the ordering of the $\lambda_i$ implies $\lambda_2^{(r)} = \alpha_2 = \lambda_2^{(r)}$. So $\lambda_2^{(r)} \leq \lambda_3^{(r)} + \lambda_4^{(r)}$ and one can decompose $\mathcal{Q}(r)$ further into $\mathcal{Q}(23)$ and $\mathcal{Q}(24)$ and a remaining term with $\lambda_1^{(r)} = \lambda_1^{(r)} = 0$, etc. Of course, for the case of three qubits one may also write down suitable values for the $\lambda_i^{(r)}$ directly, but the previous scheme can straightforwardly be extended to more qubits.

2. Secondly, for $0 \leq \mu_i \leq \lambda_i$, and where again $\lambda_1 \leq \lambda_2 + \lambda_3 + \lambda_4$, we first consider the states $\mathcal{Q}(kl)$. Their nonzero matrix elements obey $\mu_i = \lambda_i$, but, applying with some probability locally conjugate random phases (e.g. $|1\rangle_2 \mapsto e^{i\phi}|1\rangle_2$ and $|1\rangle_3 \mapsto e^{-i\phi}|1\rangle_3$) to these states
decreases the values of the $\mu_i$ (in this example for $i = 2, 3$). Therefore, one can for a given $\varrho^{(kl)}$ decrease the values of $\mu_i$ arbitrarily by local operations (in the example we can decrease e.g. the value of $\mu_3$ for $\varrho^{(12)}$ or $\mu_3$ for $\varrho^{(34)}$), and the resulting states must be biseparable. Consequently, a given $\varrho^{(\text{dia})}$ with $\lambda_1 \leq \lambda_2 + \lambda_3 + \lambda_4$ can be decomposed into biseparable states as in (i).

(iii) Further, it may happen that for a given $\varrho^{(\text{dia})}$ one has $0 \leq \mu_1 \leq \lambda_2 + \lambda_3 + \lambda_4$ but $\lambda_1 > \lambda_2 + \lambda_3 + \lambda_4$. Then we consider $\varrho'$, which is obtained from $\varrho^{(\text{dia})}$ by setting $\lambda_1 = \max\{\mu_1, \lambda_2\}$. Then, $\varrho'$ is biseparable according to (ii), and $\varrho^{(\text{dia})}$ is obtained from $\varrho'$ by mixing with the fully separable state $|000\rangle\langle000| + |111\rangle\langle111|$; hence it is biseparable.

(iv) The previous arguments prove the claim if all $\mu_i \geq 0$. If some $\mu_i$ are negative, one can prove it as follows: let $\varrho$ be a GHZ diagonal state, with some $\mu_i < 0$, which fulfills the condition of biseparability. The state $\varrho'$ that arises from $\varrho$ when all $\mu_i$ are replaced by $|\mu_i|$ fulfills the same condition, and is biseparable due to points (i)–(iii). It can be decomposed into several $\varrho^{(kl)}$; in some of them maybe we have $\mu_i(\varrho^{(kl)}) < \lambda_i(\varrho^{(kl)})$ according to points (ii) and (iii). Nevertheless, we can build out of this decomposition of $\varrho'$ a decomposition of $\varrho$ if we flip the signs of all the $\mu_i(\varrho^{(kl)})$ appropriately. An arbitrary flipping of the signs of the $\mu_i$ of a given $\varrho^{(kl)}$ can be done for each $k, l$ by local operations; hence $\varrho$ is also biseparable.

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