Multiqubit systems: highly entangled states and entanglement distribution

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Abstract
A comparison is made of various searching procedures, based upon different entanglement measures or entanglement indicators, for highly entangled multiqubits states. In particular, our present results are compared with those recently reported by Brown \textit{et al} (\textit{J. Phys. A: Math. Gen.} 2005 \textbf{38} 1119). The statistical distribution of entanglement values for the aforementioned multiqubit systems is also explored.

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1. Introduction

Quantum entanglement \cite{1} is nowadays regarded as constituting one of (if not the) most basic features of quantum mechanics \cite{2–4}. The increasing interest generated by this subject within the research community \cite{5–27} has been greatly stimulated by the discovery of novel quantum information processes \cite{2–4} (such as quantum teleportation and superdense coding) that may lead to important practical developments. The technological relevance of quantum entanglement is not limited to the information technologies, but is also at the basis of other interesting applications, such as quantum metrology \cite{5}. Besides its remarkable technological impact, current research in quantum entanglement is contributing to a deeper understanding of various basic aspects of quantum physics, such as, for instance, the foundations of quantum-statistical mechanics \cite{6, 7}. The relationship between entanglement and the dynamical evolution of multipartite quantum systems \cite{8–11} constitutes another interesting example.

Due to its great relevance, both from the fundamental and from the practical points of view, it is imperative to explore and characterize all aspects of the quantum entanglement of multipartite quantum systems. A considerable amount of research has recently been devoted to the study of multiqubit entanglement measures defined as the sum of bipartite entanglement measures over all (or an appropriate family of) the possible bi-partitions of the full system.
(14, 15, 17–26) (see also [27] for another approach, also based on bi-partitions, to multipartite entanglement). In particular, Brown et al [14] have performed a numerical search of multiqubit states exhibiting a high value of an entanglement measure defined in the aforementioned way, based upon the negativity of the system’s bi-partitions. The purpose of the present work is twofold. On the one hand, we numerically determine the distribution of entanglement values (according to four different measures of multiqubit entanglement based upon bi-partitions) of pure states of three, four and five qubits, and its relationship with important particular states, such as the $|\text{GHZ}\rangle$ state. On the other hand, we report the result of running numerical searches of multiqubit states (up to seven qubits) exhibiting high entanglement according to the alluded to four measures. The results obtained using each of these four measures are compared to each other, and also compared to those reported by Brown et al [14].

The paper is organized as follows. Some basic properties of the entanglement measures used here are reviewed in section 2. Our results concerning the distribution of multiqubit entanglement measures for systems of three, four and five qubits are reported and discussed in section 3. Our algorithm for the search of states of high entanglement is presented in section 4, and the main results obtained are discussed and compared with those reported by Brown et al. Finally, some conclusions are drawn in section 5.

2. Pure state multipartite entanglement measures based on the degree of mixedness of subsystems

Research on the properties and applications of multipartite entanglement measures has attracted considerable attention in recent years [14, 15, 17–26]. One of the first practical entanglement measures for $N$-qubit pure states $|\phi\rangle$ to be proposed was that introduced by Meyer and Wallach [17]. It was later pointed out by Brennen [18] that the measure advanced by Meyer and Wallach is equivalent to the average of all the single-qubit linear entropies,

$$Q(|\phi\rangle) = 2 \left(1 - \frac{1}{N} \sum_{k=1}^{N} \text{tr} \rho_k^2 \right).$$  

(1)

where $\rho_k, k = 1, \ldots, N$, denotes the marginal density matrix describing the $k$th qubit of the system after tracing out the rest. This quantity, often referred to as ‘global entanglement’ (GE), describes the average entanglement of each qubit of the system with the remaining $(N - 1)$-qubits. The GE measure is widely regarded as a legitimate, useful and practical $N$-qubit entanglement measure [18–22]. This measure is invariant under local unitary transformations and non-increasing on average under local quantum operations and classical communication. That is to say, $Q$ is an entanglement monotone. Another interesting feature of this measure is that it can be determined without the need for full quantum state tomography [18]. This measure proved to be useful in the study of several problems related to multipartite entanglement, such as entanglement generation by nearly random operators [19] and by operators characterized by special matrix element distributions [20], thermal entanglement in multiqubit Heisenberg models [21], and multipartite entanglement in one-dimensional time-dependent Ising models [22]. Other entanglement measures, based upon the average values of the linear entropies associated with more general partitions of the $N$-qubit systems into two subsystems (that is, involving not only the partitions of the system into a 1-qubit subsystem and an $(N-1)$-qubit subsystem) have also been recently explored [23–25]. In particular, Scott [23] studied various interesting aspects of the family of multiqubit entanglement measures given by
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Table 1. Upper bounds for the entanglement measures \( E_L, E_{VN}, E_R \) and \( E_N \).

| N  | 3   | 4   | 5   | 6   | 7   |
|----|-----|-----|-----|-----|-----|
| \( E_{L,\text{max}} \) | 1.5  | 4.25| 10  | 23  | 49.875 |
| \( E_{VN,\text{max}} \) | 3    | 10  | 25  | 66  | 154 |
| \( E_{Re,\text{max}} \) | 2.079 441 54 | 6.931 471 81 | 17.328 6795 | 45.747 7139 | 106.744 666 |
| \( E_{Neg,\text{max}} \) | 1.5  | 6.5  | 17.5 | 60.5 | 157.5 |

\[
Q_m(|\phi\rangle) = \frac{2^m}{2^m - 1} \left( 1 - \frac{m!(N-m)!}{N!} \sum_s \text{Tr} \rho_s^2 \right), \quad m = 1, \ldots, [N/2],
\]

where the sum is taken over all the subsystems \( s \) constituted by \( m \) qubits, \( \rho_s \) are the concomitant marginal density matrices, and \( [x] \) is the integer part of \( x \). The quantities \( Q_m \) correspond to the average entanglement between subsystems consisting of \( m \) qubits and the remaining \( N-m \) qubits. The measures \( Q_m \) have been applied to the study of quantum error correcting codes and to the analysis of the (multipartite) entangling power of quantum evolutions [23].

Another way of characterizing the global amount of entanglement exhibited by an \( N \)-qubit state is provided by the sum of the (bi-partite) entanglement measures associated with the \( 2^{N-1} - 1 \) possible bi-partitions of the \( N \)-qubits system [14]. These entanglement measures are given, essentially, by the degree of mixedness of the marginal density matrices associated with each bi-partition. These degrees of mixedness can be, in turn, evaluated in several ways. For instance, we can use the von Neumann entropy, the linear entropy, or a Renyi entropy of index \( q \). In what follows we are going to consider the following ways of computing the degrees of mixedness of the marginal density matrices \( \rho_i \).

- The linear entropy \( S_L = 1 - \text{Tr}[\rho_i^2] \).
- The von Neumann entropy \( S_{VN} = -\text{Tr}[\rho_i \log_2 \rho_i] \).
- The Renyi entropy with \( q \to \infty \), \( S_{\text{Renyi}}^{q \to \infty} = -\ln \lambda_{\text{max}}^k \), where \( \lambda_k \) are the eigenvalues of the marginal density matrix. This particular instance of the Renyi entropy constitutes the case (within the Renyi family) that differs the most from the von Neumann entropy [28, 29].

Besides these measures we are also going to consider the ‘negativity’ as a measure of the amount of entanglement associated with a given bi-partition. The negativity is given by

\[
\text{Neg.} = \sum |\alpha_i|,
\]

where \( \alpha_i \) are the negative eigenvalues of the partial transpose matrix associated with a given bi-partition. The global, multipartite entanglement measures associated with the sum (over all bi-partitions) of each of these four quantities are here going to be denoted, respectively, by \( E_L, E_{VN}, E_R \) and \( E_N \).

Upper bounds for the four entanglement measures \( E_L, E_{VN}, E_R \) and \( E_N \) can be established by considering an (hypothetical) \( N \)-qubits pure state such that all its marginal density matrices are fully mixed. These bounds can be seen in table 1. Note, however, that these bounds may not be reachable. For instance, there is no 4-qubit state reaching the alluded bound [15].

3. Distribution of multiqubit entanglement

In this section, we determine numerically the distribution of entanglement values corresponding to pure states of multiqubit systems randomly generated according to the Haar measure. In figures 1–3 we plot (for systems of three–five qubits respectively) the
probability densities $P$ of finding multiqubit states with given values of the entanglement measures $E_L$, $E_{VN}$, $E_R$ and $E_N$. In these figures, we also show vertical lines corresponding to the entanglement values of important particular states, such as the $N$-qubit GHZ state,

$$|\text{GHZ}\rangle = \frac{1}{\sqrt{2}}(|0\cdots0\rangle + |1\cdots1\rangle),$$

the states of high entanglement BSSB4 and BSSB5 (of four and five qubits, respectively) discovered numerically by Brown et al [14], and the 4-qubit state HS, that has been conjectured to maximize the entanglement of 4-qubit states [15] (when measuring entanglement using the sum of the marginal von Neumann entropies associated with all bi-partitions). The HS state has recently been shown to constitute a local maximum of the $E_{VN}$ entanglement measure for 4-qubit states [16].

A particularly interesting aspect of figures 1–3 is the status (as far as the present multiqubit entanglement measures are concerned) of the state GHZ with respect to the bulk of the states of the multiqubit system.

For 3-qubit systems, the $|\text{GHZ}\rangle$ state has all its single-qubit marginal density matrices complete mixed and, consequently, constitutes the state of maximum entanglement according to the measures $E_{VN}$, $E_L$, $E_N$ and $E_R$. On the other hand, the state

$$|W\rangle = \frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle),$$

according to those same measures, exhibits considerably less entanglement than $|\text{GHZ}\rangle$. However, as can clearly be appreciated in figure 1, the $W$ state is still within the most entangled 3-qubit pure states. The $W$ state is clearly more entangled than the ‘typical’ pure state of three qubits.

Figure 1. Entanglement distributions for 3-qubit states. All depicted quantities are dimensionless.
We have seen that, in the case of three qubits, the four measures $E_{VN}$, $E_L$, $E_N$ and $E_R$ lead to qualitatively similar conclusions in connection with the entanglement of the states GHZ and $W$ as compared with the entanglement exhibited by typical (pure) states. In contrast, when 4-qubit states are considered, each of the aforementioned entanglement measures yields different results. According to $E_R$, the state $|\text{GHZ}\rangle$ still has an amount of entanglement well above most pure states. According to $E_L$, the state $|\text{GHZ}\rangle$ has an entanglement a little above typical. According to $E_{VN}$, $|\text{GHZ}\rangle$ can be said to be (in terms of its entanglement value) still ‘within the bulk of pure states’, but with an amount of entanglement clearly below typical. Finally, according to $E_N$, the $|\text{GHZ}\rangle$ state exhibits less entanglement than most pure states of four qubits. It is also interesting to note that the state HS exhibits more entanglement than BSSB4 when using the measures $E_L$, $E_{VN}$ or $E_N$. In contrast, BSSB4 has a larger value of $E_R$ than HS.

For 5-qubit states, the $|\text{GHZ}\rangle$ state has less entanglement than most pure states when the entanglement is measured using $E_L$, $E_{VN}$ or $E_N$. Curiously enough, according to $E_R$ the $|\text{GHZ}\rangle$ still ranks as a 5-qubit state of rather large entanglement.

4. Search for multiqubit states of high entanglement

4.1. Searching algorithm

In the present paper, we are going to restrict our search of multiqubit states of high entanglement to pure states. In this respect our approach is a little different from that of Brown et al [14], who considered a search process within the complete space of possible states (that is, with
any degree of mixedness). The kind of search studied by Brown et al is certainly of interest and may shed some light on the structure of the 'entanglement landscape' of the full state space. However, it is reasonable to expect the states of maximum entanglement to be pure. Consequently, as far as the search of states of maximum entanglement is concerned, it seems that limiting the search to pure states is not going to reduce its efficiency. The results reported here fully confirm this expectation.

A general pure state of an $N$-qubit system can be represented as

$$|\Psi\rangle = \sum_{k=1}^{2^N} (a_k + i b_k)|k\rangle,$$

where $|k\rangle$, ($k = 1, \ldots, 2^N$) represents the states of the computational basis (that is, the $2^N$ states $|00, \ldots, 0\rangle, |10, \ldots, 0\rangle, \ldots, |11, \ldots, 1\rangle$). We start our search process with the initial state $|000\cdots0\rangle$. In other words, the initial parameters characterizing the state are $a_1 = 1$, and all the rest of the $a_i$’s and $b_i$’s are equal to zero. This initial state is fully factorizable and can thus be regarded as being ‘very distant’ from states of high entanglement. Starting with an arbitrary, random initial pure state does not alter the results of the search process. Now, at each step of the search process a new, tentative state is generated according to the following procedure. A random quantity $\Delta$ (uniformly chosen from an interval $(-\Delta_{\text{max}}, \Delta_{\text{max}})$) is added to each $a_i$ and $b_i$ (a different, independent $\Delta$ is generated for each parameter). The new state generated in this way is then normalized to 1 and its entanglement measure is computed. If the entanglement of the new state is larger than the entanglement of the previous state the new state is kept, replacing the previous one. Otherwise, the new state is rejected and a new, tentative state is generated. In order to ensure the convergence of this algorithm to a state of high entanglement, the following two rules are also implemented.
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Table 2. Numerically obtained maximum values for the entanglement measures $E_L$, $E_{VN}$, $E_R$ and $E_N$.

|        | Three qubits | Four qubits | Five qubits | Six qubits | Seven qubits |
|--------|--------------|-------------|-------------|------------|--------------|
| $E_L$  | 1.500 000   | 4.000 000   | 10.000 000  | 23.000 000 | 49.573 765   |
| $E_{VN}$ | 3.000 000   | 9.377 34  | 25.000 000  | 66.000 000 | 152.620 140 |
| $E_R$  | 2.079 441   | 5.995 47   | 17.328 678  | 45.747 705 | 91.651 820  |
| $E_N$  | 1.500 000   | 6.098 07   | 17.500 000  | 60.500 000 | 155.812 856 |

- If 500 consecutive tentative new states are rejected, the interval for the random quantity $\Delta$ is changed according to $\Delta_{\text{max}} \rightarrow \frac{\Delta_{\text{init}}}{2}$ (as the initial value for $\Delta_{\text{max}}$ we take $\Delta_{\text{init}} = 0.1$).
- When a value $\Delta_{\text{max}} \leq 1 \times 10^{-8}$ is reached the search program halts.

4.2. Results yielded by the searching algorithm

The maximum entanglement values obtained from the searching algorithm are listed in table 2. It must be stressed that the maximum values associated with different measures do not necessarily correspond to the same state. The states obtained when maximizing one particular measure do not exhibit, in general, a maximum value of the other measures. The results obtained by us after running the search algorithm several times (considering the entanglement measures $E_L$, $E_{VN}$, $E_R$ and $E_N$) can be summarized as follows.

- Among the four measures considered here, $E_L$ is computationally the easiest and quickest to evaluate. The algorithm runs faster when maximizing this measure than when maximizing any of the other three. However, in the case of four qubits most states that maximize $E_L$ do not maximize the other measures. There are many different 4-qubit states that exhibit the observed maximum value $E_L = 4$. Few of these states also exhibit the maximum value of the other entanglement measures (for instance, the value $E_{VN} = 9.377 34$).

- The measure $E_{VN}$ is computationally more expensive than $E_L$. The states obtained maximizing $E_{VN}$ also maximize $E_L$ and $E_N$. In other words, all the states that we have found that realize the observed maximum value of $E_{VN}$ realize as well the observed maxima of $E_L$ and $E_N$. In contrast, for four qubits there are many states exhibiting the observed maximum value of $E_L$ that do not reach the observed maximum value of $E_{VN}$.

- The measure $E_R$ seems to be the ‘worst’ of the four. States that maximize $E_R$ do not, in general, maximize the other measures. And, conversely, states maximizing any of the other measures do not in general maximize $E_R$.

- $E_N$ is, by far, computationally the most expensive of the measures considered here. The states maximizing this measure also maximize $E_L$ and $E_{VN}$. In this case, the situation is similar to the already-mentioned one corresponding to the measure $E_{VN}$.

The numerical values reported in the above table are the result of several search experiments that can be summarized as follows. In the case of three qubits, the numerical optimization of any of the aforementioned measures leads to the same state, the |GHZ⟩ state, and to the concomitant maxima of the entanglement measures. For four qubits, the search for states optimizing $E_{VN}$ yields a final state (equivalent to the |HS⟩ state) that also maximizes all the entanglement measures considered excepting $E_R$ (here, by ‘equivalent to the |HS⟩ state’ we mean that all the marginal density matrices of the alluded state exhibit the same entropic values as those exhibited by the corresponding marginal density matrices of |HS⟩, and also that the alluded state has, for all bipartitions, the same negativities as |HS⟩). The maximum value of $E_R$ reported in table 2 is generated by search experiments maximizing this entanglement
measure. The explicit expression of the corresponding 4-qubit state is given in table 3 (see appendix). The 4-qubit state obtained when searching for the maximum value of \(E_N\) is equivalent to that obtained when maximizing \(E_{VN}\). When conducting search experiments for 4-qubit states maximizing \(E_L\) we obtain, in most cases, states that do not reach the observed maxima of the rest of the measures. These states are not, in general, equivalent to each other. In point of fact, a different state is obtained in each run of the algorithm optimizing \(E_L\).

The 5-qubit case is similar to the 3-qubit one. The numerical search of 5-qubit states optimizing any of the aforementioned entanglement measures leads to states that exhibit the observed maxima of all these measures (which are reported in table 2). In other words, if one runs a search algorithm based upon any one of these measures, one obtains a state that exhibits all the maximum entanglement values reported in table 2. These values are those corresponding to the 5-qubit state (8).

For six qubits, the search experiments based on the maximization of either \(E_L\) or \(E_{VN}\) lead to final states exhibiting the same values of the four entanglement measures, which are reported in table 2. The search algorithm based upon the optimization of \(E_K\) yields states with lower values of the four measures than those shown in table 2. For six qubits, the search algorithm corresponding to \(E_N\) is too slow and we were not able to reach the optimal state.

Finally, in the case of seven qubits the values reported on table 2 were evaluated on the state found when numerically optimizing \(E_{VN}\) (this state is explicitly given in table 4, see appendix). When running numerical searches for 7-qubit states optimizing other measures we did not find states with entanglement values higher than those evaluated upon the state obtained when optimizing \(E_{VN}\). Let us now discuss in more detail the numerically found states of high entanglement.

### 4.2.1. Four qubits

In the case of 4-qubit systems, the extremalization processes based upon either of the measures \(E_{VN}\) or \(E_N\) always lead to states having the same entanglement values as those exhibited by the HS state discovered by Higuchi and Sudbery [15], which is given by

\[
|\text{HS}\rangle = \frac{1}{\sqrt{6}} (|1100\rangle + |0011\rangle + \omega (|1001\rangle + |0110\rangle) + \omega^2 (|1010\rangle + |0101\rangle)),
\]

with \(\omega = -\frac{1}{2} + \frac{\sqrt{3}}{2} i\). We repeated the search process starting under different, random initial conditions and always found states with entanglement values corresponding to the HS state. This constitutes convincing numerical evidence that the HS state is, at least, a local maximum of both the \(E_{VN}\) and the \(E_N\) measures. In fact, it was recently proven by Brierley and Higuchi that the HS state is indeed a local maximum for \(E_{VN}\) [16]. Higuchi and Sudbery [15] have provided analytical arguments supporting the conjecture that the HS state is also a global maximum for \(E_{VN}\), but this conjecture has not been proven yet. These authors have also proved that there is no pure state of four qubits such that all its 2-qubit marginal density matrices are completely mixed [15]. It is interesting that Brown et al [14], when performing a search process similar (but not identical) to that considered here, obtained instead of the HS state always a state (which we here call BSSB4) exhibiting values of \(E_{VN}\) and \(E_N\) smaller than those exhibited by HS. Besides some intrinsic differences in the algorithm itself, there is the fact that the main results reported here were computed starting the search process with a pure state, while Brown et al started their search with a mixed state. It is also worthwhile mentioning that we performed the searches using a FORTRAN program, while Brown et al employed a MATLAB program. When running a search algorithm maximizing the \(E_L\) measure, we obtained several different final states, some of them exhibiting values of \(E_{VN}\) larger than the value corresponding to the state BSSB4. All these findings suggest that, perhaps, the state BSSB4 has no special significance (although it is certainly a highly entangled 4-qubit state).
Its appearance when running the searching scheme developed by Brown et al seems to be just
an accident due to some special features of that algorithm.

We must mention that we also ran a search algorithm (written in the computer language
MATHEMATICA) similar to that of Brown et al (and different from that discussed in most
of the present paper), obtaining the same results as Brown et al did (that is, the algorithm
converged to a state with entanglement values corresponding to BSSB4). On the other hand,
when running an algorithm (written in MATHEMATICA) exhibiting the same basic structure
of our FORTRAN program we get the same results as those obtained with the FORTRAN code.
The main difference between our algorithm (either in the FORTRAN or the MATHEMATICA
versions) and that used by Brown et al (when particularized to pure states) is the following.
When generating new random trial states (in the ‘pure state version’ of Brown et al algorithm)
one chooses a random coefficient of the previous state, multiply the corresponding real and
imaginary parts by positive random numbers, and re-normalize the state. On the other hand, in
our algorithm (see subsection 4.1) we add random numbers (that may be positive or negative)
to the real and imaginary parts of the state’s coefficients (and then re-normalize the state).
The results of various numerical experiments done by us suggest that this difference on the
implementation of the searching algorithm accounts for the different results obtained for highly
entangled 4-qubit states.

4.2.2. Five qubits. When running our search scheme for states of five qubits, we always
obtain states exhibiting the same entanglement values as the state obtained by Brown et al
[14],

$$|BSSB5⟩ = \frac{1}{2} (|100⟩|Φ−⟩ + |010⟩|Ψ−⟩ + |100⟩|Φ+⟩ + |111⟩|Ψ+⟩) \quad (8)$$

where $Ψ± = |00⟩ ± |11⟩$ and $Φ± = |01⟩ ± |10⟩$. This state has all its marginal density matrices
(for one and two qubits) completely mixed.

4.2.3. Six qubits. In the case of six qubits, our algorithm converges to highly entangled states
exhibiting all the marginal density matrices for states of one, two, three qubits completely
mixed. In particular, we discovered the new state of high entanglement,

$$Ψ_{6qb} = \frac{1}{\sqrt{2^6}} (|000000⟩ + |111111⟩ + |000011⟩ + |111000⟩ + |001011⟩ + |110100⟩ + |010100⟩ + |101011⟩ + |011000⟩ + |100111⟩ + |010010⟩ + |101101⟩ + |001111⟩ + |110000⟩ + |110110⟩ + |010110⟩ + |100011⟩ + |011000⟩ + |101011⟩ + |001000⟩ + |110101⟩ + |000111⟩ + |100010⟩ + |001100⟩ + |111001⟩ + |011100⟩ + |110011⟩ + |000101⟩ + |100101⟩ + |010001⟩ + |110010⟩ + |010101⟩ + |101010⟩ + |011011⟩ + |101101⟩ + |001110⟩ + |111010⟩ + |011101⟩ + |101110⟩ + |001011⟩ + |100110⟩ + |010111⟩ + |110000⟩ + |011011⟩ + |101000⟩ + |001101⟩ + |110001⟩) \quad (9)$$

which, to the best of our knowledge, has not yet been reported in the literature. This state has
a rather simple structure, with all its coefficients (when expanded in the computational basis)
equal to 0 or ±1 (the same situation occurs for maximally entangled states of two, three, four
and five qubits).

4.2.4. Seven qubits. When we ran the search program for 7-qubit states of high entanglement
we found states with the following features. They all have completely mixed single-qubit
marginal density matrices. However, these states do not exhibit completely mixed 2-qubit
and 3-qubit marginal density matrices (in this sense, the present situation seems to have some
similarities with the 4-qubit case).
The high entanglement states of seven qubits that we found are characterized by 2-qubit marginal density matrices exhibiting the following entropic values:

\[
1 - \text{Tr}(\rho_i^2) = 0.744\,511\,1988 \\
S_{VN}(\rho_i) = 1.984\,1042 \\
S_{Re}^{q \to \infty}(\rho_i) = 1.248\,122\,309.
\]  

(10)  

(11)  

(12)

The 3-qubit marginal density matrices of these 7-qubit states have

\[
1 - \text{Tr}(\rho_i^2) = 0.862\,090\,188\,86 \\
S_{VN}(\rho_i) = 2.937\,397\,88 \\
S_{Re}^{q \to \infty}(\rho_i) = 1.471\,265\,9418.
\]  

(13)  

(14)  

(15)

When running our program (maximizing either \(E_{VN}\) or \(E_N\)) for 5-qubit or 6-qubit states, the search process always leads to a state whose marginal density matrices of one, two and (in the six-qubit case) three qubits are completely mixed. In contrast, this never happens when running our algorithm for 7-qubit states. The marginal density matrices of 1-qubit subsystems turn out to be maximally mixed, but not the marginal density matrices corresponding to subsystems consisting of two or three qubits. Moreover, all the runs of the algorithm for 7-qubit states yielded states with the same entropic values for the marginal statistical operators. This suggests that the case of seven qubits may have some similarities with the case of four qubits. In other words, our results constitute numerical evidence supporting the following conjecture.

**Conjecture 1.** There is no pure state of seven qubits whose marginal density matrices for subsystems of one, two or three qubits are all completely mixed.

4.2.5. The single-qubit reduced states conjecture. It was conjectured by Brown et al [14] that multiqubit states of maximum entanglement always have all their single-qubit marginal density matrices completely mixed. The results obtained by us when running the search algorithm maximizing the \(E_{VN}\) and \(E_N\) measures are consistent with the aforementioned conjecture. All the states yielded by the searching algorithm (up to systems of seven qubits) have maximally mixed single-qubit marginal density matrices. Moreover, in the case of five qubits all the states obtained also exhibited maximally mixed 2-qubit marginal density matrices. In the case of six qubits, all the states obtained had completely mixed marginal density matrices of one, two and three qubits.

5. Conclusions

In the present effort, we have investigated some aspects of the entanglement properties of multiqubit systems. We have considered global, multiqubit entanglement measures based upon the idea of considering all the possible bi-partitions of the system. For each bi-partition we computed a bi-partite entanglement measure (such as the von Neumann entropy of the marginal density matrix associated with the subsystem with a Hilbert space of lower dimensionality) and then summed the measures associated with all the bi-partitions. This approach has been widely used in the recent literature. In order to evaluate the bi-partite contributions, we considered four different quantities: the von Neumann, linear and Renyi (with \(q \to \infty\)) entropies and the negativity. Consequently, we have considered four entanglement measures.
We determined numerically, for the aforementioned four measures, the distributions of entanglement values in the Hilbert spaces of pure states of three, four and five qubits. This allowed us to determine, for instance, the entanglement status of special states (such as the $|\text{GHZ}\rangle$ state) with respect to the bulk of the state space.

We also determined, for systems of four, five, six and seven qubits, states of high entanglement using a search scheme akin, but not identical to, the one recently advanced by Brown et al. These authors performed the search process using an entanglement measure based on the negativity. We investigated the behavior of the search processes based on four different measures: the negativity, and the von Neumann, linear, and Renyi (with $q \to \infty$) entropies of the marginal density matrices associated with a bi-partition. The results obtained by us have some interesting features when compared with those reported by Brown et al. First of all, we found that a search algorithm based on the von Neumann entropy is as successful as that based upon negativity. However, the von Neumann entropy is (in general) considerably less expensive to compute than the negativity. Consequently, when initializing the search process with a pure state, it is better to use the von Neumann entropy.

In the case of states of four qubits, Brown et al. reported that their search algorithm always converged (up to local unitary transformations) to a state (here called the BSSB4 state) exhibiting less entanglement than the HS state. In contrast, our algorithm always converged to states exhibiting the same entanglement measures as those characterizing the HS state. Our results thus provide further support to the conjecture advanced by Higuchi and Sudbery that the HS state corresponds to a global entanglement maximum for 4-qubit states. Another interesting finding, going beyond the results of Brown et al., is a particular state of six qubits (discovered using our search algorithm) that has all its marginal density matrices of one, two and three qubits completely mixed. It is interesting that (in the computational basis) all the coefficients characterizing this state are (up to a global normalization constant) equal to 0 or $\pm 1$.

Finally, on the basis of the numerical evidence obtained by us when running our search algorithm for highly entangled states of seven qubits, we make the conjecture that there is no pure state of seven qubits whose marginal density matrices for subsystems of one, two or three qubits are all completely mixed.

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Appendix A

In this appendix, we present the explicit expressions for some of the states that we have introduced in the previous sections. To give the expression of a state $|\Psi\rangle$ we list the values of the coefficients $C_i$ appearing in the expansion $|\Psi\rangle = \sum C_i |i\rangle$ of the alluded state in the computational basis $\{|i\rangle\}$. 
### Table 3. Coefficients for the 4-qubit state maximizing the entanglement measure based on the Renyi entropy. This state does not maximize any other entanglement measure.

| $i$  | $C_i$ |
|------|-------|
| 0    | $(0.337 140 676 904 686, 0.174 693 405 076 796)$ |
| 1    | $(3.860 442 882 346 969 \times 10^{-02}, 6.837 682 483 380 016 \times 10^{-02})$ |
| 2    | $(5.962 390 590 615 981 \times 10^{-02}, 0.130 590 439 038 055)$ |
| 3    | $(3.780 903 708 091 862 \times 10^{-02}, 0.283 134 470 302 957)$ |
| 4    | $(0.128 308 013 031 141, 0.160 044 519 815 334)$ |
| 5    | $(-4.976 588 113 149 925 \times 10^{-02}, -0.156 794 899 004 251)$ |
| 6    | $(0.150 158 286 657 780, -0.269 632 673 631 216)$ |
| 7    | $(-0.284 880 375 838 561, 4.364 132 887 880 368 \times 10^{-02})$ |
| 8    | $(-0.291 078 649 973 983, -0.122 251 701 129 522)$ |
| 9    | $(8.597 952 221 078 008 \times 10^{-02}, -0.132 269 103 402 589)$ |
| 10   | $(-0.184 679 774 192 993, -3.521 179 357 675 151 \times 10^{-02})$ |
| 11   | $(-7.859 668 707 973 404 \times 10^{-02}, 0.285 246 180 204 626)$ |
| 12   | $(-3.120 148 147 808 102 \times 10^{-02}, 3.966 923 168 894 761 \times 10^{-02})$ |
| 13   | $(-0.352 475 250 278 756, -0.170 787 520 712 258)$ |
| 14   | $(2.666 941 273 479 068 \times 10^{-02}, -0.244 143 026 082 971)$ |
| 15   | $(0.176 830 325 000 684, -7.078 443 862 056 820 \times 10^{-02})$ |

### Table 4. Coefficients for the 7-qubit state maximizing the von Neumann entropy based entanglement measure. It also maximizes the rest of the entanglement measures used in this paper.

| $i$  | $C_i$ |
|------|-------|
| 0    | $(1.992 268 895 612 789 \times 10^{-02}, -2.048 153 299 374 923 \times 10^{-02})$ |
| 1    | $(5.733 894 334 752 334 \times 10^{-02}, 4.973 994 982 020 743 \times 10^{-03})$ |
| 2    | $(-4.620 635 677 624 599 \times 10^{-02}, 9.889 188 153 518 157 \times 10^{-02})$ |
| 3    | $(0.114 773 068 934 711, 7.803 541 807 299 509 \times 10^{-02})$ |
| 4    | $(9.358 057 357 464 943 \times 10^{-03}, 8.773 453 311 011 471 \times 10^{-02})$ |
| 5    | $(-4.517 771 306 482 277 \times 10^{-02}, 7.317 172 187 520 525 \times 10^{-02})$ |
| 6    | $(7.148 596 275 123 295 \times 10^{-02}, -6.486 415 242 189 469 \times 10^{-02})$ |
| 7    | $(8.095 549 161 110 917 \times 10^{-02}, 6.281 081 599 967 211 \times 10^{-02})$ |
| 8    | $(-0.110 934 833 126 726, -6.540 485 101 339 541 \times 10^{-02})$ |
| 9    | $(4.243 711 009 834 195, 0.111 608 997 849 607)$ |
| 10   | $(-5.324 057 236 738 998 \times 10^{-02}, -1.064 133 868 681 598 \times 10^{-02})$ |
| 11   | $(-3.199 776 618 312 627 \times 10^{-02}, 1.480 812 105 331 856 \times 10^{-02})$ |
| 12   | $(-3.484 102 446 829 533 \times 10^{-02}, 6.505 443 761 669 717 \times 10^{-02})$ |
| 13   | $(6.659 331 311 799 828 \times 10^{-02}, 2.520 078 454 850 319 \times 10^{-02})$ |
| 14   | $(2.127 875 261 481 843 \times 10^{-02}, -8.620 489 194 999 095 \times 10^{-03})$ |
| 15   | $(3.763 178 050 938 378 \times 10^{-02}, -3.257 033 322 657 695 \times 10^{-02})$ |
| 16   | $(-9.639 113 945 809 372 \times 10^{-02}, -8.706 895 542 690 339 \times 10^{-02})$ |
| 17   | $(7.213 494 811 044 056 \times 10^{-02}, 1.637 328 607 897 790 \times 10^{-02})$ |
| 18   | $(3.347 204 156 200 859 \times 10^{-03}, -4.540 542 385 699 349 \times 10^{-02})$ |
| 19   | $(5.235 538 552 827 945 \times 10^{-02}, -5.539 353 156 272 388 \times 10^{-02})$ |
| 20   | $(-5.734 329 608 600 269 \times 10^{-02}, -3.334 326 701 130 044 \times 10^{-02})$ |
| 21   | $(-2.042 578 560 682 204 \times 10^{-02}, -0.106 743 556 238 253)$ |
| 22   | $(-5.987 692 237 756 689 \times 10^{-02}, -5.035 304 599 306 584 \times 10^{-02})$ |
| 23   | $(3.304 680 530 465 200 \times 10^{-02}, 9.449 073 856 519 782 \times 10^{-02})$ |
| 24   | $(2.843 182 057 391 498 \times 10^{-02}, -2.453 794 986 457 519 \times 10^{-02})$ |
| 25   | $(-1.316 539 219 004 622 \times 10^{-02}, -4.912 228 258 199 161 \times 10^{-02})$ |
| $i$ | $C_i$ |
|-----|-------|
| 26  | $(-5.889 \times 10^{-2}, 7.627 \times 10^{-2}, 3.762 \times 10^{-2})$ |
| 27  | $(-9.712 \times 10^{-2}, 1.793 \times 10^{-2}, 3.940 \times 10^{-2})$ |
| 28  | $(0.101, 3.940, 7.627) \times 10^{-2}$ |
| 29  | $(8.351 \times 10^{-2}, -8.055 \times 10^{-2}, -8.351 \times 10^{-2})$ |
| 30  | $(3.447 \times 10^{-2}, -6.113 \times 10^{-2}, -6.113 \times 10^{-2})$ |
| 31  | $(9.951 \times 10^{-2}, 5.755 \times 10^{-2}, 9.725 \times 10^{-2})$ |
| 32  | $(-8.560 \times 10^{-2}, -4.371 \times 10^{-2}, -4.371 \times 10^{-2})$ |
| 33  | $(1.790 \times 10^{-2}, -4.609 \times 10^{-2}, -4.609 \times 10^{-2})$ |
| 34  | $(0.101, 6.494, 2.427) \times 10^{-2}$ |
| 35  | $(-2.247 \times 10^{-2}, 4.864 \times 10^{-2}, 4.864 \times 10^{-2})$ |
| 36  | $(-0.101, 3.782, 3.782) \times 10^{-2}$ |
| 37  | $(-3.152, 0.122, 0.122) \times 10^{-2}$ |
| 38  | $(3.278, 1.441, 1.441) \times 10^{-2}$ |
| 39  | $(5.216, 6.977, 6.977) \times 10^{-2}$ |
| 40  | $(8.224, 8.627, 8.627) \times 10^{-2}$ |
| 41  | $(0.154, 8.632, 8.632) \times 10^{-2}$ |
| 42  | $(7.332, -1.371, -1.371) \times 10^{-2}$ |
| 43  | $(5.208, -1.411, -1.411) \times 10^{-2}$ |
| 44  | $(3.590, 4.647, 4.647) \times 10^{-2}$ |
| 45  | $(8.697, 1.482, 1.482) \times 10^{-2}$ |
| 46  | $(1.092, 4.129, 4.129) \times 10^{-2}$ |
| 47  | $(7.674, -5.338, -5.338) \times 10^{-2}$ |
| 48  | $(-6.251, 6.425, 6.425) \times 10^{-2}$ |
| 49  | $(-8.520, -7.709, -7.709) \times 10^{-2}$ |
| 50  | $(-3.438, -2.955, -2.955) \times 10^{-2}$ |
| 51  | $(-5.277, 1.299, 1.299) \times 10^{-2}$ |
| 52  | $(0.108, 8.086, -8.086) \times 10^{-2}$ |
| 53  | $(8.106, 3.606, 3.606) \times 10^{-2}$ |
| 54  | $(1.202, 3.058, 3.058) \times 10^{-2}$ |
| 55  | $(2.485, 9.667, 9.667) \times 10^{-2}$ |
| 56  | $(6.171, -9.833, -9.833) \times 10^{-2}$ |
| 57  | $(8.806, -3.526, -3.526) \times 10^{-2}$ |
| 58  | $(6.854, -6.411, -6.411) \times 10^{-2}$ |
| 59  | $(2.066, 1.612, 1.612) \times 10^{-2}$ |
| 60  | $(1.438, 0.124, 0.124) \times 10^{-2}$ |
| 61  | $(-5.074, -5.439, -5.439) \times 10^{-2}$ |
| 62  | $(3.640, 4.594, 4.594) \times 10^{-2}$ |
| 63  | $(3.550, 8.695, 8.695) \times 10^{-2}$ |
| 64  | $(-4.773, -3.667, -3.667) \times 10^{-2}$ |
| 65  | $(2.346, -0.119, -0.119) \times 10^{-2}$ |
| 66  | $(1.493, 4.553, 4.553) \times 10^{-2}$ |
| 67  | $(5.034, 8.124, 8.124) \times 10^{-2}$ |
| 68  | $(6.802, 8.317, 8.317) \times 10^{-2}$ |
Table 4. (Continued.)

| $i$  | $C_i$                        |
|------|------------------------------|
| 77   | $(6.283 \times 10^{-02})$, $6.514 \times 10^{-02}$ |
| 78   | $(0.127 \times 10^{-02})$, $0.118 \times 10^{-02}$ |
| 79   | $(-9.788 \times 10^{-02})$, $5.354 \times 10^{-02}$ |
| 80   | $(0.117 \times 10^{-02})$, $-3.417 \times 10^{-02}$ |
| 81   | $(-9.256 \times 10^{-02})$, $-2.768 \times 10^{-02}$ |
| 82   | $(-7.424 \times 10^{-02})$, $0.671 \times 10^{-02}$ |
| 83   | $(-5.515 \times 10^{-02})$, $0.293 \times 10^{-02}$ |
| 84   | $(-3.028 \times 10^{-02})$, $0.429 \times 10^{-02}$ |
| 85   | $(-1.454 \times 10^{-02})$, $0.794 \times 10^{-02}$ |
| 86   | $(-7.121 \times 10^{-02})$, $-4.438 \times 10^{-02}$ |
| 87   | $(-3.980 \times 10^{-02})$, $8.143 \times 10^{-02}$ |
| 88   | $(8.912 \times 10^{-02})$, $1.389 \times 10^{-02}$ |
| 89   | $(9.484 \times 10^{-02})$, $-5.878 \times 10^{-02}$ |
| 90   | $(0.117 \times 10^{-02})$, $0.117 \times 10^{-02}$ |
| 91   | $(-1.169 \times 10^{-02})$, $-6.947 \times 10^{-02}$ |
| 92   | $(-6.798 \times 10^{-02})$, $-7.747 \times 10^{-02}$ |
| 93   | $(1.740 \times 10^{-02})$, $-1.809 \times 10^{-02}$ |
| 94   | $(1.885 \times 10^{-02})$, $0.631 \times 10^{-02}$ |
| 95   | $(7.520 \times 10^{-02})$, $0.446 \times 10^{-02}$ |
| 96   | $(0.117 \times 10^{-02})$, $3.066 \times 10^{-02}$ |
| 97   | $(1.127 \times 10^{-02})$, $-2.081 \times 10^{-02}$ |
| 98   | $(1.977 \times 10^{-02})$, $4.839 \times 10^{-02}$ |
| 99   | $(-0.146 \times 10^{-02})$, $1.841 \times 10^{-02}$ |
| 100  | $(2.485 \times 10^{-02})$, $-9.063 \times 10^{-02}$ |
| 101  | $(0.132 \times 10^{-02})$, $-5.308 \times 10^{-02}$ |
| 102  | $(4.288 \times 10^{-02})$, $7.033 \times 10^{-02}$ |
| 103  | $(4.876 \times 10^{-02})$, $-1.428 \times 10^{-02}$ |
| 104  | $(-3.244 \times 10^{-02})$, $8.121 \times 10^{-02}$ |
| 105  | $(2.899 \times 10^{-02})$, $0.286 \times 10^{-02}$ |
| 106  | $(5.009 \times 10^{-02})$, $-6.852 \times 10^{-02}$ |
| 107  | $(4.883 \times 10^{-02})$, $3.673 \times 10^{-02}$ |
| 108  | $(1.583 \times 10^{-02})$, $0.010 \times 10^{-02}$ |
| 109  | $(3.537 \times 10^{-02})$, $0.010 \times 10^{-02}$ |
| 110  | $(0.149 \times 10^{-02})$, $1.152 \times 10^{-02}$ |
| 111  | $(2.681 \times 10^{-02})$, $-2.650 \times 10^{-02}$ |
| 112  | $(0.099 \times 10^{-02})$, $-7.483 \times 10^{-02}$ |
| 113  | $(2.407 \times 10^{-02})$, $-2.929 \times 10^{-02}$ |
| 114  | $(3.702 \times 10^{-02})$, $5.284 \times 10^{-02}$ |
| 115  | $(-4.628 \times 10^{-02})$, $7.345 \times 10^{-02}$ |
| 116  | $(0.107 \times 10^{-02})$, $0.106 \times 10^{-02}$ |
| 117  | $(4.763 \times 10^{-02})$, $1.908 \times 10^{-02}$ |
| 118  | $(0.116 \times 10^{-02})$, $-4.314 \times 10^{-02}$ |
| 119  | $(6.120 \times 10^{-02})$, $-3.887 \times 10^{-02}$ |
| 120  | $(3.457 \times 10^{-02})$, $-7.568 \times 10^{-02}$ |
| 121  | $(6.046 \times 10^{-02})$, $-3.864 \times 10^{-02}$ |
| 122  | $(3.125 \times 10^{-02})$, $0.017 \times 10^{-02}$ |
| 123  | $(1.191 \times 10^{-02})$, $3.655 \times 10^{-02}$ |
| 124  | $(-2.612 \times 10^{-02})$, $-5.303 \times 10^{-02}$ |
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