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Highly entangled multi-qubit states with simple algebraic structure

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Abstract

Recent works by Brown *et al* (2005 *J. Phys. A: Math. Gen.* **38** 1119) and Borras *et al* (2007 *J. Phys. A: Math. Theor.* **40** 13407) have explored numerical optimization procedures to search for highly entangled multi-qubit states according to some computationally tractable entanglement measure. We present an alternative scheme based upon the idea of searching for states having not only high entanglement but also simple algebraic structure. We report results for 4, 5, 6, 7 and 8 qubits discovered by this approach, showing that *many* of such states do exist. In particular, we find a maximally entangled 6-qubit state with an algebraic structure simpler than the best results known so far. For the case of 7 qubits, we discover states with high, but not maximum, entanglement and simple structure, as well as other desirable properties. Some preliminary results are shown for the case of 8 qubits.

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1. Introduction

The concept of entanglement is intimately related to the mathematical structure of quantum mechanics, particularly as a direct consequence of linearity in tensor product Hilbert spaces. Apart from its theoretical relevance as one (if not the most) of the striking features of quantum mechanics, entanglement has been shown to enable (and play a crucial role in) practical applications such as teleportation protocols and superdense coding. It is, for this reason, often regarded as a *resource* which needs to be studied from several standpoints.

A considerable amount of research has been devoted to unveiling the mathematical structures underlying entanglement, in particular concerning its *quantification*. Properties for a good entanglement measure are reviewed and discussed in [8, 9, 15]. An alternative to the analytic approach was presented by Brown *et al* [4] and later by Borras *et al* [1].

Both works explore the application of numerical optimization techniques to search for highly entangled multi-qubit states.

In the work of Brown *et al* [4], the search is applied over the set of mixed states using the negativity of the partial transpose as a measure of entanglement. The search procedure is basically a hill-climbing algorithm with some adjustments. Such a simple form of search suffices, as the cost function which is sought to maximize (i.e. the entanglement as defined by the negativity) is known to be convex. Among the results reported are the following two 5-qubit states:

$$|\Psi''\rangle = \frac{1}{2\sqrt{2}}(|00110\rangle + |01011\rangle + |10001\rangle + |11100\rangle + i(|00101\rangle + |01000\rangle + |10010\rangle + |11111\rangle)) \tag{1}$$

$$|\Psi'''\rangle = \frac{1}{2\sqrt{2}}(|00110\rangle + |01001\rangle + |10101\rangle + |11010\rangle + i(|00000\rangle + |01111\rangle + |10011\rangle + |11100\rangle)) \tag{2}$$

which are essentially equivalent and can be reformulated as

$$|\psi_5\rangle = \tfrac{1}{2}(|001\rangle|\Phi_-\rangle + |010\rangle|\Psi_-\rangle + |100\rangle|\Phi_+\rangle + |111\rangle|\Psi_+\rangle), \tag{3}$$

where $|\Psi_\pm\rangle = \frac{1}{\sqrt{2}}|00\rangle \pm |11\rangle$ and $|\Phi_\pm\rangle = \frac{1}{\sqrt{2}}|01\rangle \pm |10\rangle$. The state $|\psi_5\rangle$ achieves the maximum possible entanglement according to the negativity measure. Muralidharan and Panigrahi [12, 13] have recently investigated the usefulness of this state for quantum teleportation, superdense coding and quantum secret sharing. In particular, perfect teleportation of arbitrary 1- and 2-qubit systems is possible, as well as superdense coding of 5 classical bits by using three qubits. (Incidentally, it is also shown how to physically produce this state in a relatively easy manner.)

In the work of Borras *et al* [1], the search is restricted to pure states of 4, 5, 6 and 7 qubits, and several measures of entanglement are investigated. The overall search algorithm is very similar to the hill-climbing scheme employed by Brown *et al*, and the authors also explore the statistical distribution of entanglement for systems of the sizes aforementioned. In the case of 6 qubits, they discovered the state

$$\begin{aligned}|\psi_6\rangle = \frac{1}{\sqrt{32}}(&|000000\rangle + |111111\rangle + |000011\rangle + |111100\rangle + |000101\rangle\\ &+ |111010\rangle + |000110\rangle + |111001\rangle + |001001\rangle + |110110\rangle\\ &+ |001111\rangle + |110000\rangle + |010001\rangle + |101110\rangle + |010010\rangle\\ &+ |101101\rangle + |011000\rangle + |100111\rangle + |011101\rangle + |100010\rangle\\ &- (|001010\rangle + |110101\rangle + |001100\rangle + |110011\rangle + |010100\rangle\\ &+ |101011\rangle + |010111\rangle + |101000\rangle + |011011\rangle + |100100\rangle\\ &+ |011110\rangle + |100001\rangle))\end{aligned} \tag{4}$$

which, as in the case of Brown *et al*'s $|\psi_5\rangle$, possesses a rather simple structure and maximum entanglement according to several measures. Choudhury *et al* [5] have also found various applications for this state, namely quantum teleportation of an arbitrary 3-qubit state and quantum state sharing of an arbitrary 2-qubit state.

In the case of 7 qubits, the authors report a highly entangled state (approximately 155.812 856, according to the negativity measure) with, apparently, no simple structure. The state is given as a list of 128 complex numbers corresponding to the coefficients of the superposition, and has all the 1-qubit density matrices completely mixed, but not the 2- and 3-qubit ones.

1.1. Motivation

Apart from theoretical repercussion, genuinely entangled states of 5 and 6 qubits have found practical applications, and new protocols based on them have been derived. In the case of 7 qubits, it is not known how to write 'nicely' the state(s) reported by Borras *et al*. This lack of structure may be a drawback in deriving protocols based on it.

The search schemes described above have proven to be very successful, but the resulting states can be difficult to process manually. In this work, we present an alternative formulation of the search where not only high entanglement is sought, but also some desired structure is imposed on the form of the outcome. As a proof-of-concept, we show how highly entangled states with a very compact form can easily be found.

2. Computationally feasible entanglement measures

All the numerical optimization approaches aforementioned rely directly upon the use of a computationally tractable measure of entanglement. For completeness and readability, we next provide a brief introduction to some of them, and particularly to the measure used in this paper. For a more in-depth treatment of the subject, we refer the reader to [8, 9, 15].

The degree of *bipartite* entanglement of a composite quantum system can be quantified in terms of the purity (or mixedness) of the reduced density matrix of one of the two subsystems: the lower the purity (or the higher the mixedness), the higher the entanglement. There is not, however, a unique way of extending this notion to systems composed of more than two subsystems. A natural alternative is to quantify multipartite entanglement among n parties as a function of the mixedness of *all* the possible bipartitions of the whole system. A common, though not unique, approach is to take the sum of the individual entanglement measures associated with the $2^{n-1}-1$ possible bipartitions of an n-qubit system [1, 4]

$$E(\rho) = \sum_s E_B(\rho_s), \tag{5}$$

where ρ is the density matrix of the n-qubit system, ρ_s is the reduced density matrix associated with subsystem s, and the sum is taken over all the possible bipartions. Common examples of bipartite entanglement measures E_B are:

(i) the linear entropy: $S_L(\rho) = 1 - \mathrm{Tr}(\rho^2)$,
(ii) the von Neumann entropy: $S_{\mathrm{VN}}(\rho) = -\mathrm{Tr}(\rho \log_2 \rho)$,
(iii) the Renyi entropy with $q \to \infty$: $S_{\mathrm{Re}}^{q\to\infty}(\rho) = -\ln\lambda_k^{\max}$, λ_k being the eigenvalues of ρ.

All these entropic measures constitute clear examples of computationally feasible measures of entanglement for *pure* states. They cannot, however, distinguish between classical and quantum correlations, and so their use for mixed states is quite limited.

Brown *et al* developed in [4] an entanglement measure for mixed states based on the negative partial transpose (NPT) criterion, which establishes as a necessary condition for separability of any density matrix that it has only non-negative eigenvalues [14]. Details about how to compute the partial transpose can be found in [4].

The *negativity*, first introduced in [17] and subsequently explored in [1, 4, 10, 16], is defined as the sum of all the negative eigenvalues of the $2^{n-1}-1$ partial transposes. The result if often negated in order to have a positive measure. We will refer to this measure as E_{NPT}. In some cases, it is convenient to have a measure normalized between 0 and 1, which can be achieved by dividing by the maximum possible entanglement. Upper bounds for the four entanglement measures discussed above can be derived by considering a hypothetical n-qubit pure state such that all its marginal density matrices are completely mixed [1]. In the case of

Table 1. Upper bounds for $|\mathbb{S}^n(V)|$ for some values of n and $|V|$.

	Number of qubits				
$\lvert V\rvert$	4	5	6	7	8
5	$2^{37.1}$	$2^{74.3}$	$2^{148.6}$	$2^{297.2}$	$2^{594.4}$
7	$2^{44.9}$	$2^{89.8}$	$2^{179.7}$	$2^{359.3}$	$2^{718.7}$
9	$2^{50.7}$	$2^{101.4}$	$2^{202.9}$	$2^{405.7}$	$2^{811.5}$
11	$2^{55.3}$	$2^{110.7}$	$2^{221.4}$	$2^{442.8}$	$2^{885.6}$
13	$2^{59.2}$	$2^{118.4}$	$2^{236.8}$	$2^{473.6}$	$2^{947.3}$

E_{NPT}, this maximum is 1.5, 6.5, 17.5, 60.5, 157.5, 504.5, 1297.5, ... for systems composed of 3, 4, 5, 6, 7, 8, 9, ... qubits. We will denote by $E_{\mathrm{NPT}}^{\mathrm{norm}}$ the normalized entanglement.

3. Searching for simplicity

3.1. Search space

We want to search for pure states having high entanglement and *simple* algebraic structure. There is not, however, a unique way to define what 'simple' means, and some of such definitions might not be computationally appropriate. For the purposes of this work, simple states will be those which can be written in a 'nice' way with respect to a given basis, i.e. states of the form

$$|\psi\rangle = \frac{1}{K}\sum_{i=0}^{2^n-1} c_i|i\rangle, \qquad (6)$$

where only a few of the coefficients c_i are non-null and, in turn, are nice to write (e.g. ± 1, $\pm i$, $\pm(1 \pm i)$,...). Even though this is quite an arbitrary definition of simplicity, it captures well the intuitive idea of what a nice-to-write state means, and, more importantly, provides a *measurable* way to determine how simple a state is, a crucial property if we are to somehow incorporate such an aspect into the search.

For the purposes of this paper, the space of 'simple' states will be given by

$$\mathbb{S}^n(V) = \left\{|\psi\rangle = \frac{1}{K}\sum_{i=0}^{2^n-1} c_i|i\rangle : c_i \in V\right\}, \qquad (7)$$

where $1/K$ is the appropriate normalization factor. The size and properties of such a space[3] strongly depend on the set V of allowed coefficients. Three examples that will be used later are $V_3 = \{0, \pm 1\}$, $V_5 = \{0, \pm 1, \pm i\}$ and $V_9 = \{0, \pm 1, \pm i, \pm(1 \pm i)\}$.

Using a simple counting argument it is not difficult to see that the size of the search space is $|\mathbb{S}^n(V)| = |V|^{2^n}$. Note, however, that some states might actually be identical up to some global phase, and therefore the previous expression is actually an upper bound on the number of useful states. The exact amount of indistinguishable states depends on the particular elements in the set V, and we will not be generally concerned about them. Table 1 shows the size of the search space for the number of qubits considered in this work and for some small values of $|V|$. The combinatorial explosion is easily recognizable in these figures, and any attempt of search by enumeration is beyond our current computational resources even for small values.

[3] Note that 'space' is used here as in 'search space' and not as in 'Hilbert space', as $\mathbb{S}^n(V)$ might not always be 1.

3.2. Fitness function

A good fitness (or cost) function should provide *guidance* through the search space towards the desired solutions, regardless of whether or not its numerical values are related to the actual cost or benefit of particular solutions. As we are interested in states having high entanglement and as many null coefficients as possible, a natural choice for the fitness function is to explicitly reward both features. We have used a fitness function of the form

$$F|\psi\rangle = E_{\mathrm{NPT}}^{\mathrm{norm}}|\psi\rangle\langle\psi| - \alpha\left(\frac{N|\psi\rangle}{2^n}\right), \tag{8}$$

where

$$N\left(\sum_{i=0}^{2^n-1} c_i|i\rangle\right) = \#\{c_i : |c_i| \neq 0\} \tag{9}$$

and $\alpha \in [0, 1]$ is a punishing factor. The term $E_{\mathrm{NPT}}^{\mathrm{norm}}|\psi\rangle\langle\psi|$ simply computes the entanglement as measured by the NPT, while the right part counts the percentage of non-null coefficients in the superposition. Note that both terms are normalized in the interval [0, 1], so α admits a natural interpretation as how much punishment is placed on the amount on non-null coefficients. Other variations around the same idea are of course possible.

3.3. Move function

The move function determines which states are reachable from a given one at any point of the search. We have defined a move function consisting of randomly choosing one of the 2^n coefficients of the state, c_i, and another, c_j, from V such that $c_i \neq c_j$. The coefficient c_i is replaced by c_j and the state vector is then renormalized. Note that each state vector has exactly $2^n(|V| - 1)$ different[4] neighbours. We will write $|\phi\rangle \leftarrow \mathrm{Move}|\psi\rangle$ to denote that state $|\phi\rangle$ is the result of moving state $|\psi\rangle$.

3.4. Search procedure

It is well known that the negativity cost function is convex [16] and its smoothness provides us with a relatively easy-to-walk search landscape. In particular, its convexity for mixed states implies that there is no chance for the search of being caught in a local optimum, even though the case for pure states is less clear. However, the trade-off between entanglement and simplicity contained in expression (8) translates into a more rugged search landscape, with lower correlation between the fitness of neighbour state vectors and, therefore, a substantial increase in the number and distribution of local optima. This suggests that very simple forms of search as those used in previous works (basically hill-climbing algorithms) are not likely to be appropriate in this case. We have verified experimentally this fact and concluded that a more powerful search technique is necessary.

Simulated annealing [11] is a well-known search heuristic inspired by the cooling processes of molten metals. It can be seen as a basic hill-climbing coupled with the probabilistic acceptance of non-improving solutions. This mechanism allows a local search that eventually can escape from local optima.

The search starts at some initial state (solution) $|\psi\rangle \in_R \mathbb{S}^n$. The algorithm employs a control parameter $T \in \mathbb{R}^+$ known as the 'temperature'. This starts at some positive value T_0 and is gradually lowered at each iteration, typically by geometric cooling: $T_{i+1} = \beta T_i$, $\beta \in [0, 1]$. At each temperature, a number MIL (Moves in Inner Loop) of neighbour states are attempted.

[4] As discussed above, some of them might be identical up to a global phase.

A candidate state $|\phi\rangle$ in the neighbourhood of $|\psi\rangle$ is obtained by applying the move function. The new state is always accepted if it is better than $|\psi\rangle$. To escape from local optima, the technique also accepts candidates which are slightly worse than the current state, meaning that its fitness is no more than $|T \ln U|$ lower, with U being a uniform random variable in (0, 1). As T is gradually lowered, this term gets closer to 0 and it becomes harder to accept worse moves.

The algorithm terminates when some stopping criterion is met, usually after executing a fixed number of inner loops or when some maximum number of consecutive inner loops without improvements have been reached. The basic algorithm is shown as follows:

$|\psi\rangle \in_R \mathbb{S}^n$
$|\psi^{\max}\rangle \leftarrow |\psi\rangle$
$T \leftarrow T_0$
repeat until stopping criterion is met
    repeat MIL *times*
        $|\phi\rangle \leftarrow \text{Move}|\psi\rangle$
        $U \in_R (0, 1)$
        if $F|\phi\rangle > F|\psi\rangle + T \ln U$ *then*
            $|\psi\rangle \leftarrow |\phi\rangle$
            if $F|\psi\rangle > F|\psi^{\max}\rangle$ *then*
                $|\psi^{\max}\rangle \leftarrow |\psi\rangle$
            endif
        endif
    endrepeat
    $T \leftarrow \beta T$
endrepeat
return $|\psi^{\max}\rangle$.

3.5. Implementation

The search scheme described above was implemented in C++, using the GNU Scientific Library [6] for complex numbers, matrix manipulations, pseudorandom number generation, eigenvalues, etc.

4. Results

We next present and discuss some results obtained for systems of 4, 5, 6, 7 and 8 qubits. A couple of states are shown for each case. These are representative of the typical outcome of the search, but *many* others have been produced by the technique.

In all the cases, the search algorithm is parameterized with 1000 moves in the internal loop (MIL) and a stop criterion consisting of 10 consecutive internal loops without improvement. For the number of qubits studied, the best results are achieved with α between 0.1 and 0.3, a starting temperature T_0 between 0.0005 and 0.001, and a cooling rate β between 0.99 and 0.999.

4.1. 4-qubit states

Higuchi and Sudbery proved in [7] that there is no 4-qubit pure state having all its marginal density matrices maximally mixed. Consequently, the theoretically maximum amount of entanglement for systems of 4 qubits (e.g., 6.5 according to the negativity measure) is unachievable. The state

$$|HS\rangle = \frac{1}{\sqrt{6}}(|1100\rangle + |0011\rangle + \omega(|1001\rangle + |0110\rangle) + \omega^2(|1010\rangle + |0101\rangle)) \tag{10}$$

where $\omega = -\frac{1}{2} + \frac{\sqrt{3}}{2}i$ is also reported in [7]. It is conjectured to be maximally entangled, having $E_{\rm NPT}|HS\rangle \approx 6.0981$. Borras *et al* claim in [1] that their search procedure consistently finds states with exactly this same amount of entanglement. In fact, the HS state is known to be a *local* maximum for the von Neumann entropy [3], and some arguments given in [7] suggest that it may have also been a *global* maximum for this measure.

In our experimentation using the set of coefficients V_5 we found the state

$$\left|\psi_4^a\right\rangle = \frac{1}{\sqrt{6}}(|1001\rangle - i(|0000\rangle - |0011\rangle + |0110\rangle + |1100\rangle + |1111\rangle)) \tag{11}$$

$$E_{\rm NPT}\left|\psi_4^a\right\rangle \approx 5.989\,631. \tag{12}$$

This state has 22 negative eigenvalues from 7 partial transposes. For the four single-index cuts, each partial transpose has a single negative eigenvalue of $-\frac{1}{2}$, and all the 1-qubit density matrices are maximally mixed. The 18 two-index partial transposes have a more complex structure, each one having 6 negative eigenvalues. None of the 2-qubit density matrices are maximally mixed.

When using the set V_9 we found the state

$$\begin{aligned}\left|\psi_4^b\right\rangle = \frac{1}{2\sqrt{6}}(&|0001\rangle - |0100\rangle + i(|1011\rangle - |1110\rangle)\\ &+ (1+i)(|0010\rangle + |1101\rangle - |0101\rangle - |0110\rangle - |1010\rangle - |1100\rangle)\\ &+ (1-i)(|1000\rangle + |1001\rangle - |0011\rangle - |0111\rangle))\end{aligned} \tag{13}$$

$$E_{\rm NPT}|\psi_4^b\rangle \approx 6.051\,660. \tag{14}$$

As in the case of $|\psi_4^a\rangle$, this state has 22 negative eigenvalues from 7 partial transposes. The four single-index cuts give a partial transpose with a single negative eigenvalue of $-\frac{1}{2}$, and all the 1-qubit density matrices are maximally mixed. The 18 two-index partial transposes have 6 negative eigenvalues each one. Again, none of the 2-qubit density matrices are maximally mixed.

The HS state is obviously more entangled than $|\psi_4^a\rangle$ and $|\psi_4^b\rangle$, yet both states (particularly the latter) do have a very high entanglement and a rather simple structure. Merely for validation purposes, we also attempted searches including both ω and ω^2 in the set of valid coefficients V. In such cases, the HS state (or states essentially equivalent to it) is easily found.

4.2. 5-qubit states

The search successfully finds 5-qubit states exhibiting maximum entanglement ($E_{\rm NPT} = 17.5$) and a rather simple algebraic structure. The following two, $|\psi_5^a\rangle$ and $|\psi_5^b\rangle$, are particular examples found using coefficients in V_5 and V_9, respectively:

$$\begin{aligned}\left|\psi_5^a\right\rangle = \frac{1}{2\sqrt{2}}(&|01010\rangle + |10011\rangle + |10110\rangle + |11000\rangle\\ &+ i(|00001\rangle - |00100\rangle + |01111\rangle - |11101\rangle))\end{aligned} \tag{15}$$

$$E_{\rm NPT}\left|\psi_5^a\right\rangle = 17.5 \tag{16}$$

$$\left|\psi_5^b\right\rangle = \tfrac{1}{4}((1+i)(|01101\rangle + |01110\rangle - |10100\rangle + |10111\rangle + |11000\rangle + |11011\rangle) + (1-i)(|00001\rangle - |00010\rangle)) \quad (17)$$

$$E_{\mathrm{NPT}}\left|\psi_5^b\right\rangle = 17.5. \quad (18)$$

Both states have 65 negative eigenvalues from 15 partial transposes. For the five single-index cuts, each partial transpose has a single negative eigenvalue of $-\frac{1}{2}$. For the ten two-index cuts, each partial transpose has six negative eigenvalues of $-\frac{1}{4}$. So

$$E_{\mathrm{NPT}}\left|\psi_5^a\right\rangle = E_{\mathrm{NPT}}\left|\psi_5^b\right\rangle = 5\cdot\tfrac{1}{2} + 10\cdot 6\cdot\tfrac{1}{4} = 17.5. \quad (19)$$

All the partial density matrices are completely mixed for both states, i.e. $\mathrm{Tr}(\rho^2) = \frac{1}{2}$ for all the 1-qubit marginal density matrices, and $\mathrm{Tr}(\rho^2) = \frac{1}{4}$ for all the 2-qubit marginal density matrices.

It is not difficult to show that these two states are equivalent under local unitary transformations, and also equivalent to Brown *et al*'s $|\psi_5\rangle$ state given by (3). All the maximally entangled 5-qubit states found in our experimentation have this form.

4.3. 6-qubit states

As with the case of 5 qubits, the search finds maximally entangled ($E_{\mathrm{NPT}} = 60.5$) 6-qubit states having a simple structure. Two examples are provided below

$$\begin{aligned}\left|\psi_6^a\right\rangle = \tfrac{1}{4}(&-|000101\rangle - |001011\rangle - |010001\rangle + |011111\rangle\\ &+ |100000\rangle + |101110\rangle - |110100\rangle + |111010\rangle\\ &+ i(|000110\rangle - |001000\rangle - |010010\rangle - |011100\rangle\\ &+ |100011\rangle - |101101\rangle + |110111\rangle + |111001\rangle))\end{aligned} \quad (20)$$

$$E_{\mathrm{NPT}}\left|\psi_6^a\right\rangle = 60.5 \quad (21)$$

$$\begin{aligned}\left|\psi_6^b\right\rangle = \tfrac{1}{4}(&|011010\rangle - |011111\rangle + |101011\rangle - |101110\rangle\\ &- |110011\rangle - |110110\rangle - |111000\rangle - |111101\rangle\\ &+ i(-|000010\rangle - |000111\rangle + |001001\rangle + |001100\rangle\\ &+ |010001\rangle - |010100\rangle - |100000\rangle + |100101\rangle))\end{aligned} \quad (22)$$

$$E_{\mathrm{NPT}}\left|\psi_6^b\right\rangle = 60.5. \quad (23)$$

Both states have 376 negative eigenvalues from 31 partial transposes. For the 6 single-index cuts, each partial transpose has a single negative eigenvalue of $-\frac{1}{2}$. For the 15 two-index cuts, each partial transpose has 6 negative eigenvalues of $-\frac{1}{4}$. For the 10 three-index cuts, each partial transpose has 28 negative eigenvalues of $-\frac{1}{8}$. So

$$E_{\mathrm{NPT}}\left|\psi_6^a\right\rangle = E_{\mathrm{NPT}}\left|\psi_6^b\right\rangle = 6\cdot\tfrac{1}{2} + 15\cdot 6\cdot\tfrac{1}{4} + 10\cdot 28\cdot\tfrac{1}{8} = 60.5. \quad (24)$$

All the partial density matrices are completely mixed for both states, i.e. $\mathrm{Tr}(\rho^2)$ being $\frac{1}{2}$, $\frac{1}{4}$ and $\frac{1}{8}$ for all the 1-qubit, 2-qubit and 3-qubit marginal density matrices, respectively.

4.3.1. A new 6-qubit state The states given by (20) and (22) are equivalent under local unitary transformations and can be reformulated as

$$|\Psi_6\rangle = \frac{1}{2}(|F_0\rangle|\Psi_-\rangle + |F_1\rangle|\Psi_+\rangle + |F_2\rangle|\Phi_-\rangle + |F_3\rangle|\Phi_+\rangle) \tag{25}$$

with $|F_0\rangle = \frac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle)$, $|F_1\rangle = \frac{1}{\sqrt{2}}(|0011\rangle + |1100\rangle)$, $|F_2\rangle = \frac{1}{\sqrt{2}}(|0110\rangle + |1001\rangle)$ and $|F_3\rangle = \frac{1}{\sqrt{2}}(|0101\rangle + |1010\rangle)$. Note that this state has an elegant description in terms of Bell pairs, since

$$\begin{aligned} &\frac{1}{\sqrt{2}}(|F_0\rangle + |F_1\rangle) = |\Psi_+\rangle|\Psi_+\rangle \\ &\frac{1}{\sqrt{2}}(|F_2\rangle + |F_3\rangle) = |\Phi_+\rangle|\Phi_+\rangle. \end{aligned} \tag{26}$$

This state has arguably a simpler algebraic structure than Borras *et al*'s $|\psi_6\rangle$ given by (4). We postpone for future work a further study of the possible relationships between both states.

4.4. 7-qubit states

It has been pointed out that entanglement in 7-qubit systems might exhibit some similarities with the case of 4 qubits. A conjecture by Borras *et al* [1] establishes that there is no pure state of 7 qubits whose marginal density matrices for subsystems of 1, 2 or 3 qubits are all *completely* mixed. If such a state would exist, its entanglement as measured by the NPT would be 157.5. In [1] it is reported that 7-qubit states with entanglement up to $E_{\mathrm{NPT}} \approx 155.812\,856$ are found. They all have completely mixed single-qubit marginal density matrices, but *not* completely mixed 2- and 3-qubit marginal density matrices.

The results found with our approach are consistent with this numerical evidence. The states $|\psi_7^a\rangle$ and $|\psi_7^b\rangle$ shown below have high (but not maximum) entanglement. Contrarily to the 7-qubit state reported in [1], these states have a remarkably simple structure and, as will be discussed later, totally mixed 1- and 2-qubit marginal density matrices.

The state

$$\begin{aligned} |\psi_7^a\rangle = \frac{1}{4\sqrt{2}}&((1+i)(|0000010\rangle + |1000101\rangle + |1011011\rangle - |0011001\rangle \\ &- |1010000\rangle - |1111101\rangle) + (1-i)(|0001100\rangle + |0010111\rangle \\ &+ |0100001\rangle + |0101111\rangle + |0110100\rangle + |0111010\rangle + |1001110\rangle \\ &+ |1100011\rangle - |1101000\rangle - |1110110\rangle)) \end{aligned} \tag{27}$$

$$E_{\mathrm{NPT}}|\psi_7^a\rangle = 152.646\,039 \tag{28}$$

has 1113 negative eigenvalues from 63 partial transposes. For the 7 single-index cuts, each partial transpose has a single negative eigenvalue of $-\frac{1}{2}$. For the 21 two-index cuts, each partial transpose has 6 negative eigenvalues of $-\frac{1}{4}$. For 21 out of the 35 three-index cuts, each partial transpose has 28 negative eigenvalues of $-\frac{1}{8}$; the remainder 14 partial transposes have each 28 negative eigenvalues, but different from $-\frac{1}{8}$.

Both the 7 single-qubit and the 21 2-qubit marginal density matrices are all completely mixed, i.e. with $\mathrm{Tr}(\rho^2)$ being $\frac{1}{2}$ and $\frac{1}{4}$, respectively. For the case of the 35 3-qubit marginal density matrices, 21 of them are completely mixed, corresponding to the following bipartitions:

$$\begin{aligned} &\{0,1,2\}, \{0,1,4\}, \{0,1,6\}, \{0,2,3\}, \{0,2,4\}, \{0,2,5\}, \{0,2,6\}, \\ &\{0,3,5\}, \{0,4,6\}, \{1,2,4\}, \{1,2,6\}, \{1,3,4\}, \{1,3,5\}, \{1,3,6\}, \\ &\{1,4,5\}, \{1,5,6\}, \{2,3,5\}, \{2,4,6\}, \{3,4,6\}, \{3,5,6\}, \{4,5,6\}. \end{aligned} \tag{29}$$

The 14 remaining marginal density matrices associated with bipartitions

$$\begin{aligned} &\{0,1,3\}, \{0,1,5\}, \{0,3,4\}, \{0,3,6\}, \{0,4,5\}, \{0,5,6\}, \{1,2,3\}, \\ &\{1,2,5\}, \{1,4,6\}, \{2,3,4\}, \{2,3,6\}, \{2,4,5\}, \{2,5,6\}, \{3,4,5\} \end{aligned} \tag{30}$$

are not completely mixed, having $\mathrm{Tr}(\rho^2) = 0.156\,250$ in all the cases except for $\{1, 4, 6\}$, which is 0.218 750.

A different 7-qubit state with high entanglement and very simple algebraic structure is

$$\begin{aligned}\left|\psi_7^b\right\rangle = \tfrac{1}{4\sqrt{2}}((1+i)(&|0011101\rangle + |0100010\rangle + |0111000\rangle + |1101100\rangle \\ &+ |1111011\rangle - |0001001\rangle - |1000111\rangle - |1110101\rangle) \\ &+ (1-i)(|0010011\rangle + |0110110\rangle + |1001010\rangle + |1010000\rangle \\ &+ |1011110\rangle - |0000100\rangle - |0101111\rangle - |1100001\rangle)) \end{aligned} \tag{31}$$

$$E_{\mathrm{NPT}}\left|\psi_7^b\right\rangle = 152.504\,073. \tag{32}$$

The analysis for $|\psi_t^b\rangle$ is completely similar to the previous case. Again, all the marginal density matrices for subsystems of 1 and 2 qubits are completely mixed. In the case of 3-qubit subsystems, the 18 marginal density matrices corresponding to bipartitions

$$\begin{aligned}&\{0,1,2\}, \{0,1,3\}, \{0,1,4\}, \{0,1,5\}, \{0,2,6\}, \{0,3,5\}, \\ &\{0,4,6\}, \{1,2,6\}, \{1,3,5\}, \{1,4,6\}, \{2,3,4\}, \{2,3,5\}, \\ &\{2,3,6\}, \{2,4,5\}, \{2,5,6\}, \{3,4,5\}, \{3,4,6\}, \{4,5,6\}\end{aligned} \tag{33}$$

are completely mixed, though not the remainder 17 corresponding to bipartitions

$$\begin{aligned}&\{0,1,6\}, \{0,2,3\}, \{0,2,4\}, \{0,2,5\}, \{0,3,4\}, \{0,3,6\}, \\ &\{0,4,5\}, \{0,5,6\}, \{1,2,3\}, \{1,2,4\}, \{1,2,5\}, \{1,3,4\}, \\ &\{1,3,6\}, \{1,4,5\}, \{1,5,6\}, \{2,4,6\}, \{3,5,6\}.\end{aligned} \tag{34}$$

The squared marginal density matrix has in all cases a trace of 0.156 250, except for the case $\{2, 4, 6\}$, which is 0.187 500.

4.5. 8-qubit states

The search for 8-qubit states is not as successful as in previous cases. An important factor in this case is definitely the computational hardness of exploring numerically the space. Each evaluation of the fitness function on a candidate state takes around 7 s. This constitutes a serious limitation to the amount of states that can be explored in reasonable time. With the computing power available to us, a typical 4-day search visits around 40 000 states (apart from the fitness evaluation, the search algorithm also imposes an overhead). In the case of 5, 6 and 7 qubits the search finishes well before 40 000 states are visited, but this seems not to be the case here. We empirically found that a possible reason for this poor performance is related to the size of the neighbourhood. According to our move function, each candidate state has $2^n(|V| - 1)$ neighbours. For a fixed V, the size of the neighbourhood increases exponentially in the number of qubits. In the case of 8 qubits, the average number of neighbour states visited before a new state is accepted is considerably higher than in previous cases, resulting in a very slow progression of the search.

According to the NPT measure, the maximum possible (attainable or not) entanglement for a 8-qubit state is 504.5. We have found states with entanglement up to around 440 and rather simple structure. As an example, the state

$$\begin{aligned}|\psi_8\rangle = \tfrac{1}{8}(&|00000010\rangle - |00000101\rangle - |00001111\rangle + |00010111\rangle + |00011010\rangle \\ &- |00011011\rangle - |00100001\rangle - |00100101\rangle + |00100110\rangle + |00101000\rangle \\ &+ |00101110\rangle + |00101111\rangle - |00110000\rangle - |00110011\rangle + |00110100\rangle \\ &- |00111100\rangle - |01000000\rangle + |01000110\rangle + |01000111\rangle - |01001010\rangle \\ &+ |01001100\rangle - |01001101\rangle + |01010001\rangle + |01010110\rangle + |01011010\rangle\end{aligned}$$

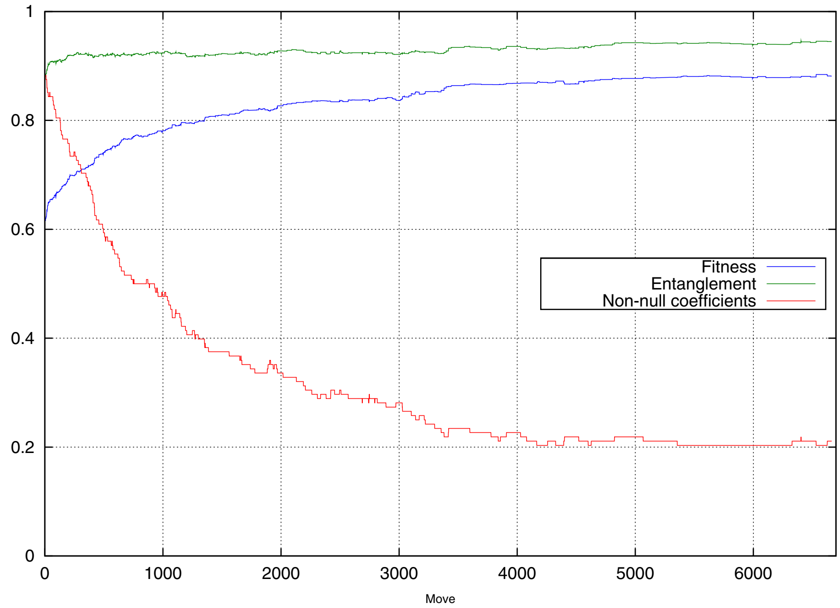

Figure 1. Typical state evolution.

$$
\begin{aligned}
&+|01100010\rangle - |01100011\rangle + |01101001\rangle + |01111001\rangle + |01111101\rangle \\
&+|01111110\rangle + |10000001\rangle + |10000111\rangle + |10001000\rangle + |10001010\rangle \\
&+|10001100\rangle - |10001110\rangle + |10010000\rangle + |10010100\rangle + |10011101\rangle \\
&+|10100010\rangle - |10101001\rangle + |10101011\rangle - |10110111\rangle + |10111001\rangle \\
&-|10111010\rangle - |10111111\rangle - |11000011\rangle - |11000101\rangle - |11001011\rangle \\
&-|11010000\rangle + |11010011\rangle + |11010100\rangle - |11011011\rangle + |11011111\rangle \\
&+|11100000\rangle + |11100100\rangle - |11101101\rangle - |11110101\rangle - |11110111\rangle \\
&+|11111000\rangle + |11111010\rangle - |11111100\rangle + |11111110\rangle) \qquad (35)
\end{aligned}
$$

has $E_{\mathrm{NPT}}|\psi_8\rangle = 439.302\,328$ and only 64 non-null coefficients equal to ± 1. The 8 single-qubit marginal density matrices are almost completely mixed, with $\mathrm{Tr}(\rho^2)$ being 0.500 488 (5 times), 0.500 977 (3 times) and 0.5 (1 times). Something similar happens for the 28 2-qubit density matrices, the average $\mathrm{Tr}(\rho^2)$ being 0.253 540. The 3- and 4-qubit marginal density matrices deviate considerably more, on average, from the expected value of a completely mixed state.

4.6. Performance and state evolution

For 5 and 6 qubits, most runs result in a maximally entangled state whenever the parameterization used for the search algorithm is appropriate. In both cases, a solution is often found in the first 4–6 cycles (i.e. the search ends after 4000–6000 generations). This constitutes a fairly rapid convergence, a typical search taking around 20–30 s for 5 qubits and 1–2 min for 6 qubits on a usual laptop. The cases of 4, 7 and 8 qubits are slightly different, as the search never converges to a maximally entangled state and the procedure ends after a certain number of consecutive non-improving cycles. A typical search resulting in a 7-qubit state with $E_{\mathrm{NPT}} \geqslant 152$ takes around 3–4 h, while the 8-qubit case requires around 4–5 days. The running time is obviously exponential in the number of qubits, and the fundamental bottleneck comes from the evaluation of the fitness function, particularly the entanglement measure.

Figure 1 shows the evolution of a typical search for 7 qubits. Apart from the fitness, both entanglement and the fraction of non-null coefficients are shown. The effect of the punishment factor in the fitness function can clearly be observed; after a few thousands evaluations, candidate states have approximately 80% of the null coefficients. The overall behaviour is identical for searches of 4, 5, 6 and 8 qubits. (In the case of 5 and 6, however, the entanglement component eventually reaches the upper bound and the search stops.)

5. Conclusions and future work

In this work, we have shown how states with a simple structure can be discovered by restricting the search to certain subspaces of interest. For 5 qubits, states equivalent to Brown *et al*'s $|\psi_5\rangle$ are easily found. In the case of 6 qubits, a new state with an algebraic structure arguably simpler than Borras *et al*'s $|\psi_6\rangle$ state has been discovered. Similarly to what has been pointed out for the latter, new teleportation and secret state sharing applications could be constructed using them. Furthermore, the fact of having at our disposal *many* of such states might enable us to devise new applications based upon the use of multiple, non-identical states having maximum entanglement.

For the case of 7 qubits, various states with high entanglement and very simple algebraic structure have been found. Even though the entanglement is not maximum, all the single- and 2-qubit marginal density matrices are completely mixed, as well as more than half of the 3-qubit marginal density matrices. These features make of them potentially useful to support some applications.

The case of 8 qubits is hard to explore numerically with our available computational resources. Although the experimentation has not been as intensive as before (and therefore the parameterization employed might not be adequate for this case), our preliminary results seem promising. Compact 8-qubit states with higher entanglement might be found with more computational resources.

In this work, we have restricted the search to *pure* multi-qubit states. Consequently, the use of the negativity of the partial transpose as a measure of entanglement is a valid but unnecessary choice. An entropic measure such as the von Neumann entropy should be enough in terms of providing adequate search guidance.

An interesting avenue for future research is related to a further work of Borras *et al* [2]. Here the authors explore the robustness of entangled states under various decoherence channels. Along these lines, we plan to study the entanglement decay of the states introduced in this paper.

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References

[1] Borras A, Plastino A R, Batle J, Zander C, Casas M and Plastino A 2007 *J. Phys. A: Math. Theor.* **40** 13407
[2] Borras A, Majtey A P, Plastino A R, Casas M and Plastino A 2009 *Phys. Rev.* A **79** 022108
[3] Brierley S and Higuchi A 2007 *J. Phys. A: Math. Theor.* **40** 8455
[4] Brown I D K, Stepney S, Sudbery A and Braunstein S L 2005 *J. Phys. A: Math. Gen.* **38** 1119
[5] Choudhury S, Muralidharan S and Panigrahi P K 2009 *J. Phys. A: Math. Theor.* **42** 115303
[6] Galassi M *et al* 2008 *GNU Scientific Library Reference Manual* 3rd edn ISBN 0954612078 http://www.gnu.org/software/gsl/
[7] Higuchi A and Sudbery A 2000 *Phys. Lett.* A **273** 213
[8] Horodecki M, Horodecki P and Horodecki R 2000 *Phys. Rev. Lett.* **84** 2014 (arXiv:quant-ph/9908065)
[9] Horodecki M 2001 Entanglement measures *Quantum Inf. Comput.* **1** 3–26 (arXiv:quant-ph/9908065)
[10] Kendon V M, Nemoto K and Munro W J 2002 *J. Mod. Opt.* **49** 1709 (arXiv:quant-ph/0106023)
[11] Kirkpatrick S, Gelatt C D Jr and Vecchi M P 1983 *Science* **220** 671–80
[12] Muralidharan S and Panigrahi P K 2008 *Phys. Rev.* A **77** 032321 (arXiv:quant-ph/07083785)
[13] Muralidharan S and Panigrahi P K 2008 Perfect teleportation and superdense coding through an asymmetric five qubit state arXiv:quant-ph/08023484
[14] Peres A 1996 *Phys. Rev. Lett.* **77** 8
[15] Plenio M B and Virmani S 2006 An introduction to entanglement measures arXiv:quant-ph/0504163
[16] Vidal G and Werner R F 2002 *Phys. Rev.* A **65** 032314 (arXiv:quant-ph/0102117)
[17] Życzkowski K, Horodecki P, Sanpera A and Lewenstein M 1998 *Phys. Rev.* A **58** 883 (arXiv:quant-ph/9804024)