Searching for highly entangled multi-qubit states

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classification: **02.60.Pn**: Numerical optimization; **03.65.Ud**: Entanglement and quantum nonlocality; **03.67.Mn** Entanglement production, characterization, and manipulation

Abstract.

We present a simple numerical optimisation procedure to search for highly entangled states of 2, 3, 4 and 5 qubits. We develop a computationally tractable entanglement measure based on the negative partial transpose (NPT) criterion, which can be applied to quantum systems of an arbitrary number of qubits. The search algorithm attempts to optimise this entanglement cost function to find the maximal entanglement in a quantum system.

We present highly entangled 4 qubit and 5 qubit states discovered by this search. We show that the 4 qubit state is not quite as entangled, according to two separate measures, as the conjectured maximally entangled Higuchi-Sudbery state. Using this measure, these states are more highly entangled than the 4-qubit and 5-qubit GHZ states.

We also present a conjecture about the NPT measure, inspired by some of our numerical results, that the single-qubit reduced states of maximally entangled states are all totally mixed.

1. Introduction

There are known examples of maximally and highly entangled quantum states of 2 and 3 qubits. Yet for multipartite entanglement of 4 qubits and more, the mathematical structure of the entangled states is less clear. The 4 qubit *Higuchi-Sudbery state* is conjectured, but not known, to be maximally entangled (at least in some measures of entanglement).

There is an alternative to the analytic approach. Faced with finding an optimum in a complicated, mathematically intractable space, we at least have an arsenal of numerical search and optimisation techniques to hand.

In this paper we apply numerical search techniques to hunt down highly entangled multi-qubit states. This work is exploratory in studying multipartite maximal entanglement across all possible partitionings of the state.

2. Entanglement measures and cost functions

In order to perform a search, we need a *cost function*: a measure of the amount of entanglement in a quantum state. There are several entanglement measures, and their usefulness depends on the type of analysis to be done. Properties for a good entanglement measure are reviewed in [Horodecki *et al.* 2000], [Horodecki 2001]; not all entanglement measures display all these properties.

2.1. Requirements

We want an entanglement measure for a very specific purpose: to be used as a cost function in a numerical search algorithm for highly entangled states. This puts certain constraints on the function, but also allows certain freedoms.

- The cost function must be computationally tractable. It will be evaluated many thousands of times during each search run. Most proposed entanglement measures in the literature are computationally intractable.
- The cost function must define a searchable landscape. It must not be so rugged or discontinuous that the search algorithm is unable to use the information in the cost function to find improved solutions.
- The cost function must be suitable for mixed as well as pure states.
- The cost function must correspond closely to agreed entanglement measures at high entanglement, where the search is aiming, but can be rather more approximate at low entanglement, since we are not searching for such states.

2.2. Negative Partial Transpose

The partial transpose of a density matrix ρ can be used to determine whether the mixed quantum state represented by ρ is separable. As a result it can also be used to detect entanglement in ρ.

Consider a mixed state ρ_{AB}, composed of subsystems A and B. The *partial transpose* of ρ with respect to subsystem A is

$$\left(\rho^{T_A}\right)_{m\,\mu,n\nu} = \rho_{n\,\mu,m\nu} \tag{1}$$

[Peres 1996] proves that a necessary condition for separability is that the partial transpose of ρ has only non-negative eigenvalues. This is also known as the *positive partial transpose* (PPT) test. Conversely, if the partial transpose of ρ has one or more negative eigenvalues then the system is inseparable and contains some degree of entanglement. Such states have a *non-positive partial transpose* (NPPT).

The *Peres-Horodecki criterion* states that PPT is a necessary and *sufficient* condition for bipartite states to be separable for Hilbert spaces of size 2×2 and 2×3. In other cases PPT is only a necessary condition for separability and [Horodecki 1997] shows the existence of entangled PPT states. Entangled states which maintain positive partial transpose are known as *bound entangled states*.

We are not worried by this lack of sufficiency, however. We are interested only in highly entangled states, so a measure that fails to spot a few lesser entangled states is not of concern. Given the simplicity and computability of the partial transpose condition, we choose to use a cost function based on it, namely the *negativity* introduced by [Życzkowski *et al.* 1998] and investigated by [Vidal & Werner 2002], who demonstrated its monotonicity under local operations and classical communication (LOCC), and its convexity. This measure of entanglement was also used in numerical explorations of multipartite states by [Kendon *et al.* 2002].

2.3. Negative Partial Transpose definition

Consider an n qubit state in the form

$$|\psi\rangle = \sum_{k=0}^{2^n-1} c_k \, |k\rangle \tag{2}$$

where the $c_k \in \mathbb{C}$ obey the normalisation condition. Each k is a basis state $|a_1 a_2 \ldots a_n\rangle$, where $a_1 a_2 \ldots a_n$ is the binary representation of the integer k, with $a_i \in \{0,1\}$.

Construct a density operator of a mixed state ρ using N pure states of the same form as $|\psi\rangle$:

$$\rho = \sum_{j=1}^{N} p_j \, |\psi_j\rangle \langle \psi_j| \tag{3}$$

Expand this out in terms of the individual coefficients.

$$\begin{aligned}
\rho &= \sum_{j=1}^{N} p_j \sum_{a_1 \ldots a_n = 0}^{1} c^{j}_{a_1 \ldots a_n} \, |a_1 \ldots a_n\rangle \sum_{a'_1 \ldots a'_n = 0}^{1} c^{j\,*}_{a'_1 \ldots a'_n} \, \langle a'_1 \ldots a'_n| \qquad (4)\\
&= \sum_{j=1}^{N} p_j \sum_{\substack{a_1 \ldots a_n = 0\\ a'_1 \ldots a'_n = 0}}^{1} d^{j}_{a_1 \ldots a_n a'_1 \ldots a'_n} \, |a_1 \ldots a_n\rangle \langle a'_1 \ldots a'_n| \qquad (5)
\end{aligned}$$

where $d^{j}_{a_1 \ldots a_n a'_1 \ldots a'_n} = c^{j}_{a_1 \ldots a_n} c^{j\,*}_{a'_1 \ldots a'_n}$.

Now construct the partial transpose of ρ with respect to the index i (also known as the cut set $\{i\}$). This achieved by transposing the bits a_i and a'_i in the basis states and reconstructing the new matrix $\rho^{T_{\{i\}}}$

$$\begin{aligned}
\rho^{T_{\{i\}}} &= \sum_{j=1}^{N} p_j \sum_{\substack{a_1 \ldots a_n = 0\\ a'_1 \ldots a'_n = 0}}^{1} d^{j}_{a_1 \ldots a_i \ldots a_n a'_1 \ldots a'_i \ldots a'_n} \, |a_1 \ldots a'_i \ldots a_n\rangle \langle a'_1 \ldots a_i \ldots a'_n| \qquad (6)\\
&= \sum_{j=1}^{N} p_j \sum_{\substack{a_1 \ldots a_n = 0\\ a'_1 \ldots a'_n = 0}}^{1} d^{j}_{a_1 \ldots a'_i \ldots a_n a'_1 \ldots a_i \ldots a'_n} \, |a_1 \ldots a_i \ldots a_n\rangle \langle a'_1 \ldots a'_i \ldots a'_n| \qquad (7)
\end{aligned}$$

The partial transpose with respect to a larger set of indices (larger *cut set*) is constructed similarly, by transposing the bits corresponding to each index in the set.

We can then calculate the eigenvalues of this new matrix $\rho^{T_{\{i\}}}$ to see if it has any negative eigenvalues indicating entanglement.

2.4. The relevant cut sets

Each density operator has 2^n different partial transposes. The density operator can be transposed with respect to each subset of indices, or *cut*, taken from the n qubit *cut set*. If the n qubit computational basis is in the form $|a_1 a_2 \ldots a_n\rangle$ then the cut set is the power set $2^{\{a_1, a_2, \ldots, a_n\}}$.

Even for an entangled system, some cuts might exhibit no negative eigenvalues. For example, a system of two individually entangled, but jointly separable subsystems.

Additionally, the more negative eigenvalues, the more entangled the state. Since we want a measure of entanglement, we should investigate all the possible cuts.

In practice, however, it is unnecessary to compute the partial transpose with respect to every cut, since certain cuts are equivalent. Only $2^{n-1}-1$ of the 2^n partial transposes need to be calculated.

Consider the partial transpose of ρ with respect to index 1, $\rho^{T_{\{1\}}}$. Calculating the complementary cut with respect to all the other indices together, $\{2 \ldots n\}$, is redundant, because $\rho^{T_{\{1\}}}$ and $\rho^{T_{\{2 \ldots n\}}}$ have the same eigenvalues. We can neglect the other complementary cuts similarly, leaving 2^{n-1} cut sets.

Additionally, we do not need to consider the trivial partial transpose with respect to the empty cut, $\rho^{T_{\{\varnothing\}}}$, since this is the original density matrix, which is known to have no negative eigenvalues.

Hence we need consider only $2^{n-1} - 1$ partial transposes to find all the negative eigenvalues.

2.5. The cost function

Once we have all partial transposes with respect to all necessary cuts then any negative eigenvalues of these new matrices detect entanglement in the state ρ.

There are $2^{n-1} - 1$ sets of 2^n eigenvalues (not necessarily unique). We take the negation of the sum of all the negative eigenvalues as our cost function $E_{\mathrm{NPT}}(\rho)$, a measure of entanglement in a given quantum state ρ. (We negate the sum in order to make the result positive. This helps to make the terminology clearer: we seek to maximise the cost function in order to maximise the entanglement.) The larger E becomes, the greater the amount of entanglement ρ contains.

It is more conventional to define an entanglement measure to lie between zero (no entanglement) and one (maximally entangled). We could achieve this by normalising with respect to the maximally entangled state, and use $E_{\mathrm{NPT}}(\rho)/E_{\mathrm{NPT}}^{max}$. However, the value E_{NPT}^{max} is unknown for the cases of interest (it is in part what our search is attempting to discover). Such normalisation is unnecessary in our numerical explorations, where we simply need a monotonic function. Hence we choose to maximise the negated sum of negative eigenvalues, E_{NPT}.

2.6. NPT Entanglement of GHZ states

The n-qubit GHZ state $|\psi_{GHZ}\rangle_n = \frac{1}{\sqrt{2}}(|0\rangle_n + |1\rangle_n)$ has a simple form of this NPT entanglement measure.

In every cut, there is a partial transpose containing a 4×4 block like

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{8}$$

(multiplied by $\frac{1}{2}$) and with all other entries zero. So each cut has eigenvalues $-\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$. Since we take into acount the $2^{n-1}-1$ distinct cuts, we have

$$E_{NPT}\,|\psi_{GHZ}\rangle_n = \tfrac{1}{2}(2^{n-1}-1) \tag{9}$$

2.7. Limits of Entanglement

We use known results of maximally entangled states of 2 and 3 qubits to provide insights into our chosen entanglement cost function.

The Peres-Horodecki criterion guarantees that a separable state has no negative eigenvalues and hence the entanglement measure $E_{\mathrm{NPT}} = 0$ for separable states.

2.7.1. 2 qubits. Consider the maximally entangled 2 qubit state

$$|\psi_+\rangle = \frac{1}{\sqrt{2}}\left(|00\rangle + |11\rangle\right) \tag{10}$$

Constructing the density operator of $|\psi_+\rangle$ gives

$$\begin{aligned}\rho &= |\psi_+\rangle\langle\psi_+| \\ &= \tfrac{1}{2}\left(|00\rangle\langle 00| + |00\rangle\langle 11| + |11\rangle\langle 00| + |11\rangle\langle 11|\right)\end{aligned} \tag{11}$$

For 2 qubits the $2^{2-1}-1 = 1$ cut is $\{1\}$. The partial transpose with respect this cut is

$$\rho^{T_{\{1\}}} = \tfrac{1}{2}\left(|00\rangle\langle 00| + |10\rangle\langle 01| + |01\rangle\langle 10| + |11\rangle\langle 11|\right) \tag{12}$$

$\rho^{T_{\{1\}}}$ has a single negative eigenvalue of $-\frac{1}{2}$. So $E_{\mathrm{NPT}}\,|\psi_+\rangle = 0.5$.

2.7.2. 3 qubits. We can determine a limit for 3 qubit maximal entanglement from the GHZ and W states. For 3 qubits the $2^{3-1}-1 = 3$ cuts are $\{1\}$, $\{2\}$, and $\{3\}$. Our entanglement cost function yields different values for entanglement for $|\psi_{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ and for $|\psi_W\rangle = \frac{1}{\sqrt{3}}(|000\rangle + |010\rangle + |001\rangle)$.

We have $E_{\mathrm{NPT}}\,|\psi_{GHZ}\rangle = 1.5$. Each W-state transpose has a single negative eigenvalue of $-\frac{\sqrt{2}}{3}$, and so $E_{\mathrm{NPT}}\,|\psi_W\rangle = \sqrt{2} \approx 1.4142$. For three qubits, 1.5 is the maximal possible entanglement value, since there are only single cuts (one qubit against two), and the maximal amount in these single cuts is $\frac{1}{2}$.

We examine whether our search procedure for maximal entanglement tends to the limit of 1.5 and hence a GHZ state, or a limit of $\sqrt{2}$ and hence a W-state.

2.7.3. 4 qubits. The $2^4 - 1 = 7$ cuts for 4 qubit partial transposes are $\{1\}$, $\{2\}$, $\{3\}$, $\{4\}$, $\{1,2\}$, $\{1,3\}$, $\{1,4\}$.

We have $E_{\mathrm{NPT}}\,|\psi_{GHZ}\rangle_4 = \frac{7}{2} = 3.5$.

The highly entangled 4 qubit Higuchi-Sudbery (HS) state is conjectured to be maximally entangled [Higuchi & Sudbery 2000]. The state is

$$\begin{aligned}|\psi_{HS}\rangle = \tfrac{1}{\sqrt{6}}\Big(&|1100\rangle + |0011\rangle + \omega(|1001\rangle + |0110\rangle) \\ &+ \omega^2(|1010\rangle + |0101\rangle)\Big)\end{aligned} \tag{13}$$

where $\omega = -\frac{1}{2} + \frac{\sqrt{3}}{2} i$.

This gives $E_{\mathrm{NPT}} \, |\psi_{HS}\rangle \approx 6.0981$. Our aim is to see if our search technique can equal, or better, this value.

2.7.4. 5 qubits. The $2^5 - 1 = 15$ cuts for 5 qubit partial transposes are $\{1\}$, $\{2\}$, $\{3\}$, $\{4\}$, $\{5\}$, $\{1,2\}$, $\{1,3\}$, $\{1,4\}$, $\{1,5\}$, $\{2,3\}$, $\{2,4\}$, $\{2,5\}$, $\{3,4\}$, $\{3,5\}$, $\{5,5\}$.

We have $E_{\mathrm{NPT}} \, |\psi_{GHZ}\rangle_5 = \frac{15}{2} = 7.5$.

Our aim is to see if our search technique can find a highly entangled 5 qubit state.

3. The Search

3.1. The search algorithm

There are several numerical optimisation techniques available (such as hill climbing, simulated annealing, or genetic algorithms), of differing sophistication. Which to use depends on the structure of the search space defined by the cost function.

The negativity cost function is convex [Vidal & Werner 2002]. So it is relatively smooth, and increasing towards the surface of the hypersphere defined by the state vectors. This suggests the simplest form of search, hill climbing, since the convexity means that is no chance of being caught in a mixed state local optimum. It remains to be seen if the search gets caught in a pure state local optimum on the surface of the search hypersphere. We use hill climbing to maximise $E_{\mathrm{NPT}}(\rho)$. The hill climbing algorithm involves repeatedly making a small random change to the current best solution, and accepting the changed solution if it is better.

3.2. The search space

The cost function is defined on density matrices, so these constitute the search space. Looking at equation 3, there are two clear possibilities: confining the search to pure states with $N = 1$, or allowing mixed states with $N > 1$.

Using pure states is equivalent to searching on the surface of a hypersphere, whilst mixed states allow movement through the interior of the hypersphere, too. We know that there are multiple different entanglement maxima on the hypersurface (for example, in the 3 qubit case corresponding to the GHZ and W-states), which might potentially lead to the problem of getting trapped at an uninteresting local optimum.

So our initial search space comprised mixed states, with $N = 2^n$ being sufficient to span the space. It transpires that the search very rapidly converges to (close to) the hypersurface of pure states, so we also experimented with a pure state search space, with $N = 1$ (section 3.6.1).

3.3. The move function

The move function defines how to choose the next point in the search space.

For the mixed state case, the move function choses a random one of the N state vectors ψ_j, and a random one of its (complex) components, c_i^j, and multiplies its real and imaginary components by the current (real) values of the move sizes δ_{re} and δ_{im}. The state vector is then renormalised. The probability p_j is multiplied by the current value of the move size δ_p and then the probabilities are renormalised.

The various move sizes are each set to a random number between 0.5 and 1.5, and changed if there have been too many consecutive rejected moves. (We note that hill climbing, along with most other search algorithms, becomes less efficient as it gets close to an optimum, since each random move choice becomes more likely to point in the wrong direction. This problem increases as the number of dimensions increases.)

3.4. The implementation

We used Matlab 6.5 to implement all the matrix manipulations. Outer products, eigenvalues, complex numbers, and so on, are built in. All we had to implement was the partial transpose definition, the random state initialisation, and the move function.

The move size is set to a random number uniformly distributed in the interval $(1-\alpha, 1+\alpha)$, with $\alpha = 0.5$. This is changed to a new random number in the same interval if there have been 500 consecutive rejected moves. The search terminates once there are 10000 consecutive rejected moves. The search algorithm is as follows:

initialise N random state vectors ψ_j, probabilities p_j
construct initial density matrix $\rho := \rho_0$
calculate eigenvalues and hence $E := E_0$
$\alpha := 0.5$;
$\delta_{re} :\in (1-\alpha, 1+\alpha)$; $\delta_{im} :\in (1-\alpha, 1+\alpha)$; $\delta_p :\in (1-\alpha, 1+\alpha)$;
$t_0 := 0$; $t_i := 0$;
while $t_0 < 10000$
    while $t_i < 500$
        apply move function to give ψ', ρ'
        calculate eigenvalues and hence E'
        if $E' > E$ **then** accept move ($\psi := \psi'$; $E := E'$; $t_0 := 0$; $t_i := 0$)
            else reject move ($++t_0$; $++t_i$)
    endwhile
    $t_i := 0$; reset δs
endwhile
return ψ, E

Some optimisations are included. If a probability drops below 10^{-10}, it is set to zero, and that case drops out of further consideration. If the real or imaginary part of a coefficient drops below 10^{-2}, it is set to zero. At the end of a search, the result is hand-tweaked, setting any remaining small coefficients to zero, and used as the input to a further run, to see whether that improves the result. If appropriate, some algebraic simplification of the result is then performed.

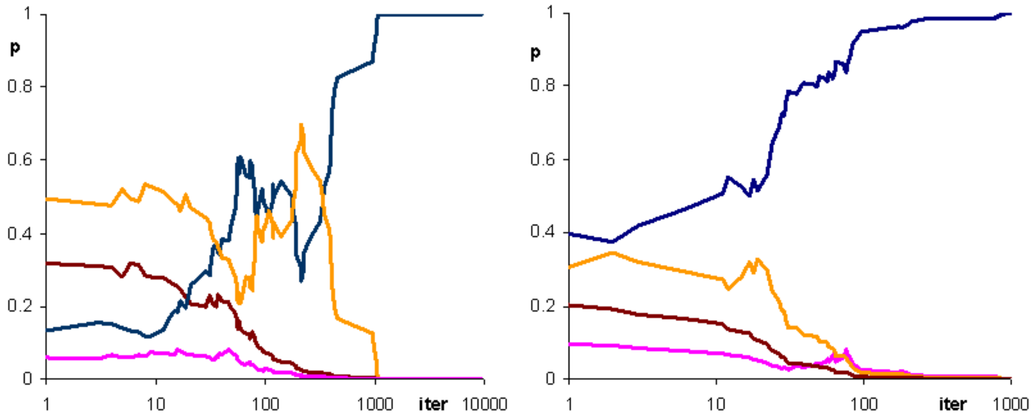

Figure 1. Patterns of probability evolution during a search, from an initial mixed state with random probabilities p_j (eqn 3). At the end of the search, one probability is 1, and the other have dropped to zero, indicating a final pure state. (a) atypically, the initial maximum probability state does not eventually dominate (b) more typically, the initial maximum probability state eventually dominates

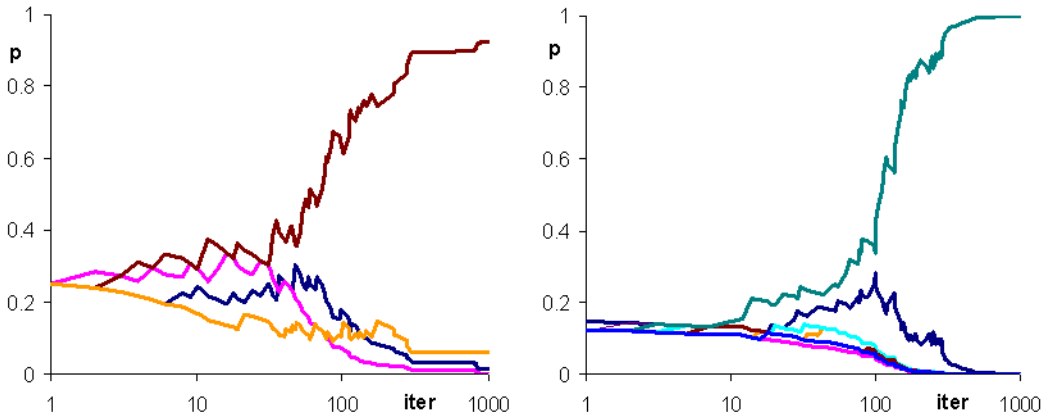

Figure 2. Typical patterns of probability evolution during a search, from an initial mixed state with equal probabilities p_j (eqn 3). (a) typical 2-qubit search (b) typical 3-qubit search

3.5. Validation

For 2 and 3 qubits, the search discovers the known states, both when started randomly, and when started close to the known solutions.

For 3 qubits, when started randomly it discovers the maximal GHZ state, rather than the W state. When started close to the W state, it does converge to that state.

For 4 qubits, when started close to the HS state, it converges to that state.

3.6. Performance

Runs typically converge in 10000–50000 generations. Most runs result in some highly entangled state. Using Matlab 6.5 on a Pentium PC, typically a 2 qubit search takes 3–5 CPU seconds; a 3 qubit search takes 10–20 CPU seconds; a 4 qubit search takes 3–6 CPU minutes; a 5 qubit search takes 2–4 CPU hours. The running time is exponential in the number of qubits.

3.6.1. Probability evolution. Convergence to a pure state (all but one probability p_j tending to zero) is to be expected, because of the convexity of the negativity function [Vidal & Werner 2002]. All the mixed state searches very rapidly converge to a pure state, in approximately 1000 generations. Using a random spread of initial probabilities for the N state vectors nearly always results in the largest initial probability eventually dominating (figure 1). Using uniform initial probabilities still results in one probability dominating after a relatively small number of generations compared to the total number for convergence (figure 2). We note that [Wei *et al.* 2003] have performed a more refined investigation of two-qubit states, searching for the most entangled state (under various measures of entanglement) with given purity.

Based on the observed rapidity of the convergence, we experimented with starting from an initial random single pure state. The converged results were essentially the same, with some increase in efficiency (in the calculation of the density matrix). We conclude that we are no more likely to escape a local optimum on the search hypersphere surface by starting in a mixed state than a pure state. However, we need not fear such local optima: we are searching for highly entangled states (good local optima), not only maximally entangled states (global optima).

3.6.2. State evolution. Using the move function with $\delta \in (0.5, 1.5)$, the states typically converge to a near optimum fairly rapidly (figures 3, 4). It can be seen that, even close to the converged result, the movement can be quite large. However, causing the value of α to decrease as the search progresses, to force the move function to take smaller steps, has no appreciable effect on the results.

4. Results

4.1. A highly entangled 4-qubit state

4.1.1. A new state. The search procedure resulted (after algebraic simplification) in the following two highly entangled states

$$\begin{aligned} |\,\Psi\rangle \; &= \tfrac{1}{2\sqrt{2}}(i\,|\,0010\rangle + (1+i)\,|\,0101\rangle + |\,0110\rangle \\ &\qquad + (1+i)\,|\,1000\rangle + |\,1011\rangle + i\,|\,1111\rangle) \\ E_{\mathrm{NPT}}\,|\,\Psi\rangle &= 5.9142 \end{aligned} \tag{14}$$

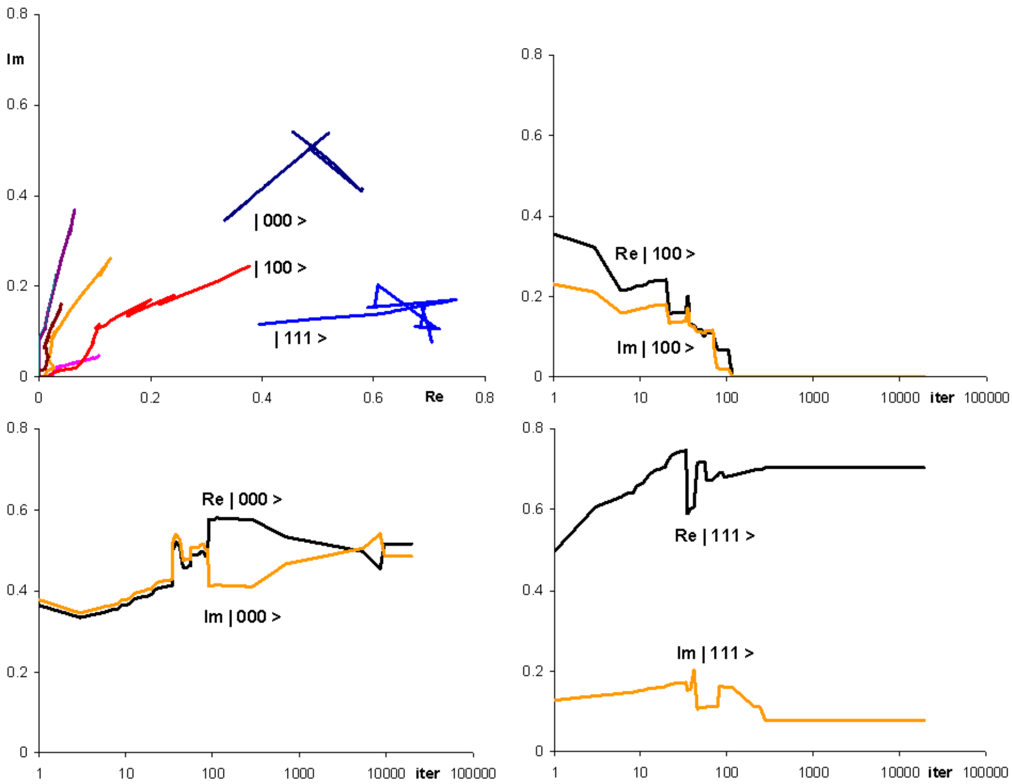

Figure 3. Typical pattern of evolution of the eventually dominant state component during a 3-qubit search, here converging to (near to) the state $\frac{1+i}{2}\,|\,000\rangle + \frac{1}{\sqrt{2}}\,|\,111\rangle$. (a) Argand diagram showing evolution of all state components. (b–d) Evolution of the real and imaginary parts of selected components, as a function of iteration number (log scale). The coincident changing of real and imaginary parts is due to renormalisation of the state vector after one of the other components is changed.

$$\begin{aligned} |\,\Psi'\rangle &= \tfrac{i}{2}(|\,0001\rangle + |\,1111\rangle) \\ &\qquad + \tfrac{1}{2\sqrt{2}}(|\,0100\rangle + |\,1010\rangle + i\,\,|\,0110\rangle + i\,\,|\,1000\rangle) \\ E_{\mathrm{NPT}}\,|\,\Psi'\rangle &= 5.9142 \end{aligned} \tag{15}$$

These states are essentially equivalent, and can be reformulated as

$$|\,\psi_4\rangle = \tfrac{1}{2}\left(|\,0000\rangle + |\,{+011}\rangle + |\,1101\rangle + |\,{-110}\rangle\right) \tag{16}$$

where $|\,+\rangle = \frac{1}{\sqrt{2}}(|\,0\rangle + |\,1\rangle)$ and $|\,-\rangle = \frac{1}{\sqrt{2}}(|\,0\rangle - |\,1\rangle)$.

The state has 22 negative eigenvalues from 7 partial transposes. For the four single-index cuts, the partial transposes each have a single negative eigenvalue of $-\frac{1}{2}$. One of the two-index cuts has six negative eigenvalues of $-\frac{1}{4}$; the other two two-index cuts each have negative eigenvalues of $-\frac{1}{4\sqrt{2}}$ (4 times), $-\frac{2+\sqrt{2}}{8}$ and $-\frac{2-\sqrt{2}}{8}$. So

$$E_{\mathrm{NPT}}\,|\,\psi_4\rangle = 2 + \sqrt{2} \approx 5.9142 \tag{17}$$

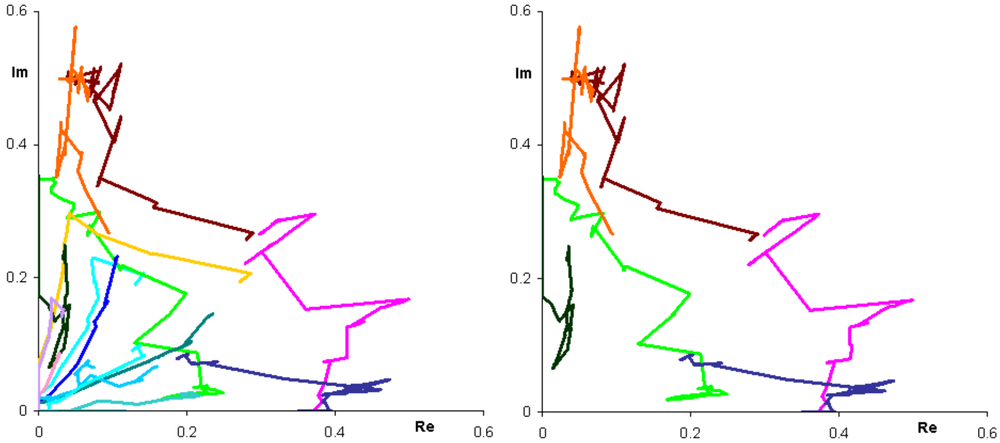

Figure 4. Evolution of a highly entangled 4-qubit state, $|\Psi'\rangle$ (section 4.1.1) (a) evolution of all 16 components. (b) evolution of 6 components that do not vanish: two end near $\frac{i}{2}$, two end at $\frac{1}{2\sqrt{2}}$, and two end at $\frac{i}{2\sqrt{2}}$.

4.1.2. Comparison with the GHZ state. We have $E_{\rm NPT}\,|\psi_{GHZ}\rangle_4 = \frac{7}{2} = 3.5$. Hence the state $|\psi_4\rangle$ is more entangled, according to the NPT measure.

Note that [Chen 2004] claims that the GHZ states are the maximally entangled states. Our result emphasises that maximal entanglement is relative to the particular measure of entanglement chosen [Wei *et al.* 2003]. Indeed, with repect to our NPT measure, the state $|\psi_{GHZ}\rangle_4$ is not even a local maximum: there are nearby states with a higher NPT entanglement measure.

4.1.3. Comparison with the Higuchi-Sudbery state. The HS state also has 22 negative eigenvalues from 7 partial transposes. For the four single-index cuts, the partial transposes also each have a single negative eigenvalue of $-\frac{1}{2}$. But each of the three two-index cuts have three negative eigenvalues of $-\frac{1}{2\sqrt{3}}$ and three of $-\frac{1}{6}$. So

$$E_{\rm NPT}\,|\psi_{HS}\rangle = 2 + \tfrac{3}{2}\sqrt{3} \approx 6.0981 \tag{18}$$

Hence the HS state is more entangled, according to the NPT measure, yet $|\psi_4\rangle$ does have a very high measure of entanglement.

When the state $|\psi_{HS}\rangle$ was conjectured to be maximally entangled, the entanglement measure used involved taking the average von Neumann entropy of 2 qubit subsystems [Higuchi & Sudbery 2000], $E_{VN} = \frac{1}{3}(E_{AB}+E_{AC}+E_{AD})$, where $E_{XY} = -Tr(\rho_{XY}\log\rho_{XY})$. (For comparison, the von Neumann entropy of the GHZ state is $\log_2 2$ (that is, 1) for every cut.) The HS state is more entangled than state $|\psi_4\rangle$ using this measure, too:

$$E_{VN}\,|\psi_{HS}\rangle = 1 + \tfrac{1}{2}\log_2 3 \approx 1.7925 \tag{19}$$

$$E_{VN}\,|\psi_4\rangle = \tfrac{5}{2} - \tfrac{1}{2\sqrt{2}}\log_2(3+\sqrt{2}) \approx 1.7426 \tag{20}$$

$$E_{VN}\,|GHZ\rangle_4 = 1 \tag{21}$$

This is another example of a computationally feasible entanglement measure on a pure state 4 qubit system. (We do not use this measure in our numerical searches, however, because we also look at mixed states. The von Neumann entropy measure cannot distinguish between classical and quantum correlations, and so would not help us secure information about the features we were attempting to capture.)

4.1.4. Observation on the Higuchi-Sudbery state. Since for some reason our search procedure did not converge to the HS state from a random starting point, we deliberately seeded the search with an initial state at, and one near, the HS state. Those searches did converge to the HS state, implying that it is at least a *local* maximum with respect to the NPT entanglement measure. The HS state is also a local maximum with respect to the entropy measure‡.

4.2. A highly entangled 5-qubit state

4.2.1. A new state. The search procedure resulted (after algebraic simplification) in the following two highly entangled states

$$\begin{aligned} |\Psi''\rangle &= \tfrac{1}{2\sqrt{2}}(|00110\rangle + |01011\rangle + |10001\rangle + |11100\rangle \\ &\qquad + i(|00101\rangle + |01000\rangle + |10010\rangle + |11111\rangle)) \\ E_{\mathrm{NPT}}\,|\Psi''\rangle &= 17.5 \end{aligned} \tag{22}$$

$$\begin{aligned} |\Psi'''\rangle &= \tfrac{1}{2\sqrt{2}}(|00110\rangle + |01001\rangle + |10101\rangle + |11010\rangle \\ &\qquad + i(|00000\rangle + |01111\rangle + |10011\rangle + |11100\rangle)) \\ E_{\mathrm{NPT}}\,|\Psi'''\rangle &= 17.5 \end{aligned} \tag{23}$$

These states are essentially equivalent, and can be reformulated as

$$|\psi_5\rangle = \tfrac{1}{2}\left(|000\rangle\,|\Phi_-\rangle + |010\rangle\,|\Psi_-\rangle + |100\rangle\,|\Phi_+\rangle + |111\rangle\,|\Psi_+\rangle\right) \tag{24}$$

where $|\Psi_\pm\rangle = |00\rangle \pm |11\rangle$ and $|\Phi_\pm\rangle = |01\rangle \pm |10\rangle$.

For the five single-index cuts the partial transposes each have a single negative eigenvalue of $-\frac{1}{2}$. Each of the 10 two-index cuts have six negative eigenvalues of $-\frac{1}{4}$.

4.2.2. Comparison with the GHZ state. We have $E_{\mathrm{NPT}}\,|\psi_{GHZ}\rangle_5 = \frac{15}{2} = 7.5$. Hence the state $|\psi_5\rangle$ is more entangled, according to the NPT measure.

Recall that the von Neumann entropy for a GHZ state is 1 for every cut. The von Neumann entropy of $|\psi_5\rangle$ is also 1 for the single index cuts, but it is 2 for the two-index cuts. So the state $|\psi_5\rangle$ is more highly entangled than the GHZ state, according to the von Neumann entropy measure too.

We note that the von Neumann entropies of $|\psi_5\rangle$ reflect the fact that in every cut, the reduced states are as mixed as they can be, that is, the state of the smaller subset of qubits is totally mixed — something that has been shown to be impossible for four qubits [Higuchi & Sudbery 2000].

‡ A. Higuchi, private communication 2004

5. Conjecture

We note that for 2 qubit Bell states, the 3 qubit GHZ states (but not the W state), the conjectured maximally entangled 4 qubit HS state, and our highly entangled 5 quibit $|\psi_5\rangle$ state, the single index cut partial transposes all have a single negative eigenvalue of $-\frac{1}{2}$. This is because the single-qubit reduced states are all totally mixed. Based on this partial numerical evidence, we *conjecture* that this continues to hold for higher numbers of qubits. That is

Conjecture 1 *For an n qubit state maximally entangled with respect to the NPT entanglement measure, all single-qubit reduced states are totally mixed.*

Note that we conjecture this to be a necessary, but not a sufficient, condition for maximum entanglement: our highly entangled but not maximally entangled state $|\psi_4\rangle$, and the non-maximally entangled states $|GHZ\rangle_4$ and $|GHZ\rangle_5$, also enjoy this property.

6. Conclusions

Numerical search has proved to be a richly rewarding topic.

We have successfully found a near-maximally entangled 4-qubit state (equation 16), and a highly entangled 5-qubit state (equation 24), using the E_{NPT} cost function. This cost function can be used to investigate higher numbers of qubits, but the expense of doing so increases exponentially (both in the size of matrices being manipulated, and in the number of cuts to be calculated).

Our numerical investigations support the conclusion that the conjectured maximally entangled HS state is at least a *local* maximum. Also, under our NPT measure, the GHZ states of 4 and 5-qubits are neither maximally entangled, nor even local maxima.

We have posed a conjecture that the single-qubit reduced states of maximally entangled states are all totally mixed.

7. Acknowledgments

Thanks to Viv Kendon for suggesting the use of the NPT criterion and its properties; to Lieven Clarisse for drawing our attention to some relevant literature; to Charles Fox for the use of his quantum computation functions for Matlab; and to the anonymous referee for helpful comments.

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