How entangled can two couples get?*

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Abstract

We describe a pure state of four qubits whose single-qubit density matrices are all maximally mixed and whose average entanglement as a system of two pairs of qubits appears to be maximal.

1 Introduction

In a system of two qubits the state

\[
|C_2\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)
\]

(1.1)

is, on all counts, the most entangled of all pure states. It gives the greatest violation of Bell inequalities, it has the largest entropy of entanglement, and its one-party reduced states are both maximally mixed. All of these properties determine it uniquely up to local unitary transformations.

A pure state of three qubits with similar properties is the GHZ state

\[
|C_3\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle).
\]

(1.2)

This state has the maximum value of pure 3-party entanglement, as measured by Wootters’s 3-tangle [3, 2], and its one-particle reduced density matrices

\textsuperscript{*}See ref. [8].
are all maximally mixed. Like the two-qubit state $|C_2\rangle$, it is characterised uniquely, up to local unitary transformations, by the latter property \[5\].

The obvious $n$-party generalisation is the “Schrödinger cat” state

$$|C_n\rangle = \frac{1}{\sqrt{2}}(|00\cdots0\rangle + |11\cdots1\rangle). \quad (1.3)$$

Like $|C_2\rangle$ and $|C_3\rangle$, this state has the property that its one-party reduced states are all maximally mixed. On the strength of this, $|C_n\rangle$ is sometimes called the “maximally entangled” pure state of $n$ qubits. For $n > 3$, however, not all states with this property are locally equivalent, and it is not clear that $|C_n\rangle$ is really the most entangled of them. Here we examine the case $n = 4$, show that there are 4-qubit states which are more entangled than $|C_4\rangle$, and attempt to find the most entangled among them.

A four-qubit system can be regarded, in three different ways, as a system of two pairs of qubits, and one can ask how entangled are these pairs. In the state $|C_4\rangle$ this entanglement is not maximal: each pair $X, Y$ of the four qubits $A, B, C, D$ is not in the maximally mixed state but exhibits correlations, all two-qubit density matrices being

$$\rho_{XY} = \frac{1}{2}(|00\rangle\langle00| + |11\rangle\langle11|). \quad (1.4)$$

But there do exist pure states of four qubits in which four of the six two-qubit reduced density matrices are maximally mixed. (We note that these density matrices come in pairs: if the reduced state of one pair is maximally mixed, so is that of the complementary pair.) For example, the state

$$|\Psi\rangle = \frac{1}{2}(|0000\rangle + |0111\rangle + |1001\rangle + |1110\rangle) \quad (1.5)$$

has two-qubit density matrices

$$\rho_{AB} = \rho_{AC} = \rho_{BD} = \rho_{CD} = \frac{1}{4}\mathbf{1},$$
$$\rho_{AD} = \frac{1}{2}(|++\rangle\langle++| + |--\rangle\langle--|),$$
$$\rho_{BC} = \frac{1}{2}(|00\rangle\langle00| + |11\rangle\langle11|),$$

where

$$|\pm\rangle = \frac{1}{\sqrt{2}}(|0\rangle \pm |1\rangle). \quad (1.6)$$

The one-qubit reduced density matrices of $|\Psi\rangle$ are all maximally mixed. But $|\Psi\rangle$ is not locally equivalent to the cat state $|C_4\rangle$, for it has different values...
from that state of the entanglement entropies $E_{AB}, E_{AC}, E_{BD}, E_{CD}$, which are invariants under local unitary transformations. (We write

$$ E_{XY} = - \text{tr}(\rho_{XY} \log_2 \rho_{XY}), \quad \rho_{XY} = \text{tr}_Z \ketbra{\Psi}{\Psi} \quad (1.7) $$

where $\{W, X, Y, Z\} \text{ is a permutation of } \{A, B, C, D\}$. In fact [7], the state $\ket{\Psi}$ cannot be asymptotically reversibly converted into any collection of the states $\ket{C_n}$ for $n = 2, 3, 4$.

It is natural to wonder whether there is a still more entangled state in which the reduced density matrices of all six pairs of qubits are maximally entangled. In Section 2 we will show that there is no such state of four qubits. The situation changes, however, if particles with larger state spaces are considered, and we will show that a system of four four-state particles does have pure states with this property.

In Section 3 we ask what is the maximum two-pair entanglement possible for a system of four qubits. Taking as a measure the average entanglement entropy $\langle E_2 \rangle = \frac{1}{3}(E_{AB} + E_{AC} + E_{AD})$, we exhibit a pure state $\ket{M_4}$ with a greater value of this quantity than the state (1.5); we show that $\langle E_2 \rangle$ has a stationary value at $\ket{M_4}$, and present evidence that this is a global maximum.

## 2 Non-existence of maximal entanglement between all pairs of pairs

**Theorem 1.** There is no pure state of four qubits whose two-qubit density matrices are all multiples of the identity.

**Proof.** Write the four-qubit state $\ket{\Psi}$ as

$$ \ket{\Psi} = \sum_{i,j,k,l=0,1} t^{ijkl} \ket{i} \ket{j} \ket{k} \ket{l} $$

The tensor $t^{ijkl}$ can be regarded as a $4 \times 4$ matrix in three different ways:

$$ t^{ijkl} = \frac{1}{2}(U_1)^{ij}_{kl} = \frac{1}{2}(U_2)^{ik}_{jl} = \frac{1}{2}(U_3)^{il}_{jk} $$

and the requirement of maximal entanglement is that $U_1, U_2$ and $U_3$ should all be unitary matrices.

\footnote{This question has been studied by Gisin and Bechmann-Pasquinucci [4] for the general case of $n$ qubits, but under the restriction that the states are symmetric under permutations of the qubits. This is an unnatural requirement in this context, since it is not invariant under local unitary transformations.}
We show first that by local unitary transformations we can arrange that the coordinates of $|\Psi\rangle$ satisfy

$$t^{1000} = t^{0100} = t^{0010} = t^{0001} = 0.$$ 

To do this, we find normalised states $|\alpha\rangle, |\beta\rangle, |\gamma\rangle, |\delta\rangle$ which maximise $N = |\langle\Psi|\alpha\rangle|\beta\rangle|\gamma\rangle|\delta\rangle|^2$. Such states certainly exist, since $N(\alpha, \beta, \gamma, \delta)$ is a continuous function on the compact space $S^3 \times S^3 \times S^3 \times S^3$. Change basis in each of the single-qubit spaces so that $|\alpha\rangle|\beta\rangle|\gamma\rangle|\delta\rangle$ becomes the basis state $|0000\rangle$; then $N = |t^{0000}|^2$. But if $t^{1000}$ were non-zero we could change basis for states of the first qubit so as to increase $|t^{0000}|$; since we have maximised it, we must have $t^{1000} = 0$. Similarly $t^{0100} = t^{0010} = t^{0001} = 0$.

The matrices $U_1, U_2, U_3$ which have to be unitary are now

$$
\begin{pmatrix}
t^{0000} & 0 & 0 & t^{0011} \\
0 & t^{0101} & t^{0110} & t^{0111} \\
0 & t^{1001} & t^{1010} & t^{1011} \\
t^{1000} & t^{1101} & t^{1110} & t^{1111}
\end{pmatrix},
\begin{pmatrix}
t^{0000} & 0 & 0 & t^{0101} \\
0 & t^{0011} & 0 & t^{0110} \\
0 & t^{0101} & t^{1001} & t^{1010} \\
t^{0110} & t^{1101} & t^{1110} & t^{1111}
\end{pmatrix},
\begin{pmatrix}
t^{0000} & 0 & 0 & t^{1110} \\
0 & t^{0011} & 0 & t^{1110} \\
0 & t^{0111} & t^{1011} & t^{1111} \\
t^{1100} & t^{1111} & t^{1110} & t^{1111}
\end{pmatrix}.
$$

Hence the following three conditions must hold:

1. $t^{0011} = 0$ or $t^{0111} = t^{1011} = 0$;
2. $t^{0101} = 0$ or $t^{0111} = t^{1101} = 0$;
3. $t^{0110} = 0$ or $t^{0111} = t^{1110} = 0$.

Following the branching consequences of these, and requiring that the matrices are unitary, leads to a conclusion of the form that three $2 \times 2$ matrices

$$
\begin{pmatrix}
a & b \\
c & d
\end{pmatrix},
\begin{pmatrix}
b & e \\
f & c
\end{pmatrix},
\begin{pmatrix}
a & e \\
f & d
\end{pmatrix}
$$

must all be unitary. In this situation all the matrix elements must be non-zero: if, for example, $a = 0$, then $d = 0$ and $b, c, e, f$ would all have unit modulus, which is impossible if the second matrix is to be unitary. Now unitarity gives

$$a = -\frac{bd}{e} = -\frac{ce}{f},$$

so

$$b\bar{f} = e\bar{c}.$$ 

But

$$b\bar{f} + e\bar{c} = 0,$$

so $b\bar{f} = e\bar{c} = 0$, which is impossible. □
Four-party states with this property do exist, however, if the individual parties have more independent states. For example, suppose each party has a 4-dimensional state space; then the (non-normalised) state with coordinates

\[ t_{ijkl} = \begin{cases} 
1 & \text{if } i = j = k = l \text{ or } (i, j, k, l) \text{ is an even permutation of } (1, 2, 3, 4) \\
0 & \text{otherwise}
\end{cases} \]

has every two-qubit density matrix equal to a multiple of the identity.

We note that the method introduced in this proof can be used to define a canonical form for any multipartite pure state, in which a maximal number of coordinates are zero. This can be regarded as a generalisation of the Schmidt decomposition of a bipartite state. Details can be found in [1].

3 A Maximally Entangled Four-qubit State?

Given that a four-qubit state cannot have maximal entropy of entanglement for every two-qubit subset, we now ask what is the greatest possible average for such entropies, i.e. we seek to maximise

\[ \langle E_2 \rangle = \frac{1}{6} (E_{AB} + E_{AC} + E_{AD} + E_{BC} + E_{BD} + E_{CD}) = \frac{1}{3} (E_{AB} + E_{AC} + E_{AD}). \]

The second equality holds because complementary pairs have equal entropy.

We have not been able to solve this problem analytically. We will adopt a heuristic approach, using an (indefensible) analogy with the two-qubit system to obtain a candidate maximally entangled state and then showing that \( \langle E_2 \rangle \) is indeed stationary at this state and appears to be maximal.

Maximally entangled states of two qubits like \( |\Psi^-\rangle \) are often referred to as “singlet” states, since an example of such a state is the state of two spin-\( \frac{1}{2} \) particles with zero total angular momentum. This description is not invariant under local unitary transformations, which need not preserve the total angular momentum. Nevertheless, let us take this as a hint in investigating four-qubit states. A system of four spin-\( \frac{1}{2} \) particles has two independent singlet states. The most symmetric combination of these, in the sense that all of its two-qubit density matrices are unitarily equivalent, is locally equivalent to

\[ |M_4\rangle = \frac{1}{\sqrt{6}} \left[ |0011\rangle + |1100\rangle + \omega(|1010\rangle + |0101\rangle) + \omega^2(|1001\rangle + |0110\rangle) \right], \]

where \( \omega = e^{2\pi i/3} \), or to \( \overline{|M_4\rangle} \), the complex conjugate of \( |M_4\rangle \) in the computation basis. Note that this state is not symmetric between the qubits but
belongs to a two-dimensional representation of the permutation group, the
other state in the representation being $\ket{M_4}$.

The two-qubit density matrices of $\ket{M_4}$ are

$$\rho_{AB} = \rho_{AC} = \rho_{AD} = \frac{1}{6} \left( \ket{00}\bra{00} + \ket{11}\bra{11} + \ket{\Phi_+}\bra{\Phi_+} + \frac{1}{2}\ket{\Phi_-}\bra{\Phi_-} \right) \quad (3.1)$$

where

$$\ket{\Phi_\pm} = \frac{1}{\sqrt{2}} (\ket{10} \pm \ket{01})$$

(in angular momentum terms, the two-qubit reduced states are equal mix-
tures of a singlet and a maximally mixed triplet). Hence the entangleme
entropies are

$$E_{AB} = E_{AC} = E_{AD} = 1 + \frac{1}{2} \log_2 3.$$  

Comparing with the cat state $\ket{C_4}$, for which

$$E_{AB} = E_{AC} = E_{AD} = 1,$$

and the state of $\ket{\psi}$, for which

$$E_{AB} = E_{AC} = 2, \quad E_{AD} = 1,$$

we see that $\ket{M_4}$ has a greater value of $\langle E_2 \rangle$ than either.

We will now show that the function $\langle E_2 \rangle$ is stationary at $\ket{M_4}$. To simplify
the calculation, we consider the functions $E_{XY}$ defined by (1.7) for all state
vectors $\ket{\psi}$, though these functions coincide with the entropies only when
$\ket{\psi}$ is normalised. Suppose $\ket{\psi}$ changes by $\ket{\delta\psi}$. Because the trace makes
the operators behave as if they commuted, the consequent change in $E_{XY}$ is
given by

$$\delta E_{XY} = - \text{tr} \left[ \rho_{XY} \log_2(e\rho_{XY}) \right].$$

At $\ket{\psi} = \sqrt{6}\ket{M_4}$ we find

$$\delta E_{AB} = \text{Re} \left[ - \langle \psi \delta\psi \rangle \log_2(3e^2) + \langle \psi \delta\psi \rangle \log_2 3 \right],$$

$$\delta E_{AC} = \text{Re} \left[ - \langle \psi \delta\psi \rangle \log_2(3e^2) + \omega \langle \psi \delta\psi \rangle \log_2 3 \right],$$

$$\delta E_{AD} = \text{Re} \left[ - \langle \psi \delta\psi \rangle \log_2(3e^2) + \omega^2 \langle \psi \delta\psi \rangle \log_2 3 \right],$$

where $\langle \overline{\psi} \rangle$ is the complex conjugate of $\ket{\psi}$ in the computation basis. Hence
the gradient of the average $\langle E_2 \rangle$ in the real 32-dimensional space of all state
vectors is in the direction of $\ket{\psi}$:

$$\delta \langle E_2 \rangle = - \log_2(3e^2) \text{Re} \langle \psi \delta\psi \rangle.$$
Thus \( \langle E_2 \rangle \) is stationary at \(|\Psi\rangle\) for variations on the sphere of vectors with the same norm as \(|\Psi\rangle\). But each \( E_{XY} \), as given by (1.7), is linearly related to the true entropy of entanglement, so the average two-party entropy is stationary at \(|M_4\rangle\).

We have searched numerically for states which maximise \( \langle E_2 \rangle \) starting from several arbitrarily chosen states. All the states we have obtained in this manner are locally equivalent to \(|M_4\rangle\) or \(|\overline{M}_4\rangle\).

## 4 Robustness of the entanglement

One of the criteria for maximal entanglement suggested in [4] is that the entanglement should be maximally fragile: a measurement on any one of the qubits destroys the entanglement between the remaining qubits. This is true of the cat state (1.3) if the measurement projects onto the computation basis \(|0\rangle, |1\rangle\}. Projection onto the basis \{|+, |−\rangle\} defined in (1.6), however, leaves the remaining qubits in a cat state.

The state constructed in the previous section behaves in the opposite way to the cat state: measurement of one qubit leaves the other three qubits in an entangled state, and the amount of entanglement afterwards is independent of what measurement is performed. To be precise, projection of one qubit onto a computation basis state leaves the remaining qubits in one of the entangled states

\[
\frac{1}{\sqrt{3}} \left( |011\rangle + \omega |101\rangle + \omega^2 |110\rangle \right) \quad (4.1)
\]

or

\[
\frac{1}{\sqrt{3}} \left( |100\rangle + \omega |010\rangle + \omega^2 |001\rangle \right). \quad (4.2)
\]

These states, which are clearly locally equivalent, have recently been identified as having maximal average two-qubit entanglement in a certain sense [5]. Projection onto any other state of the first qubit leaves the other three qubits in another state which is locally equivalent to the above. This follows from the fact that the state \(|M_4\rangle\) is an SU(2) singlet, so that the unitary transformation from the computation basis to any other basis of one qubit can be undone by performing the same transformation on the other three qubits.

Thus the entanglement of the state \(|M_4\rangle\) is robust. Any carelessness by the holder of any one of the qubits, resulting in an uncontrolled decoherence of that qubit, does not completely destroy the entanglement of the remaining qubits, and always leaves them with the same amount of entanglement.
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