On maximal entanglement between two pairs in four-qubit pure states

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Abstract
We show that the state with the highest known average two-particle von
Neumann entanglement entropy proposed by Sudbery and one of the authors
gives a local maximum of this entropy. We also show that this is not the case
for an alternative highly entangled state proposed by Brown *et al*.

PACS numbers: 03.67.Mn, 03.65.Ta, 03.65.Ud, 03.65.Db

1. Introduction

The characterization of multi-particle entanglement is a major open problem that is particularly
significant for the study of quantum computation and many-body physics [1]. One of the ways
in which entanglement can be understood is by way of reference to a 'maximally' entangled
state. This target state can then be used, for example, to determine the largest rate at which
it is possible to distill pure maximally entangled states from a supply of mixed states using
only LOCC [2]. An obvious condition for maximal entanglement in the case of pure states
is that all one-qubit-reduced density matrices are maximally mixed. For two- and three-qubit
systems this leads to a unique state [3] (up to local unitary operations). However this is not
true for a system with more than three qubits. For example, the states

$$|\phi_1\rangle = \tfrac{1}{\sqrt{2}}(|0000\rangle + |1111\rangle)$$
$$|\phi_2\rangle = \tfrac{1}{2}(|0000\rangle + |0111\rangle + |1001\rangle + |1110\rangle)$$

have the property that all one-party-reduced density matrices are maximally mixed; yet these
two states are not locally equivalent. One may then ask which states also have maximally
mixed two-party-reduced density matrices. However, Sudbery and one of the authors (AH)
have shown that it is not possible for all two-qubit-reduced density matrices of a pure four-
qubit state to be maximally mixed [4]. Nevertheless, they found a state which appears to
maximize the average von Neumann entropy of two-qubit-reduced density matrices, which
will be denoted by E_2 in this paper. They showed that this state is a stationary point of the

function E_2, but it is not known whether this state indeed gives the maximum of E_2. In this paper we show that this state gives at least a local maximum of E_2.

Given four qubits A, B, C and D the von Neumann entropy of the two-party-reduced states is

$$E_{XY} = -\text{tr}(\rho_{XY} \log_2 \rho_{XY}), \tag{1}$$

where $\rho_{XY} = \text{tr}_{ZW}|\psi\rangle\langle\psi|$ with W, X, Y, Z being a permutation of the four systems. The average entropy of two-qubit-reduced density matrices is defined by

$$E_2 \equiv \tfrac{1}{6}(E_{AB} + E_{AC} + E_{AD} + E_{BC} + E_{BD} + E_{CD})$$
$$= \tfrac{1}{3}(E_{AB} + E_{AC} + E_{AD}).$$

This quantity can naturally be taken as a measure of the entanglement between two pairs in pure four-qubit states.

There are other approaches to quantifying multi-partite entanglement that are applicable to a general mixed state. A measure for a general composite system has been introduced by Yukalov [5] using the ratio of norms of an entangling operator and of a disentangling operator in the relevant disentangled Hilbert space. The entanglement of a four-qubit system can also be studied using the entropy of the reduced three-particle system and the strong subaddativity inequality [6]. Brown *et al* have considered the partial transpose with respect to all possible partitions of the state [7]. These measures are more general than E_2 in so much as they are applicable to mixed states. In this paper, we only consider pure states and, therefore, the average entropy is a suitable measure of entanglement.

The four-qubit state proposed in [4],

$$|M_4\rangle = \tfrac{1}{\sqrt{6}}[|0011\rangle + |1100\rangle + \omega(|0101\rangle + |1010\rangle) + \overline{\omega}(|0110\rangle + |1001\rangle)],$$

where $\omega = \exp(2i\pi/3)$ is a third root of unity, has the highest known average two-qubit bipartite entanglement [4, 7]. It is also an element of the orbit of SLOCC operations that has maximal four-partite entanglement [8]. Together with its complex conjugate, it also provides a basis for the space of singlets contained in a four-qubit Hilbert space [9].

The entropy E_{XY} measures the entanglement between systems XY and WZ, i.e. it measures entanglement between pairs. The entropy of the one-party-reduced density matrices measures the entanglement between individual systems and the rest of the state. Another way in which entanglement could manifest itself in a four-qubit system is the entanglement between any two individual systems. For example, the entanglement between X and Y is measured by regarding ρ_{XY} as a (mixed) state in its own right. There are various bipartite entanglement measures for mixed states. One that is commonly used for multipartite states is the concurrence, since for this measure there is an inequality, the CKW inequality, which gives an upper bound on the bipartite entanglement in terms of one-party entanglement [10, 11]. Namely

$$C_{AB}^2 + C_{AC}^2 + C_{AD}^2 \leqslant C_{A(BCD)}^2, \tag{2}$$

where $C_{A(BCD)}$ denotes the concurrence across the partition $A : BCD$, where the qubits BCD are regarded as one eight-dimensional qudit. Since $\rho_{ABCD} = |M_4\rangle\langle M_4|$ is pure, one has $C_{A(BCD)} = 2\sqrt{\det(\rho_A)} = 1$.

It is interesting to note that $|M_4\rangle$ contains no bipartite entanglement, that is, ρ_{AY} is separable[1] for all Y. Moreover, the states ρ_{AY} are on the boundary of separable states. This can be seen by writing ρ_{AY} in the form

$$\rho_{AY} = \frac{\left(1 - \tfrac{1}{3}\right)}{4}\mathbb{I} + \frac{1}{3}|\Phi_-\rangle\langle\Phi_-|,$$

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[1] ρ_{AY} is a mixed state, and so separability here means that it can be written as the convex sum of unentangled pure states.

where $|\Phi_-\rangle = \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle)$, i.e. as a Werner state with $x = \frac{1}{3}$ [12, 13]. Therefore, the left-hand side of equation (2) is zero while the right-hand side is one. This can be thought of as saying that A shares none of its entanglement with its neighbours, i.e. the entanglement between AY and WZ does not come from the separate entanglement of A with W or Z in the state $|M_4\rangle$.

The authors of [4] conjectured that $|M_4\rangle$ gives a maximum of the average two-qubit bipartite entanglement. By considering the first variation, δE_{XY}, they were able to show that E_2 is stationary at $|M_4\rangle$. In this paper, we will consider the second variation of the average entropy and demonstrate that the state $|M_4\rangle$ indeed gives a local maximum. We will also consider another highly entangled state proposed in [7] and show that this state is in fact not a stationary point of our measure, thus illustrating that maximal entanglement is dependent on the measure used.

2. Varying the entropy

We consider variations of the state near $|M_4\rangle$ with the varied states characterized by several small parameters. In general, suppose we vary a four-qubit state $|\psi\rangle$ in second-order approximation as

$$|\psi\rangle \to |\psi'\rangle = |\psi\rangle + |\delta\psi\rangle + |\delta^2\psi\rangle,$$

where $|\delta\psi\rangle$ and $|\delta^2\psi\rangle$ are of first and second orders, respectively, in the small parameters characterizing the variations. From the normalization condition $\langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle = 1$, we obtain

$$2\,\mathrm{Re}\langle\delta\psi|\psi\rangle = 0 \tag{3}$$

at first order and

$$2\,\mathrm{Re}\langle\delta^2\psi|\psi\rangle + \langle\delta\psi|\delta\psi\rangle = 0 \tag{4}$$

at second order.

In order to find the first and second variations of the entropy, we need the following lemma.

Lemma 2.1. *For any function $f(A)$ of a matrix A that can be written as a power series, consider variations of A with small parameters, $A \mapsto A + \delta A + \delta^2 A$, to second order in these parameters. Then to second order the corresponding variation $\mathrm{tr}[f(A)] \mapsto \mathrm{tr}[f(A)] + \delta\mathrm{tr}[f(A)] + \delta^2\mathrm{tr}[f(A)]$ is given by*

$$\delta\mathrm{tr}[f(A)] = \mathrm{tr}[\delta A \cdot f'(A)],$$
$$\delta^2\mathrm{tr}[f(A)] = \mathrm{tr}\left[\delta^2 A \cdot f'(A) + \tfrac{1}{2}\delta A \cdot \delta f'(A)\right].$$

Proof. Since $f(A)$ can be written as a power series, it is enough to show these formulae for $f(A) = A^n$. We obtain first-order terms in the variation of A^n by replacing one of the A's by δA. Thus, $\delta\,\mathrm{tr}A^n = n\,\mathrm{tr}[\delta A \cdot A^{n-1}]$. This proves the first formula. We get second-order terms by replacing one of A's by a $\delta^2 A$ or by replacing two A's by two δA's. Thus,

$$\delta^2\mathrm{tr}A^n = n\mathrm{tr}[\delta^2 A \cdot A^{n-1}] + \frac{n}{2}\sum_{k=0}^{n-2}\mathrm{tr}[\delta A \cdot A^k \cdot \delta A \cdot A^{n-k-2}]$$

$$= \mathrm{tr}[\delta^2 A \cdot n A^{n-1}] + \frac{1}{2}\mathrm{tr}[\delta A \cdot \delta(n A^{n-1})].$$

(One can perhaps convince oneself of the need for the factor $1/2$ in the second term by noting that the number of ways to replace two A's by two δA's is $n(n-1)/2$.) This proves the second formula. $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\quad\Box$

Letting $A = 1 - \rho_{XY}$ and $f(A) = (1 - A)\log(1 - A) = \rho_{XY}\log\rho_{XY}$ in this lemma, and using the normalization conditions $\text{tr}[\delta\rho_{XY}] = \text{tr}[\delta^2\rho_{XY}] = 0$, we obtain the first- and second-order variations of E_{XY} defined by (1) as

$$\delta E_{XY} = -\frac{1}{\log 2}\,\text{tr}[\delta\rho_{XY}\log\rho_{XY}], \tag{5}$$

$$\delta^2 E_{XY} = -\frac{1}{\log 2}\,\text{tr}\left[\delta^2\rho_{XY}\log\rho_{XY} + \frac{1}{2}\delta\rho_{XY}\delta\log\rho_{XY}\right], \tag{6}$$

where

$$\rho_{XY} = \text{tr}_{ZW}(|\psi\rangle\langle\psi|),$$
$$\delta\rho_{XY} = \text{tr}_{ZW}(|\delta\psi\rangle\langle\psi| + |\psi\rangle\langle\delta\psi|),$$
$$\delta^2\rho_{XY} = \text{tr}_{ZW}(|\delta^2\psi\rangle\langle\psi| + |\psi\rangle\langle\delta^2\psi| + |\delta\psi\rangle\langle\delta\psi|).$$

3. An alternative highly entangled state

In [7], Brown *et al* have considered multi-partite entanglement across all possible partitions of a state and calculated the sum of all negative eigenvalues when the partial-transpose function is applied and sought to maximize this over all possible states. In the four-qubit case, their numerical search found the state

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

where $|+\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $|-\rangle = \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. Here we consider whether the state $|\psi_4\rangle$ gives a local maximum of E_2 as a measure of entanglement.

We start by noting that ρ_{AC} is maximally mixed and that the eigenvalues of ρ_{AB} and ρ_{AD} are both equal to

$$\left\{\frac{2+\sqrt{2}}{8}, \frac{2+\sqrt{2}}{8}, \frac{2-\sqrt{2}}{8}, \frac{2-\sqrt{2}}{8}\right\}.$$

Comparing the average two-qubit entanglement of this state with that of $|M_4\rangle$, we see that the state $|\psi_4\rangle$ has lower two-party average von Neumann entanglement [7]. Namely

$$E_2(|\psi_4\rangle) = \tfrac{5}{2} - \tfrac{1}{2\sqrt{2}}\log_2(3 + \sqrt{2}) \approx 1.7426,$$
$$E_2(|M_4\rangle) = 1 + \tfrac{1}{2}\log_2 2 \approx 1.7925.$$

We will now show that the state $|\psi_4\rangle$ in fact does not give a local maximum of E_2 by demonstrating that it is not a stationary point. The first-order variation of E_2 is given by

$$3\delta E_2 = \delta E_{AB} + \delta E_{AC} + \delta E_{AD}.$$

Since ρ_{AC} is maximally mixed, we have $\delta E_{AC} = 0$ by (5) and the first-order normalization condition. In order to diagonalize ρ_{AB} and ρ_{AD} we use the bases $\{|u_\pm\rangle, |v_\pm\rangle\}$ and $\{|w_\pm\rangle, |x_\pm\rangle\}$, respectively, where

$$|u_\pm\rangle = (\sqrt{2}\mp 1)|10\rangle \pm |00\rangle, \qquad |v_\pm\rangle = (\sqrt{2}\pm 1)|11\rangle \mp |01\rangle,$$
$$|w_\pm\rangle = (\sqrt{2}\mp 1)|10\rangle \mp |00\rangle, \qquad |x_\pm\rangle = (\sqrt{2}\pm 1)|11\rangle \pm |01\rangle.$$

Therefore we can now write

$$\rho_{AB} = \rho_{AD} = \frac{1}{8} \begin{bmatrix} 2+\sqrt{2} & & & \\ & 2-\sqrt{2} & & \\ & & 2+\sqrt{2} & \\ & & & 2-\sqrt{2} \end{bmatrix}$$

$$= (2-\sqrt{2})\frac{\mathbb{I}}{8} + \frac{\sqrt{2}}{4}\begin{bmatrix} 1 & & & \\ & 0 & & \\ & & 1 & \\ & & & 0 \end{bmatrix}.$$

Hence, by (5) and the normalization condition,

$$\delta E_2 \propto \text{tr}[\delta\rho_{AB}(|u_+\rangle\langle u_+| + |v_+\rangle\langle v_+|) + \delta\rho_{AD}(|w_+\rangle\langle w_+| + |x_+\rangle\langle x_+|)]$$
$$= \langle u_+|\delta\rho_{AB}|u_+\rangle + \langle v_+|\delta\rho_{AB}|v_+\rangle + \langle w_+|\delta\rho_{AD}|w_+\rangle + \langle x_+|\delta\rho_{AD}|x_+\rangle.$$

Consider a variation of the form

$$|\delta\psi\rangle = \alpha|0011\rangle + \beta|1011\rangle.$$

Then the normalization condition requires that $\text{Re}\{\alpha + \beta\} = 0$. We find

$$\delta\rho_{AB} = \tfrac{1}{\sqrt{2}}(|00\rangle + |10\rangle)(\overline{\alpha}\langle 00| + \overline{\beta}\langle 10|) + \tfrac{1}{\sqrt{2}}(\alpha|00\rangle + \beta|10\rangle)(\langle 00| + \langle 10|),$$

and hence

$$\langle u_+|\delta\rho_{AB}|u_+\rangle = 2\text{Re}[\alpha + \beta(\sqrt{2}-1)],$$

$$\langle v_+|\delta\rho_{AB}|v_+\rangle = 0.$$

Similarly,

$$\langle w_+|\delta\rho_{AD}|w_+\rangle = 0,$$

$$\langle x_+|\delta\rho_{AD}|x_+\rangle = 2\text{Re}[\alpha(\sqrt{2}+1) + \beta(2\sqrt{2}+3)].$$

Therefore, for the variations considered here we have

$$\delta E_2 \propto \text{Re}[\alpha(2+\sqrt{2}) + \beta(2+3\sqrt{2})].$$

Hence, by putting $\alpha = -\beta = \varepsilon$ for a small $\varepsilon \in \mathbb{R}$—note that the normalization condition $\text{Re}(\alpha + \beta) = 0$ is satisfied—we have $\delta E_2 \neq 0$. Therefore the state $|\psi_4\rangle$ cannot give a local maximum of E_2.

4. The second-order variations

We now return to the state $|M_4\rangle$ and show that it gives a local maximum of E_2, that is, $\delta^2 E_{AB} + \delta^2 E_{AC} + \delta^2 E_{AD} < 0$. Let us write $\delta^2\rho_{XY} = \kappa_{XY} + \sigma_{XY}$, where

$$\sigma_{XY} = \text{tr}_{WZ}(|\delta\psi\rangle\langle\delta\psi|),$$

$$\kappa_{XY} = \text{tr}_{WZ}(|\delta^2\psi\rangle\langle\psi| + |\psi\rangle\langle\delta^2\psi|).$$

Then,

$$-\log 2 \sum_Y \delta^2 E_{AY} = \sum_Y \text{tr}\left(\kappa_{AY}\log\rho_{AY} + \sigma_{AY}\log\rho_{AY} + \frac{1}{2}\delta\rho_{AY}\delta\log\rho_{AY}\right), \tag{7}$$

where $Y = B, C$ and D. Our task now is to show that the right-hand side of this equation is positive definite for all nontrivial variations of the state $|\psi\rangle = |M_4\rangle$ satisfying the normalization conditions (3) and (4). We will deal with each term in (7) separately.

4.1. The first two terms in the expansion

We note that $\log \rho_{AY} = \log 3 \cdot |\Phi_-\rangle\langle\Phi_-| - \log 6 \cdot \mathbb{I}$, where $|\Phi_-\rangle = \frac{1}{\sqrt{2}}(|10\rangle - |01\rangle)$, for all Y, and that

$$\mathrm{tr}(\kappa_{AB}|\Phi_-\rangle\langle\Phi_-|) = \mathrm{Re}(\langle\delta^2\psi|\psi\rangle - \langle\delta^2\psi|\overline{\psi}\rangle),$$

$$\mathrm{tr}(\kappa_{AC}|\Phi_-\rangle\langle\Phi_-|) = \mathrm{Re}(\langle\delta^2\psi|\psi\rangle - \overline{\omega}\langle\delta^2\psi|\overline{\psi}\rangle),$$

$$\mathrm{tr}(\kappa_{AD}|\Phi_-\rangle\langle\Phi_-|) = \mathrm{Re}(\langle\delta^2\psi|\psi\rangle - \omega\langle\delta^2\psi|\overline{\psi}\rangle),$$

where $|\overline{\psi}\rangle$ is the complex conjugate of $|\psi\rangle = |M_4\rangle$ in the computation basis, as was shown in [4] in the context of first-order variation. Hence, using the normalization condition (4), we find the first term of (7) as

$$\sum_Y \mathrm{tr}(\kappa_{AY} \log \rho_{AY}) = 3 \log 2\sqrt{3} \cdot \langle\delta\psi|\delta\psi\rangle.$$

We now consider the second term in (7). We have

$$\mathrm{tr}(\sigma_{XY} \log \rho_{XY}) = \mathrm{tr}(\sigma_{XY} \log 3 \cdot |\Phi_-\rangle\langle\Phi_-| - \sigma_{XY} \log 6 \cdot \mathbb{I})$$

$$= \log 3 \cdot \mathrm{tr}[(\mathrm{tr}_{WZ}|\delta\psi\rangle\langle\delta\psi|)|\Phi_-\rangle\langle\Phi_-|] - \log 6 \cdot \langle\delta\psi|\delta\psi\rangle$$

$$= \log 3 \sum_{i,j=0}^{1} |(\langle\Phi_-|_{XY}\langle ij|_{WZ})|\delta\psi\rangle|^2 - \log 6 \cdot \langle\delta\psi|\delta\psi\rangle.$$

Hence,

$$\sum_Y \mathrm{tr}(\sigma_{AY} \log \rho_{AY}) = -3 \log 6 \cdot \langle\delta\psi|\delta\psi\rangle + F_{AB} + F_{AC} + F_{AD},$$

where

$$F_{XY} = \log 3 \sum_{i,j=0}^{1} |(\langle\Phi_-|_{XY}\langle ij|_{WZ})|\delta\psi\rangle|^2.$$

Thus

$$\sum_Y \mathrm{tr}[(\kappa_{AY} + \sigma_{AY}) \log \rho_{AY}] = -3 \log\sqrt{3} \cdot \langle\delta\psi|\delta\psi\rangle + F_{AB} + F_{AC} + F_{AD}$$

$$\geqslant -\frac{3}{2} \log 3 \cdot \langle\delta\psi|\delta\psi\rangle,$$

because $F_{AB} + F_{AC} + F_{AD} \geqslant 0$. This motivates us to define

$$P \equiv \sum_Y \mathrm{tr}[\delta\rho_{AY}\delta \log \rho_{AY}] - 3 \log 3 \cdot \langle\delta\psi|\delta\psi\rangle. \tag{8}$$

Then, if $P > 0$ for all nontrivial variations, $\delta^2 E_2$ is negative definite and the state $|M_4\rangle$ gives a local maximum of E_2. We will show this fact with a certain convenient parametrization of variations.

4.2. The third term in the expansion

The following lemma will be useful in analysing the variation $\delta \log \rho_{XY}$.

Lemma 4.1. *Provided that the eigenvalues of A are positive and less than 1, we have*

$$\delta \log A = \int_0^1 [\mathbb{I} - t(\mathbb{I} - A)]^{-1}\delta A[\mathbb{I} - t(\mathbb{I} - A)]^{-1} \, \mathrm{d}t.$$

Proof. We expand $\log A$ as

$$\log A = \log(\mathbb{I} - (\mathbb{I} - A)) = -\sum_{n=1}^{\infty} \frac{(\mathbb{I} - A)^n}{n}.$$

Then

$$\delta \log A = \sum_{n=1}^{\infty} \sum_{m=0}^{n-1} \frac{(\mathbb{I} - A)^m \delta A (\mathbb{I} - A)^{n-m-1}}{n}$$

$$= \sum_{n'=0}^{\infty} \sum_{m=0}^{\infty} \frac{(\mathbb{I} - A)^m \delta A (\mathbb{I} - A)^{n'}}{n' + m + 1},$$

where we have let $n' = n - m - 1$. Noting the elementary integral,

$$\int_0^1 t^{n'+m} \mathrm{d}t = \frac{1}{n' + m + 1},$$

we find

$$\delta \log A = \int_0^1 \sum_{n'=0}^{\infty} \sum_{m=0}^{\infty} [t(\mathbb{I} - A)]^m \delta A [t(\mathbb{I} - A)]^{n'} \, \mathrm{d}t$$

$$= \int_0^1 \sum_{m=0}^{\infty} [t(\mathbb{I} - A)]^m \delta A \sum_{n'=0}^{\infty} [t(\mathbb{I} - A)]^{n'} \, \mathrm{d}t$$

$$= \int_0^1 [\mathbb{I} - t(\mathbb{I} - A)]^{-1} \delta A [\mathbb{I} - t(\mathbb{I} - A)]^{-1} \, \mathrm{d}t$$

as required. $\qquad\square$

We use this lemma with $A = \rho$, where ρ is a density matrix. Since ρ is Hermitian, we can choose a basis in which $\rho = \mathrm{diag}\{\lambda_1, \ldots, \lambda_n\}$. We can apply this lemma if $0 < \lambda_i < 1$ for all i. Note that the state $|M_4\rangle$ has this property. If $\lambda_i \neq \lambda_j$, we have

$$(\delta \log \rho)_{ij} = \int_0^1 \frac{\delta_{ik}}{1 - t(1 - \lambda_i)} \delta \rho_{kl} \frac{\delta_{lj}}{1 - t(1 - \lambda_j)} \, \mathrm{d}t$$

$$= \int_0^1 \left(\frac{X}{1 - t(1 - \lambda_i)} + \frac{Y}{1 - t(1 - \lambda_j)} \right) \delta \rho_{ij} \, \mathrm{d}t,$$

where $X = \frac{1-\lambda_i}{\lambda_j - \lambda_i}$ and $Y = \frac{1-\lambda_j}{\lambda_i - \lambda_j}$. Hence, for $\lambda_i \neq \lambda_j$,

$$(\delta \log \rho)_{ij} = \frac{1}{\lambda_j - \lambda_i} \log\left(\frac{\lambda_j}{\lambda_i} \right) \delta \rho_{ij}. \tag{9}$$

If $\lambda_i = \lambda_j$, then

$$(\delta \log \rho)_{ij} = \int_0^1 \frac{\delta \rho_{ij}}{(1 - t(1 - \lambda_i))^2} \, \mathrm{d}t$$

$$= \frac{\delta \rho_{ij}}{\lambda_i}. \tag{10}$$

(This formula can also be obtained by letting $\lambda_j \to \lambda_i$ in (9).) We now apply these formulae to the variation $\delta \log \rho_{XY}$.

To ease the notation we let $\delta \rho_{AB} = (a_{ij}^{(1)})$, $\delta \rho_{AC} = (a_{ij}^{(2)})$ and $\delta \rho_{AD} = (a_{ij}^{(3)})$. We will use the basis $S = \{|O\rangle, |I\rangle, |+\rangle, |-\rangle\} = \{|00\rangle, |11\rangle, |\Phi_+\rangle, |\Phi_-\rangle\}$, where $|\Phi_\pm\rangle = 2^{-1/2}$ $(|10\rangle - |01\rangle)$. Thus, for example, $a_{OI}^{(1)} = \langle O|\delta \rho_{AB}|I\rangle$. Since $\lambda_1 = \lambda_2 = \lambda_3 = 1/6$ and

$\lambda_4 = 1/2$ for each ρ_{AY}, we have, by applying (9) and (10),

$$\text{tr}(\delta\rho_{AB}\delta\log\rho_{AB}) = \sum_{ij} K_{ij}\left|a_{ij}^{(1)}\right|^2,$$

$$\text{tr}(\delta\rho_{AC}\delta\log\rho_{AC}) = \sum_{ij} K_{ij}\left|a_{ij}^{(2)}\right|^2,$$

$$\text{tr}(\delta\rho_{AD}\delta\log\rho_{AD}) = \sum_{ij} K_{ij}\left|a_{ij}^{(3)}\right|^2,$$

where

$$K = \begin{pmatrix} 6 & 6 & 6 & 3\log 3 \\ 6 & 6 & 6 & 3\log 3 \\ 6 & 6 & 6 & 3\log 3 \\ 3\log 3 & 3\log 3 & 3\log 3 & 2 \end{pmatrix}.$$

In order to proceed further, we need to explicitly parameterize the variations $|\delta\Psi\rangle$. Thus, we write

$$\begin{aligned}|\delta\Psi\rangle = {} & \epsilon_{0000}|0000\rangle + \epsilon_{1111}|1111\rangle + \epsilon_{0011}|0011\rangle + \epsilon_{1100}|1100\rangle + \omega(\epsilon_{1010}|1010\rangle + \epsilon_{0101}|0101\rangle) \\ & + \omega^2(\epsilon_{1001}|1001\rangle + \epsilon_{0110}|0110\rangle) \\ & + \epsilon_{0111}|0111\rangle + \epsilon_{1011}|1011\rangle + \epsilon_{1101}|1101\rangle + \epsilon_{1110}|1110\rangle \\ & + z(|1000\rangle + |0100\rangle + |0010\rangle + |0001\rangle).\end{aligned}$$

Note that we have included only one term with 'three 0's' out of four possible terms. This is because all other terms can be eliminated by local unitary transformations to first order. We derive additional constraints on the variations by noting that if the effect of the variation is to change the relative phase in any one of the qubits, then our new state $|\psi'\rangle$ is locally equivalent to $|M_4\rangle$. Let us write

$$\begin{aligned}\epsilon_{0011} - \epsilon_{1100} &= x_1 + iy_1, & \epsilon_{1100} + \epsilon_{0011} &= X_1 + iY_1, \\ \epsilon_{0101} - \epsilon_{1010} &= x_2 + iy_2, & \epsilon_{1010} + \epsilon_{0101} &= X_2 + iY_2, \\ \epsilon_{0110} - \epsilon_{1001} &= x_3 + iy_3, & \epsilon_{1001} + \epsilon_{0110} &= X_3 + iY_3.\end{aligned}$$

The first-order variation in the relative phase within the first qubit results in the change in $y_1 + y_2 + y_3$. Similarly, the phase variations in the second and third qubits change the values of $-y_1 + y_2 + y_3$ and $y_1 - y_2 + y_3$, respectively. Hence, for any variation, we can always find an equivalent variation satisfying

$$y_1 = y_2 = y_3 = 0 \tag{11}$$

by adjusting these phases. In the same way we find that an overall change of phase, $|M_4\rangle \to e^{i\theta}|M_4\rangle$, can be used to impose the condition

$$Y_1 + Y_2 + Y_3 = 0. \tag{12}$$

Thus, we have 21 real parameters (after imposing the normalization condition) in our space of variations. Since the dimensionality of the space of locally inequivalent states is 18 (see, e.g., [16]) in a neighbourhood of a generic state, three dimensions are redundant. This discrepancy is due to the fact that the state $|M_4\rangle$ remains unchanged if all qubits are transformed by the same $SU(2)$ matrix; thus, the dimensionality of the orbit of the local unitary transformations of the state $|M_4\rangle$ is 10, which is smaller than the dimensionality of this orbit for a generic state by 3. We have eliminated all variations that reduce to infinitesimal local unitary transformations, but the set of physically equivalent variations is generically three dimensional. It would be

possible to eliminate this redundancy by using canonical forms [14, 15] though we have chosen not to do so.

With the condition (11) imposed, the quantity P defined by (8) can be written as

$$P = P_1 + P_2 + P_3 + P_4,$$

where

$$P_1 = 12 \sum_{\alpha=1}^{3} |a_{OI}^{(\alpha)}|^2 - 3 \log 3 (|\epsilon_{0000}|^2 + |\epsilon_{1111}|^2), \tag{13}$$

$$P_2 = \sum_{\alpha=1}^{3} \left[12 (|a_{I+}^{(\alpha)}|^2 + |a_{O+}^{(\alpha)}|^2) + 6 \log 3 (|a_{I-}^{(\alpha)}|^2 + |a_{O-}^{(\alpha)}|^2) \right]$$
$$- 3 \log 3 (|\epsilon_{0111}|^2 + |\epsilon_{1011}|^2 + |\epsilon_{1101}|^2 + |\epsilon_{1110}|^2 + 4|z|^2), \tag{14}$$

$$P_3 = 6 \log 3 \sum_{\alpha=1}^{3} |a_{+-}^{(\alpha)}|^2 - \frac{3}{2} \log 3 (x_1^2 + x_2^2 + x_3^2), \tag{15}$$

$$P_4 = \sum_{\alpha=1}^{3} \left[6 (|a_{OO}^{(\alpha)}|^2 + |a_{II}^{(\alpha)}|^2 + |a_{++}^{(\alpha)}|^2) + 2|a_{--}^{(\alpha)}|^2 \right] - \frac{3}{2} \log 3 \sum_{\alpha=1}^{3} (X_\alpha^2 + Y_\alpha^2). \tag{16}$$

We will show that (i) $P_1 > 0$ if either ϵ_{0000} or ϵ_{1111} is nonzero, (ii) $P_2 > 0$ if any of $\epsilon_{0111}, \epsilon_{1011}, \epsilon_{1101}, \epsilon_{1110}$ or z is nonzero, (iii) $P_3 > 0$ if any of x_α's is nonzero and (iv) $P_4 > 0$ if any or X_α's or Y_α's is nonzero. This will imply that P is positive definite.

4.2.1. Positivity of P_1. The only terms relevant here are $a_{OI}^{(\alpha)}$'s. These are given by

$$\sqrt{6} a_{OI}^{(1)} = \langle O|\delta\rho_{AB}|I\rangle = \langle \delta\psi|II\rangle + \langle OO|\delta\psi\rangle = \overline{\epsilon_{1111}} + \epsilon_{0000},$$
$$\sqrt{6} a_{OI}^{(2)} = \langle O|\delta\rho_{AC}|I\rangle = \omega\langle \delta\psi|II\rangle + \overline{\omega}\langle OO|\delta\psi\rangle = \omega\overline{\epsilon_{1111}} + \overline{\omega}\epsilon_{0000},$$
$$\sqrt{6} a_{OI}^{(3)} = \langle O|\delta\rho_{AD}|I\rangle = \overline{\omega}\langle \delta\psi|II\rangle + \omega\langle OO|\delta\psi\rangle = \overline{\omega}\overline{\epsilon_{1111}} + \omega\epsilon_{0000}.$$

Thus we have

$$\sum_{\alpha=1}^{3} |a_{OI}^{(\alpha)}|^2 = \frac{1}{2} (|\epsilon_{0000}|^2 + |\epsilon_{1111}|^2).$$

Hence by (13)

$$P_1 = (6 - 3 \log 3)(|\epsilon_{0000}|^2 + |\epsilon_{1111}|^2),$$

which is positive if either ϵ_{0000} or ϵ_{1111} is nonzero.

4.2.2. Positivity of P_2. We find the relevant $a_{ij}^{(1)}$'s as

$$\sqrt{6} a_{I+}^{(1)} = -\frac{1}{\sqrt{2}} (\epsilon_{1101} + \epsilon_{1110}) + \sqrt{2}\overline{z}, \qquad \sqrt{6} a_{I-}^{(1)} = -\sqrt{\frac{3}{2}} i(\epsilon_{1110} - \epsilon_{1101}),$$
$$\sqrt{6} a_{O+}^{(1)} = \frac{1}{\sqrt{2}} (\overline{\epsilon_{0111}} + \overline{\epsilon_{1011}}) - \sqrt{2} z, \qquad \sqrt{6} a_{O-}^{(1)} = \frac{1}{\sqrt{2}} (\overline{\epsilon_{1011}} - \overline{\epsilon_{0111}}).$$

Hence,

$$12 |a_{I+}^{(1)}|^2 + 6 \log 3 |a_{I-}^{(1)}|^2 = |\epsilon_{1101} + \epsilon_{1110} - 2\overline{z}|^2 + \frac{3}{2} \log 3 |\epsilon_{1101} - \epsilon_{1110}|^2,$$
$$12 |a_{O+}^{(1)}|^2 + 6 \log 3 |a_{O-}^{(1)}|^2 = |\epsilon_{1011} + \epsilon_{0111} - 2\overline{z}|^2 + \frac{1}{2} \log 3 |\epsilon_{1011} - \epsilon_{0111}|^2.$$

The corresponding quantities involving $a_{ij}^{(2)}$'s and $a_{ij}^{(3)}$ can be obtained similarly as follows:

$$12\left|a_{I+}^{(2)}\right|^2 + 6\log 3\left|a_{I-}^{(2)}\right|^2 = |\epsilon_{1011} + \epsilon_{1110} - 2\omega^2\bar{z}|^2 + \tfrac{3}{2}\log 3|\epsilon_{1011} - \epsilon_{1110}|^2,$$

$$12\left|a_{O+}^{(2)}\right|^2 + 6\log 3\left|a_{O-}^{(2)}\right|^2 = |\epsilon_{1101} + \epsilon_{0111} - 2\omega^2\bar{z}|^2 + \tfrac{1}{2}\log 3|\epsilon_{1101} - \epsilon_{0111}|^2,$$

$$12\left|a_{I+}^{(3)}\right|^2 + 6\log 3\left|a_{I-}^{(3)}\right|^2 = |\epsilon_{1011} + \epsilon_{1101} - 2\omega\bar{z}|^2 + \tfrac{3}{2}\log 3|\epsilon_{1011} - \epsilon_{1101}|^2,$$

$$12\left|a_{O+}^{(3)}\right|^2 + 6\log 3\left|a_{O-}^{(3)}\right|^2 = |\epsilon_{1110} + \epsilon_{0111} - 2\omega\bar{z}|^2 + \tfrac{1}{2}\log 3|\epsilon_{1110} - \epsilon_{0111}|^2.$$

From these equations we find

$$P_2 = \left(1 - \tfrac{1}{2}\log 3\right)\left(|\epsilon_{0111} + \epsilon_{1011}|^2 + |\epsilon_{0111} + \epsilon_{1101}|^2 + |\epsilon_{0111} + \epsilon_{1110}|^2\right)$$
$$+ \left(1 - \tfrac{1}{2}\log 3\right)\left(|\epsilon_{1011} + \epsilon_{1101}|^2 + |\epsilon_{1011} + \epsilon_{1110}|^2 + |\epsilon_{1101} + \epsilon_{1110}|^2\right)$$
$$+ \log 3(|\epsilon_{1011} - \epsilon_{1101}|^2 + |\epsilon_{1011} - \epsilon_{1110}|^2 + |\epsilon_{1101} - \epsilon_{1110}|^2) + 24\left(1 - \tfrac{1}{2}\log 3\right)|z|^2.$$

It is clear that the right-hand side is positive unless ϵ_{0111}, ϵ_{1011}, ϵ_{1101}, ϵ_{1110} and z all vanish[2].

4.2.3. Positivity of P_3. We have

$$2\sqrt{6}a_{+-}^{(1)} = -2(x_2 + x_3) - \sqrt{3}\mathrm{i}(x_2 - x_3),$$

and $a_{+-}^{(2)}$ and $a_{+-}^{(3)}$ are obtained from this by cyclic permutations $2 \to 3 \to 1$ and $3 \to 2 \to 1$, respectively. Hence,

$$\left|a_{+-}^{(1)}\right|^2 + \left|a_{+-}^{(2)}\right|^2 + \left|a_{+-}^{(3)}\right|^2 = \tfrac{1}{12}\left(7x_1^2 + 7x_2^2 + 7x_3^2 + x_2x_3 + x_3x_1 + x_1x_2\right).$$

Thus, P_3 given by (15) is

$$P_3 = \frac{\log 3}{2}\left(4x_1^2 + 4x_2^2 + 4x_3^2 + x_2x_3 + x_3x_1 + x_1x_2\right),$$

which is positive if x_1, x_2 or x_3 is nonzero.

4.2.4. Positivity of P_4. We have

$$\sqrt{6}a_{OO}^{(1)} = \epsilon_{0011} + \overline{\epsilon_{0011}} = X_1 + x_1, \qquad \sqrt{6}a_{II}^{(1)} = \epsilon_{1100} + \overline{\epsilon_{1100}} = X_1 - x_1.$$

Hence

$$6\left|a_{OO}^{(1)}\right|^2 + 6\left|a_{II}^{(1)}\right|^2 = 2\left(X_1^2 + x_1^2\right).$$

Similarly,

$$6\left|a_{OO}^{(2)}\right|^2 + 6\left|a_{II}^{(2)}\right|^2 = 2\left(X_2^2 + x_2^2\right), \qquad 6\left|a_{OO}^{(3)}\right|^2 + 6\left|a_{II}^{(3)}\right|^2 = 2\left(X_3^2 + x_3^2\right).$$

Thus,

$$6\sum_{\alpha=1}^{3}\left(\left|a_{OO}^{(\alpha)}\right|^2 + \left|a_{II}^{(\alpha)}\right|^2\right) \geqslant 2\sum_{\alpha=1}^{3} X_\alpha^2. \tag{17}$$

The remaining 'diagonal terms' are

$$-\sqrt{6}a_{++}^{(1)} = \mathrm{Re}\{\omega(\epsilon_{1010} + \epsilon_{0101}) + \bar{\omega}(\epsilon_{0110} + \epsilon_{1001})\},$$

$$-\sqrt{2}a_{--}^{(1)} = \mathrm{Im}\{\omega(\epsilon_{1010} + \epsilon_{0101}) - \bar{\omega}(\epsilon_{0110} + \epsilon_{1001})\}.$$

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[2] The expression for P_2 is not symmetric under permutations of four qubits involving the first qubit. However, $\delta^2 E_2$ itself is symmetric under such permutations thanks to the contribution from $F_{AB} + F_{AC} + F_{AD}$ (which we have discarded because it is positive definite). This must be the case because the average two-partite von Neumann entanglement entropy E_2 has this symmetry.

The coefficients $a_{++}^{(2)}$ and $a_{--}^{(2)}$ $\left(a_{++}^{(3)}\right.$ and $\left.a_{--}^{(3)}\right)$ are obtained from the expressions for $a_{++}^{(1)}$ and $a_{--}^{(1)}$ by interchanging the second and third (fourth) qubits. Remembering the definitions $\epsilon_{1010} + \epsilon_{0101} = X_2 + iY_2$ and $\epsilon_{1001} + \epsilon_{0110} = X_3 + iY_3$, we obtain

$$6\left|a_{++}^{(1)}\right|^2 + 2|a_{--}^{(1)}|^2 = X_2^2 + Y_2^2 + X_3^2 + Y_3^2 + 2(X_2 X_3 - Y_2 Y_3).$$

We find similarly

$$6\left|a_{++}^{(2)}\right|^2 + 2|a_{--}^{(2)}|^2 = X_3^2 + Y_3^2 + X_1^2 + Y_1^2 + 2(X_3 X_1 - Y_3 Y_1),$$

$$6\left|a_{++}^{(3)}\right|^2 + 2|a_{--}^{(3)}|^2 = X_1^2 + Y_1^2 + X_2^2 + Y_2^2 + 2(X_1 X_2 - Y_1 Y_2).$$

By combining these formulae and (17) with the definition (16) of P_4, we have

$$\begin{aligned} P_4 \geqslant \left(4 - \tfrac{3}{2}\log 3\right)\left(X_1^2 + X_2^2 + X_3^2\right) &+ 2(X_2 X_3 + X_3 X_1 + X_1 X_2) \\ &+ \left(2 - \tfrac{3}{2}\log 3\right)\left(Y_1^2 + Y_2^2 + Y_3^2\right) - 2(Y_2 Y_3 + Y_3 Y_1 + Y_1 Y_2). \end{aligned}$$

Finally, the use of the condition $Y_1 + Y_2 + Y_3 = 0$ leads to

$$\begin{aligned} P_4 \geqslant [(X_2 + X_3)^2 + (X_3 + X_1)^2 + (X_1 + X_2)^2] \\ + \left(2 - \tfrac{3}{2}\log 3\right)\left(X_1^2 + X_2^2 + X_3^2\right) + 3(2 - \log 3)\left(Y_1^2 + Y_1 Y_2 + Y_2^2\right). \end{aligned}$$

Thus, $P_4 > 0$ unless X_α's and Y_α's all vanish. This completes the proof that $\delta^2 E_2$ at $|M_4\rangle$ is negative definite[3]. Hence, the state $|M_4\rangle$ indeed gives a local maximum of the average two-partite von Neumann entanglement entropy.

Acknowledgments

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[3] It is possible to prove $\delta^2 E_2 < 0$ without the condition $Y_1 + Y_2 + Y_3 = 0$. In that case, one needs to evaluate the positive contribution $F_{AB} + F_{AC} + F_{AD}$ to $\sum_Y \text{tr}[\sigma_{AY} \log \rho_{AY}]$.