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# A study of two-qubit density matrices with fermionic purifications 

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Received 22 August 2008
Published 10 November 2008
Online at stacks.iop.org/JPhysA/41/505304


#### Abstract

We study 12 parameter families of two-qubit density matrices, arising from a special class of two-fermion systems with four single-particle states or alternatively from a four-qubit state with amplitudes arranged in an antisymmetric matrix. We calculate the Wootters concurrences and the negativities in a closed form and study their behavior. We use these results to show that the relevant entanglement measures satisfy the generalized Coffman-Kundu-Wootters formula of distributed entanglement. An explicit formula for the residual tangle is also given. The geometry of such density matrices is elaborated in some detail. In particular, an explicit form for the Bures metric is given.


PACS numbers: $03.67 . \mathrm{Mn}, 03.65 . \mathrm{Ud}, 03.65 . \mathrm{Ta}$

## 1. Introduction

Entanglement is the basic resource of quantum information processing [1]. As such it has to be quantified and its structure characterized. For entanglement quantification one uses special classes of entanglement measures which are real-valued functions on the states. Pure and mixed state entanglement and its quantification in its bipartite form is a well-understood phenomenon. Moreover, on the geometry and structure of entangled states associated with such systems a large number of interesting results are available [2].

For example, for pure states of bipartite systems the classification of different entanglement types is effected by the Schmidt decomposition. If the Schmidt decomposition is known, from the Schmidt numbers one can form the von-Neumann entropy [3] as a good measure characterizing bipartite entanglement. For quantifying mixed state entanglement no such general method exists. For the special case of two qubits as a measure of entanglement we have the celebrated formula of Hill and Wootters [4] for the bipartite concurrence $\mathcal{C}$ and the associated entanglement of formation. The structure of this measure of entanglement
was studied in many different papers ${ }^{1}$. Its structure has been related to antilinear operators [5], combs and filters [6], and has also been generalized to rebits [7]. Explicit expressions for different special classes of density matrices and a comparison with other measures of entanglement have been given [8-10].

In this paper we would like to study the structure of special 12-parameter families of twoqubit density matrices for which the mixed state concurrences can be calculated in a closed form. Such density matrices can be regarded as reduced ones coming from some larger system with special properties. In order to motivate our choice for this larger system we consider an example. If we consider a three-qubit state $|\psi\rangle \in \mathbf{C}^{2} \otimes \mathbf{C}^{2} \otimes \mathbf{C}^{2}$, then after calculating any of the reduced density matrices, e.g., $\varrho_{12}=\operatorname{Tr}_{3}(|\psi\rangle\langle\psi|)$ we are left with a two-qubit density matrix of a very special structure. For example in this case $\varrho_{12}$ is of rank two, and this observation enables an explicit calculation of the mixed state concurrence in terms of the amplitudes of the three-qubit state $|\psi\rangle$. This result forms the basis of further important developments, namely the derivation of the Coffman-Kundu-Wootters relation of distributed entanglement [11].

Proceeding by analogy we expect that four-qubit states of special structure might provide us with further interesting examples of that kind. Let us consider a four-qubit state $|\Psi\rangle \in \mathbf{C}^{2} \otimes \mathbf{C}^{2} \otimes \mathbf{C}^{2} \otimes \mathbf{C}^{2}$. A class of two-qubit density matrices arises after forming the reduced density matrices such as $\varrho_{12}=\operatorname{Tr}_{34}(|\Psi\rangle\langle\Psi|)$. However, density matrices of that kind are still too general to have a characteristic structure. Hence as an extra constraint we impose an antisymmetry condition on the amplitudes of

$$
\begin{equation*}
|\Psi\rangle=\sum_{i j k l=0}^{1} \Psi_{i j k l}|i j k l\rangle \tag{1}
\end{equation*}
$$

as

$$
\begin{equation*}
\Psi_{i j k l}=-\Psi_{k l i j}, \tag{2}
\end{equation*}
$$

i.e., we impose antisymmetry in the first and second pairs of indices.

An alternative (and more physical) way is the one of imposing such constraints on the original Hilbert space $H \simeq \mathbf{C}^{16}$ which renders to have a tensor product structure on one of its six dimensional subspaces $\mathcal{H}$ of the form

$$
\begin{equation*}
\mathcal{H}=\left(\mathbf{C}^{2} \otimes \mathbf{C}^{2}\right) \wedge\left(\mathbf{C}^{2} \otimes \mathbf{C}^{2}\right) \tag{3}
\end{equation*}
$$

where $\wedge$ refers to antisymmetrization. As we know quantum tensor product structures are observable-induced [12], hence in order to specify our system with a tensor product structure of equation (3) we have to specify the experimentally accessible interactions and measurements that account for the admissible operations we can perform on our system. For example we can realize our system as a pair of fermions with four single-particle states where a part of the admissible operations is local unitary transformations of the form

$$
\begin{equation*}
|\Psi\rangle \mapsto(U \otimes V) \otimes(U \otimes V)|\Psi\rangle, \quad U, V \in U(2), \quad|\Psi\rangle \in \mathcal{H} \tag{4}
\end{equation*}
$$

Taken together with equation (2) this transformation rule clearly indicates that the first, second, third and fourth subsystems form two indistinguishable subsystems of fermionic type.

The aim of the present paper is to study the interesting structure of the reduced density matrices of the form $\varrho_{i j}, i<j, i, j=1,2,3,4$, arising from fermionic states that are elements of the tensor product structure as shown by equation (3). We can alternatively coin the term that these density matrices are those with fermionic purifications.
${ }^{1}$ For a nice summary see the relevant chapter of [2].

The organization of the paper is as follows. In section 2 we present our parametrized family of density matrices we wish to study. Using suitable local unitary transformations we transform this family to a canonical form. In section 3 based on these results we calculate the Wootters concurrence, the negativity and the purity. We give a formula for the upper bound of negativity for a given concurrence. (We prove it in appendix.) In section 4 we analyze the structure of these quantities and discuss how they are related to each other. In particular, we prove that the relevant entanglement measures associated with our four-qubit state satisfy the generalized Coffman-Kundu-Wootters inequality of distributed entanglement [13]. For the residual tangle we derive an explicit formula, containing two from the four algebraically independent four-qubit invariants. In section 5 we investigate the Bures geometry of this special subclass of two-qubit density matrices. We show that thanks to our purifications being fermionic an explicit formula for the Bures metric with a hyperbolic structure can be obtained. The conclusions and some comments are left for section 6.

## 2. The density matrix

Let us parametrize the six amplitudes of our normalized four-qubit state $|\Psi\rangle$ of equation (1) with the antisymmetry property of equation (2) as

$$
\begin{equation*}
\Psi_{i j k l}=\frac{1}{2}\left(\varepsilon_{i k} \mathcal{A}_{j l}+\mathcal{B}_{i k} \varepsilon_{j l}\right) \tag{5}
\end{equation*}
$$

where $\mathcal{A}$ and $\mathcal{B}$ are symmetric matrices of the form
$\mathcal{A}=\left(\begin{array}{cc}z_{1}-\mathrm{i} z_{2} & -z_{3} \\ -z_{3} & -z_{1}-\mathrm{i} z_{2}\end{array}\right)=\varepsilon(\mathbf{z} \overline{\boldsymbol{\sigma}}), \quad \mathcal{B}=\left(\begin{array}{cc}w_{1}-\mathrm{i} w_{2} & -w_{3} \\ -w_{3} & -w_{1}-\mathrm{i} w_{2}\end{array}\right)=\varepsilon(\mathbf{w} \overline{\boldsymbol{\sigma}})$,
where $\mathbf{z}, \mathbf{w} \in \mathbf{C}^{3}, \mathbf{w} \boldsymbol{\sigma}=w_{1} \sigma_{1}+w_{2} \sigma_{2}+w_{3} \sigma_{3}$, with the usual $\sigma_{i}$ Pauli matrices,

$$
\varepsilon=\left(\begin{array}{cc}
0 & 1  \tag{7}\\
-1 & 0
\end{array}\right)
$$

and the overline refers to complex conjugation.
It is straightforward to check that the normalization condition of the state $|\Psi\rangle$ takes the form

$$
\begin{equation*}
\|\Psi\|^{2} \equiv\|\mathbf{w}\|^{2}+\|\mathbf{z}\|^{2}:=1 \tag{8}
\end{equation*}
$$

The density matrices we wish to study are arising as reduced ones of the form

$$
\begin{equation*}
\varrho \equiv \varrho_{12}=\operatorname{Tr}_{34}(|\Psi\rangle\langle\Psi|) \tag{9}
\end{equation*}
$$

Note that since the subsystems (12) and (34) are by definition indistinguishable we also have $\varrho=\varrho_{12}=\varrho_{34}$.

A calculation of the trace yields the following explicit form for $\varrho$,

$$
\begin{equation*}
\varrho=\frac{1}{4}(\mathbf{1}+\Lambda) \tag{10}
\end{equation*}
$$

where 1 denotes the $4 \times 4$ identity matrix and $\Lambda$ is the traceless matrix

$$
\begin{align*}
& \Lambda:=\mathbf{x} \sigma \otimes I+I \otimes \mathbf{y} \sigma+\mathbf{w} \boldsymbol{\sigma} \otimes \overline{\mathbf{z}} \sigma+\overline{\mathbf{w}} \boldsymbol{\sigma} \otimes \mathbf{z} \sigma,  \tag{11}\\
& \mathbf{x}:=\mathrm{iw} \times \overline{\mathbf{w}}, \quad \mathbf{y}:=\mathrm{i} \mathbf{z} \times \overline{\mathbf{z}}, \tag{12}
\end{align*}
$$

where $I$ is the $2 \times 2$ identity matrix. Note that $\mathbf{x}, \mathbf{y} \in \mathbf{R}^{3}$ and $\mathbf{x w}=\mathbf{x} \overline{\mathbf{w}}=\mathbf{y z}=\mathbf{y} \overline{\mathbf{z}}=0$. Due to this, and the identities

$$
\begin{equation*}
|\mathbf{x}|^{2}=\|\mathbf{w}\|^{4}-\mathbf{w}^{2} \overline{\mathbf{w}}^{2}, \quad|\mathbf{y}|^{2}=\|\mathbf{z}\|^{4}-\mathbf{z}^{2} \overline{\mathbf{z}}^{2}, \tag{13}
\end{equation*}
$$

it can be checked that $\Lambda$ satisfies the identity

$$
\begin{equation*}
\Lambda^{2}=\left(1-\eta^{2}\right) \mathbf{1} \tag{14}
\end{equation*}
$$

where

$$
\begin{align*}
& \eta \equiv\left|\mathbf{w}^{2}-\mathbf{z}^{2}\right|,  \tag{15}\\
& 0 \leqslant \eta \leqslant 1 \tag{16}
\end{align*}
$$

Note that the quantity $\eta$ is just the Schliemann-measure of entanglement for two-fermion systems with four single-particle states [14, 15]. Indeed, our density matrix $\varrho$ (with a somewhat different parametrization) can alternatively be obtained [15] as a reduced one arising from such fermionic systems after a convenient global $U(4)$, and a local $U(2) \times U(2)$ transformation of the form $I \otimes \sigma_{2}$.

Now by employing suitable local unitary transformations we would like to obtain a canonical form for $\varrho$. According to equation (4) the transformations operating on subsystems 12 or equivalently 34 are of the form $U \otimes V \in U(2) \times U(2)$.

As a first step let us consider the unitary transformation

$$
\begin{equation*}
U(\hat{\mathbf{u}}, \alpha):=\mathrm{e}^{\mathrm{i} \frac{\alpha}{2} \hat{\mathbf{u}} \sigma}=\cos \left(\frac{\alpha}{2}\right) I+\mathrm{i} \sin \left(\frac{\alpha}{2}\right) \hat{\mathbf{u}} \sigma, \tag{17}
\end{equation*}
$$

which is a spin- $\frac{1}{2}$ representation of an $S U(2)$ rotation around the axis $\hat{\mathbf{u}} \in \mathbf{R}^{3}(|\hat{\mathbf{u}}|=1)$ with an angle $\alpha$. A special rotation from $\mathbf{x}$ to $\mathbf{x}^{\prime}\left(\mathbf{x}^{\prime} \neq-\mathbf{x}\right)$ can be written as

$$
\begin{align*}
& U(\hat{\mathbf{u}}, \alpha)^{\dagger}(\mathbf{x} \sigma) U(\hat{\mathbf{u}}, \alpha)=\mathbf{x}^{\prime} \sigma,  \tag{18}\\
& U(\hat{\mathbf{u}}, \alpha)=\frac{1}{\sqrt{2 \mathbf{x}^{2}\left(\mathbf{x}^{2}+\mathbf{x x}^{\prime}\right)}}\left(\mathbf{x}^{2} I+(\mathbf{x} \sigma)\left(\mathbf{x}^{\prime} \sigma\right)\right),  \tag{19}\\
& \hat{\mathbf{u}}=\frac{\mathbf{x} \times \mathbf{x}^{\prime}}{\left|\mathbf{x} \times \mathbf{x}^{\prime}\right|}, \quad \alpha=\arccos \left(\frac{\mathbf{x} \mathbf{x}^{\prime}}{\mathbf{x x}}\right) . \tag{20}
\end{align*}
$$

Employing this, we can rotate the vector $\mathbf{x}$ to the direction of the coordinate axis $z$. In this case

$$
\begin{align*}
& r:=|\mathbf{x}|  \tag{21}\\
& U_{\mathbf{x}}:=\frac{1}{\sqrt{2 r\left(r+x_{3}\right)}}\left(r I+(\mathbf{x} \boldsymbol{\sigma}) \sigma_{3}\right),  \tag{22}\\
& U_{\mathbf{x}}^{\dagger}(\mathbf{x} \boldsymbol{\sigma}) U_{\mathbf{x}}=r \sigma_{3} . \tag{23}
\end{align*}
$$

Moreover, using equation (19) it can be checked that due to the special form of $\mathbf{x}$ (see equation (12)), the above transformation rotates the third component of $\mathbf{w}$ into zero

$$
\begin{align*}
& U_{\mathbf{x}}^{\dagger}(\mathbf{w} \boldsymbol{\sigma}) U_{\mathbf{x}}=\mathbf{w}^{\prime} \boldsymbol{\sigma},  \tag{24}\\
& \mathbf{w}^{\prime}=\mathbf{w}-\frac{\mathbf{w} \mathbf{x}^{\prime}}{r^{2}+\mathbf{\mathbf { x x } ^ { \prime }}}\left(\mathbf{x}+\mathbf{x}^{\prime}\right)=\left[\begin{array}{c}
w_{1}-\frac{x_{1}}{r+x_{3}} w_{3} \\
w_{2}-\frac{x_{2}}{r+x_{3}} w_{3} \\
0
\end{array}\right] . \tag{25}
\end{align*}
$$

A similar set of transformations can be applied to $\mathbf{y} \boldsymbol{\sigma}$

$$
\begin{equation*}
s:=|\mathbf{y}| \tag{26}
\end{equation*}
$$

$$
\begin{align*}
& V_{\mathbf{y}}:=\frac{1}{\sqrt{2 s\left(s+y_{3}\right)}}\left(s I+(\mathbf{y} \boldsymbol{\sigma}) \sigma_{3}\right),  \tag{27}\\
& V_{\mathbf{y}}^{\dagger}(\mathbf{y} \boldsymbol{\sigma}) V_{\mathbf{y}}=s \sigma_{3}  \tag{28}\\
& V_{\mathbf{y}}^{\dagger}(\mathbf{z} \boldsymbol{\sigma}) V_{\mathbf{y}}=\mathbf{z}^{\prime} \boldsymbol{\sigma},  \tag{29}\\
& \mathbf{z}^{\prime}=\mathbf{z}-\frac{\mathbf{z} \mathbf{y}^{\prime}}{s^{2}+\mathbf{y} \mathbf{y}^{\prime}}\left(\mathbf{y}+\mathbf{y}^{\prime}\right)=\left[\begin{array}{c}
z_{1}-\frac{y_{1}}{s+y_{3}} z_{3} \\
z_{2}-\frac{y_{2}}{s+y_{3}} z_{3} \\
0
\end{array}\right] \tag{30}
\end{align*}
$$

Obviously, every $U \in U(2)$ unitary transformation acting on an arbitrary $\mathbf{a} \in \mathbf{C}^{3}$ as $U^{\dagger} \mathbf{a} \sigma U=\mathbf{a}^{\prime} \boldsymbol{\sigma}$ preserves $\mathbf{a}^{2}$ and $\|\mathbf{a}\|^{2}$, since $\mathbf{a}^{2}=-\operatorname{det}(\mathbf{a} \boldsymbol{\sigma})$, and $\|\mathbf{a}\|^{2}=\frac{1}{2} \operatorname{Tr}\left((\mathbf{a} \sigma)^{\dagger}(\mathbf{a} \sigma)\right)$. Hence

$$
\begin{array}{ll}
\mathbf{w}^{\prime 2}=\mathbf{w}^{2}, & \mathbf{z}^{\prime 2}=\mathbf{z}^{2}, \\
\left\|\mathbf{w}^{\prime}\right\|^{2}=\|\mathbf{w}\|^{2}, & \left\|\mathbf{z}^{\prime}\right\|^{2}=\|\mathbf{z}\|^{2} \tag{32}
\end{array}
$$

and

$$
\begin{equation*}
\eta^{\prime}=\eta \tag{33}
\end{equation*}
$$

are invariant under local $U(2) \times U(2)$ transformations. (The entanglement measure $\eta$ is also invariant under the larger group of $U(4)$ transformations.)

Now by employing the local $U(2) \times U(2)$ transformations $U_{\mathbf{x}} \otimes V_{\mathbf{y}}$, our density matrix can be cast into the form,

$$
\begin{align*}
& \varrho^{\prime}=\left(U_{\mathbf{x}} \otimes V_{\mathbf{y}}\right)^{\dagger} \varrho\left(U_{\mathbf{x}} \otimes V_{\mathbf{y}}\right)=\frac{1}{4}\left(\mathbf{1}+\Lambda^{\prime}\right)  \tag{34}\\
& \Lambda^{\prime}=r \sigma_{3} \otimes I+I \otimes s \sigma_{3}+\mathbf{w}^{\prime} \boldsymbol{\sigma} \otimes \overline{\mathbf{z}}^{\prime} \boldsymbol{\sigma}+\overline{\mathbf{w}}^{\prime} \boldsymbol{\sigma} \otimes \mathbf{z}^{\prime} \boldsymbol{\sigma} \tag{35}
\end{align*}
$$

where $\Lambda^{\prime}$ has the special form

$$
\Lambda^{\prime}=\left[\begin{array}{cccc}
\alpha_{3} & 0 & 0 & \alpha_{1}-\mathrm{i} \alpha_{2}  \tag{36}\\
0 & \beta_{3} & \beta_{1}-\mathrm{i} \beta_{2} & 0 \\
0 & \beta_{1}+\mathrm{i} \beta_{2} & -\beta_{3} & 0 \\
\alpha_{1}+\mathrm{i} \alpha_{2} & 0 & 0 & -\alpha_{3}
\end{array}\right]
$$

with the quantities $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbf{R}^{3}$ defined as

$$
\begin{array}{ll}
\boldsymbol{\alpha}=\left[\begin{array}{c}
\xi_{1}-\xi_{2} \\
\zeta_{1}+\zeta_{2} \\
r+s
\end{array}\right], \quad \boldsymbol{\beta}=\left[\begin{array}{c}
\xi_{1}+\xi_{2} \\
\zeta_{1}-\zeta_{2} \\
r-s
\end{array}\right], \\
\xi_{1}=w_{1}^{\prime} \bar{z}_{1}^{\prime}+\bar{w}_{1}^{\prime} z_{1}^{\prime}, & \zeta_{1}=w_{2}^{\prime} \bar{z}_{1}^{\prime}+\bar{w}_{2}^{\prime} z_{1}^{\prime}, \\
\xi_{2}=w_{2}^{\prime} \bar{z}_{2}^{\prime}+\bar{w}_{2}^{\prime} z_{2}^{\prime}, & \zeta_{2}=w_{1}^{\prime} \bar{z}_{2}^{\prime}+\bar{w}_{1}^{\prime} z_{2}^{\prime} . \tag{39}
\end{array}
$$

Thanks to the special shape of $\Lambda$, we can regard $\varrho^{\prime}$ as the direct sum of two $2 \times 2$ blocks, i.e. $(I+\boldsymbol{\alpha} \boldsymbol{\sigma})$ and $(I+\boldsymbol{\beta} \boldsymbol{\sigma})$. Having obtained the canonical form of our reduced density matrix $\varrho$, now we turn to the calculation of the corresponding entanglement measures.

## 3. Measures of entanglement for the density matrix

### 3.1. Concurrence

In this section we calculate the Wootters concurrence of our density matrix $\varrho$ defined in equations (10)-(12). This quantity is defined as

$$
\begin{equation*}
\mathcal{C}=\max \left\{0, \lambda_{1}-\lambda_{2}-\lambda_{3}-\lambda_{4}\right\} \tag{40}
\end{equation*}
$$

where $\lambda_{1} \geqslant \lambda_{2} \geqslant \lambda_{3} \geqslant \lambda_{4}$ are the square roots of the eigenvalues of the matrix $\varrho \tilde{\varrho}$ where

$$
\begin{equation*}
\tilde{\varrho}=\left(\sigma_{2} \otimes \sigma_{2}\right) \bar{\varrho}\left(\sigma_{2} \otimes \sigma_{2}\right) \tag{41}
\end{equation*}
$$

This matrix (the Wootters spin-flip of $\varrho$ ) is known to have real non-negative eigenvalues. Moreover, the important point is that $\mathcal{C}$ is an $S L(2, \mathbf{C}) \times S L(2, \mathbf{C})$ invariant [6], hence we can use the canonical form we obtained in the previous section via using the transformation $U_{\mathbf{x}} \otimes V_{\mathbf{y}} \in S U(2) \times S U(2) \subset S L(2, \mathbf{C}) \times S L(2, \mathbf{C})$ for its calculation.

It is straightforward to check that $16 \varrho^{\prime} \varrho^{\prime}$ has the same X-shape as $\varrho^{\prime}$, with the blocks $\left(\tilde{\alpha}_{0} I+\tilde{\boldsymbol{\alpha}} \boldsymbol{\sigma}\right)$ and $\left(\tilde{\beta}_{0} I+\tilde{\boldsymbol{\beta}} \boldsymbol{\sigma}\right)$ where $\tilde{\alpha}_{\mu}, \tilde{\beta}_{\nu} \mu, \nu=0,1,2,3$ are quadratic in $\boldsymbol{\alpha}, \boldsymbol{\beta}$ :
$\tilde{\alpha}_{\mu}=\left[\begin{array}{c}1+\alpha_{1}^{2}+\alpha_{2}^{2}-\alpha_{3}^{2} \\ 2 \alpha_{1}-\mathrm{i} 2 \alpha_{2} \alpha_{3} \\ 2 \alpha_{2}+\mathrm{i} 2 \alpha_{3} \alpha_{1} \\ 0\end{array}\right] \in \mathbf{C}^{4}, \quad \tilde{\beta}_{v}=\left[\begin{array}{c}1+\beta_{1}^{2}+\beta_{2}^{2}-\beta_{3}^{2} \\ 2 \beta_{1}-\mathrm{i} 2 \beta_{2} \beta_{3} \\ 2 \beta_{2}+\mathrm{i} 2 \beta_{3} \beta_{1} \\ 0\end{array}\right] \in \mathbf{C}^{4}$.
The eigenvalues of the blocks $\left(\tilde{\alpha}_{0} I+\tilde{\boldsymbol{\alpha}} \boldsymbol{\sigma}\right)$ and $\left(\tilde{\beta}_{0} I+\tilde{\boldsymbol{\beta}} \boldsymbol{\sigma}\right)$ are $\tilde{\alpha}_{0} \pm \sqrt{\tilde{\boldsymbol{\alpha}}^{2}}$ and $\tilde{\beta}_{0} \pm \sqrt{\tilde{\boldsymbol{\beta}}^{2}}$, respectively. Now, we can express these with the help of the quantities $\boldsymbol{\alpha}, \boldsymbol{\beta}$ of (42) and get the eigenvalues of $\varrho^{\prime} \varrho^{\prime}$ in the form

$$
\begin{equation*}
\Lambda_{i}=\left\{\frac{1}{16}\left(\sqrt{\alpha_{1}^{2}+\alpha_{2}^{2}} \pm \sqrt{1-\alpha_{3}^{2}}\right)^{2}, \frac{1}{16}\left(\sqrt{\beta_{1}^{2}+\beta_{2}^{2}} \pm \sqrt{1-\beta_{3}^{2}}\right)^{2}\right\} \tag{43}
\end{equation*}
$$

Now, using equations (37)-(39), we have to express these as functions of our original quantities $\mathbf{z}^{2}, \mathbf{w}^{2},\|\mathbf{z}\|^{2}$ and $\|\mathbf{w}\|^{2}$. A straightforward calculation shows that

$$
\begin{align*}
& \alpha_{1}^{2}+\alpha_{2}^{2}=2\left\|\mathbf{w}^{\prime}\right\|^{2}\left\|\mathbf{z}^{\prime}\right\|^{2}+\mathbf{w}^{\prime 2} \overline{\mathbf{z}}^{\prime 2}+\overline{\mathbf{w}}^{\prime 2} \mathbf{z}^{\prime 2}-2 r s \\
& \beta_{1}^{2}+\beta_{2}^{2}=2\left\|\mathbf{w}^{\prime}\right\|^{2}\left\|\mathbf{z}^{\prime}\right\|^{2}+\mathbf{w}^{\prime 2} \overline{\mathbf{z}}^{\prime 2}+\overline{\mathbf{w}}^{\prime 2} \mathbf{z}^{\prime 2}+2 r s  \tag{44}\\
& 1-\alpha_{3}^{2}=2\left\|\mathbf{w}^{\prime}\right\|^{2}\left\|\mathbf{z}^{\prime}\right\|^{2}+\mathbf{w}^{\prime 2} \overline{\mathbf{w}}^{\prime 2}+\mathbf{z}^{\prime 2} \overline{\mathbf{z}}^{\prime 2}-2 r s \\
& 1-\beta_{3}^{2}=2\left\|\mathbf{w}^{\prime}\right\|^{2}\left\|\mathbf{z}^{\prime}\right\|^{2}+\mathbf{w}^{\prime 2} \overline{\mathbf{w}}^{\prime 2}+\mathbf{z}^{\prime 2} \overline{\mathbf{z}}^{\prime 2}+2 r s
\end{align*}
$$

The formulae above are expressed in terms of quantities invariant under our transformation yielding the canonical form (see equations (31) and (32)), hence we can simply omit the primes. Hence by using equations (13) and (15) we can establish that

$$
\begin{equation*}
\alpha_{1}^{2}+\alpha_{2}^{2}=1-\alpha_{3}^{2}-\eta^{2}, \quad \beta_{1}^{2}+\beta_{2}^{2}=1-\beta_{3}^{2}-\eta^{2} \tag{45}
\end{equation*}
$$

For further use, denote

$$
\begin{equation*}
\gamma_{+}:=r+s \equiv \alpha_{3}, \quad \gamma_{-}:=r-s \equiv \beta_{3} . \tag{46}
\end{equation*}
$$

With these, the square roots of the eigenvalues of $\varrho \tilde{\varrho}$ are
$\lambda_{i}=\sqrt{\Lambda_{i}}=\left\{\frac{1}{4}\left(\sqrt{1-\gamma_{+}^{2}} \pm \sqrt{1-\gamma_{+}^{2}-\eta^{2}}\right), \frac{1}{4}\left(\sqrt{1-\gamma_{-}^{2}} \pm \sqrt{1-\gamma_{-}^{2}-\eta^{2}}\right)\right\}$.
The biggest one of these is $\lambda_{\max }=\frac{1}{4}\left(\sqrt{1-\gamma_{-}^{2}}+\sqrt{1-\gamma_{-}^{2}-\eta^{2}}\right)$ and after subtracting the others from it, we get finally the nice formula for the concurrence

$$
\begin{equation*}
\mathcal{C}(\varrho)=\max \left\{0, \frac{1}{2}\left(\sqrt{1-\gamma_{-}^{2}-\eta^{2}}-\sqrt{1-\gamma_{+}^{2}}\right)\right\} \tag{48}
\end{equation*}
$$

with the quantities defined in equations (12), (15), (21), (26) and (46) containing our basic parameters $\mathbf{w}$ and $\mathbf{z}$ of $\varrho$. One can easily check by the definitions (46) that the surface dividing the entangled and separable states in the space of these density matrices is a special deformation of the $\eta=0$ Klein-quadric [15] given by the equation

$$
\begin{equation*}
\eta^{2}=4 r s \tag{49}
\end{equation*}
$$

This can also be seen from the formula (52) of negativity, see in the following subsection.

### 3.2. Negativity

Another entanglement-measure which we can calculate for $\varrho$ is the negativity. It is related to the notion of partial transpose and the criterion of Peres [17]. It is defined by the smallest eigenvalue of the partially transposed density matrix as follows [2, 8]:

$$
\begin{equation*}
\mathcal{N}(\varrho)=\max \left\{0,-2 \mu_{\min }\right\} \tag{50}
\end{equation*}
$$

Since the eigenvalues of a complex $4 \times 4$ matrix are invariant under $U(4)$ transformation, we can use again the $S U(2) \times S U(2) \subset U(4)$-transformed $\varrho^{\prime}$ of equation (34).

Denote by $\varrho^{\prime T_{2}}$ the partial transpose of $\varrho^{\prime}$ with respect to the second subsystem. This operation results in the transformation $\Lambda^{\prime T_{2}}=r \sigma_{3} \otimes I+I \otimes s \sigma_{3}+\mathbf{w}^{\prime} \boldsymbol{\sigma} \otimes\left(\overline{\mathbf{z}}^{\prime} \boldsymbol{\sigma}\right)^{T}+\overline{\mathbf{w}^{\prime}} \boldsymbol{\sigma} \otimes\left(\mathbf{z}^{\prime} \boldsymbol{\sigma}\right)^{T}$, i.e., only $z_{2}^{\prime}$ changes to $-z_{2}^{\prime}$. By virtue of this, retaining the definitions (38) and (39) of $\xi_{1}, \xi_{2}, \zeta_{1}, \zeta_{2}$, and redefining $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbf{R}^{3}$ of equation (37) as

$$
\boldsymbol{\alpha}=\left[\begin{array}{c}
\xi_{1}+\xi_{2}  \tag{51}\\
\zeta_{1}-\zeta_{2} \\
r+s
\end{array}\right], \quad \boldsymbol{\beta}=\left[\begin{array}{c}
\xi_{1}-\xi_{2} \\
\zeta_{1}+\zeta_{2} \\
r-s
\end{array}\right]
$$

the calculation proceeds as in section 3.1. The eigenvalues of $\varrho^{T_{2}}$ are $\mu_{i}=\left\{\frac{1}{4}(1 \pm|\boldsymbol{\alpha}|)\right.$, $\left.\frac{1}{4}(1 \pm|\boldsymbol{\beta}|)\right\}$, and a straightforward calculation shows that $\boldsymbol{\alpha}^{2}=1-\eta^{2}+4 r s$ and $\boldsymbol{\beta}^{2}=1-\eta^{2}-4 r s$. Hence one can see that the negativity of $\varrho$ is

$$
\begin{equation*}
\mathcal{N}(\varrho)=\max \left\{0, \frac{1}{2}\left(\sqrt{1-\eta^{2}+4 r s}-1\right)\right\} \tag{52}
\end{equation*}
$$

with the usual conventions of equations (15), (21) and (26).

### 3.3. Comparison of concurrence and negativity

For a two-qubit density matrix we can write the following inequalities between the concurrence and the negativity,

$$
\begin{equation*}
\sqrt{(1-\mathcal{C})^{2}+\mathcal{C}^{2}}-(1-\mathcal{C}) \leqslant \mathcal{N} \leqslant \mathcal{C} \tag{53}
\end{equation*}
$$

which are known from a paper of Audenaert et al [8]. Our special case with fermionic correlations may give extra restrictions between concurrence and negativity, so we can pose the question, whether we can replace inequality (53) by a stronger one.

Figure 1 shows the result of a numerical calculation. The gray field denotes the possible entangled states of the (10)-form on the $\mathcal{C}-\mathcal{N}$ plane. The upper bound of these can be analytically determined, and it can be proven (see the appendix) that the following inequality holds for $\mathcal{N}$ :

$$
\begin{equation*}
\sqrt{(1-\mathcal{C})^{2}+\mathcal{C}^{2}}-(1-\mathcal{C}) \leqslant \mathcal{N} \leqslant \frac{1}{2}\left(\sqrt{2-(1-2 \mathcal{C})^{2}}-1\right) \leqslant \mathcal{C} \tag{54}
\end{equation*}
$$

To see that this upper bound is the tightest, consider the special case when $\mathbf{w}=\mathbf{z}$. These states realize the boundary, so the second inequality in (54) turns to equality. (In this case $\eta=0$, $r=s, \gamma_{+}=2 r, \gamma_{-}=0$, and for entangled states, $\mathcal{C}=\frac{1}{2}\left(1-\sqrt{1-4 r^{2}}\right), \mathcal{N}=\frac{1}{2}\left(\sqrt{1+4 r^{2}}-1\right)$.


Figure 1. Range of value of negativity for a given concurrence, with its boundaries, as in (54).

These depend only on $r$, which can be expressed from $\mathcal{C}$, thus we can express the negativity of these states with their concurrence and get back the curve of the upper bound.)

It can be seen, by calculating the intersection of the corresponding curves of (54), that for maximally entangled states $\mathcal{C}\left(\varrho_{\max }\right)=\frac{1}{2}$, and $\mathcal{N}\left(\varrho_{\max }\right)=\frac{\sqrt{2}-1}{2}$. We can study the behavior of these states: from the concurrence formula (48) one can see that

$$
\begin{equation*}
\mathcal{C}=\frac{1}{2} \quad \Longleftrightarrow \quad\left(\eta^{2}=0, \gamma_{-}^{2}=0 \text { and } \gamma_{+}^{2}=1\right) . \tag{55}
\end{equation*}
$$

The first two of these constraints hold, if and only if $\mathbf{w}^{2}=\mathbf{z}^{2}$, and $r=s$, because of (15), (13) and (46). If $\mathbf{w}^{2}=\mathbf{z}^{2}$ then $r=s$ and $\|\mathbf{w}\|^{2}=\|\mathbf{z}\|^{2}=\frac{1}{2}$ are equivalent, and if $r=s$ then $\gamma_{+}^{2}=4 r^{2}=1,\|\mathbf{w}\|^{4}-\left|\mathbf{w}^{2}\right|^{2}=\frac{1}{4}$ and it follows that $\mathbf{w}^{2}=0$ :

$$
\begin{equation*}
\mathcal{C}=\mathcal{C}_{\max }=\frac{1}{2} \quad \Longleftrightarrow \quad\left(\|\mathbf{w}\|^{2}=\|\mathbf{z}\|^{2}=\frac{1}{2} \text { and } \mathbf{w}^{2}=\mathbf{z}^{2}=0\right) \tag{56}
\end{equation*}
$$

Since the transformation (34) on $\varrho$ preserves the quantities appearing here, we can easily calculate the canonical form (34) of the maximally entangled state $\varrho^{\prime}$. Let us choose an ansatz of the form (25) and (30) for $\mathbf{w}_{\text {max }}^{\prime}$ and $\mathbf{z}_{\text {max }}^{\prime}$ as $\mathbf{w}_{\text {max }}^{\prime}=\frac{1}{\sqrt{2}}\left[\cos (\alpha) \mathrm{e}^{\mathrm{i} \varphi_{1}}, \sin (\alpha) \mathrm{e}^{\mathrm{i} \varphi_{2}}, 0\right]^{T}$ and $\mathbf{z}_{\max }^{\prime}=\frac{1}{\sqrt{2}}\left[\cos (\beta) \mathrm{e}^{\mathrm{i} \psi_{1}}, \sin (\beta) \mathrm{e}^{\mathrm{i} \psi_{2}}, 0\right]^{T}$. These satisfy the first constraint of (56), and from the second it follows that $\cos \alpha=\sin \alpha=\frac{1}{\sqrt{2}}$ and $\varphi_{1}=\varphi_{2}-\frac{\pi}{2}=: \varphi$ and the same for $\mathbf{z}_{\text {max }}^{\prime}$ :

$$
\mathbf{w}_{\max }^{\prime}=\frac{1}{2} \mathrm{e}^{\mathrm{i} \varphi}\left[\begin{array}{l}
1  \tag{57}\\
\mathrm{i} \\
0
\end{array}\right], \quad \mathbf{z}_{\max }^{\prime}=\frac{1}{2} \mathrm{e}^{\mathrm{i} \psi \psi}\left[\begin{array}{l}
1 \\
\mathrm{i} \\
0
\end{array}\right] .
$$

Then for the density matrix with maximal concurrence we get the expression

$$
\varrho_{\max }^{\prime}=\frac{1}{4}\left[\begin{array}{clll}
\frac{3}{2} & 0 & 0 & 0  \tag{58}\\
0 & 1 & \mathrm{e}^{\mathrm{i} \delta} & 0 \\
0 & \mathrm{e}^{-\mathrm{i} \delta} & 1 & 0 \\
0 & 0 & 0 & \frac{1}{2}
\end{array}\right]
$$

with $\delta=\varphi-\psi$ being the only parameter characterizing this maximally entangled density matrix.

### 3.4. Purity

The purity measures the degree of mixedness of a density matrix. For our $\varrho$ thanks to the special property of $\Lambda$ (see in equation (14)) it can easily be calculated. We have the result

$$
\begin{align*}
& \operatorname{Tr} \varrho^{2}=\frac{1}{4}\left(2-\eta^{2}\right),  \tag{59}\\
& \frac{1}{4} \leqslant \operatorname{Tr} \varrho^{2} \leqslant \frac{1}{2} \tag{60}
\end{align*}
$$

by virtue of equation (16). The participation ratio is by definition

$$
\begin{equation*}
R=\frac{1}{\operatorname{Tr} \varrho^{2}}=\frac{4}{2-\eta^{2}} \tag{61}
\end{equation*}
$$

## 4. Relating different measures of entanglement

Now we would like to discuss the physical meaning of our quantities derived in the previous section. First let us note that the

$$
\begin{align*}
& \varrho_{1}=\operatorname{Tr}_{234}(|\Psi\rangle\langle\Psi|)=\operatorname{Tr}_{2}\left(\varrho_{12}\right)=\operatorname{Tr}_{2}(\varrho)=\frac{1}{2}(I+\mathbf{x} \boldsymbol{\sigma})  \tag{62}\\
& \varrho_{2}=\operatorname{Tr}_{134}(|\Psi\rangle\langle\Psi|)=\operatorname{Tr}_{1}\left(\varrho_{12}\right)=\operatorname{Tr}_{1}(\varrho)=\frac{1}{2}(I+\mathbf{y} \boldsymbol{\sigma}) \tag{63}
\end{align*}
$$

reduced density matrices describe the entanglement properties of subsystems 1 and 2 to the rest of the system described by the four-qubit state $|\Psi\rangle$. It is well known that the measures describing how much these subsystems are entangled with the rest are $\mathcal{C}_{1(234)}^{2}=4 \operatorname{Det}\left(\varrho_{1}\right)$ and $\mathcal{C}_{2(134)}^{2}=4 \operatorname{Det}\left(\varrho_{2}\right)$. Due to equations (62) and (63) these quantities are

$$
\begin{equation*}
0 \leqslant \mathcal{C}_{1(234)}^{2}=1-r^{2} \leqslant 1, \quad 0 \leqslant \mathcal{C}_{2(134)}^{2}=1-s^{2} \leqslant 1 \tag{64}
\end{equation*}
$$

Clearly, since $\varrho_{1}=\varrho_{3}$ and $\varrho_{2}=\varrho_{4}$, we also have

$$
\begin{equation*}
\mathcal{C}_{3(124)}^{2}=\mathcal{C}_{1(234)}^{2}, \quad \mathcal{C}_{4(123)}^{2}=\mathcal{C}_{2(134)}^{2} \tag{65}
\end{equation*}
$$

Moreover, we already know that $\varrho_{12}=\varrho_{34}=\varrho$. A straightforward calculation of the two-partite density matrices $\varrho_{14}$ and $\varrho_{23}$ shows that they again have the form of equation (10) with the sign of $\mathbf{w}$ being changed in the first case and the vectors $\mathbf{w}$ and $\mathbf{z}$ are exchanged in the second. Since these transformations do not change the value of the concurrence, we have

$$
\begin{equation*}
\mathcal{C}_{12}^{2}=\mathcal{C}_{14}^{2}=\mathcal{C}_{23}^{2}=\mathcal{C}_{34}^{2} . \tag{66}
\end{equation*}
$$

Now the only two-qubit density matrices we have not discussed yet are the ones $\varrho_{13}$ and $\varrho_{24}$. Their form is
$\left(\varrho_{13}\right)_{i k i^{\prime} k^{\prime}}=\frac{1}{2}\left(\|\mathbf{z}\|^{2} \varepsilon_{i k} \varepsilon_{i^{\prime} k^{\prime}}+\mathcal{B}_{i k} \overline{\mathcal{B}}_{i^{\prime} k^{\prime}}\right), \quad\left(\varrho_{24}\right)_{j l j^{\prime} l^{\prime}}=\frac{1}{2}\left(\|\mathbf{w}\|^{2} \varepsilon_{j l} \varepsilon_{j^{\prime} l^{\prime}}+\mathcal{A}_{j l} \overline{\mathcal{A}}_{j^{\prime} l^{\prime}}\right)$.
Recall now that the (4) transformation property of our four-qubit state gives rise to the corresponding ones for the reduced density matrices

$$
\begin{equation*}
\varrho_{13} \mapsto(U \otimes U) \varrho_{13}(\bar{U} \otimes \bar{U}), \quad \varrho_{24} \mapsto(V \otimes V) \varrho_{24}(\bar{V} \otimes \bar{V}) \tag{68}
\end{equation*}
$$

For $U, V \in S U(2)$ we have $V \varepsilon V^{t}=U \varepsilon U^{t}=\varepsilon$, hence the tensors occurring in equation (67) transform as

$$
\begin{equation*}
\varepsilon \mapsto \varepsilon, \quad \mathcal{A} \mapsto V \mathcal{A} V^{t}, \quad \mathcal{B} \mapsto U \mathcal{B} U^{t} \tag{69}
\end{equation*}
$$

Using the definition (6) of $\mathcal{A}$ we have for example

$$
\begin{equation*}
V \mathcal{A} V^{t}=\varepsilon \bar{V} \overline{\mathbf{z}} V^{t}=\varepsilon \overline{V \overline{\mathbf{z}} \sigma V^{\dagger}}=\varepsilon \overline{\overline{\mathbf{z}^{\prime}} \boldsymbol{\sigma}}=\varepsilon \mathbf{z}^{\prime} \bar{\sigma}, \tag{70}
\end{equation*}
$$

where by choosing $V \equiv V_{\mathbf{y}}^{\dagger}$ of equation (27) we get for $\mathbf{z}^{\prime}$ the form (30). Finally these manipulations yield for $\varrho_{24}$ the canonical form

$$
\varrho_{24}=\frac{1}{2}\left(\begin{array}{cccc}
\kappa_{0}+\kappa_{3} & 0 & 0 & \kappa_{1}-\mathrm{i} \kappa_{2}  \tag{71}\\
0 & \|\mathbf{w}\|^{2} & -\|\mathbf{w}\|^{2} & 0 \\
0 & -\|\mathbf{w}\|^{2} & \|\mathbf{w}\|^{2} & 0 \\
\kappa_{1}+\mathrm{i} \kappa_{2} & 0 & 0 & \kappa_{0}-\kappa_{3}
\end{array}\right)
$$

where
$\kappa_{0}=\left\|\mathbf{z}^{\prime}\right\|^{2}=\|\mathbf{z}\|^{2}, \quad-\kappa_{1}=\left|z_{1}^{\prime}\right|^{2}-\left|z_{2}^{\prime}\right|^{2}, \quad-\kappa_{2}=2 \operatorname{Re}\left(z_{1}^{\prime} \overline{z_{2}^{\prime}}\right), \quad-\kappa_{3}=2 \operatorname{Im}\left(z_{1}^{\prime} \overline{z_{2}^{\prime}}\right)$.
Note that

$$
\begin{equation*}
\kappa_{0}^{2}=\kappa_{1}^{2}+\kappa_{2}^{2}+\kappa_{3}^{2}=\|\mathbf{z}\|^{4}, \tag{73}
\end{equation*}
$$

hence the eigenvalues of $\varrho_{24}$ are $\|\mathbf{w}\|^{2},\|\mathbf{z}\|^{2}, 0,0$, i.e., our mixed state is of rank two. The structure of $\varrho_{13}$ is similar to the roles of $\mathbf{w}$ and $\mathbf{z}$ exchanged. Following the same steps as in section 3.1, we get for the corresponding squared concurrences the following expressions:

$$
\begin{equation*}
\mathcal{C}_{13}^{2}=\left(\|\mathbf{z}\|^{2}-\left|\mathbf{w}^{2}\right|\right)^{2}, \quad \mathcal{C}_{24}^{2}=\left(\|\mathbf{w}\|^{2}-\left|\mathbf{z}^{2}\right|\right)^{2} \tag{74}
\end{equation*}
$$

Let us now understand the meaning of the invariant $\eta$ from the four-qubit point of view. It is known that we have four algebraically independent $S L(2, \mathbf{C})^{\otimes 4}$ invariants $[16,18]$ denoted by $H, L, M$ and $D$. These are quadratic, quartic, quartic and sextic invariants of the complex amplitudes $\Psi_{i j k l}$, respectively. The invariants $H$ and $L$ are given by the expressions

$$
\begin{equation*}
H=\Psi_{0} \Psi_{15}-\Psi_{1} \Psi_{14}-\Psi_{2} \Psi_{13}+\Psi_{3} \Psi_{12}-\Psi_{4} \Psi_{11}+\Psi_{5} \Psi_{10}+\Psi_{6} \Psi_{9}-\Psi_{7} \Psi_{8} \tag{75}
\end{equation*}
$$

and

$$
L=\operatorname{Det}\left(\begin{array}{cccc}
\Psi_{0} & \Psi_{1} & \Psi_{2} & \Psi_{3}  \tag{76}\\
\Psi_{4} & \Psi_{5} & \Psi_{6} & \Psi_{7} \\
\Psi_{8} & \Psi_{9} & \Psi_{10} & \Psi_{11} \\
\Psi_{12} & \Psi_{13} & \Psi_{14} & \Psi_{15}
\end{array}\right)
$$

where instead of the binary one we used the decimal labeling. For the explicit form of the remaining two invariants $M$ and $D$ see the paper of Luque and Thibon [16]. A straightforward calculation shows that for our four-qubit state we have $M=D=0$, however,

$$
\begin{equation*}
H=-\frac{1}{2}\left(\mathbf{z}^{2}+\mathbf{w}^{2}\right), \quad L=\frac{1}{16}\left(\mathbf{z}^{2}-\mathbf{w}^{2}\right)^{2} \tag{77}
\end{equation*}
$$

hence

$$
\begin{equation*}
|L|=\frac{1}{16} \eta^{2} . \tag{78}
\end{equation*}
$$

For convenience we also introduce the quantity

$$
\begin{equation*}
\sigma \equiv\left|\mathbf{w}^{2}+\mathbf{z}^{2}\right|=2|H| \tag{79}
\end{equation*}
$$

Hence $\eta=\left|\mathbf{w}^{2}-\mathbf{z}^{2}\right|$ and $\sigma=\left|\mathbf{w}^{2}+\mathbf{z}^{2}\right|$ are related to the only nonvanishing four-qubit invariants $L$ and $H$. Using the definitions of these quantities and equation (13) one can check that
$\mathcal{C}_{13}^{2}=s^{2}+\frac{1}{2}\left(\eta^{2}+\sigma^{2}\right)-2\left\|\mathbf{z}^{2}\right\|\left|\mathbf{w}^{2}\right|, \quad \mathcal{C}_{24}^{2}=r^{2}+\frac{1}{2}\left(\eta^{2}+\sigma^{2}\right)-2\left\|\mathbf{w}^{2}\right\|\left|\mathbf{z}^{2}\right|$.
Hence we have the inequality

$$
\begin{equation*}
\mathcal{C}_{13}^{2}+\mathcal{C}_{24}^{2} \leqslant s^{2}+r^{2}+\eta^{2}+\sigma^{2} . \tag{81}
\end{equation*}
$$

Moreover, since $\mathcal{C}_{12}^{2}=\mathcal{C}_{14}^{2}$ after taking the square of equation (48) we get

$$
\begin{equation*}
\mathcal{C}_{12}^{2}+\mathcal{C}_{14}^{2}=1-r^{2}-s^{2}-\frac{1}{2} \eta^{2}-\sqrt{\left(1-\eta^{2}-\gamma_{-}^{2}\right)\left(1-\gamma_{+}^{2}\right)} . \tag{82}
\end{equation*}
$$

Combining this result with equations (64) and (80) we obtain

$$
\begin{equation*}
\mathcal{C}_{12}^{2}+\mathcal{C}_{13}^{2}+\mathcal{C}_{14}^{2}+\Sigma_{1}=\mathcal{C}_{1(234)}^{2} \quad \mathcal{C}_{12}^{2}+\mathcal{C}_{23}^{2}+\mathcal{C}_{24}^{2}+\Sigma_{2}=\mathcal{C}_{2(134)}^{2} \tag{83}
\end{equation*}
$$

where

$$
\begin{align*}
& \Sigma_{1}=2\|\mathbf{z}\|^{2}\left|\mathbf{w}^{2}\right|+\sqrt{\left(\frac{1}{2} \sigma^{2}+p_{+}\right)\left(\frac{1}{2} \sigma^{2}+p_{-}\right)}-\frac{1}{2} \sigma^{2}  \tag{84}\\
& \Sigma_{2}=2\|\mathbf{w}\|^{2}\left|\mathbf{z}^{2}\right|+\sqrt{\left(\frac{1}{2} \sigma^{2}+p_{+}\right)\left(\frac{1}{2} \sigma^{2}+p_{-}\right)}-\frac{1}{2} \sigma^{2} \tag{85}
\end{align*}
$$

Here

$$
\begin{equation*}
p_{ \pm}=2\|\mathbf{z}\|^{2}\|\mathbf{w}\|^{2} \pm \frac{1}{2}\left(4 r s-\eta^{2}\right) . \tag{86}
\end{equation*}
$$

Note that by virtue of equation (13) $p_{-}$is non-negative. Moreover according to equation (52) for nonseparable states $\left(\varrho_{12}, \varrho_{14}, \varrho_{34}, \varrho_{23}\right)$ we have nonzero negativity, hence $4 r s>\eta^{2}$ and thus $p_{+}$is also non-negative. In this case the residual tangles $\Sigma_{1}$ and $\Sigma_{2}$ as defined by equations (84) and (85) are positive as they should be, hence the generalized Coffman-Kundu-Wootters inequalities of distributed entanglement [11, 13] hold,

$$
\begin{equation*}
\mathcal{C}_{12}^{2}+\mathcal{C}_{13}^{2}+\mathcal{C}_{14}^{2} \leqslant \mathcal{C}_{1(234)}^{2} \quad \mathcal{C}_{12}^{2}+\mathcal{C}_{23}^{2}+\mathcal{C}_{24}^{2} \leqslant \mathcal{C}_{2(134)}^{2} \tag{87}
\end{equation*}
$$

For separable states we have $\mathcal{C}_{12}=\mathcal{C}_{14}=\mathcal{C}_{34}=\mathcal{C}_{23}=0$ and a calculation shows that the inequalities (87) in the form $\mathcal{C}_{13}^{2} \leqslant \mathcal{C}_{1(234)}^{2}$ and $\mathcal{C}_{24}^{2} \leqslant \mathcal{C}_{2(134)}^{2}$ still hold with the residual tangles

$$
\begin{equation*}
\Sigma_{1}=2\|\mathbf{z}\|^{2}\left(\left|\mathbf{w}^{2}\right|+\|\mathbf{w}\|^{2}\right) \quad \Sigma_{2}=2\|\mathbf{w}\|^{2}\left(\left|\mathbf{z}^{2}\right|+\|\mathbf{z}\|^{2}\right) \tag{88}
\end{equation*}
$$

Equations (84), (85) and (88) show the structure of the residual tangle. Unlike in the well-known three-qubit case these quantities among others contain two invariants $\eta$ and $\sigma$ characterizing four-partite correlations. The role of $\sigma$ (which for a general four-qubit state is a permutation-invariant) is to be compared with the similar role, the permutation invariant three-tangle $\tau_{123}=4|\mathcal{D}|$ plays (an $S L(2, \mathbf{C})^{\otimes 3}$ invariant) within the three-qubit context. ( $\mathcal{D}$ is Cayley's hyperdeterminant [11].) An important difference to the three-qubit case is that the residual tangles $\Sigma_{1,2}$ seem to be lacking the important entanglement monotone property. However, according to a conjecture [20] the sum $\Sigma_{1}+\Sigma_{2}$ could be an entanglement monotone. We hope that our explicit form will help to settle this issue at least for our special four-qubit state of equations (1) and (2).

## 5. Bures metric

As we have emphasized our density matrix $\varrho$ can be regarded as a reduced density matrix of a two-particle system on $\left(\mathbf{C}^{2} \otimes \mathbf{C}^{2}\right) \wedge\left(\mathbf{C}^{2} \otimes \mathbf{C}^{2}\right)$, meaning

$$
\begin{equation*}
\varrho=\Psi \Psi^{\dagger} \tag{89}
\end{equation*}
$$

where $\Psi$ is the $4 \times 4$ antisymmetric matrix occurring in equation (76). In the space of such fermionic purifications of our density matrix the curve $\Psi(t)$ is horizontal, when the differential equation

$$
\begin{equation*}
\dot{\Psi}^{\dagger} \Psi=\Psi^{\dagger} \dot{\Psi} \tag{90}
\end{equation*}
$$

holds. We can satisfy this equation by the ansatz

$$
\begin{equation*}
\dot{\Psi}=G \Psi, \quad G=G^{\dagger} \tag{91}
\end{equation*}
$$

for some $G=G^{\dagger}$, so that

$$
\begin{equation*}
\mathrm{d} \varrho=\{G, \varrho\} \tag{92}
\end{equation*}
$$

We can define the Bures metric on the space of density matrices as follows [2]:

$$
\begin{equation*}
\mathrm{d} s_{B}^{2}=\frac{1}{2} \operatorname{Tr}(G \mathrm{~d} \varrho) \tag{93}
\end{equation*}
$$

Let us now take into account the condition $\Psi^{T}=-\Psi$. Taking the transpose of equation (90), we get

$$
\begin{equation*}
\Psi^{T} \dot{\Psi}^{\dagger T}=\dot{\Psi}^{T} \Psi^{\dagger T}, \quad \Psi \dot{\Psi}^{\dagger}=\dot{\Psi} \Psi^{\dagger} \tag{94}
\end{equation*}
$$

Using this result, we get a simpler formula for $\mathrm{d} \varrho$ :

$$
\begin{equation*}
\mathrm{d} \varrho=\dot{\Psi} \Psi^{\dagger}+\Psi \dot{\Psi}^{\dagger}=2 G \Psi \Psi^{\dagger}=2 G \varrho \tag{95}
\end{equation*}
$$

and to get $G$, we only have to invert $\varrho$. A calculation of the eigenvalues of $\varrho$ shows that they are of the form [15]

$$
\begin{equation*}
\lambda_{ \pm}=\frac{1}{4}\left(1 \pm \sqrt{1-\eta^{2}}\right) \tag{96}
\end{equation*}
$$

Hence $\varrho$ is nonsingular iff $\eta \neq 0$ (i.e. iff $|L| \neq 0$ ). In the following we consider this case.
For nonsingular density matrices by virtue of equation (14), $\varrho^{-1}$ can be calculated easily

$$
\begin{equation*}
\varrho^{-1}=\frac{4}{\eta^{2}}(\mathbf{1}-\Lambda), \tag{97}
\end{equation*}
$$

hence

$$
\begin{equation*}
G=\frac{1}{2} \mathrm{~d} \varrho \varrho^{-1}=\frac{1}{2 \eta^{2}}(\mathrm{~d} \Lambda-\mathrm{d} \Lambda \Lambda), \tag{98}
\end{equation*}
$$

and the Bures metric

$$
\begin{equation*}
\mathrm{d} s_{B}^{2}=\frac{1}{4 \eta^{2}} \operatorname{Tr}(\mathrm{~d} \Lambda \mathrm{~d} \Lambda-\mathrm{d} \Lambda \Lambda \mathrm{~d} \Lambda) \tag{99}
\end{equation*}
$$

Since $\Lambda$ is idempotent and traceless, one can see that the trace of the second term equals zero: $2 \operatorname{Tr}(\mathrm{~d} \Lambda \Lambda \mathrm{~d} \Lambda)=\operatorname{Tr}\left(\mathrm{d} \Lambda \mathrm{d}\left(\Lambda^{2}\right)\right)=\operatorname{Tr}\left(\mathrm{d} \Lambda \mathrm{d}\left(-\eta^{2}\right) \mathbf{1}\right)=0$. Let us introduce the quantities $f_{i j}=w_{i} \bar{z}_{j}+\bar{w}_{i} z_{j}$. With this notation we have

$$
\begin{equation*}
\mathrm{d} s_{B}^{2}=\frac{1}{\eta^{2}}\left(\mathrm{~d} x_{i} \mathrm{~d} x_{i}+\mathrm{d} y_{j} \mathrm{~d} y_{j}+\mathrm{d} f_{i j} \mathrm{~d} f_{i j}\right) \tag{100}
\end{equation*}
$$

(Summation on $i, j=1,2,3$ is implied.) Moreover, a calculation shows that $\eta^{2}=1-$ $\left(x_{i} x_{i}+y_{j} y_{j}+f_{i j} f_{i j}\right)$, so after putting the quantities $x_{i}, y_{j}, f_{i j}$ into a 15 -component vector $\mathbf{k} \in \mathbf{R}^{15}$ our final result is the nice formula

$$
\begin{equation*}
\mathrm{d} s_{B}^{2}=\frac{1}{1-\mathbf{k}^{2}} \mathrm{~d} \mathbf{k}^{2}=\frac{1}{4} \eta^{2}\left[\frac{4 \mathrm{~d} \mathbf{k}^{2}}{\left(1-\mathbf{k}^{2}\right)^{2}}\right] . \tag{101}
\end{equation*}
$$

Let us compare this formula with that obtained for the Bures metric of one-qubit density matrices arising as a reduced density matrix from a pair of distinguishable qubits [19],

$$
\begin{equation*}
\mathrm{d} l_{B}^{2}=\frac{1}{4 \cosh ^{2} \beta}\left(\mathrm{~d} \beta^{2}+\sinh ^{2} \beta \mathrm{~d} \Omega^{2}\right) \tag{102}
\end{equation*}
$$

where $1-C^{2}=\tanh ^{2} \beta$ with $C$ the pure state concurrence for two qubits, and $d \Omega^{2}$ is the usual line element on the two-sphere $S^{2}$ expressed by the angular coordinates $\vartheta$ and $\varphi$. Since the space of one-qubit density matrices is the Bloch-ball $\mathbf{B}^{3}$ this parametrization provides a map between the upper sheets of the double-sheeted hyperboloids $\mathbf{H}^{3}$ and $\mathbf{B}^{3}$. The standard metric on $\mathbf{H}^{3}$ is just $\mathrm{d} \beta^{2}+\sinh ^{2} \beta \mathrm{~d} \Omega^{2}$. Hence we see that the Bures metric is up to the conformal
factor $C^{2} / 4$, which is just the standard metric on the upper sheet of the double-sheeted hyperboloid $H^{3}$. However, using the stereographic projection one can show that

$$
\begin{equation*}
\mathrm{d} \beta^{2}+\sinh ^{2} \beta \mathrm{~d} \Omega^{2}=\frac{4 \mathrm{~d} \mathbf{R}^{2}}{\left(1-\mathbf{R}^{2}\right)^{2}} \tag{103}
\end{equation*}
$$

where $R_{1}, R_{2}$ and $R_{3}$ can alternatively be used to parametrize $\mathbf{B}^{3}$. Hence we can write

$$
\begin{equation*}
\mathrm{d} l_{B}^{2}=\frac{1}{4} C^{2}\left[\frac{4 \mathrm{~d} \mathbf{R}^{2}}{\left(1-\mathbf{R}^{2}\right)^{2}}\right], \tag{104}
\end{equation*}
$$

where the metric on the right is the standard Poincare metric on the unit ball which is now just the Bloch-ball. Comparing this equation with our previous expression of equation (101) we see that it is up to the conformal factor $\eta^{2} / 4$, which is just the Poincaré metric on the Poincaré ball $\mathbf{B}^{15}$. We emphasize, however, that unlike the usual one-qubit mixed state where all the Bloch parameters characterizing the density matrix are independent, here the 15 parameters associated with the vector $\mathbf{k}$ are subject to nontrivial constraints. These constraints describe some nontrivial embedding of the space of nonsingular density matrices $\mathcal{D}$ into the Bloch-ball $\mathbf{B}^{15}$ with our Bures metric of equation (101).

## 6. Conclusions

In this paper we investigated the structure of a 12-parameter family of two-qubit density matrices with fermionic purifications. Our starting point was a four-qubit state with a special antisymmetry constraint imposed on its amplitudes. Such states are elements of the space $\left(\mathbf{C}^{2} \otimes \mathbf{C}^{2}\right) \wedge\left(\mathbf{C}^{2} \otimes \mathbf{C}^{2}\right)$ and the admissible local operations are of the form $(U \otimes V) \otimes(U \otimes V) \in S L(2, \mathbf{C})^{\otimes 4}$. Our density matrices are arising as the reduced ones $\varrho=\varrho_{12}=\operatorname{Tr}_{34}(|\Psi\rangle\langle\Psi|)$. Since the 12 subsystem is indistinguishable from the 34 one we have $\varrho_{12}=\varrho_{34}$. We obtained an explicit form for $\varrho$ in terms of the six independent complex amplitudes $\mathbf{w}$ and $\mathbf{z}$ of our four-qubit states. Employing local unitary transformations of the form $U \otimes V \in S U(2) \times S U(2) \subset S L(2, \mathbf{C}) \times S L(2, \mathbf{C})$ we derived the canonical form for $\varrho$. This form enabled an explicit calculation for different entanglement measures. We have calculated the Wootters concurrence, the negativity and the purity. The quantities occurring in these formulae (and some additional ones) are subject to monogamy relations of distributed entanglement similar to those showing up in the Coffman-Kundu-Wootters relations for three qubits. They characterize the entanglement trade-off between different subsystems. We have the entanglement measures $\eta$ and $\sigma$ describing the intrinsically four-partite correlations, quantities (Wootters concurrences) keeping track the mixed state entanglement of the bipartite subsystems embedded in the four-qubit one. Finally, we have the independent quantities $\mathcal{C}_{1(234)}^{2}$ and $\mathcal{C}_{2(134)}^{2}$ measuring how much subsystems 1 and 2 are entangled individually to the rest. We derived explicit formulae displaying how these important quantities are related. Last we have studied in some detail the Bures geometry underlying the structure of these density matrices. We have shown that the constraint of antisymmetry makes it possible to obtain a nice explicit formula for the Bures metric reminiscent of those known from hyperbolic geometry [21].

## Acknowledgments

One of us (PL) would like to express his gratitude to Professor Werner Scheid for his warm hospitality at the Department of Theoretical Physics of the Justus Liebig University of Giessen where part of this work was completed. Financial support from the Országos Tudományos Kutatási Alap (OTKA) (grant nos: T046868, T047041 and T038191) is gratefully acknowledged.

## Appendix. Upper bound of negativity

In this fermionic-correlated case, defined by equations (10)-(12) and (15), we can prove the following inequality:

Theorem. For all entangled $\varrho$ :

$$
\begin{equation*}
\mathcal{N}(\varrho) \leqslant \frac{1}{2}\left(\sqrt{2-(1-2 \mathcal{C}(\varrho))^{2}}-1\right) \tag{A.1}
\end{equation*}
$$

Proof. Insert equations (48) and (52) into (A.1):
$\frac{1}{2}\left(\sqrt{1-\eta^{2}+4 r s}-1\right) \leqslant \frac{1}{2}\left(\sqrt{2-\left(1-\sqrt{1-\gamma_{-}^{2}-\eta^{2}}+\sqrt{1-\gamma_{+}^{2}}\right)^{2}}-1\right)$,
after some algebra, we can rearrange the terms:
$0 \leqslant 2 \eta^{2}-2+\gamma_{-}^{2}+\gamma_{+}^{2}-4 r s+2 \sqrt{1-\gamma_{-}^{2}-\eta^{2}}-2 \sqrt{1-\gamma_{+}^{2}}+2 \sqrt{1-\gamma_{-}^{2}-\eta^{2}} \sqrt{1-\gamma_{+}^{2}}$.

It follows from the definition (46) that $\gamma_{+}^{2}-4 r s=\gamma_{-}^{2}$. With this:
$0 \leqslant-\left(1-\gamma_{-}^{2}-\eta^{2}\right)+\sqrt{1-\gamma_{-}^{2}-\eta^{2}}-\sqrt{1-\gamma_{+}^{2}}+\sqrt{1-\gamma_{-}^{2}-\eta^{2}} \sqrt{1-\gamma_{+}^{2}}$.
The right-hand side is factorizable:

$$
\begin{equation*}
0 \leqslant\left(\sqrt{1-\gamma_{-}^{2}-\eta^{2}}-\sqrt{1-\gamma_{+}^{2}}\right)\left(1-\sqrt{1-\gamma_{-}^{2}-\eta^{2}}\right) \tag{A.5}
\end{equation*}
$$

The second parenthesis is obviously positive. For entangled states $\mathcal{C}(\varrho)>0$, and the first parenthesis is proportional to the concurrence, which is strictly positive.

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