Maximally entangled mixed states of two qubits

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(Received 22 December 2000; published 15 June 2001)

We consider mixed states of two qubits and show under which global unitary operations their entanglement is maximized. This leads to a class of states that is a generalization of the Bell states. Three measures of entanglement are considered: entanglement of formation, negativity, and relative entropy of entanglement. Surprisingly all states that maximize one measure also maximize the others. We give a complete characterization of these generalized Bell states and prove that these states for fixed eigenvalues are all equivalent under local unitary transformations. Furthermore we characterize all nearly entangled states closest to the maximally mixed state and derive a lower bound on the volume of separable mixed states.

DOI: 10.1103/PhysRevA.64.012316 PACS number(s): 03.67.−a, 03.65.Ud, 89.70.+c

In this paper we investigate how much entanglement in a mixed two-qubit system can be created by global unitary transformations. The class of states for which no more entanglement can be created by global unitary operations is clearly a generalization of the class of Bell states to mixed states, and gives strict bounds on how the degree of mixing of a state limits its entanglement. This question is of considerable interest as entanglement is the magic ingredient of quantum information theory and experiments always deal with mixed states. Recently, Ishizaka and Hiroshima [1] independently considered the same question. They proposed a class of states and conjectured that the entanglement of formation [2] and the negativity [3] of these states could not be increased by any global unitary operation. Here we rigorously prove their conjecture and furthermore prove that the states they proposed are the only ones having the property of maximal entanglement.

Closely related to the issue of generalized Bell states is the question of characterizing the set of separable density matrices [5], as the entangled states closest to the maximally mixed state necessarily have to belong to the proposed class of maximal entangled mixed states. We can thus give a complete characterization of all nearly entangled states lying on the boundary of the sphere of separable states surrounding the maximally mixed state. As a by-product this gives an alternative derivation of the well-known result of Zyczkowski *et al.* [3] that all states for which the inequality $\mathrm{Tr}(\rho^2)\leqslant\frac{1}{3}$ holds are separable.

The original motivation of this paper was the following question: given a single quantum-mechanical system consisting of two spin-$\frac{1}{2}$ systems, i.e., two qubits, in a given state, how can one maximize the entanglement of these qubits using only unitary operations? If not only unitary operations but also measurements were allowed, it is clear that a Von Neumann measurement in the Bell basis would immediately yield a singlet. Here, however, we restrict ourselves to unitary operations. Obviously, these unitary operations must be global ones, that is, acting on the system as a whole, since any reasonable measure of entanglement must be invariant under local unitary operations, acting only on single qubits. As measures of entanglement, the entanglement of formation (EOF) [2], the negativity [3], and the relative entropy of entanglement [4] were chosen.

The entanglement of formation of mixed states is defined variationally as $E_f(\rho)=\min_{\{\psi_i\}}\Sigma_i p_i E(\psi_i)$ where $\rho=\Sigma_i p_i \psi_i \psi_i^\dagger$. For 2×2 systems the EOF is well characterized by introducing the concurrence C [2]:

$$E_f(\rho)=f(C(\rho))=H\left(\frac{1+\sqrt{1-C^2}}{2}\right), \tag{1}$$

$$C(\rho)=\max(0,\sigma_1-\sigma_2-\sigma_3-\sigma_4). \tag{2}$$

Here $\{\sigma_i\}$ are the square roots of the eigenvalues of the matrix A arranged in decreasing order,

$$A=\rho S\rho^* S, \tag{3}$$

$$S=\sigma_y\otimes\sigma_y. \tag{4}$$

$H(x)$ is Shannon's entropy function and σ_y is the Pauli matrix. It can be shown that $f(C)$ is convex and monotonically increasing. Using some elementary linear algebra it is furthermore easy to prove that the numbers $\{\sigma_i\}$ are equal to the singular values [8] of the matrix $\sqrt{\rho}^T S\sqrt{\rho}$. Here we use the notation $\sqrt{\rho}=\Phi\Lambda^{1/2}$ given $\Phi\Lambda\Phi^\dagger$, the eigenvalue decomposition of ρ.

The concept of negativity of a state is closely related to the well-known Peres condition for separability of a state [6]. If a state is separable (disentangled), then the partial transpose of the state is again a valid state, i.e., it is positive. For 2×2 systems, this condition is also sufficient [7]. It turns out that the partial transpose of a nonseparable state has one negative eigenvalue. From this, a measure for entanglement follows: the *negativity* of a state [3] is equal to the trace norm of its partial transpose. We will adopt the definition of negativity as twice the absolute value of this negative eigenvalue:

$$E_N(\rho)=2\max(0,-\lambda_4), \tag{5}$$

where λ_4 is the minimal eigenvalue of ρ^{T_A}. In the case of two qubits, this is equivalent to the trace norm of the partial transpose up to an affine mapping.

The relative entropy of entanglement was proposed by Vedral and Plenio [4] as a measure of entanglement motivated by the classical concept of Kullback-Leibler distance between probability distributions. This measure has very nice properties, such as being a good upper bound for the entanglement of distillation. It is variationally defined as

$$E_R(\rho)=\min_{\sigma\in D}\mathrm{Tr}(\rho\log\rho-\rho\log\sigma), \tag{6}$$

where D represents the convex set of all separable density operators.

We now state our main result.

Theorem 1. Let the eigenvalue decomposition of ρ be

$$\rho=\Phi\Lambda\Phi^{\dagger},$$

where the eigenvalues $\{\lambda_i\}$ are sorted in nonascending order. The entanglement of formation is maximized if and only if a global unitary transformation of the form

$$U=(U_1\otimes U_2)\begin{pmatrix}0&0&0&1\\ 1/\sqrt{2}&0&1/\sqrt{2}&0\\ 1/\sqrt{2}&0&-1/\sqrt{2}&0\\ 0&1&0&0\end{pmatrix}D_{\phi}\Phi^{\dagger}$$

is applied to the system, where U_1 and U_2 are local unitary operations and D_{ϕ} is a unitary diagonal matrix. This same global unitary transformation is the unique transformation maximizing the negativity and the relative entropy of entanglement. The entanglement of formation and negativity of the new state $\rho'=U\rho U^{\dagger}$ are then given by

$$E_f(\rho')=f(\max(0,\lambda_1-\lambda_3-2\sqrt{\lambda_2\lambda_4})),$$

$$E_N(\rho')=\max(0,\sqrt{(\lambda_1-\lambda_3)^2+(\lambda_2-\lambda_4)^2}-\lambda_2-\lambda_4),$$

respectively, while the expression for the relative entropy of entanglement is given by

$$\begin{aligned}E_R(\rho')=&\,\mathrm{Tr}(\rho\log\rho)-\lambda_1\log[(1-a)/2]\\ &-\lambda_2\log\{[a+b+2(\lambda_2-\lambda_4)]/4\}\\ &-\lambda_3\log[(1-b)/2]-\lambda_4\log\{[a+b\\ &-2(\lambda_2-\lambda_4)]/4\},\end{aligned}$$

$$a=[d-\sqrt{d^2-4(1-\lambda_1)(1-\lambda_3)(\lambda_2-\lambda_4)^2}]/[2(1-\lambda_3)],$$

$$b=[d-\sqrt{d^2-4(1-\lambda_1)(1-\lambda_3)(\lambda_2-\lambda_4)^2}]/[2(1-\lambda_1)],$$

$$d=\lambda_2+\lambda_4+(\lambda_2-\lambda_4)^2.$$

The class of generalized Bell states is defined as the states ρ' thus obtained. These states are the maximally entangled mixed states (MEMS's).

We now present the complete proof of this theorem. The cases of entanglement of formation, negativity, and relative entropy of entanglement will be treated independently. We start with the entanglement of formation.

As the function $f(x)$ is monotonically increasing, maximizing the EOF is equivalent to maximizing the concurrence. The problem is now reduced to finding

$$C_{\max}=\max_{U\in U(4)}(0,\sigma_1-\sigma_2-\sigma_3-\sigma_4) \tag{7}$$

with $\{\sigma_i\}$ the singular values of

$$Q=\Lambda^{1/2}\Phi^T U^T S U\Phi\Lambda^{1/2}. \tag{8}$$

Now, Φ, U, and S are unitary, and so is any product of them. It then follows that

$$C_{\max}\leqslant\max_{V\in U(4)}(0,\sigma_1-\sigma_2-\sigma_3-\sigma_4) \tag{9}$$

with $\{\sigma_i\}$ the singular values of $\Lambda^{1/2}V\Lambda^{1/2}$. The inequality becomes an equality if there is a unitary matrix U such that the optimal V can be written as $\Phi^T U^T S U\Phi$. A necessary and sufficient condition for this is that the optimal V be symmetric ($V=V^T$): as S is symmetric and unitary, it can be written as a product $S_1^T S_1$, with S_1 again unitary. This is known as the Takagi factorization of S [8]. This factorization is not unique: left-multiplying S_1 by a complex orthogonal matrix O ($O^T O=\mathbb{1}$) also yields a valid Takagi factor. An explicit form of S_1 is given by

$$S_1=\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&1&0\\ -1&0&0&1\\ 0&-i&i&0\\ i&0&0&i\end{pmatrix}. \tag{10}$$

If V is symmetric it can also be factorized like this: $V=V_1^T V_1$. It is now easy to see that any U of the form

$$U=S_1^{\dagger}OV_1\Phi^{\dagger}, \tag{11}$$

with O real orthogonal, indeed yields $V=V_1^T V_1$.

To proceed, we need two inequalities concerning singular values of matrix products. Henceforth, singular values as well as eigenvalues will be sorted in nonascending order. The following inequality for singular values is well known [9].

Lemma 1. Let $A\in M_{n,r}(\mathbb{C})$, $B\in M_{r,m}(\mathbb{C})$. Then,

$$\sum_{i=1}^{k}\sigma_i(AB)\geqslant\sum_{i=1}^{k}\sigma_i(A)\sigma_i(B), \tag{12}$$

for $k=1,\ldots,q=\min\{n,r,m\}$.

Less known is the following result by Wang and Xi [10]

Lemma 2. Let $A\in M_n(\mathbb{C})$, $B\in M_{n,m}(\mathbb{C})$, and $1\leqslant i_1<\cdots<i_k\leqslant n$. Then

$$\sum_{t=1}^{k}\sigma_{i_t}(AB)\geqslant\sum_{t=1}^{k}\sigma_{i_t}(A)\sigma_{n-t+1}(B). \tag{13}$$

Set $n=4$ in both inequalities. Then put $k=1$ in the first, and $k=3$, $i_1=2$, $i_2=3$, $i_3=4$ in the second. Subtracting the inequalities then gives

$$\sigma_1(AB)-[\sigma_2(AB)+\sigma_3(AB)+\sigma_4(AB)]\leqslant\sigma_1(A)\sigma_1(B)-\sigma_2(A)\sigma_4(B)-\sigma_3(A)\sigma_3(B)-\sigma_4(A)\sigma_2(B).$$

Furthermore, let $A=\Lambda^{1/2}$ and $B=V\Lambda^{1/2}$, with Λ positive diagonal and with the diagonal elements sorted in nonascending order. Thus, $\sigma_i(A)=\sigma_i(B)=\sqrt{\lambda_i}$. This gives

$$[\sigma_1-(\sigma_2+\sigma_3+\sigma_4)](\Lambda^{1/2}V\Lambda^{1/2})\leqslant\lambda_1-(2\sqrt{\lambda_2\lambda_4}+\lambda_3).$$

It is easy to see that this inequality becomes an equality if and only if V is equal to the permutation matrix

$$\begin{pmatrix}1&0&0&0\\0&0&0&1\\0&0&1&0\\0&1&0&0\end{pmatrix} \tag{14}$$

multiplied by an arbitrary unitary diagonal matrix D_ϕ. Therefore, we have proven

$$\max_{V\in U(4)}[\sigma_1-(\sigma_2+\sigma_3+\sigma_4)](\Lambda^{1/2}V\Lambda^{1/2})=\lambda_1-(2\sqrt{\lambda_2\lambda_4}+\lambda_3). \tag{15}$$

We can directly apply this to the problem at hand. The optimal V is indeed symmetric, so that it can be decomposed as $V=V_1^TV_1$. A possible Takagi factor is

$$V_1=\begin{pmatrix}1&0&0&0\\0&1/\sqrt{2}&0&1/\sqrt{2}\\0&0&1&0\\0&i/\sqrt{2}&0&-i/\sqrt{2}\end{pmatrix}. \tag{16}$$

The optimal unitary operations U are thus all of the form $U=S_1^\dagger OV_1D_\phi^{1/2}\Phi^\dagger$ with O an arbitrary orthogonal matrix. It has to be emphasized that the diagonal matrix D_ϕ will not have any effect on the state $\rho'=U\Phi\Lambda\Phi^\dagger U^\dagger$.

To proceed we exploit a well-known accident in Lie group theory:

$$\mathrm{SU}(2)\otimes\mathrm{SU}(2)\cong\mathrm{SO}(4). \tag{17}$$

It now happens that the unitary matrix S_1 is exactly of the form for making $S_1(U_1\otimes U_2)S_1^\dagger$ real for arbitrary $\{U_1,U_2\}\in\mathrm{SU}(2)$. It follows that $S_1(U_1\otimes U_2)S_1^\dagger$ is orthogonal and thus is an element of SO(4). Conversely, each element $Q\in\mathrm{SO}(4)$ can be written as $Q=S_1(U_1\otimes U_2)S_1^\dagger$. On the other hand the orthogonal matrices with determinant equal to -1 can all be written as orthogonal matrices with determinant 1 multiplied by a fixed matrix of determinant -1. Some calculations reveal that

$$S_1^\dagger\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&-1\end{pmatrix}V_1=(\sigma_y\otimes\sigma_y)S_1^\dagger V_1\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&1\end{pmatrix}.$$

We conclude that for each $O\in O(4)$ and D_ϕ unitary diagonal, there exist $U_1,U_2\in\mathrm{SU}(2)$ and $D_{\phi'}$ unitary diagonal, such that $U=S_1^\dagger OV_1D_\phi\Phi^\dagger=(U_1\otimes U_2)S_1^\dagger V_1D_{\phi'}\Phi^\dagger$.

It is now easy to check that a unitary transformation produces maximal entanglement of formation if and only if it is of the form

$$(U_1\otimes U_2)\begin{pmatrix}0&0&0&1\\1/\sqrt{2}&0&1/\sqrt{2}&0\\1/\sqrt{2}&0&-1/\sqrt{2}&0\\0&1&0&0\end{pmatrix}D_\phi\Phi^\dagger. \tag{18}$$

This completes the proof of the first part of Theorem 1.

We now proceed to prove the second part of Theorem 1 concerning the negativity. This proof is based on the Rayleigh-Ritz variational characterization of the minimal eigenvalue of a Hermitian matrix:

$$\lambda_{\min}(\rho^{T_A})=\min_{x:\|x\|=1}\mathrm{Tr}\,\rho^{T_A}|x\rangle\langle x|=\min_{x:\|x\|=1}\mathrm{Tr}\,\rho(|x\rangle\langle x|)^{T_A}. \tag{19}$$

The eigenvalue decomposition of $(|x\rangle\langle x|)^{T_A}$ can best be deduced from its singular-value decomposition. Let $\tilde{x}$ denote a reshaping of the vector x to a 2×2 matrix with $\tilde{x}_{ij}=\langle e^i\otimes e^j|x\rangle$. Introducing the permutation matrix $P_0=\Sigma_{ij}e^{ij}\otimes e^{ji}$, the partial transpose can be written as follows:

$$(|x\rangle\langle x|)^{T_A}=P_0(\tilde{x}\otimes\tilde{x}^\dagger). \tag{20}$$

The proof of this statement is elementary. We denote the Schmidt decomposition of the vector $|x\rangle$ by

$$\tilde{x}=U_1\Sigma U_2^\dagger, \tag{21}$$

where the diagonal elements of Σ are given by σ_1,σ_2. Since x is normalized we can parameterize these as cos (α) and sin (α) with $0\leqslant\alpha\leqslant\pi/4$ (to maintain the ordering). We get

$$(|x\rangle\langle x|)^{T_A}=P_0(U_1\otimes U_2)(\Sigma\otimes\Sigma)(U_2\otimes U_1)^\dagger. \tag{22}$$

This clearly is a singular-value decomposition. The explicit eigenvalue decomposition can now be calculated using the basic property of P_0 that $P_0(A\otimes B)=(B\otimes A)P_0$ for arbitrary A,B. It is then easy to check that the eigenvalue decomposition of $(|x\rangle\langle x|)^{T_A}$ is given by

$$(|x\rangle\langle x|)^{T_A}=V(x)D[\alpha(x)]V(x)^\dagger, \tag{23}$$

where $D[\alpha(x)]$ is the diagonal matrix with eigenvalues $(\sigma_1^2,\sigma_1\sigma_2,\sigma_2^2,-\sigma_1\sigma_2)$ and

$$V(x)=(U_1(x)\otimes U_2(x))\begin{pmatrix}1&0&0&0\\0&1/\sqrt{2}&0&1/\sqrt{2}\\0&1/\sqrt{2}&0&-1/\sqrt{2}\\0&0&1&0\end{pmatrix}. \tag{24}$$

For the problem at hand, we have to minimize the minimal eigenvalue of $(U\rho U^\dagger)^{T_A}$ over all possible $U\in U(4)$. Thus, we have to minimize

$$\min_{U,x}\operatorname{Tr}U\Phi\Lambda\Phi^\dagger U^\dagger(x)D[\alpha(x)]V(x)^\dagger = \min_\alpha\min_W\operatorname{Tr}\Lambda W^\dagger D(\alpha)W, \tag{25}$$

where we have absorbed the eigenvector matrix Φ of ρ, as well as $V(x)^\dagger$, into U, yielding W. Now, the minimization over W can be done by writing the trace in components

$$g(\alpha)=\operatorname{Tr}\Lambda W^\dagger D(\alpha)W=\sum_{i,j}d_j(\alpha)|W_{ji}|^2\lambda_i=d(\alpha)^TJ(W)\lambda, \tag{26}$$

where $d(\alpha)$ and λ denote the vectors containing the diagonal elements of $D(\alpha)$ and Λ, respectively. $J(W)$ is a doubly stochastic matrix formed from W by taking the modulus squared of every element. The minimum over all W is attained when $J(W)$ is a permutation matrix; this follows from Birkhoff's theorem [8], which says that the set of doubly stochastic matrices is the convex closure of the set of permutation matrices, and also from the fact that our object function is linear. Since the components of σ and λ are sorted in descending order and λ is positive, the permutation matrix yielding the minimum for any α is the matrix

$$J_0=\begin{pmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{pmatrix}. \tag{27}$$

Thus W has to be chosen equal to J_0 multiplied by a diagonal unitary matrix D_ϕ. Hence, the minimum over W is given by $\Sigma_{j=1}^4\lambda_jd_{4+1-j}(\alpha)$. Minimizing over α gives, after a few basic calculations,

$$\cos(2\alpha)=\frac{\lambda_2-\lambda_4}{\sqrt{(\lambda_1-\lambda_3)^2+(\lambda_2-\lambda_4)^2}},$$

$$g(\alpha)=[\lambda_2+\lambda_4-\sqrt{(\lambda_1-\lambda_3)^2+(\lambda_2-\lambda_4)^2}]/2.$$

This immediately yields the conjectured formula for the optimal negativity.

We now have to find the U for which this optimum is reached. As $V(x)^\dagger U\Phi=W$, it follows that the optimal unitary transformation U is given by $U=V(x)J_0D_\phi\Phi^\dagger$:

$$U=(U_1\otimes U_2)\begin{pmatrix}0&0&0&1\\1/\sqrt{2}&0&1/\sqrt{2}&0\\1/\sqrt{2}&0&-1/\sqrt{2}&0\\0&1&0&0\end{pmatrix}D_\phi\Phi^\dagger. \tag{28}$$

This is exactly the same U as in the case of entanglement of formation.

Next we move to the third part of Theorem 1 concerning the relative entropy of entanglement. We first prove two lemmas.

Lemma 3. Consider the class of superoperators

$$\mathcal{T}(\rho)=\sum_i a_iU_i\rho U_i^\dagger,$$

where all U_i are unitary, and the a_i form a distribution. Then, for any state ρ that is invariant under $\mathcal{T}$, we have for the relative entropy

$$S(\rho\|\sigma)\geqslant S(\rho\|\mathcal{T}^\dagger(\sigma)).$$

Proof. The proof of this lemma is heavily inspired by Theorem 6 in [11]. From $S(\rho)=S(\mathcal{T}(\rho))$, we find

$$\begin{aligned}S(\rho\|\sigma)&=\operatorname{Tr}\rho\log\rho-\operatorname{Tr}\rho\log\sigma\\&=\operatorname{Tr}\rho\log\rho-\operatorname{Tr}\mathcal{T}(\rho)\log\sigma\\&=\operatorname{Tr}\rho\log\rho-\sum_i a_i\operatorname{Tr}U_i\rho U_i^\dagger\log\sigma\\&=\operatorname{Tr}\rho\log\rho-\sum_i a_i\operatorname{Tr}\rho\log(U_i^\dagger\sigma U_i)\\&\geqslant\operatorname{Tr}\rho\log\rho-\operatorname{Tr}\rho\log\Big(\sum_i a_iU_i^\dagger\sigma U_i\Big)\\&=S(\rho\|\mathcal{T}^\dagger(\sigma)),\end{aligned}$$

where at the $\geqslant$ relation we have used the subadditivity of the relative entropy with respect to its second argument.

Lemma 4. For ρ of the form $\rho=U\Lambda U^\dagger$ with

$$U=\begin{pmatrix}0&0&0&1\\1/\sqrt{2}&0&1/\sqrt{2}&0\\1/\sqrt{2}&0&-1/\sqrt{2}&0\\0&1&0&0\end{pmatrix}$$

and Λ containing the ordered eigenvalues of ρ,

$$E_R(\rho)=\min_{\sigma\in D\cap\mathrm{MEMS}}S(\rho\|\sigma),$$

where MEMS is the class of maximally entangled mixed states.

Proof. Define the superoperator

$$\mathcal{T}(\rho) = V\,\mathrm{diag}(V^\dagger \rho V) V^\dagger.$$

Here, diag(ρ) is the superoperator that sets all off-diagonal elements of ρ equal to zero while keeping the diagonal ones intact. This superoperator can also be written as

$$\mathrm{diag}(\rho) = \sum_i P_i \rho P_i / 2^n,$$

where P_i runs through all possible diagonal matrices having only $+1$ or -1 on their diagonal [12]. It follows that $\mathcal{T}$ is of the form mentioned in Lemma 1 and, furthermore, that it is a self-dual superoperator, i.e., $\mathcal{T}^\dagger = \mathcal{T}$.

It is obvious that all MEMS's (with $U_1 = U_2 = \mathbb{1}$) are left invariant by $\mathcal{T}$. We will now show that any such $\mathcal{T}$ maps separable states to separable states. Consider the pure product states only; if the proposition is valid for pure product states, it will be valid for all separable states (by linearity). The most general pure product state has the state vector $\psi = (ac, ad, bc, bd)$, with a,b,c,d complex numbers. Then, since

$$V^\dagger \psi = ((ad+bc)/\sqrt{2}, bd, (ad-bc)/\sqrt{2}, ac),$$

$$\mathcal{T}(\psi\psi^\dagger) = V\,\mathrm{diag}(V^\dagger \psi\psi^\dagger V) V^\dagger = V \Lambda V^\dagger,$$

where the diagonal elements of Λ are, in order,

$$(|(ad+bc)/\sqrt{2}|^2, |bd|^2, |(ad-bc)/\sqrt{2}|^2, |ac|^2).$$

As these values are not necessarily sorted, $\mathcal{T}(\psi\psi^\dagger)$ need not be a MEMS. However, it is still possible to apply the formula for the negativity of MEMS's which says that

$$E_N(\rho) = \max(0, \sqrt{(\lambda_1 - \lambda_3)^2 + (\lambda_2 - \lambda_4)^2} - \lambda_2 - \lambda_4).$$

As can be easily checked, the validity of this formula does not rely on the ordering of the λ_i, as long as each λ_i pertains to the ith column of V. In particular, using

$$\lambda_1 - \lambda_3 = 2\,\mathrm{Re}[ab(cd)^*],$$

$$\lambda_2 \pm \lambda_4 = |bd|^2 \pm |ac|^2,$$

we get for the negativity of $\mathcal{T}(\psi\psi^\dagger)$

$$E_N[\mathcal{T}(\psi\psi^\dagger)] = \max(0, F)$$

with

$$\begin{aligned} F &= \sqrt{(\lambda_1 - \lambda_3)^2 + (\lambda_2 - \lambda_4)^2} - (\lambda_2 + \lambda_4) \\ &= \sqrt{4\,\mathrm{Re}[ab(cd)^*]^2 + |bd|^4 + |ac|^4 - 2|abcd|^2} \\ &\quad - (|bd|^2 + |ac|^2) \\ &= \sqrt{|bd|^4 + |ac|^4 + 2|abcd|^2 - 4\,\mathrm{Im}[ab(cd)^*]^2} \\ &\quad - (|bd|^2 + |ac|^2) \\ &= \sqrt{(|bd|^2 + |ac|^2)^2 - 4\,\mathrm{Im}[ab(cd)^*]^2} - (|bd|^2 + |ac|^2) \\ &\leqslant 0. \end{aligned}$$

Hence, $\mathcal{T}(\psi\psi^\dagger)$ is separable, as we set out to prove, so that $\mathcal{T}$ maps separable states to separable states.

From the previous discussion it also follows that states of the form $V\Lambda V^\dagger$ are separable if and only if the eigenvalues satisfy

$$\sqrt{(\lambda_1 - \lambda_3)^2 + (\lambda_2 - \lambda_4)^2} - \lambda_2 - \lambda_4 \leqslant 0. \tag{29}$$

Furthermore, states $V\Lambda V^\dagger$ are obviously invariant under $\mathcal{T}$. Hence, letting σ traverse all separable states of this form generates the same set of states $\mathcal{T}(\sigma)$ as letting σ traverse all separable states without restriction. Therefore,

$$\begin{aligned} E_R(\rho) &= \min_{\lambda \in D} S(\rho \| \sigma) \\ &\geqslant \min_{\sigma \in D} S(\rho \| \mathcal{T}(\sigma)) \\ &= \min_{\sigma = V\Lambda V^\dagger \in D} S(\rho \| \sigma). \end{aligned}$$

Comparing the first and the third lines, we immediately see that the inequality must be an equality.

Actually, an even stronger result holds, as we can restrict ourselves in this minimization to states $\sigma = V\Lambda V^\dagger \in D$ where the diagonal elements appear in descending order ($\lambda_1 \geqslant \lambda_2 \geqslant \lambda_3 \geqslant \lambda_4$). In other words, σ may be taken from the set of separable MEMS's. To see this, note that, as ρ and σ are both MEMS's,

$$S(\rho \| \sigma) = \sum_i p_i (\log p_i - \log \lambda_i),$$

where the p_i are the sorted eigenvalues of ρ, and λ_i are the not necessarily sorted eigenvalues of σ. It is easy to see that one always gets a lower relative entropy by permuting the λ_i into descending order [12]. This ends the proof of Lemma 4.

It is now easy to prove the last part of Theorem 1: Because the σ are restricted to separable MEMS's, this means that, for any global unitary U, $U\sigma U^\dagger$ is still separable. Hence,

$$\begin{aligned} E_R(\rho) &= \min_{\sigma \in D \cap \mathrm{MEMS}} S(\rho \| \sigma) \\ &= \min_{\sigma \in D \cap \mathrm{MEMS}} S(U\rho U^\dagger \| U\sigma U^\dagger) \\ &\geqslant \min_{U\sigma U^\dagger \in D} S(U\rho U^\dagger \| U\sigma U^\dagger) \\ &= E_R(U\rho U^\dagger), \end{aligned}$$

where the inequality arises because the minimization domain has been enlarged.

The explicit calculation of the relative entropy of entanglement of the maximally entangled mixed states is now a tedious but straightforward exercise, whose result is quoted in the theorem. This completes the proof of Theorem 1. □

Let us now analyze more closely this class of generalized Bell states. We already know that U is unique up to local unitary transformations. It is easy to check that the ordered

eigenvalues of the generalized Bell states for given entanglement of formation $f(C)$ are parametrized by two independent variables α and β:

$$0 \leqslant \alpha \leqslant 1,$$

$$\beta \geqslant \sqrt{1-\alpha^2/9} - \sqrt{\tfrac{8}{9}}\,\alpha,$$

$$\beta \leqslant \min\left(\sqrt{(1+C)/(1-C) - \alpha^2/9} - \sqrt{\tfrac{2}{9}}\,\alpha, \sqrt{3-\alpha^2} - \sqrt{2}\,\alpha\right),$$

$$\lambda_1 = 1 - \frac{1-C}{6}(3+\beta^2),$$

$$\lambda_2 = \frac{1-C}{6}(\alpha+\sqrt{2}\beta)^2,$$

$$\lambda_3 = \frac{1-C}{6}[3-(\sqrt{2}\alpha+\beta)^2],$$

$$\lambda_4 = \frac{1-C}{6}\alpha^2. \tag{30}$$

For a given EOF there is thus, up to local unitary transformations, a two-dimensional manifold of maximally entangled states. In the case of concurrence $C=1$ the upper and the lower bounds on β become equal and the unique pure Bell states arise. Another observation is the fact that λ_4 of all generalized Bell states is smaller then $\frac{1}{6}$. This implies that, if the smallest eigenvalue of any two-qubit state exceeds $\frac{1}{6}$, the state is separable.

A natural question is now how to characterize the entangled states closest to the maximally mixed state. A sensible metric is given by the Frobenius norm $\|\rho - \mathbb{1}\|_2 = \sqrt{\Sigma_i \lambda_i^2 - 1/4}$. This norm is dependent only on the eigenvalues of ρ and it is thus sufficient to consider the generalized Bell states at the boundary of entangled states where both the concurrence and the negativity become zero. This can be solved using the method of Lagrange multipliers. A straightforward calculation leads to a one-parameter family of solutions:

$$0 \leqslant x \leqslant \tfrac{1}{6},$$

$$\lambda_1 = \tfrac{1}{3} + \sqrt{x(\tfrac{1}{3}-x)}, \quad \lambda_2 = \tfrac{1}{3} - x,$$

$$\lambda_3 = \tfrac{1}{3} - \sqrt{x(\tfrac{1}{3}-x)}, \quad \lambda_4 = x. \tag{31}$$

The Frobenius norm $\|\rho - \mathbb{1}\|_2$ for all these states on the boundary of the sphere of separable states is given by the number $\sqrt{\frac{1}{12}}$. This criterion is exactly equivalent to the well-known criterion of Zyczkowski *et al.* [3]: $\mathrm{Tr}\rho^2 = \frac{1}{3}$. Here, however, we have the additional benefit of knowing exactly all the entangled states on this boundary as these are the generalized Bell states with eigenvalues given by Eq. (31). Furthermore, Zyczkowski *et al.* [3] proposed a lower bound on the volume of separable states by considering the ball of states that remain separable under all global unitary transformations. Clearly, the criterion $\Sigma_i \lambda_i^2 \leqslant \frac{1}{3}$ can be strengthened to $\lambda_1 - \lambda_3 - 2\sqrt{\lambda_2 \lambda_4} \leqslant 0$. Some tedious integration then leads to a better lower bound for the volume of separable states relative to the volume of all states: 0.3270 (as opposed to 0.3023 of [3]).

Further interesting properties of the maximally entangled mixed states include the fact that the states with maximal entropy for given entanglement all belong to this class. This will be reported elsewhere.

In conclusion, we have generalized the concept of pure Bell states to mixed states of two qubits. We have proved that the entanglement of formation, the negativity, and the relative entropy of entanglement of these generalized Bell states cannot be increased by applying any global unitary transformation. Whether their entanglement of distillation is also maximal is an interesting open problem.

We thank Lieven Vandersypen for bringing the problem to our attention, and J. Dehaene, L. De Lathauwer, K. Zyczkowski, and especially T. De Bie for valuable comments. This work was supported by the Flemish Government through the Research Council K. U. Leuven, Concerted Research Action Mefisto-666, FWO Projects No. G.0240.99 and No. G.0256.97 and Research Communities ICCoS and ANMMM and IWT Project EUREKA 2063-IMPACT and STWW. Financial support was also provided the Belgian State through Grants No. IUAP P4-02 and No. IUAP P4-2, and the Sustainable Mobility Program Project No. MD/01/24; by the European Commission through TMR Networks ALAPEDES and System Identification and the Brite/Euram Thematic Network NICONET; and by contract from ISMC, Data4S, Electrabel, Laborelec, Verhaert, and Europay.

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