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Maximally entangled mixed states of two qubits

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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. Two measures of entanglement are considered: entanglement of formation and negativity. Surprisingly all states that maximize one measure also maximize the other. We will give a complete characterization of these generalized Bell states and prove that these states for fixed eigenvalues are all equivalent under local unitary transformations. We will furthermore characterize all nearly entangled states closest to the maximally mixed state.

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In this letter 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, those latter restricted to pure states. 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 prove their conjecture and furthermore prove that the states they proposed are the only ones having the property of maximal entanglement.

Closely related to these generalized Bell states is the question of characterizing the set of separable density matrices [4], 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 byproduct this gives an alternative derivation of the well known result of Zyczkowski et al. [3] that all states for which the inequality $\mathrm{Tr}(\rho^2) \leq 1/3$ holds are separable.

The original motivation of this Letter was the following question: given a single quantum mechanical system consisting of two spin-1/2 systems, i.e. two qubits, in a given state, how can one maximize the entanglement of these qubits using only 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] and negativity [3] were chosen.

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

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

$$C(\rho) = \max(0, \sigma_1 - \sigma_2 - \sigma_3 - \sigma_4) \quad (2)$$

where $\{\sigma_i\}$ are the square roots of the eigenvalues of the matrix A

$$A = \rho S \rho^* S \quad (3)$$

$$S = \sigma_y \otimes \sigma_y. \quad (4)$$

Here $H(x)$ is Shannon's entropy function, the eigenvalues are arranged in decreasing order and σ_y is the Pauli matrix. It can be shown that $f(C)$ is convex and monotonously increasing. Using some elementary linear algebra it is furthermore easy to prove that the numbers $\{\sigma_i\}$ are equal to the singular values [7] of the matrix $\sqrt{\rho}^T S \sqrt{\rho}$. Here we use the notation $\sqrt{\rho} = \Phi \Lambda^{1/2}$ with $\Phi \Lambda \Phi^\dagger$ 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 [5]. 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 [6]. It turns out that the partial transpose of a non-separable state has one negative eigenvalue. From this, a measure for entanglement follows: the *negativity* of a state [3] is twice the absolute value of this negative eigenvalue:

$$E_N(\rho) = 2\max(0, -\lambda_4), \quad (5)$$

where λ_4 is the minimal eigenvalue of ρ^{T_A}.

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 non-ascending order. Then both the entanglement of formation and the *negativity are 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. The entanglement of formation and negativity of the new state $\rho' = U\rho U^\dagger$ are then given by

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

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

respectively.

The class of generalized Bell states is defined as the states ρ' thus obtained.

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

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

$$C_{\max} = \max_{U\in U(4)} (0, \sigma_1 - \sigma_2 - \sigma_3 - \sigma_4) \tag{6}$$

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

$$Q = \Lambda^{1/2}\Phi^T U^T S U \Phi \Lambda^{1/2}. \tag{7}$$

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

$$C_{max} \le \max_{V\in U(4)} (0, \sigma_1 - \sigma_2 - \sigma_3 - \sigma_4) \tag{8}$$

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 [7]. This factorization is not unique: left-multiplying S_1 with 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:

$$S_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 1 \\ 0 & -i & i & 0 \\ i & 0 & 0 & i \end{pmatrix}. \tag{9}$$

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

$$U = S_1^\dagger O V_1 \Phi^\dagger, \tag{10}$$

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 non-ascending order. The following inequality for singular values is well-known [8]:

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

$$\sum_{i=1}^k \sigma_i(AB) \le \sum_{i=1}^k \sigma_i(A)\sigma_i(B), \tag{11}$$

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

Less known is the following result by Wang and Xi [9]:

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

$$\sum_{t=1}^k \sigma_{i_t}(AB) \ge \sum_{t=1}^k \sigma_{i_t}(A)\sigma_{n-t+1}(B). \tag{12}$$

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:

$$\sigma_1(AB) - (\sigma_2(AB) + \sigma_3(AB) + \sigma_4(AB)) \le$$
$$\sigma_1(A)\sigma_1(B) - \sigma_2(A)\sigma_4(B) - \sigma_3(A)\sigma_3(B) - \sigma_4(A)\sigma_2(B)$$

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

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

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

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} \tag{13}$$

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

$$\max_{V\in U(4)} (\sigma_1 - (\sigma_2 + \sigma_3 + \sigma_4))(\Lambda^{1/2}V\Lambda^{1/2}) = \lambda_1 - (2\sqrt{\lambda_2\lambda_4} + \lambda_3). \tag{14}$$

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

$$V_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 0 & 1 & 0 \\ 0 & i/\sqrt{2} & 0 & -i/\sqrt{2} \end{pmatrix} \quad (15)$$

The optimal unitary operations U are thus all of the form: $U = S_1^\dagger O V_1 D_\phi^{1/2} \Phi^\dagger$ 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 :

$$SU(2) \otimes SU(2) \cong SO(4). \quad (16)$$

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 $\{U_1, U_2\} \in SU(2)$. 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 $Q \in SO(4)$ 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 an orthogonal matrix 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 $U_1, U_2 \in SU(2)$ and $D_{\phi'}$ unitary diagonal, such that $U = S_1^\dagger O V_1 D_\phi \Phi^\dagger = (U_1 \otimes U_2) S_1^\dagger V_1 D_{\phi'} \Phi^\dagger$.

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

$$(U_1 \otimes U_2) \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} D_\phi \Phi^\dagger. \quad (17)$$

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

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

$$\begin{aligned} \lambda_{min}(\rho^{T_A}) &= \min_{x:||x||=1} \operatorname{Tr} \rho^{T_A} |x\rangle\langle x| \\ &= \min_{x:||x||=1} \operatorname{Tr} \rho (|x\rangle\langle x|)^{T_A} \end{aligned} \quad (18)$$

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 $P_0 = \sum_{ij} e^{ij} \otimes e^{ji}$, the partial transpose can be written as follows:

$$(|x\rangle\langle x|)^{T_A} = P_0(\tilde{x} \otimes \tilde{x}^\dagger). \quad (19)$$

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

$$\tilde{x} = U_1 \Sigma U_2^\dagger, \quad (20)$$

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

$$(|x\rangle\langle x|)^{T_A} = P_0(U_1 \otimes U_2)(\Sigma \otimes \Sigma)(U_2 \otimes U_1)^\dagger. \quad (21)$$

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:

$$(|x\rangle\langle x|)^{T_A} = V(x) D(\alpha(x)) V(x)^\dagger \quad (22)$$

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

$$V(x) = (U_1(x) \otimes U_2(x)) \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1/\sqrt{2} & 0 & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (23)$$

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:

$$\begin{aligned} &\min_{U,x} \operatorname{Tr} U\Phi\Lambda\Phi^\dagger U^\dagger V(x) D(\alpha(x)) V(x)^\dagger \\ &\qquad = \min_\alpha \min_W \operatorname{Tr} \Lambda W^\dagger D(\alpha) W, \end{aligned} \quad (24)$$

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

$$\begin{aligned} g(\alpha) &= \operatorname{Tr} \Lambda W^\dagger D(\alpha) W \\ &= \sum_{i,j} d_j(\alpha) |W_{ji}|^2 \lambda_i \\ &= d(\alpha)^T J(W) \lambda, \end{aligned} \quad (25)$$

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 [7], which says that the set of doubly-stochastic matrices is the convex closure of the set of permutation matrices, and also of 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

$$J_0 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \qquad (26)$$

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 $\sum_{j=1}^4 \lambda_j d_{4+1-j}(\alpha)$. Minimizing over α gives, after a few basic calculations:

$$\cos(2\alpha) = \frac{\lambda_2 - \lambda_4}{\sqrt{(\lambda_1-\lambda_3)^2 + (\lambda_2-\lambda_4)^2}}$$
$$g(\alpha) = \left(\lambda_2 + \lambda_4 - \sqrt{(\lambda_1-\lambda_3)^2 + (\lambda_2-\lambda_4)^2}\right)/2.$$

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 $U = V(x)J_0 D_\phi \Phi^\dagger$:

$$U = (U_1 \otimes U_2) \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1/\sqrt{2} & 0 & 1/\sqrt{2} & 0 \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix} D_\phi \Phi^\dagger \qquad (27)$$

This is exactly the same U as in the case of entanglement of formation. This completes the proof of the Theorem. □

Let us now analyze more closely the newly defined 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 parameterized by two independent variables α and β:

$$\begin{aligned}
&0 \le \alpha \le 1 \\
&\beta \ge \sqrt{1-\frac{\alpha^2}{9}} - \sqrt{\frac{8}{9}}\alpha \\
&\beta \le \min\left(\sqrt{\frac{1+C}{1-C} - \frac{\alpha^2}{9}} - \sqrt{\frac{2}{9}}\alpha, \sqrt{3-\alpha^2} - \sqrt{2}\alpha\right) \\
&\lambda_1 = 1 - \frac{1-C}{6}(3+\beta^2) \\
&\lambda_2 = \frac{1-C}{6}(\alpha + \sqrt{2}\beta)^2 \\
&\lambda_3 = \frac{1-C}{6}(3 - (\sqrt{2}\alpha + \beta)^2) \\
&\lambda_4 = \frac{1-C}{6}\alpha^2
\end{aligned} \qquad (28)$$

For 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 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 $1/6$. This implies that if the smallest eigenvalue of whatever two-qubit state exceeds $1/6$, this state is separable.

A natural question is now to characterize the entangled states closest to the maximally mixed state. A sensible metric is given by the Frobenius norm $||\rho - \mathbb{1}|| = \sqrt{\sum_i \lambda_i^2 - 1/4}$. This norm is only dependent on the eigenvalues of ρ and it is thus sufficient to consider the generalized Bell states at the boundary 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:

$$\begin{aligned}
&0 \le x \le \frac{1}{6} \\
&\lambda_1 = \frac{1}{3} + \sqrt{x\left(\frac{1}{3} - x\right)} \qquad \lambda_2 = \frac{1}{3} - x \\
&\lambda_3 = \frac{1}{3} - \sqrt{x\left(\frac{1}{3} - x\right)} \qquad \lambda_4 = x
\end{aligned} \qquad (29)$$

The Frobenius norm $||\rho - \mathbb{1}||$ for all these states on the boundary of the sphere of separable states is given by the number $\sqrt{1/12}$. This criterion is exactly equivalent to the well-known criterion of Zyczkowski et al. [3]: $\mathrm{Tr}\,\rho^2 = 1/3$. 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 the previous formula.

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

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