On the fidelity of mixed states of two qubits.

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We consider a single copy of a mixed state of two qubits and show how its fidelity or maximal singlet fraction is related to the entanglement measures concurrence and negativity. We characterize the extreme points of the convex set of states with constant fidelity, and use this to prove tight lower and upper bounds on the fidelity for a given amount of entanglement.

The concept of fidelity [1], also called maximal singlet fraction [2], is of central importance in the field of quantum information theory. It is defined as as the maximal overlap of the state with a maximally entangled state (ME)

$$F(\rho) = \max_{|\psi\rangle=\mathrm{ME}} \langle\psi|\rho|\psi\rangle. \quad (1)$$

An explicit value for the fidelity has been derived by Horodecki [3]. If one considers the real 3×3 matrix $\tilde{R} = \mathrm{Tr}\,(\rho\sigma_i \otimes \sigma_j)$ with $\{\sigma_i, i = 1..3\}$ the Pauli matrices, then

$$F(\rho) = \frac{1+\lambda_1+\lambda_2-\mathrm{Sgn}(\det(\tilde{R}))\lambda_3}{4}$$

with $\{\lambda_i\}$ the ordered singular values of $\tilde{R}$ and $\mathrm{Sgn}(\det(\tilde{R}))$ the sign of the determinant of $\tilde{R}$.

The concept of fidelity appears in the context of entanglement distillation [1, 4] where it quantifies how close a state is to a maximally entangled one, and in the context of teleportation [5] where it quantifies the quality of the teleportation that can be achieved with the given state. Due to the linearity and the convexity of the definition (1), this measure has very nice properties that make it also possible to derive upper bounds for the entanglement of distillation [6].

Despite the importance of the concept of fidelity, no rigorous comparison appears to have been made before between the value of the fidelity on one side and entanglement measures on the other side. This paper aims at filling this gap and gives explicit tight lower and upper bounds of the fidelity for given concurrence [7] and negativity [8].

At first we will explicitly derive the possible range of values of the fidelity in function of its concurrence [7] or entanglement of formation. Next we show that the states that minimize (maximize) the fidelity for given values of the entanglement of formation are also extremal for given negativity [8]. Following [9, 10], we use the following definition of negativity:

$$N(\rho) = \max\left(0, -2\lambda_{\min}(\rho^{\Gamma})\right)$$

with $\lambda_{\min}$ the minimal eigenvalue of the partial transpose of ρ denoted as ρ^{Γ}.

Theorem 1 *Given a mixed state of two qubits ρ with negativity equal to N and concurrence equal to C, then its fidelity F is bounded above by*

$$F \leq \frac{1+N}{2} \leq \frac{1+C}{2}.$$

Moreover, the first inequality becomes an equality iff $N = C$, and this condition is equivalent to the condition that the eigenvector corresponding to the negative eigenvalue of the partial transpose of ρ is maximally entangled.

Proof: The fidelity of a state ρ is given by

$$\max_{U_A,U_B\in SU(2)} \mathrm{Tr}\left((U_A\otimes U_B)|\psi\rangle\langle\psi|(U_A\otimes U_B)^{\dagger}\rho\right) =$$

$$\frac{1}{2}\max_{U_A,U_B} \mathrm{Tr}\left(\left(\begin{array}{cccc}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{array}\right)(U_A\otimes U_B^*)^{\dagger}\rho^{\Gamma}(U_A\otimes U_B^*)\right)$$

with $|\psi\rangle = (|00\rangle+|11\rangle)/\sqrt{2}$. An upper bound is readily obtained by extending the maximization over all unitaries instead of all local unitaries, and it follows that $F \leq \mathrm{Tr}\left(\rho^{\Gamma}\right) = (1+N)/2$. Equality is achieved iff the eigenvector of $\rho^{T_{\Gamma}}$ corresponding to the negative eigenvalue is maximally entangled. As shown in [10], this condition is exactly equivalent to the condition for N to reach its upper bound C, which ends the proof. □

Note that the upper bound is achieved for all pure states.

A more delicate and technical reasoning is needed to obtain a tight lower bound on the fidelity. We will need the following lemma:

Lemma 1 *Consider the density operator ρ and the real 3×3 matrix $\tilde{R}$ with coefficients $\tilde{R}_{ij} = \mathrm{Tr}\,(\rho\sigma_i\otimes\sigma_j)$ with $1 \leq i,j \leq 3$. Then ρ is as a convex sum (i.e. mixture) of rank 2 density operators all having exactly the same coefficients $\tilde{R}_{ij}$.*

Proof: Consider the real 4×4 matrix R with coefficients $R_{\alpha\beta} = \mathrm{Tr}\left(\rho \sigma_\alpha \otimes \sigma_\beta\right)$, parameterized as

$$R = \begin{pmatrix} 1 & x_1 \; x_2 \; x_3 \\ y_1 & \\ y_2 & \tilde{R} \\ y_3 & \end{pmatrix}.$$

If ρ is full rank, then a small perturbation on the values $\{x_i\}, \{y_i\}$ will still yield a full rank density operator. Consider a perturbation on $x_1' = x_1 + \epsilon$ and the corresponding ρ'. As the set of density operators is compact, there will exist a lower bound $lb < 0$ and an upper bound $ub > 0$ such that ρ' is positive iff $lb < \epsilon < ub$. Call ρ_{lb}, ρ_{ub} the rank three density operator obtained when $\epsilon = lb$ and $\epsilon = ub$ respectively. It is easy to see that $\rho = (ub\rho_{lb} + lb\rho_{ub})/(lb + ub)$, such that it is proven that a rank four density operator can always be written as a convex sum of two rank three density operators with the same corresponding $\tilde{R}$.

Consider now ρ rank three and its associated "square root" $\rho = XX^\dagger$ with X a 4×3 matrix. A small perturbation of the form $\rho' = \rho + \epsilon XQX^\dagger$, with Q an arbitrary hermitian 3×3 matrix $Q = \sum_{i=1}^{9} q_i G_i$ and G_i generators of U(3), will still yield a state of rank three. Moreover, there always exists a non-trivial Q such that $\tilde{R}$ is left unchanged by this perturbation. This is indeed the case if the following set of equations is fulfilled:

$$\sum_i q_i \mathrm{Tr}\left(G_i X^\dagger (\sigma_\alpha \otimes \sigma_\beta) X\right) = 0$$

for $(\alpha, \beta) = (0, 0)$ and $\alpha, \beta \geq 1$. It can easily be verified that this set of 10 equations only contains at most 8 independent ones irrespective of the 4×3 matrix X , and as Q has nine independent parameters there always exists at least one non-trivial solution to this set of homogeneous equations. A similar reasoning as in the full rank case then implies that one can always tune ϵ such that ρ can be written as a convex sum of two rank two density operators with the same $\tilde{R}$, which concludes the proof. $\square$

This lemma is interesting if one wants to maximize a convex measure of a density operator (such as the entropy or an entanglement monotone) under the constraint that the fidelity is fixed: indeed, the fidelity is only a function of $\tilde{R}$, and by the previous lemma we immediately know that states with maximal entropy for given fidelity will have rank two. Note that exactly the same reasoning applies when one wants to maximize a convex measure under the constraint that the CHSH Bell-violation is fixed [8], as this CHSH Bell-violation is also solely a function of $\tilde{R}$. This is in exact correspondence with the results derived in [8], where it was proven that the states exhibiting the minimal amount of Bell violation for given entanglement of formation are rank 2.

We are now ready to prove a tight lower bound on the fidelity:

Theorem 2 *Given a mixed state of two qubits ρ with concurrence equal to C, then a tight lower bound for its fidelity F is given by:*

$$F \geq \max\left(\frac{1+C}{4}, C\right).$$

Proof: A direct consequence of lemma (1) is that to find states with minimal fidelity for given concurrence (i.e. maximal concurrence for given fidelity), it is sufficient to look at states of rank two. Consider therefore a rank 2 state ρ and associated to it the real 4×4 matrix R with coefficients $R_{\alpha\beta} = \mathrm{Tr}\left(\sigma_\alpha \otimes \sigma_\beta \rho\right)$. As shown in [8, 10, 11, 12], if R is multiplied right and left by proper orthochronous Lorentz transformations leaving the $(0,0)$-element equal to 1, then a new state is obtained with the same concurrence. Moreover the fidelity of a state ρ is variationally defined as

$$F(\rho) = \min_{O_A, O_B \in SO(3)} \mathrm{Tr}\left(M \begin{pmatrix} 1 & 0 \\ 0 & O_A \end{pmatrix} R \begin{pmatrix} 1 & 0 \\ 0 & O_B^T \end{pmatrix}\right)$$

with $M = \mathrm{diag}(1, -1, -1, -1)$ (M is the representation of the singlet in the R-picture). The minimal fidelity for given concurrence can therefore be obtained by minimizing the following constrained cost-function over all proper orthochronous Lorentz transformations L_1, L_2:

$$K = \mathrm{Tr}\left(M L_1 R L_2^T\right) - \lambda \mathrm{Tr}\left(L_1 R L_2^T \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}\right).$$

Note that λ is a Lagrange constraint. Without loss of generality we can assume that the lower 3×3 block $\tilde{R}$ of R is diagonal and of the form $\tilde{R} = \mathrm{diag}(-|s_1|, -|s_2|, -s_3)$ with $|s_1| \geq |s_2| \geq |s_3|$, as this is precisely the form needed for maximizing the fidelity over all local unitary operations. The cost-function K can be differentiated over L_1, L_2 by introducing the generators of the Lorentz group (see e.g.[8]), and this immediately yields the optimality conditions $(\lambda = 0, MRM = R^T)$ or $(\lambda = 2, R = R^T)$. Note however that the above argument breaks down in the case that $|s_2| = -s_3$. Indeed, the fidelity cannot be differentiated in this case as for example a perturbation of s_3 of the form $s_3' = s_3 + \epsilon$ always leads to a perturbation of the fidelity $F' = F + |\epsilon|$. In this case the conditions $x_2 = y_2, x_3 = y_3$ or $x_2 = -y_2, x_3 = -y_3$ vanish, and if also $|s_1| = |s_2| = -s_3$ there are no optimality conditions on $\{x_i, y_i\}$ left.

Let us first treat the case with R symmetric and $s_1 \geq s_2 \geq |s_3|$:

$$R = \begin{pmatrix} 1 & x_1 & x_2 & x_3 \\ x_1 & -s_1 & 0 & 0 \\ x_2 & 0 & -s_2 & 0 \\ x_3 & 0 & 0 & -s_3 \end{pmatrix}.$$

The condition that ρ corresponding to this state is rank 2 implies that all 3×3 minors of ρ are equal to zero. Due to the conditions $s_1 \geq s_2 \geq |s_3|$, it can easily be shown that a state of rank 2 (and not of rank 1!) is obtained iff $x_1 = 0 = x_2$ and $x_3 = \pm\sqrt{(1-s_1)(1-s_2)}$ and $1 - s_1 - s_2 + s_3 = 0$. In this case the concurrence is equal to $C = s_2$ and the fidelity is given by $F = (s_1 + s_2)/2$, and the constraints become $1 \geq s_1 \geq s_2 \geq (1-s_1)/2$ what implies that $C \geq 1/3$. The minimal fidelity for given concurrence occurs when $s_1 = s_2$ and then $C = F$ which gives the lower bound of the theorem in the case of $C \geq 1/3$.

Let us now consider the case where $R = MR^TM$:

$$R = \begin{pmatrix} 1 & x_1 & x_2 & x_3 \\ -x_1 & -s_1 & 0 & 0 \\ -x_2 & 0 & -s_2 & 0 \\ -x_3 & 0 & 0 & -s_3 \end{pmatrix}$$

with again $s_1 \geq s_2 \geq |s_3|$. Let us first note that, due to the symmetry, R has a Lorentz singular value decomposition [11] of the form $R = L_1\Sigma\tilde{M}ML_1^TM$ with Σ of the form $\mathrm{diag}(|\sigma_0|, -|\sigma_1|, -|\sigma_2|, -|\sigma_3|)$ and $\tilde{M}$ of the form $\mathrm{diag}(1,1,1,1)$ or $\mathrm{diag}(1,-1,-1,1)$ or $\mathrm{diag}(1,-1,1,-1)$ or $\mathrm{diag}(1,1,-1,-1)$. It follows that $\mathrm{Tr}\,(R) = \mathrm{Tr}\left(\Sigma\tilde{M}\right)$, and due to the ordering of the Lorentz singular values, $\tilde{M}$ has to be equal to the identity if $\mathrm{Tr}\,(R) \leq 0$. But $\mathrm{Tr}\,(\Sigma)$ is just $-2C$ with C the concurrence of the state, and $\mathrm{Tr}\,(R) = 2 - 4F$ with F the fidelity of the state. Therefore it holds that $F = (1+C)/2$ if $\mathrm{Tr}\,(R) \leq 0$ which corresponds to the upper bound of the fidelity. Therefore only the case where $\mathrm{Tr}\,(R) > 0$ has to be considered for finding lower bounds of the fidelity. The condition that the state be rank 2 (and not rank 1) immediately yields: $x_3 = 0$, $s_1 + s_2 - s_3 = 1$ and $s_1 + s_2 = x_1^2/(1-s_2) + x_2^2/(1-s_1)$. If we only consider the case with $\mathrm{Tr}\,(R) > 0$, it holds that $s_3 < 0$ and the inequality constraints become $(1-s_1)/2 \leq s_2 \leq (1-s_1) \leq 2/3$. The concurrence can again be calculated analytically and is given by $C = (1-s_1-s_2-s_3)/2$, and it follows that $F = (1-C)/2$. Note that the inequality constraints limit C to be in the interval $C \in \{0, 1/3\}$, and so this bound is less stringent then the one stated in the theorem.

Let us now move to the degenerate case where $s_1 > s_2 = -s_3$:

$$R = \begin{pmatrix} 1 & x_1 & x_2 & x_3 \\ y_1 & -s_1 & 0 & 0 \\ y_2 & 0 & -s_2 & 0 \\ y_3 & 0 & 0 & s_2 \end{pmatrix}.$$

As $s_1 > s_2$, optimality requires $x_1 = \pm y_1$. We first treat the case $x_1 = y_1$. Defining $\alpha = x_3/y_3$, a set of necessary and sufficient conditions for being rank 2 is given by:

$$\begin{aligned} 0 &= x_1 = y_1 \\ 0 &= x_2 + \alpha y_2 \\ 0 &= \alpha^2 - \alpha\frac{1-s_1}{s_2} + 1 \\ 0 &= (x_2^2 + x_3^2) - \alpha s_2(1+s_1). \end{aligned}$$

Under these conditions the concurrence can again be calculated exactly and is given by $C = s_2$, while the fidelity is given by $F = (1+s_1)/4$. Note that the above set of equations only has a solution if $(1-s_1)/2 \geq s_2$, implying that $C \leq 1/3$. The fidelity will now be minimal when $s_2 = s_1$, and then $F = (1+C)/4$ which is the second bound stated in the theorem.

Let us now consider the degenerate case with $s_1 > s_2 = -s_3$ but $x_1 = -y_1$. The rank 2 condition implies that $s_1 + 2s_2 = 1$ and $x_2 = -y_2$ and $x_3 = y_3$. Some straightforward algebra leads to the condition

$$4\frac{1-s_1}{1+s_1}x_1^2 + 1 - s_1^2 - 2x_2^2 - 2x_3^2 = 0.$$

Taking into account the constraints, the concurrence is again given by $C = s_2 = (1-s_1)/2$ and bounded above by $1/3$, while the fidelity if equal to $F = (1+s_1)/4 = (1-C)/2$. This bound always exceeds the previously derived bound $F \geq (1+C)/4$ for $C \leq 1/3$, and is therefore useless.

It only remains to consider the case where $s_1 = s_2 = -s_3$:

$$R = \begin{pmatrix} 1 & x_1 & x_2 & x_3 \\ y_1 & -s_1 & 0 & 0 \\ y_2 & 0 & -s_1 & 0 \\ y_3 & 0 & 0 & s_1 \end{pmatrix}.$$

Defining $\alpha = x_1/y_1$, the rank 2 constraint leads to the following set of necessary and sufficient conditions:

$$\begin{aligned} 0 &= x_2 - \alpha y_2 \\ 0 &= x_3 + \alpha y_3 \\ 0 &= s_1\alpha^2 + \alpha(1-s_1) + s_1 \\ 0 &= \alpha(x_1^2 + x_2^2 + x_3^2) + s_1(1+s_1). \end{aligned}$$

The inequality constraint reads $s_1 \leq 1/3$, and the concurrence can again be calculated exactly and is given by $C = s_1$. Therefore the fidelity of these states obeys the relation $F = (1+C)/4$ for $C \leq 1/3$, which is the sharp lower bound. $\square$

It might be interesting to note that all rank 2 states minimizing the fidelity for given concurrence are quasi-distillable [2, 11] and have one separable and one entangled eigenvector. More specifically, the states minimizing the fidelity for $C \leq 1/3$ are, up to local unitaries, of the form

$$\rho = \begin{pmatrix} \frac{1+C}{2} & 0 & 0 & 0 \\ 0 & \frac{1-C+\sqrt{1-2C-3C^2}}{4} & -\frac{C}{2} & 0 \\ 0 & -\frac{C}{2} & \frac{1-C-\sqrt{1-2C-3C^2}}{4} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix},$$

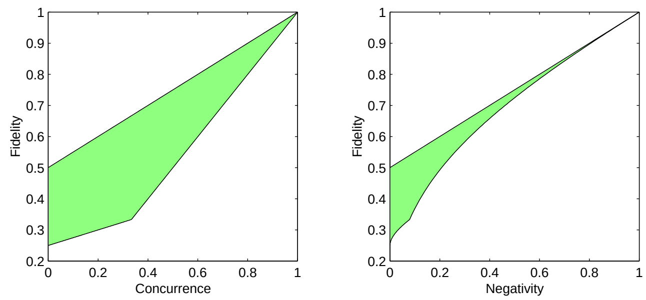

FIG. 1: Range of values of the fidelity for given concurrence and negativity.

and those for $C \geq 1/3$ of the form

$$\rho = \begin{pmatrix} 1-C & 0 & 0 & 0 \\ 0 & C/2 & -C/2 & 0 \\ 0 & -C/2 & C/2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Exactly the same states also minimize the fidelity for given negativity. This leads to the following sharp bounds for the fidelity versus negativity:

$$\begin{aligned} F &\geq \frac{1}{4} + \frac{1}{8}\left(N + \sqrt{5N^2 + 4N}\right) \\ F &\geq \sqrt{2N(N+1)} - N \\ F &\leq \frac{1+N}{2}. \end{aligned}$$

The first condition applies when $N \leq (\sqrt{5}-2)/3$ and the second when $N \geq (\sqrt{5}-2)/3$. A plot of these bounds is given in figure (1). One observes that the difference between the lower bound and the upper bound in terms of the negativity becomes very small ($\simeq \epsilon^2/16$) for large negativity $N = 1 - \epsilon$. Moreover the fidelity is always larger then $1/2$ if the negativity exceeds $(\sqrt{2}-1)/2$.

In conclusion, we derived a tight upper bound for the fidelity for given value of the concurrence and fidelity, and we identified all states for which this upper bound is saturated. Next we have characterized the extreme points of the convex set of states with given fidelity, and this enabled us to derive tight lower bounds on the fidelity for given amount of entanglement.

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