Maximally entangled mixed states under nonlocal unitary operations in two qubits

Satoshi Ishizaka * and Tohya Hiroshima†

Fundamental Research Laboratories, System Devices and Fundamental Research, NEC Corporation, 34 Miyukigaoka, Tsukuba, Ibaraki 305-8501, Japan

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We propose mixed states in two qubits that have a property that the amount of entanglement of these states cannot be increased by any unitary transformation. The property is proven when the rank of the states is less than 4, and confirmed numerically in the other general cases. The corresponding entanglement of formation specified by its eigenvalues gives an upper bound of that for density matrices with the same eigenvalues. Further, as a simple application of the upper bound of the entanglement of formation, we analyze the entanglement of formation of the state generated by a decohered controlled-NOT gate in the spin-boson model.

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Entanglement (or inseparability) is one of the most striking features of quantum mechanics and an important resource for most applications of quantum information. In quantum computers, the quantum information stored in quantum bits (qubits) is processed by operating quantum gates. Multibit quantum gates, such as the controlled-NOT gate, are particularly important, since these gates can create entanglement between qubits.

In recent years, quantification of the amount of entanglement has attracted much attention, and a number of measures, such as the entanglement of formation [1], negativity [2,3], and relative entropy of entanglement [4], have been proposed. When the system of the qubits is in a pure state, the amount of entanglement can be changed through the gate operations from zero in separable states to unity in maximally entangled states. Most of the quantum algorithms are designed for such ideal pure states. When the system is maximally mixed, however, we cannot receive any benefit from entanglement in the quantum computation, since the density matrix of the system (unit matrix) is invariantly separable under any unitary transformation or gate operations. Recently, a question about NMR quantum computation has been proposed [5], since the states in the vicinity of the maximally mixed state are also always separable, as is the case of the present NMR experiments.

In all realistic systems, the mixture of the density matrix describing the qubits is inevitably increased by the coupling between the qubits and its surrounding environment. Therefore, it is extremely important to understand the nature of entanglement for general mixed states between two extremes of pure states and a maximally mixed state.

In this paper, we try to answer a simple question of how much the increase of the mixture limits the amount of entanglement to be generated by the gate operation, or equivalently, by unitary transformation. To this end, we propose a class of mixed states in bipartite 2×2 systems (two qubits). The states in this class show a property of having a maximum amount of entanglement in the sense that the entanglement of formation (and even negativity) of these states cannot be increased by any (local or nonlocal) unitary transformation. The property is rigorously proven in the case in which the rank of the states is less than 4, and confirmed numerically in the case of rank 4. The corresponding entanglement of formation specified by its eigenvalues gives an upper bound of that for density matrices with the same eigenvalues.

The entanglement of formation (EOF) [1] for a pure state is defined as the von Neumann entropy of the reduced density matrix. The EOF of a mixed state is defined as $E_F(\rho) = \min \Sigma_i p_i E_F(\psi)$, where the minimum is taken over all possible decompositions of ρ into pure states $\rho = \Sigma_i p_i |\psi_i\rangle\langle\psi_i|$. The analytical form for EOF in 2×2 systems is given by [6]

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

with $H(x)$ being Shannon's entropy function. The concurrence C is given by

$$C = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\}, \tag{2}$$

where λ's are the square root of eigenvalues of $\rho\tilde{\rho}$ in decreasing order. The spin-flipped density matrix $\tilde{\rho}$ is defined as

$$\tilde{\rho} = \sigma_y^A \otimes \sigma_y^B \rho^* \sigma_y^A \otimes \sigma_y^B, \tag{3}$$

where * denotes the complex conjugate in the computational basis. Since E_F is a monotonic function of C, the maximum of C corresponds to the maximum of E_F.

The states we propose are those obtained by applying any *local* unitary transformation to

$$M = p_1|\Psi^-\rangle\langle\Psi^-| + p_2|00\rangle\langle00| + p_3|\Psi^+\rangle\langle\Psi^+| + p_4|11\rangle\langle11|, \tag{4}$$

where $|\Psi^\pm\rangle = (|01\rangle \pm |10\rangle)/\sqrt{2}$ are Bell states, and $|00\rangle$ and $|11\rangle$ are product states orthogonal to $|\Psi^\pm\rangle$. Here, p_i's are eigenvalues of M in decreasing order ($p_1 \geqslant p_2 \geqslant p_3 \geqslant p_4$), and $p_1+p_2+p_3+p_4=1$. These include states such as

*Email address: isizaka@frl.cl.nec.co.jp

†Email address: tohya@frl.cl.nec.co.jp

$$\rho = p_1|\Phi^-\rangle\langle\Phi^-| + p_2|01\rangle\langle 01| + p_3|\Phi^+\rangle\langle\Phi^+| + p_4|10\rangle\langle 10|, \tag{5}$$

where $|\Phi^\pm\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}$ are also Bell states, and include those that are obtained by exchanging $|\Psi^-\rangle \leftrightarrow |\Psi^+\rangle$, $|00\rangle \leftrightarrow |11\rangle$ in Eq. (4), or $|\Phi^-\rangle \leftrightarrow |\Phi^+\rangle$, $|01\rangle \leftrightarrow |10\rangle$ in Eq. (5). Since entanglement is preserved by local unitary transformation, all these states have the same concurrence of

$$C^* = \max\{0, C^*(p_i)\},$$
$$C^*(p_i) \equiv p_1 - p_3 - 2\sqrt{p_2 p_4}. \tag{6}$$

The concurrence C^* is maximum among density matrices with the same eigenvalues, at least when the density matrices have a rank less than 4 $(p_4 = 0)$. The proof is as follows:

(1) Rank 1 case $(p_2 = p_3 = p_4 = 0)$. In this case, Eq. (4) is reduced to $M = |\Psi^-\rangle\langle\Psi^-|$, which obviously has the maximum concurrence of unity.

(2) Rank 2 case $(p_3 = p_4 = 0)$. Any density matrices of two qubits (not necessarily rank 2) can be expressed as [7]

$$\rho = q|\psi\rangle\langle\psi| + (1-q)\rho_{\text{sep}}, \tag{7}$$

where $|\psi\rangle$ is an entangled state and ρ_{sep} is a separable density matrix. The convexity of the concurrence [8] implies that

$$C(\rho) \leqslant qC(|\psi\rangle\langle\psi|) + (1-q)C(\rho_{\text{sep}}) = qC(|\psi\rangle\langle\psi|). \tag{8}$$

Since ρ_{sep} is a positive operator, q is equal to or less than the maximum eigenvalue of ρ, and thus

$$C(\rho) \leqslant p_1. \tag{9}$$

The equality is satisfied when $|\psi\rangle$ is a maximally entangled *pure* state and an eigenvector of ρ with the eigenvalue of p_1. The upper bound in Eq. (9) coincides with C^* for $p_3 = p_4 = 0$.

(3) Rank 3 case $(p_4 = 0)$. Any rank 3 density matrices can be decomposed into two density matrices by simply decomposing their eigenvalues as

$$\rho = (1 - 3p_3)\rho_2 + 3p_3\rho_3, \tag{10}$$

where the eigenvalues of ρ_2 are

$$\left\{\frac{p_1 - p_3}{1 - 3p_3}, \frac{p_2 - p_3}{1 - 3p_3}, 0, 0\right\}, \tag{11}$$

and eigenvalues of ρ_3 are $\{1/3, 1/3, 1/3, 0\}$. According to Lemma 3 in Ref. [3],

$$\operatorname{Tr}\rho^2 \leqslant \frac{1}{3} \Rightarrow \rho \text{ is separable.} \tag{12}$$

Since the purity of ρ_3 is 1/3, ρ_3 is always separable. Therefore, convexity of the concurrence implies that

$$C(\rho) \leqslant (1 - 3p_3)C(\rho_2) \leqslant p_1 - p_3. \tag{13}$$

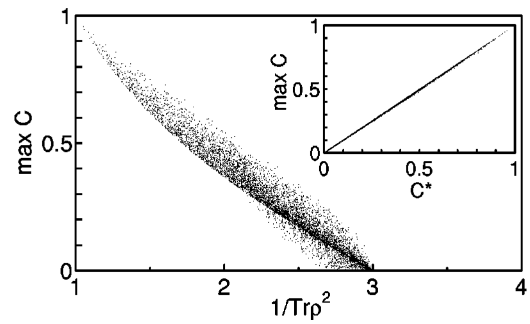

FIG. 1. Numerically obtained maximum concurrence for random density matrices as a function of the participation ratio and C^* (inset).

Here, we have used that, as shown above, the maximum concurrence of rank 2 density matrices is its maximum eigenvalue. The upper bound in Eq. (13) again coincides with C^* for $p_4 = 0$.

In order to check whether C^* is maximum, even in general $p_4 \neq 0$ cases, we have performed a numerical calculation whose scheme is similar to that in Refs. [9,3,10]. We have generated 10 000 density matrices in a diagonal form with four random eigenvalues distributed uniformly [3]. The maximum concurrence has been obtained among 1 000 000 density matrices generated by multiplying random unitary matrices in the circular unitary ensemble [11] to each of 10 000 diagonal matrices. The results are shown in Fig. 1 where the maximum concurrence is plotted as a function of the participation ratio $(R = 1/\operatorname{Tr}\rho^2)$.

When the density matrix is close to the pure state $(R = 1)$, the maximum concurrence is also close to unity, as expected. For $R \geqslant 3$, the states are always separable [Eq. (12)] and the maximum is zero. In the region of $1 < R < 3$, the maximum tends to decrease with an increase of R, but the points are rather broadly distributed. The same data are plotted as a function of C^* in the inset of Fig. 1. All points are very closely distributed along the straight line of $C = C^*$, and none of the points are present on the higher side of the line. This numerical result strongly supports the hypothesis that C^* gives an upper bound of the concurrence, even in the general cases of $p_4 \neq 0$.

Accepting the hypothesis implies that all the states satisfying $C^*(p_i) \leqslant 0$ become automatically separable. This condition of separability is looser than Eq. (12). In fact, $C^*(p_i) \leqslant 0$ is only a necessary condition of $\operatorname{Tr}\rho^2 \leqslant 1/3$. The difficulty with the rigorous proof of the hypothesis, if it is true, might relate to the difficulty in completely understanding the separable-inseparable boundary in the 15-dimensional space of the density matrices due to its complex structure. We emphasize again that the numerical result strongly supports the truth of the hypothesis.

It should be noted here that, when the eigenvalues of a density matrix satisfy a relation, C^* is indeed maximum, even for $p_4 \neq 0$. The rank 4 density matrices satisfying $C(p_i) \geqslant 0$ are decomposed as

$$\rho = (p_1 - p_3 - 2\sqrt{p_2 p_4})|1\rangle\langle 1| + \rho_4, \tag{14}$$

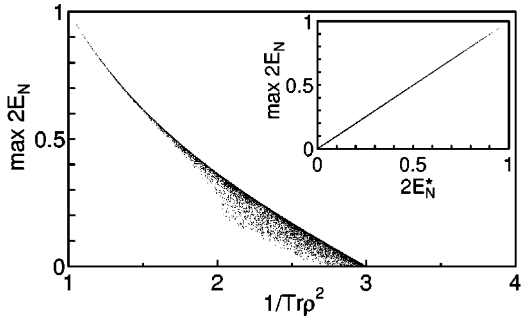

FIG. 2. The same as Fig. 1, but negativity is plotted.

where $|1\rangle$ is an eigenvector of ρ, and the eigenvalues of ρ_4 (not normalized) are $\{p_3+2\sqrt{p_2p_4},p_2,p_3,p_4\}$. When the eigenvalues of ρ satisfy

$$p_3=p_2+p_4-\sqrt{p_2p_4},\tag{15}$$

the purity of (normalized) ρ_4 is equal to 1/3 and ρ_4 becomes always separable. Therefore, using the convexity of the concurrence again, the upper bound of the concurrence is proven to be C^* for density matrices satisfying Eq. (15) (and $p_1-p_3-2\sqrt{p_2p_4}\geqslant 0$). When $p_2=p_3=p_4(\leqslant 1/4)$, M is reduced to the Werner state [12]:

$$M=p_1|\Psi^-\rangle\langle\Psi^-|+\frac{1-p_1}{3}(|\Psi^+\rangle\langle\Psi^+|+|\Phi^-\rangle\langle\Phi^-| +|\Phi^+\rangle\langle\Phi^+|),\tag{16}$$

whose eigenvalues satisfy Eq. (15). Therefore, it was proven that the EOF of the Werner state cannot be increased by any unitary transformation.

It is worth testing whether the states we propose have maximum entanglement in the other entanglement measures. It has been shown that a positive partial transpose is a necessary condition for separability [2], and that it is also a sufficient condition for 2×2 and 2×3 systems [13]. In 2×2 systems, when the density matrix is entangled, its partial transpose has only one negative eigenvalue [14]. The modulus of the negative eigenvalue (E_N) is a kind of entanglement measure, and two times E_N agrees with the negativity introduced in Ref. [3]. We have performed a numerical calculation similar to that for Fig. 1, and obtained a maximum of E_N for 10 000 random density matrices. In the inset of Fig. 2 those are plotted as a function of

$$\begin{aligned}2E_N^*&=\max\{0,2E_N^*(p_i)\},\\ 2E_N^*(p_i)&\equiv -p_2-p_4+\sqrt{(p_1-p_3)^2+(p_2-p_4)^2},\end{aligned}\tag{17}$$

which is the negativity of M. None of the points are present on the higher side of a straight line of $E_N=E_N^*$, as in the case of the concurrence. While it has been shown that two measures (EOF and negativity) do not induce the same ordering of density matrices with respect to the amount of entanglement [9], the above numerical results suggest that M has the maximum amount of entanglement in both measures.

As mentioned in the introduction, it will be natural to attribute the upper bound of entanglement, which is well described by $C^*(p_i)$ and $E_N^*(p_i)$, to the increase of the degree of the mixture of the states. In this sense, $C^*(p_i)$ and $2E_N^*(p_i)$ (both are distributed in the range of $[-1/2,1]$) each can be considered as one of the measures characterizing the degree of mixture, such as the purity (or participation ratio), von Neumann entropy, Renyi entropy, and so on.

Finally, as a simple application of the upper bound of EOF,

$$E_F(\rho)\leqslant H\left(\frac{1+\sqrt{1-C^{*2}}}{2}\right),\tag{18}$$

we consider the situation generating entangled states by using the quantum gate consisting of two qubits, more concretely a controlled-NOT (CNOT) gate. In realistic situations the coupling between the gate and its surrounding environment is inevitably present. The entire system consisting of the gate plus its environment happens to be entangled by the coupling, and the mixture of the reduced density matrix describing the gate will inevitably be increased.

In order to treat such decohered CNOT gates, we adopt the spin-boson model [15,16], where each qubit is described as a spin-$\frac{1}{2}$ system, and the environment is expressed as an ensemble of independent bosons. As the model of the CNOT gate, we choose the simplest Hamiltonian:

$$H_G=-\frac{R}{4}(1-\sigma_{cz})\otimes\sigma_{tx},\tag{19}$$

where c and t denotes the control-bit and target-bit, respectively. The state change after $t=h/(2R)$ corresponds to the change in the CNOT operation. In this paper, we demonstrate two types of gate-environment couplings. These are

$$\begin{aligned}H_{GE}^{(1)}&=-\sigma_{cz}\sum_k B_k(a_k^\dagger+a_k),\\ H_{GE}^{(2)}&=-\frac{1}{2}(1-\sigma_{cz})\otimes\sigma_{tx}\sum_k B_k(a_k^\dagger+a_k),\end{aligned}\tag{20}$$

where a_k is an annihilation operator of a boson in the environment. $H_{GE}^{(1)}$ describes the situation in which only the control-bit couples with the environment. $H_{GE}^{(2)}$ may describe the situation in which the gate operation is achieved by irradiating a optical pulse that contains a noise coherent over the qubits as well as the pulse itself. For these phase-damping couplings, the time evolution of the reduced density matrix describing the gate is analytically solved [17] by assuming the product initial state for the entire density matrix:

$$\rho_{\mathrm{tot}}(0)=\rho(0)\otimes\rho_E,\tag{21}$$

where ρ_E is the thermal equilibrium density matrix of the environment. Since we pay attention only to the generation of the entangled state, the initial state of the CNOT gate is chosen to be the pure state of $(|0\rangle_c+|1\rangle_c)\otimes|0\rangle_t$.

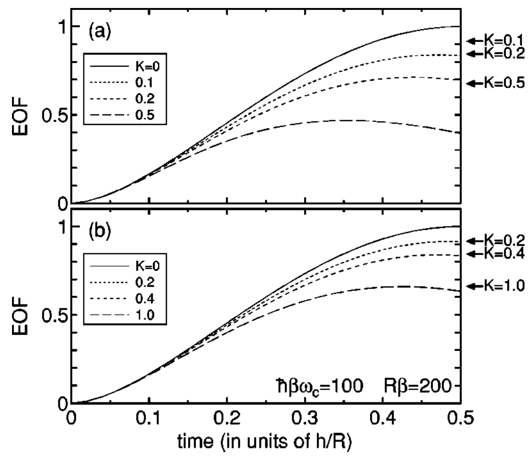

FIG. 3. EOF as a function of time in a decohered CNOT gate for several values of the coupling strength. ω_c is the cut-off frequency of the ohmic environmental mode, and β is the inverse temperature. (a) $H_{GE}^{(1)}$ coupling and (b) $H_{GE}^{(2)}$ coupling.

The time development of the EOF for several values of the coupling strength $K[\propto \Sigma_k B_k^2 \delta(\omega - \omega_k)]$ is shown in Fig. 3 for the (a) $H_{GE}^{(1)}$ and (b) $H_{GE}^{(2)}$ coupling. The values of the coupling strength K are chosen such that the values of the fidelity of the output state to the desired state in the absence of the decoherence are roughly 0.95, 0.9, and 0.8, which are common to Figs. 3(a) and 3(b). It is interesting to note that, while the fidelity is the same in two cases of coupling, the amount of the entanglement is significantly different.

The upper bound of the EOF [Eq. (18)] for each coupling strength is shown by an arrow on the right-hand side of each panel for comparison. In the present model, the rank of the resultant reduced density matrix is always less than 4, and Eq. (18) gives the strict (proven) bound. Since the EOF of a state has the physical meaning of the asymptotic number of Bell pairs required to prepare the state by using only local quantum operations and classical communication (LQCC), comparing the difference in the EOF will make sense. In Fig. 3(a), the EOF is considerably lower than the corresponding upper bound, while the EOF almost agrees with the upper bound in Fig. 3(b). Therefore, with respect to the function generating entangled states, the performance of the CNOT gate shown in Fig. 3(b) is already optimal (or saturated) in the sense that there is no other way to further increase the amount of the entanglement than to avoid an increase of the mixture of the output density matrix, and thus avoid the decoherence itself. On the other hand, for the CNOT gate shown in Fig. 3(a), there is room for improvement of the performance in principle, although we cannot show the detailed methods here.

To conclude, we propose mixed states in two qubits, which have a property that the amount of entanglement of these states cannot be increased by any unitary operation. The property is proven when the rank of the states is less than 4, and when the states satisfy a special relation such as the Werner state. The results of the numerical calculations strongly support a hypothesis that these mixed states are indeed maximally entangled even in general cases. It should be noted finally that a class of mixed states, whose probabilistic increase of the EOF of the single copy cannot be achieved by any LQCC protocol, has been proposed [18,19]. The Werner state belongs to this class, and at the same time belongs to the class we propose in the present paper. Therefore, the Werner state has the property of having a maximum amount of entanglement in both nonlocal unitary transformation and LQCC protocol. It will be extremely important to seek out the *maximally entangled mixed states* as well as the measure in systems with a larger dimension, for understanding the nature of entanglement of general mixed states and for the progress of the quantum information science and its applications.

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