# Numerical analysis of capacities for two-qubit unitary operations

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We present numerical results on the capacities of two-qubit unitary operations for performing communication and creating entanglement. The capacities for communication considered are based upon the increase in Holevo information of an ensemble. Our results indicate that the capacity may be accurately estimated using ensemble sizes and ancilla dimensions of 4. In addition, the calculated values of these capacities were close to, and in some cases equal to, the similarly defined entangling capacities; this result indicates connections between these capacities.

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## I. INTRODUCTION

A nonlocal operation is one that operates on two subsystems, and cannot be expressed as a tensor product of operations on the individual subsystems. Such operations occur when the subsystems evolve under an interaction Hamiltonian. Nonlocal operations may be used to create entanglement between two subsystems, and also to perform classical communication. In fact, it is not possible to achieve these tasks without an interaction. In characterizing quantum operations, it is important to determine the capacities for creating entanglement or performing communication.

Shared classical information may be considered to be the classical equivalent of entanglement. Therefore it is reasonable to consider the process of classical communication to be the classical equivalent of entanglement creation, and one may expect that there is a close relationship between the capacities for these two tasks. In this paper we make a direct numerical comparison between the capacities for entanglement creation and classical communication.

The capacities of unitary operations for creating entanglement have been studied extensively [1–8]. It is relatively straightforward to determine the entanglement capacity for infinitesimal operations [3]. For finite operations, most results are restricted to numerical results for classes of two-qubit operations [6]. We study the same classes of operations here, and the results we present for the entanglement reproduce those given in Ref. [6], except for some data points where our results are more accurate.

The capacities for classical communication were initially considered for simple unitary operations, such as the CNOT and SWAP operations [9,10]. It is straightforward to analyze the capacities for these operations, because they allow error-free communication. In contrast, more general operations may allow some (possibly large) probability of error, so it is necessary to take this into account in the definition of the capacity. Bennett *et al.* [11] introduced asymptotic capacities, where the average communication when the operation is performed a very large number of times is considered. When the operation is performed a large number of times, it is possible to use error correcting techniques to reduce the probability of error to be arbitrarily small.

It is not feasible to calculate these asymptotic capacities directly from their definitions. However, it is shown in Ref. [11] that the unidirectional capacity is equal to an alternative definition of the capacity based on the Holevo information. This result means that it is possible to calculate this capacity. The capacity based on the Holevo information is still difficult to calculate, as the definition potentially allows unlimited ensemble size and ancilla dimensions. However, it is reasonable that this capacity may be accurately estimated for moderate ancilla dimensions and ensemble size. In particular, it would be reasonable to conjecture that:

*Conjecture 1*. For a unitary operation $U$ that acts upon two subsystems of dimension $d$, the Holevo capacities may be estimated accurately using ancillas of dimension $d$ and ensembles with $d^2$ states.

As motivation for this conjecture, note that ancillas of dimension $d$ are sufficient for one of the entangling capacities [12], and an ensemble size of $d^2$ is sufficient for qudit channels [13]. In this paper we numerically test this conjecture for a range of two-qubit operations, and show that the ancilla dimension required is larger.

Another interesting problem is the relationship between the communication and entanglement capacities. In previous work [11,14,15] it was shown that there are a number of inequalities between these capacities. If the communication capacities were equal to the entanglement capacities, this would indicate deep connections between them. The results in Refs. [11,14,15] are not sufficient to show equality, though they do suggest that the capacities may be close. Therefore it is reasonable to make the second conjecture:

*Conjecture 2*. For a unitary operation $U$ that acts upon two subsystems, the Holevo capacities may be estimated from similarly defined entangling capacities.

In this paper we give numerical evidence supporting this conjecture. Note that in these two conjectures we have not specified how accurate an estimation is required. We will refine this point in the conclusions.

This paper is organized as follows. In Sec. II we review the definitions of entanglement and classical communication capacities, and in Sec. III discuss the relations between these capacities. We give numerical results for the communication capacity based on the Holevo information obtained for initial ensembles with zero Holevo information in Sec. IV. We compare this capacity to the entanglement that may be created from initial states that have zero entanglement. We then present analytic results for these capacities in Sec. V. In Sec. VI we give results for the increase in Holevo information for general initial ensembles. These capacities are compared to the increase in entanglement for arbitrary initially entangled states. We conclude in Sec. VII.

## II. DEFINITIONS

First we provide definitions for the various capacities. Throughout this paper we divide the system into two subsystems, $A$ and $B$, and denote the Hilbert spaces by $\mathcal{H}_A$ and $\mathcal{H}_B$. The party in possession of subsystem $A$ will be referred to as Alice and the party in possession of subsystem $B$ will be referred to as Bob. The subsystems $A$ and $B$ are divided into further subsystems:

$$\mathcal{H}_A = \mathcal{H}_{A_{\mathrm{anc}}} \otimes \mathcal{H}_{A_U}, \quad \mathcal{H}_B = \mathcal{H}_{B_U} \otimes \mathcal{H}_{B_{\mathrm{anc}}}. \tag{1}$$

The operation $U$ acts only upon $\mathcal{H}_{A_U} \otimes \mathcal{H}_{B_U}$, and the Hilbert spaces $\mathcal{H}_{A_{\mathrm{anc}}}$ and $\mathcal{H}_{B_{\mathrm{anc}}}$ are ancillas. Each of these Hilbert spaces has finite dimension, which we denote by $d$ with the appropriate subscripts. For example, $d_{A_U} = \dim \mathcal{H}_{A_U}$ and $d_B = \dim \mathcal{H}_B$. For cases where the dimensions $d_{A_U}$ and $d_{B_U}$ are equal (as in Conjecture 1), we take $d = d_{A_U} = d_{B_U}$.

There are two main ways of defining capacities for entanglement. The first is the entanglement that may be obtained when the initial state is pure and unentangled:

$$E_U \equiv \sup_{|\phi\rangle_A \in \mathcal{H}_A, |\chi\rangle_B \in \mathcal{H}_B} E(U|\phi\rangle_A|\chi\rangle_B). \tag{2}$$

The quantity $E(\cdots)$ is the entropy of entanglement $E(|\Psi\rangle) = S[\mathrm{Tr}_A(|\Psi\rangle\langle\Psi|)]$, where $S(\rho) = -\mathrm{Tr}(\rho \log \rho)$. Throughout we employ logarithms to base 2, so the entanglement is expressed in units of ebits. The second definition is the maximum increase in entanglement when the initial state may be an arbitrary pure entangled state:

$$\Delta E_U \equiv \sup_{|\psi\rangle_{AB} \in \mathcal{H}_A \otimes \mathcal{H}_B} [E(U|\psi\rangle_{AB}) - E(|\psi\rangle_{AB})]. \tag{3}$$

There are also a number of additional ways of defining the entanglement capacity. One can allow mixed states, and use the entanglement of formation as the entanglement measure. Alternatively, the entanglement of formation may be used as the initial entanglement measure, and the distillable entanglement as the final entanglement measure. Another alternative definition is based on the average entanglement that may be obtained in the limit that the operation is performed a large number of times. These alternative definitions are discussed in Ref. [11], and it is shown that they are equal to the maximum increase in entanglement as defined in Eq. (3). Therefore we do not separately consider them in this study.

In the numerical search, it is not possible to consider ancilla spaces with arbitrarily large dimension. For the results presented below, equal ancilla dimensions were used, and this common dimension is indicated by a superscript. For example, $\Delta E_U^{(4)}$ is the maximum change in entanglement when the ancilla spaces are of dimension 4. When we refer to multiple results with different ancilla dimensions we use a superscript asterisk. We omit the superscript in the case of $E_U$ when $d_{A_{\mathrm{anc}}} \geqslant d_{A_U}$ and $d_{B_{\mathrm{anc}}} \geqslant d_{B_U}$, because this is known to be sufficient to achieve the capacity [12].

The classical communication capacities that we consider are based upon the Holevo information of ensembles. An ensemble is a set of states $\{|\Phi_i\rangle_{AB}\}$ that are supplied with probabilities $p_i$. Each state $|\Phi_i\rangle_{AB}$ is a pure state shared between Alice and Bob, and Alice chooses the index $i$. The ensemble is denoted by $\mathcal{E} = \{p_i, |\Phi_i\rangle_{AB}\}$. We also define the ensemble of reduced density matrices possessed by Bob as

$$\mathsf{E} = \mathrm{Tr}_A\, \mathcal{E} = \{p_i, \rho_i\}, \tag{4}$$

where $\rho_i = \mathrm{Tr}_A|\Phi_i\rangle_{AB}\langle\Phi_i|$. The Holevo information of the ensemble $\mathsf{E}$ is given by

$$\chi(\mathsf{E}) = S(\bar{\rho}) - \sum_i p_i S(\rho_i), \tag{5}$$

where $\bar{\rho} = \Sigma_i p_i \rho_i$. From the Holevo-Schumacher-Westmoreland theorem [16,17], the Holevo information gives the average communication that may be performed from Alice to Bob by coding over multiple states.

Similarly to the case for entanglement, we may define capacities based on the maximum change in Holevo information. One definition that we will use is the maximum final Holevo information when the initial ensemble has zero Holevo information. For the initial ensemble, we have an initial state $|\psi\rangle_{AB}$, and Alice encodes $i$ by applying a local unitary operation $V_i$. For the capacity, the supremum is taken over the initial state $|\psi\rangle_{AB}$, the encoding operations $V_i$ and the probabilities $p_i$:

$$\chi_U = \sup_{p_i, V_i, |\psi\rangle_{AB}} \chi(p_i, \mathrm{Tr}_A\, U V_i |\psi\rangle_{AB}). \tag{6}$$

We use the notation convention that $\mathrm{Tr}_A|\phi\rangle \equiv \mathrm{Tr}_A|\phi\rangle\langle\phi|$. Note that the initial state $|\psi\rangle_{AB}$ may contain entanglement, though the encoding operations $V_i$ are restricted to be local. This definition is equivalent to the capacity $\Delta\chi_U^{(1,\varnothing)}$ as defined in Ref. [11].

One may also define the maximum change in Holevo information when the initial ensemble is arbitrary:

$$\Delta\chi_U = \sup_{\mathcal{E}} [\chi(\mathrm{Tr}_A\, U\mathcal{E}) - \chi(\mathrm{Tr}_A\, \mathcal{E})]. \tag{7}$$

Here we are using the notation conventions

$$U\mathcal{E} \equiv \{p_i, U|\Phi_i\rangle\}, \tag{8}$$

$$\mathrm{Tr}_X\, \mathcal{E} \equiv \{p_i, \mathrm{Tr}_X(|\Phi_i\rangle)\}. \tag{9}$$

This capacity is equivalent to the capacity $\Delta\chi_U^{(1,*)}$ defined in Ref. [11]. As shown in Ref. [11], this capacity is equal to the average entanglement-assisted communication that may be performed from Alice to Bob. Therefore this quantity may be interpreted as the asymptotic communication capacity, just as $\Delta E_U$ may be interpreted as the asymptotic entanglement capacity.

It is also possible to interpret $\chi_U$ in terms of asymptotic capacities. The capacity $\chi_U$ gives the Holevo information after a single application of the operation $U$. This communication can not actually be performed for a single ensemble; it is necessary to code over multiple states to perform this average communication. Therefore $\chi_U$ may be interpreted as the asymptotic communication capacity with the restriction that the applications of $U$ are performed on distinct input states that are not entangled with each other, rather than allowing the output of one application of $U$ to be used as part of the input to another application of $U$, as in the general case.

One may also consider capacities where the initial ensembles are restricted to being unentangled. We will denote the capacities analogous to $\chi_U$ and $\Delta\chi_U$ but with initially unentangled states using primes. In particular

$$\chi'_U = \sup_{p_i,|\phi_i\rangle_A,|\chi\rangle_B} \chi(p_i, \mathrm{Tr}_A\, U|\phi_i\rangle_A|\chi\rangle_B),$$

$$\Delta\chi'_U = \sup_{p_i,|\phi_i\rangle_A,|\chi_i\rangle_B}\left[\chi(p_i,\mathrm{Tr}_A\, U|\phi_i\rangle_A|\chi_i\rangle_B) - S\left(\sum_i p_i|\chi_i\rangle_B\langle\chi_i|\right)\right]. \quad (10)$$

In this study we primarily consider the capacities where entangled initial states are allowed. However, the capacities $\chi'_U$ and $\Delta\chi'_U$ are useful as it is more straightforward to derive analytic results for them.

In the case of $\chi'_U$, it is easily seen that Conjecture 1 is correct. To show this, first note that the ancilla for Bob need have dimension no larger than $d_{B_U}$. This can be seen immediately, because in the Schmidt decomposition of $|\chi\rangle_B$ the number of terms is no larger than $d_{B_U}$. In addition, from convexity the capacity will be maximized for unentangled states in $\mathcal{H}_{A_U}$, so the ancilla $\mathcal{H}_{A_{\mathrm{anc}}}$ may be omitted. For a given $|\chi\rangle_B$ the operation $U$ defines a quantum channel with the initial state in $\mathcal{H}_{A_U}$ as the input. Therefore the capacity is maximized with no more than $d_{A_U}^2$ states in the ensemble [13]. This derivation is provided in more detail in the Appendix. For the other capacities it is also possible to restrict the number of states required in the ensemble for given ancilla dimensions (see the Appendix). However, we have not found a way of limiting the ancilla dimensions required in these cases.

In the numerical results presented for $\chi'_U$, we use the ancilla dimensions and ensemble sizes sufficient to obtain the capacity. For the other Holevo capacities we use superscripts to indicate the number of states in the ensemble and the dimension of the ancilla spaces (we take $d_{A_{\mathrm{anc}}}=d_{B_{\mathrm{anc}}}$). For example, $\Delta\chi_U^{(2,4)}$ is the maximum change in Holevo information for two states in the ensemble and ancillas with dimension 4. We use a superscript asterisk to refer to multiple capacities with different ancilla dimensions or ensemble sizes. It must be emphasized that our use of superscripts in this paper differs from that in Ref. [11].

## III. RELATIONS BETWEEN CAPACITIES

There are many relationships between the various capacities that enable one to derive inequalities. For example, it is clear that restricting the initial states to be unentangled does not increase the maximum change in entanglement. Similarly, restricting the initial ensembles to have no correlations or be unentangled does not increase the maximum change in Holevo information. Therefore we have

$$E_U \leqslant \Delta E_U, \quad \chi'_U \leqslant \chi_U \leqslant \Delta\chi_U, \quad \Delta\chi'_U \leqslant \Delta\chi_U. \quad (11)$$

For two-qubit operations it has been shown that it is possible to derive ensembles for increasing the Holevo information from a state related to $\Delta E_U$ [14,15]. In particular, if $|\psi\rangle_{AB}$ is a state such that the entanglement is decreased by $\Delta E_U$ under operation $U$, then we construct the ensemble $\{1/4, \sigma_i\otimes\sigma_i|\psi\rangle_{AB}\}$, where the $\sigma_i$ are Pauli operators for $i\in\{1,2,3\}$ and $\sigma_0$ is the identity. The Holevo information of this ensemble is increased by $\Delta E_U$ under operation $U$. This result is sufficient to show that

$$\Delta\chi_U \geqslant \Delta E_U \quad (12)$$

for two-qubit operations. In this paper we show that $\chi_U \geqslant E_U$, though this derivation does not appear to have a simple interpretation.

There is a subtlety in this derivation, in that it is possible that the supremum $\Delta E_U$ is not achieved for any initial state. In that case, it is possible to obtain states such that the decrease in entanglement is at least $\Delta E_U - \epsilon$, for any $\epsilon > 0$. The corresponding increase in the Holevo information of the ensemble would be $\geqslant \Delta E_U - \epsilon$. As $\epsilon$ may be made arbitrarily small, it is still the case that $\Delta\chi_U \geqslant \Delta E_U$.

It can also be shown that $\Delta\chi_U \leqslant \Delta E_U + \Delta E_{U^\dagger}$. This was shown in Ref. [11] using the result that $\Delta\chi_U$ is equal to the unidirectional entanglement-assisted communication capacity. It can also be shown in a more direct way as follows. For any $\epsilon > 0$, let $\{p_i, |\psi_i\rangle_{AB}\}$ be an ensemble such that the Holevo information is increased by at least $\Delta\chi_U - \epsilon$. Then we have

$$\Delta\chi_U - \epsilon \leqslant S\left(\sum_i p_i\, \mathrm{Tr}_A\, U|\psi_i\rangle_{AB}\right) - S\left(\sum_i p_i\, \mathrm{Tr}_A|\psi_i\rangle_{AB}\right) - \sum_i p_i[S(\mathrm{Tr}_A\, U|\psi_i\rangle_{AB}) - S(\mathrm{Tr}_A|\psi_i\rangle_{AB})]. \quad (13)$$

By taking the initial state $\Sigma_i\sqrt{p_i}|i\rangle_{A'}|\psi_i\rangle_{AB}$, the change in entanglement would be

$$S\left(\sum_i p_i\, \mathrm{Tr}_A\, U|\psi_i\rangle_{AB}\right) - S\left(\sum_i p_i\, \mathrm{Tr}_A|\psi_i\rangle_{AB}\right) \leqslant \Delta E_U. \quad (14)$$

Similarly, by taking the initial state $|\psi_i\rangle_{AB}$, the change in entanglement is

$$S(\mathrm{Tr}_A\, U|\psi_i\rangle_{AB}) - S(\mathrm{Tr}_A\, |\psi_i\rangle_{AB}) \geqslant -\Delta E_{U^\dagger}. \quad (15)$$

Therefore Eq. (13) gives

$$\Delta\chi_U - \epsilon \leqslant \Delta E_U + \sum_i p_i \Delta E_{U^\dagger} = \Delta E_U + \Delta E_{U^\dagger}. \quad (16)$$

As this is true for arbitrary $\epsilon > 0$, we have $\Delta\chi_U \leqslant \Delta E_U + \Delta E_{U^\dagger}$. In the case of two-qubit operations, $\Delta E_U = \Delta E_{U^\dagger}$, so we have the bounds

$$2\Delta E_U \geqslant \Delta\chi_U \geqslant \Delta E_U. \quad (17)$$

In the case where the initial states are restricted to being unentangled, it is possible to derive additional relations. In that case, we have $S(\mathrm{Tr}_A|\psi_i\rangle_{AB})=0$, so we obtain

$$\Delta\chi'_U - \epsilon \leqslant S\left(\sum_i p_i \,\mathrm{Tr}_A\, U|\psi_i\rangle_{AB}\right) - S\left(\sum_i p_i \,\mathrm{Tr}_A\, |\psi_i\rangle_{AB}\right) \leqslant \Delta E_U. \quad (18)$$

As this is true for all $\epsilon>0$, $\Delta\chi'_U\leqslant\Delta E_U$. For the capacity $\chi'_U$, let $\{p_i,|\phi_i\rangle_A|\chi\rangle_B\}$ be an ensemble that achieves the capacity to within $\epsilon$. Then

$$\chi'_U - \epsilon \leqslant S\left(\sum_i p_i \,\mathrm{Tr}_A\, U|\phi_i\rangle_A|\chi\rangle_B\right) - \sum_i p_i S(\mathrm{Tr}_A\, U|\phi_i\rangle_A|\chi\rangle_B). \quad (19)$$

Using the initial unentangled state

$$\sum_i \sqrt{p_i}|i\rangle_{A_{\mathrm{anc}}}|\phi_i\rangle_{A_U}|\chi\rangle_B, \quad (20)$$

the final entanglement is

$$S\left(\sum_i p_i \,\mathrm{Tr}_A\, U|\phi_i\rangle_A|\chi\rangle_B\right) \leqslant E_U. \quad (21)$$

Therefore $\chi'_U-\epsilon\leqslant E_U$ for all $\epsilon>0$, so $\chi'_U\leqslant E_U$.

In the case of controlled-$U$ operations, it is possible to show the inequalities in the opposite direction. A controlled-$U$ operation is one of the form

$$U = \sum_i |\psi_i\rangle_{A_U}\langle\psi_i| \otimes U_i, \quad (22)$$

where the $|\psi_i\rangle_{A_U}$ are an orthogonal basis for $\mathcal{H}_{A_U}$, and the $U_i$ are unitary. Consider an initial unentangled state $|\phi\rangle_A|\chi\rangle_B$ such that the final entanglement is at least $E_U-\epsilon$. The state $|\phi\rangle_A$ may be expanded as $\Sigma_{ij}\lambda_{ij}|\varphi_i\rangle_{A_{\mathrm{anc}}}|\psi_j\rangle_{A_U}$, so the final state is

$$\sum_{ij} \lambda_{ij}|\varphi_i\rangle_{A_{\mathrm{anc}}}|\psi_j\rangle_{A_U}U_j|\chi\rangle_B. \quad (23)$$

Applying $U$ to the ensemble $\{|\lambda_{ij}|^2,|\varphi_i\rangle_{A_{\mathrm{anc}}}|\psi_j\rangle_{A_U}|\chi\rangle_B\}$ results in $\{|\lambda_{ij}|^2,|\varphi_i\rangle_{A_{\mathrm{anc}}}|\psi_j\rangle_{A_U}U_j|\chi\rangle_B\}$. The Holevo information of this ensemble is

$$S\left(\sum_{ij} |\lambda_{ij}|^2 U_j|\chi\rangle_B\langle\chi|U_j^\dagger\right) \leqslant \chi'_U. \quad (24)$$

As this is equal to the entanglement of the state $U|\phi\rangle_A|\chi\rangle_B$, we have $E_U-\epsilon\leqslant\chi'_U$ for all $\epsilon>0$, so $E_U\leqslant\chi'_U$. As we previously showed $E_U\geqslant\chi'_U$, we have, for controlled-$U$ operations, $E_U=\chi'_U$.

Similarly, for the case of $\Delta E_U$, let $|\phi\rangle_{AB}$ be an initial state such that the increase in entanglement is at least $\Delta E_U-\epsilon$. This state may be expressed as

$$|\phi\rangle_{AB} = \sum_{ij} \lambda_{ij}|\varphi_i\rangle_{A_{\mathrm{anc}}}|\psi_j\rangle_{A_U}|\chi_{ij}\rangle_B, \quad (25)$$

where the $\lambda_{ij}$ are real and $\Sigma_{ij}\lambda_{ij}^2=1$, but the $|\chi_{ij}\rangle$ are not mutually orthogonal. The change in entanglement under the operation $U$ is then

$$S\left(\sum_{ij} \lambda_{ij}^2 U_j|\chi_{ij}\rangle_B\langle\chi_{ij}|U_j^\dagger\right) - S\left(\sum_{ij} \lambda_{ij}^2|\chi_{ij}\rangle_B\langle\chi_{ij}|\right) \geqslant \Delta E_U - \epsilon. \quad (26)$$

Now consider the initial ensemble $\{\lambda_{ij}^2,|\varphi_i\rangle_{A_{\mathrm{anc}}}|\psi_j\rangle_{A_U}|\chi_{ij}\rangle_B\}$. This ensemble gives a change in Holevo information equal to the change in entanglement for $|\phi\rangle_{AB}$. Therefore we have $\Delta\chi'_U\geqslant E_U-\epsilon$ for all $\epsilon>0$, so $\Delta\chi'_U\geqslant E_U$. As we have shown $\Delta\chi'_U\leqslant E_U$, we have, for controlled-$U$ operations, $\Delta E_U=\Delta\chi'_U$.

## IV. CAPACITIES FOR ZERO INITIAL HOLEVO INFORMATION

It is clear that the capacity $\chi_U$ is an analogous quantity for communication to $E_U$ for entanglement; similarly $\Delta\chi_U$ is analogous to $\Delta E_U$. Although it is possible to derive inequalities for these quantities analytically, these results are not sufficient to determine whether these capacities are equal. In this section we perform a direct numerical comparison between the two capacities $\chi_U$ and $E_U$. In addition we present results for the simplest capacity $\chi'_U$. We then derive analytic results for these capacities in Sec. V. In Sec. VI we numerically compare the capacities $\Delta\chi_U$ and $\Delta E_U$.

In this paper we concentrate on two-qubit unitary operations. It is not possible to perform calculations for the entire range of two-qubit operations. To make the problem feasible, we only consider a limited number of examples of two-qubit operations. In particular, we consider operations of the form

$$U_1(\alpha) = U_d(\alpha,0,0), \quad (27)$$

$$U_2(\alpha) = U_d(\alpha,\alpha,0), \quad (28)$$

$$U_3(\alpha) = U_d(\alpha,\alpha,\alpha), \quad (29)$$

where

$$U_d(\alpha_1,\alpha_2,\alpha_3) = e^{-i(\alpha_1\sigma_1\otimes\sigma_1+\alpha_2\sigma_2\otimes\sigma_2+\alpha_3\sigma_3\otimes\sigma_3)}. \quad (30)$$

The operations $U_1$, $U_2$, and $U_3$ correspond to the CNOT, double CNOT (DCNOT), and SWAP families of operations considered in Ref. [6].

In order to consider the complete range of two-qubit unitary operations in the case of the entanglement, it is sufficient to consider operations of the form (30), with $\pi/4\geqslant\alpha_1\geqslant\alpha_2\geqslant\alpha_3\geqslant0$ [5]. This derivation relies on the fact that any two-qubit unitary operation may be simplified to one of the form (30) with $\pi/4\geqslant\alpha_1\geqslant\pm\alpha_2\geqslant\alpha_3\geqslant0$ using local operations [3,5,18,19]. In addition to using local operations, the derivation in Ref. [5] relies on the fact that the entanglement capabilities of $U$ and $U^*$ are identical (which implies that all the $\alpha_i$ may be taken to be positive).

Similarly, for the Holevo information, $\chi(\mathrm{Tr}_A\mathcal{E})=\chi(\mathrm{Tr}_A\mathcal{E}^*)$ and $\chi(\mathrm{Tr}_A U\mathcal{E})=\chi(\mathrm{Tr}_A U^*\mathcal{E}^*)$. Thus the capacities of $U$ and $U^*$ to increase the Holevo information are identical. Therefore, in order to obtain results for the complete range of two-qubit unitary operations, it is sufficient to consider operations of the form (30) with $\pi/4\geqslant\alpha_1\geqslant\alpha_2\geqslant\alpha_3\geqslant0$ in the cases of both the entanglement and the Holevo information.

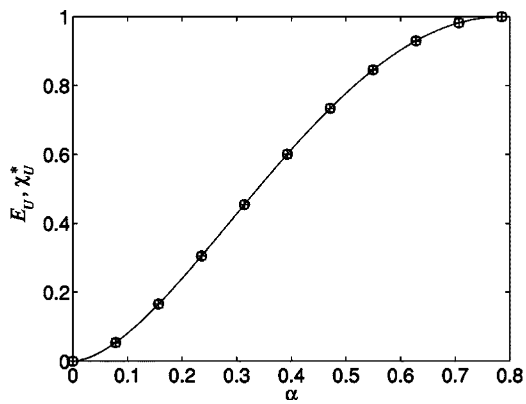


FIG. 1. Capacities with zero initial entanglement or Holevo information for the operation $U_1$. The values of $E_U$ are shown as the solid line, and the values of $\chi_U'$, $\chi_U^{(2,1)}$, $\chi_U^{(4,4)}$ are shown as the circles, plusses and squares, respectively (these symbols overlap and are not separately visible).

This restriction on the values of the $\alpha_i$ defines a three-dimensional region of values. For most results in this paper we do not consider the entire region; however, the operations $U_1$, $U_2$, and $U_3$ which we consider form three lines on the boundaries of this region.

The numerical results for $E_U$, $\chi_U'$, and $\chi_U^*$ for the operation $U_1$ are shown in Fig. 1. It was found that, for $U_1$, the capacity $E_U$ was achieved without ancilla, in agreement with Ref. [5]. The values of $\chi_U^*$ were determined with no ancilla and two states in the ensemble, as well as with ancillas of dimension 4 and four states in the ensemble. It was found that the results in these two cases were identical, indicating that, for $U_1$, a final Holevo information equal to the asymptotic capacity $\chi_U$ may be achieved without ancillas and with an ensemble consisting of two states.

In addition, note that there is no difference between the results obtained for $E_U$ and $\chi_U$. These results strongly indicate that $E_U = \chi_U$ for the operation $U_1$. We also find that $E_U = \chi_U'$ for $U_1$. This result may be predicted from the results of Sec. III, because operations of the form $U_1$ are equivalent to controlled-$U$ operations [21].

Numerical results for $E_U$, $\chi_U'$, and $\chi_U^*$ for the operations $U_2$ and $U_3$ are shown in Figs. 2 and 3, respectively. In both cases, we find that $\chi_U'$ is well below the other capacities. For $U_2$, the capacity $\chi_U^*$ is increased for ancilla dimensions higher than 2. For an ancilla dimension of 2, the value of $\chi_U^{(4,2)}$ is less than $E_U$ for many of the samples. The values of $\chi_U^{(4,3)}$ are larger, but still less than $E_U$. When the ancilla dimension is increased to 4, we find that $\chi_U^{(4,4)}$ is equal to $E_U$, just as in the case of $U_1$.

For $U_3$, the results are similar, except that for some of the samples $\chi_U^*$ is slightly larger than $E_U$. For $\alpha = \pi/40$, $2\pi/40$, and $3\pi/40$, the values of both $\chi_U^{(4,3)}$ and $\chi_U^{(4,4)}$ are larger than $E_U$. This difference is small, less than 0.02, but it is sufficient to demonstrate that $E_U$ is not equal to $\chi_U$ for $U_3$. For the other samples we find that $\chi_U^{(4,4)}$ is equal to $E_U$.

For both $U_2$ and $U_3$ calculations have been performed for an ancilla dimension of 8 and an ensemble size of 8, and in both cases it was found that $\chi_U^{(8,8)}$ is unchanged from $\chi_U^{(4,4)}$.

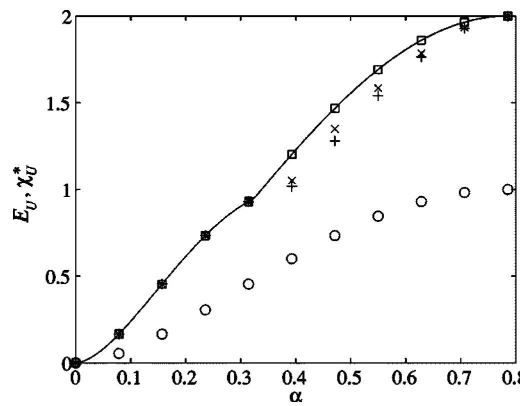


FIG. 2. Capacities with zero initial entanglement or Holevo information for the operation $U_2$. The values of $E_U$ are shown as the solid line, and the values of $\chi_U'$, $\chi_U^{(4,2)}$, $\chi_U^{(4,3)}$, and $\chi_U^{(4,4)}$ are shown as the circles, plusses, crosses, and squares, respectively.

These results indicate that, for all three classes of operation tested, a final Holevo information equal to the asymptotic capacity $\chi_U$ may be achieved with ancillas of dimension 4 and an ensemble size of 4.

Our results also indicate that for two of the classes of operation tested, $U_1$ and $U_2$, $\chi_U$ is equal to $E_U$. For the operation $U_3$, it is possible to obtain slightly higher values of $\chi_U^*$, demonstrating that $\chi_U$ is not equal to $E_U$ for this operation. Nevertheless, the results still indicate that $\chi_U$ is close to $E_U$ for this operation.

## V. ANALYTIC RESULTS FOR ENSEMBLES

In the numerical results for $E_U$ presented in the previous section it was found that the maximal values were obtained for initial states in one of two forms:

$$|01\rangle, \quad (|00\rangle + |11\rangle)(|00\rangle + |11\rangle)/2. \tag{31}$$

Here we use the convention that, where there are four subsystems, these are $A_{\rm anc}$, $A_U$, $B_U$, and $B_{\rm anc}$. Where there are

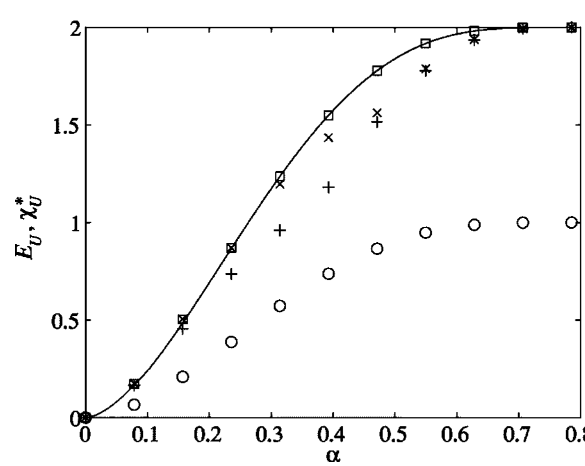


FIG. 3. Capacities with zero initial entanglement or Holevo information for the operation $U_3$. The values of $E_U$ are shown as the solid line, and the values of $\chi_U'$, $\chi_U^{(4,2)}$, $\chi_U^{(4,3)}$, and $\chi_U^{(4,4)}$ are shown as the circles, plusses, crosses, and squares, respectively.

two subsystems, these are simply $A_U$ and $B_U$. It has been found numerically that the maximal final *linear* entropy is obtained for one of the two states (31) [5]. To test this hypothesis for the case of the entropy of entanglement, the value of $E_U$ was determined for operations $U_d(\alpha_1,\alpha_2,\alpha_3)$ such that $\pi/4 \geqslant \alpha_1 \geqslant \alpha_2 \geqslant \alpha_3 \geqslant 0$. Recall that this range of operations is sufficient to characterize the capacities for all two-qubit unitaries. Step sizes of $\pi/4000$ for each of the $\alpha_i$ were used, and in each case one of the initial states in Eq. (31) gave a final entanglement as large as the maximum obtained numerically. This is compelling evidence that, for two-qubit unitaries, the maximum final entropy of entanglement is always obtained for one of these two states.

Next we show that, provided the maximum final entropy is obtained for one of the initial states (31), $\chi_U \geqslant E_U$. To show this result, we first determine the entanglement obtained for the initial states in Eq. (31). To determine these entanglements, we use the expression given by Ref. [12]:

$$\begin{aligned} U_d(\alpha_1,\alpha_2,\alpha_3) &= (c_1c_2c_3 + is_1s_2s_3)\sigma_0 \otimes \sigma_0 + (c_1s_2s_3 \\ &\quad + is_1c_2c_3)\sigma_1 \otimes \sigma_1 + (s_1c_2s_3 + ic_1s_2c_3)\sigma_2 \\ &\quad \otimes \sigma_2 + (s_1s_2c_3 + ic_1c_2s_3)\sigma_3 \otimes \sigma_3, \end{aligned} \tag{32}$$

where $s_i = \sin \alpha_i$ and $c_i = \cos \alpha_i$. Using this expression it may be shown that the two final entanglements obtained are

$$H(\cos^2 \alpha_+, \sin^2 \alpha_+), \quad H(\mu_+, \mu_-, \nu_+, \nu_-), \tag{33}$$

where $\alpha_\pm = \alpha_1 \pm \alpha_2$,

$$\mu_\pm = (\sin^2 \alpha_+ + \sin^2 \alpha_-)/2 \pm \sin \alpha_+ \sin \alpha_- \cos(2\alpha_3),$$

$$\nu_\pm = (\cos^2 \alpha_+ + \cos^2 \alpha_-)/2 \pm \cos \alpha_+ \cos \alpha_- \cos(2\alpha_3), \tag{34}$$

and the function $H$ is the entropy of the arguments

$$H(\lambda_1,\ldots,\lambda_N) = -\sum_{n=1}^{N} \lambda_n \log \lambda_n. \tag{35}$$

Next we consider two different ensembles:

$$\mathcal{E}_1 = \{1/2, (|011\rangle \pm |100\rangle)/\sqrt{2}\},$$

$$\mathcal{E}_2 = \{1/4, \sigma_i[|0\rangle(|00\rangle + |11\rangle) + |1\rangle(|02\rangle + |13\rangle)]/2\}, \tag{36}$$

where $\sigma_i$ acts upon subsystem 1 and $i \in \{0,1,2,3\}$. Here we use the convention that subsystems 1, 2, and 3 are $A_U$, $B_U$, and $B_{\rm anc}$, respectively. In the first case subsystem 3 is a qubit, and in the second case subsystem 3 is a four-level ancilla.

Considering ensemble $\mathcal{E}_1$ first, applying $U_d(\alpha_1,\alpha_2,\alpha_3)$ gives the two alternative states

$$(c_+|011\rangle + s_+|101\rangle \pm c_+|100\rangle \pm s_+|010\rangle)/\sqrt{2}, \tag{37}$$

where

$$c_\pm = e^{\mp i\alpha_3} \cos \alpha_\pm, \quad s_\pm = ie^{\mp i\alpha_3} \sin \alpha_\pm. \tag{38}$$

We find that the reduced density matrices for Bob are

$$\frac{1}{2}\begin{bmatrix} |c_+|^2 & \pm s_+^* c_+ & 0 & 0 \\ \pm s_+ c_+^* & |s_+|^2 & 0 & 0 \\ 0 & 0 & |s_+|^2 & \pm s_+ c_+^* \\ 0 & 0 & \pm s_+^* c_+ & |c_+|^2 \end{bmatrix}. \tag{39}$$

Both of these have entropy 1, but the average density matrix has entropy $H(|c_+|^2, |s_+|^2) + 1$. Thus the final Holevo information is the same as the final entanglement for the initial state $|01\rangle$.

For the ensemble $\mathcal{E}_2$, the four states obtained are (ignoring a trivial global phase for $|\psi_2\rangle$)

$$\begin{aligned} |\psi_{0/3}\rangle &= [c_+(|011\rangle \pm |102\rangle) + s_+(|101\rangle \pm |012\rangle) \\ &\quad + c_-(|000\rangle \pm |113\rangle) + s_-(|110\rangle \pm |003\rangle)]/2, \end{aligned}$$

$$\begin{aligned} |\psi_{1/2}\rangle &= [c_+(|100\rangle \pm |013\rangle) + s_+(|010\rangle \pm |103\rangle) \\ &\quad + c_-(|111\rangle \pm |002\rangle) + s_-(|001\rangle \pm |112\rangle)]/2. \end{aligned} \tag{40}$$

It is straightforward to verify that each of these states is maximally entangled, so the reduced density matrix has entropy of 1. The average reduced density matrix for Bob has entropy $H(\mu_+, \mu_-, \nu_+, \nu_-) + 1$, resulting in a total Holevo information of $H(\mu_+, \mu_-, \nu_+, \nu_-)$.

Therefore if the maximal entanglement is obtained for one of the two initial states in Eq. (31), then $\chi_U \geqslant E_U$. Given the compelling numerical evidence that the maximal entanglement is always obtained for one of these two initial states, our results show that $\chi_U \geqslant E_U$ for two-qubit unitaries. However, this result is not proven due to the reliance on numerical results.

There is also a relatively simple ensemble for which the final Holevo information is greater than $E_U$ for some $U$. It is given by

$$\begin{aligned} \mathcal{E}_3 = \{1/3, H_i[&|1\rangle(|00\rangle + |11\rangle + |02\rangle) \\ &- |0\rangle(|10\rangle + |01\rangle - |12\rangle)]/\sqrt{6}\}, \end{aligned} \tag{41}$$

where $H_i$ acts upon subsystem 1 and $i \in \{0,1,2\}$. $H_0$ is the identity, $H_1$ is the Hadamard operator, and $H_2$ has the matrix representation

$$H_2 = \frac{1}{\sqrt{2}}\begin{bmatrix} -1 & 1 \\ 1 & 1 \end{bmatrix}. \tag{42}$$

As before, subsystems 1, 2, and 3 are $A_U$, $B_U$, and $B_{\rm anc}$, respectively. It can be verified numerically that the Holevo information obtained for this ensemble agrees with that displayed in Fig. 3.

In the case of the operation $U_1$, it is not necessary to rely on the numerical results. In this case it has been proven that the maximal entanglement is obtained for either of the two initial states in Eq. (31) [5]. Alternatively, this result may be deduced from the fact that operations of the form $U_1$ are equivalent to controlled-$U$ operations [21], so $\chi'_U = E_U$. As $\chi'_U \leqslant \chi_U$, this proves that $\chi_U \geqslant E_U$ for $U_1$.

To understand this result in terms of ensembles, the maximum entanglement is obtained for the initial state $|01\rangle$. Using the method given in Sec. III we may derive the ensemble

$\mathcal{E}_3=\{1/2,(|0\rangle\pm|1\rangle)|1\rangle/\sqrt{2}\}$ from this state. It is easily verified that this ensemble gives the final entanglement $H(\cos^2\alpha,\sin^2\alpha)$. Therefore, in the case of $U_1$, there is a simple explanation of the result $\chi_U \geqslant E_U$ in terms of ensembles. However, we do not have a similar explanation for the general case.

An aspect of the results for $\chi'_U$ that may be explained is that $\chi'_U$ does not exceed 1. In general the Holevo information can be no more than $\log d_{A_U}$ higher than the initial entanglement. This result may be shown in the following way:

$$\begin{aligned}\chi(p_i,\mathrm{Tr}_A\, UV_i|\psi\rangle_{AB}) &\leqslant \chi(p_i,\mathrm{Tr}_{A_{\mathrm{anc}}}\, UV_i|\psi\rangle_{AB})\\ &\leqslant S\left(\sum_i p_i \mathrm{Tr}_{A_{\mathrm{anc}}} UV_i|\psi\rangle_{AB}\right)\\ &= S\Big(\mathrm{Tr}_{A_{\mathrm{anc}}}\sum_i p_i V_i|\psi\rangle_{AB}\langle\psi|V_i^\dagger\Big)\\ &\leqslant S\Big(\mathrm{Tr}_{A_{\mathrm{anc}}B}\sum_i p_i V_i|\psi\rangle_{AB}\langle\psi|V_i^\dagger\Big)\\ &\quad + S(\mathrm{Tr}_A|\psi\rangle_{AB})\\ &\leqslant \log d_{A_U} + E(|\psi\rangle_{AB}). \qquad (43)\end{aligned}$$

Here $E(|\psi\rangle_{AB})$ is the entanglement of the initial state. This result is related to superdense coding. In particular, it is known that when transmitting a qudit, the information communicated can be no larger than $\log d$ plus the initial entanglement [20].

From this result it is clear that using unentangled states for two-qubit unitaries will not allow a capacity above one bit. Although we find that $\chi'_U=E_U$ for controlled-$U$ operations, we cannot expect this result for more general operations, because $E_U$ may be higher than $\log d_{A_U}$.

## VI. CAPACITIES FOR ARBITRARY INITIAL ENSEMBLES

Next we consider the capacities $\Delta\chi_U$ and $\Delta E_U$. These capacities are more general, in that arbitrary initial states or ensembles are allowed. Analytic results for the relation between these capacities were derived in Refs. [14,15]. It was proven that, for two-qubit unitary operations, $\Delta\chi_U \geqslant \Delta E_U$. If a change in the entanglement of $\Delta E_U$ is obtained with a particular ancilla dimension, then an increase in Holevo information equal to $\Delta E_U$ may be obtained with the same ancilla dimension, and with four states in the ensemble.

In principle it is possible that there is no finite ancilla dimension that achieves $\Delta E_U$, and instead $\Delta E_U$ is approached in the limit of large ancilla dimension. However, in practice it has been found that, for two-qubit unitary operations, it appears to be possible to achieve $\Delta E_U$ with an ancilla dimension of 2 [6]. This means that it should be possible to achieve an increase in Holevo information of $\Delta E_U$ with an ancilla dimension of 2.

The capacities $\Delta\chi^*_U$ and $\Delta E^*_U$ are shown for the operation $U_1$ in Fig. 4. It was found that the entanglement capacity $\Delta E^*_U$ did not increase beyond that for no ancilla as the ancilla dimension was increased up to 5, in agreement with the result given in Ref. [6].

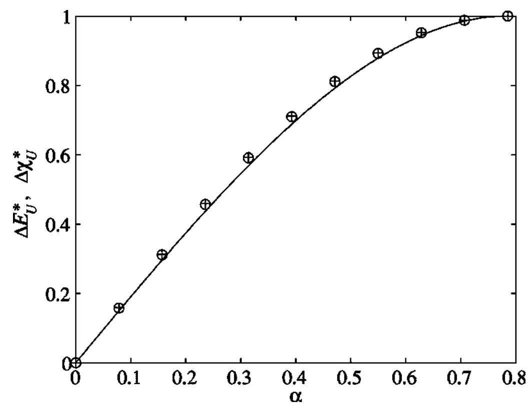


FIG. 4. Capacities with arbitrary initial states or ensembles for the operation $U_1$. The values of $\Delta E^{(1)}_U$ and $\Delta E^{(2)}_U$ are shown as the solid line, and the values of $\Delta\chi^{(2,1)}_U$ and $\Delta\chi^{(2,2)}_U$ are shown as the circles and plusses, respectively.

The capacities $\Delta\chi^*_U$ without ancilla and with ancillas of dimension 2 are shown in Fig. 4. In both cases these capacities are for ensembles with two states. It was found that, even without ancilla, the capacity $\Delta\chi^*_U$ is greater than the values calculated for $\Delta E^*_U$. The only cases where there is equality are the trivial cases where $\alpha=0$ or $\pi/4$. These results strongly indicate that, for some unitary operations, there is the strict inequality $\Delta\chi_U > \Delta E_U$.

In addition, the capacity $\Delta\chi^*_U$ is slightly increased by adding an ancilla. This is not so visible in Fig. 4; to make this difference visible, the differences between the capacities $\Delta\chi^*_U$ with ancilla and the capacities with no ancilla $\Delta\chi^{(2,1)}_U$ are plotted in Fig. 5. It can be seen that there is a small but significant increase in $\Delta\chi^*_U$ when an ancilla is allowed.

There are further increases as the ancilla dimension is increased to 3, 4, or 5 (see Fig. 6). These results suggest that there is no finite ancilla dimension for which the capacity is equal to the asymptotic capacity $\Delta\chi_U$. However, each increase in the capacity with the ancilla dimension is smaller than the previous, indicating that the results calculated here should be a good approximation of $\Delta\chi_U$.

Calculations were also performed with four-dimensional ancillas and four states in the ensemble, and without ancillas

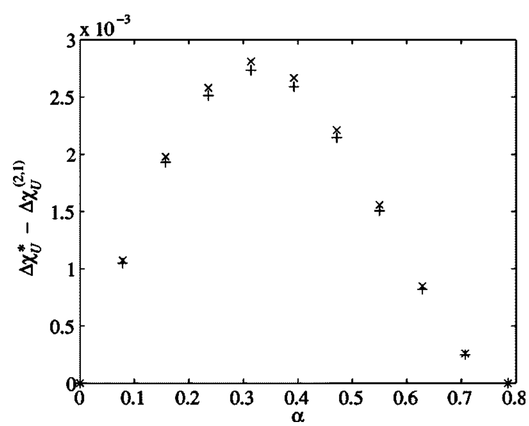


FIG. 5. The differences between $\Delta\chi^*_U$ and $\Delta\chi^{(2,1)}_U$ for the operation $U_1$. The values of $\Delta\chi^{(2,2)}_U-\Delta\chi^{(2,1)}_U$ and $\Delta\chi^{(2,3)}_U-\Delta\chi^{(2,1)}_U$ are shown as the plusses and crosses, respectively.

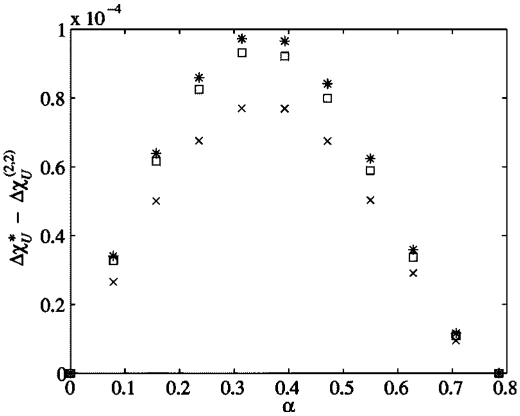


FIG. 6. The differences between $\Delta\chi_U^*$ and $\Delta\chi_U^{(2,2)}$ for the operation $U_1$. The values of $\Delta\chi_U^{(2,3)}-\Delta\chi_U^{(2,2)}$, $\Delta\chi_U^{(2,4)}-\Delta\chi_U^{(2,2)}$, and $\Delta\chi_U^{(2,5)}-\Delta\chi_U^{(2,2)}$ are shown as the crosses, squares, and asterisks, respectively.

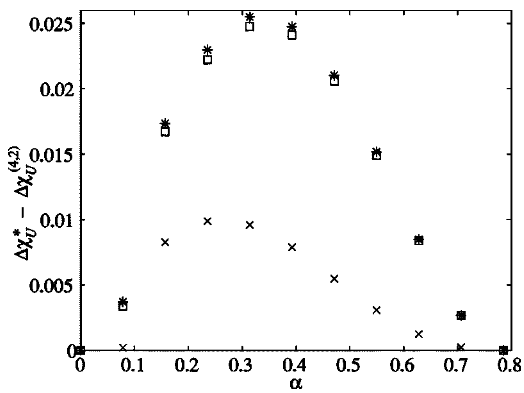


FIG. 8. The differences between $\Delta\chi_U^*$ and $\Delta\chi_U^{(4,2)}$ for the operation $U_2$. The values of $\Delta\chi_U^{(4,3)}-\Delta\chi_U^{(4,2)}$, $\Delta\chi_U^{(4,4)}-\Delta\chi_U^{(4,2)}$, and $\Delta\chi_U^{(4,5)}-\Delta\chi_U^{(4,2)}$ are shown as the crosses, squares, and asterisks, respectively.

and eight states in the ensemble. In both cases it was found that there was no increase in the capacity above that for two states in the ensemble.

The results for $\Delta\chi_U^*$ and $\Delta E_U^*$ for the operation $U_2$ are shown in Fig. 7. In each case shown, ensembles with four states were used. In the case without ancilla, it was found that $\Delta\chi_U^{(4,1)}$ and $\Delta E_U^{(1)}$ were equal. When an ancilla is included, there is a significant increase in both $\Delta\chi_U^*$ and $\Delta E_U^*$. In particular, these have a maximum of 2, rather than 1 as in the case without ancilla.

Note also that the value of $\Delta E_U^*$ is increased when an ancilla is added for each of the values of $\alpha$ except the trivial points at $\alpha=0$ and $\pi/4$. In contrast, for the data shown in Ref. [6] there was no visible increase in $\Delta E_U^*$ when the ancilla was included for another three data points (at $\alpha=\pi/40$, $2\pi/40$, and $3\pi/40$). The data points given in Ref. [6] appear to correspond to the local maximum for the solution with no ancilla, rather than the global maximum.

It was found that using ancilla dimensions above 2 up to an ancilla dimension of 5 did not increase $\Delta E_U^*$, in agreement with Ref. [6]. When the ancilla was included, $\Delta\chi_U^*$ was slightly greater than $\Delta E_U^*$, just as in the case of the operation $U_1$. In addition, it was found that $\Delta\chi_U^*$ was further increased as the ancilla dimension was increased beyond 2 (see Fig. 8). In this case the difference is somewhat greater, being around 0.02 rather than $10^{-4}$, but the values still appear to be converging for large ancilla dimension. Calculations were also performed for an ancilla dimension of 2 and an ensemble size of 8. It was found that no increases in $\Delta\chi_U^*$ were obtained with this increase in the ensemble size.

The results for $U_3$ are shown in Figs. 9 and 10. All results here are for ensembles with four states. In this case it was found that, if the ancillas had dimension 2, the values of $\Delta\chi_U^{(4,2)}$ and $\Delta E_U^{(2)}$ were identical. In other respects the results were similar to those for the operation $U_2$. The value of $\Delta E_U^*$ was not increased by increasing the ancilla dimension above 2, as for the operations $U_1$ and $U_2$. The value of $\Delta\chi_U^*$ was increased for larger ancilla dimensions, so for these larger ancilla dimensions $\Delta\chi_U^*$ was not equal to $\Delta E_U^*$. Also, for an ancilla dimension of 2, there was no increase in $\Delta\chi_U^*$ when the ensemble size was increased to 8.

To summarize, our results strongly indicate that $\Delta\chi_U$ is strictly greater than $\Delta E_U$ for most two-qubit unitary opera-

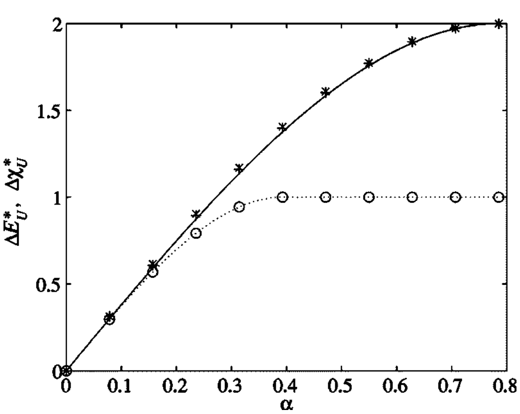


FIG. 7. Capacities with arbitrary initial states or ensembles for the operation $U_2$. The values of $\Delta E_U^{(1)}$ and $\Delta E_U^{(2)}$ are shown as the dotted and solid lines, respectively, and the values of $\Delta\chi_U^{(4,1)}$, $\Delta\chi_U^{(4,2)}$, and $\Delta\chi_U^{(4,3)}$ are shown as the circles, plusses, and crosses, respectively.

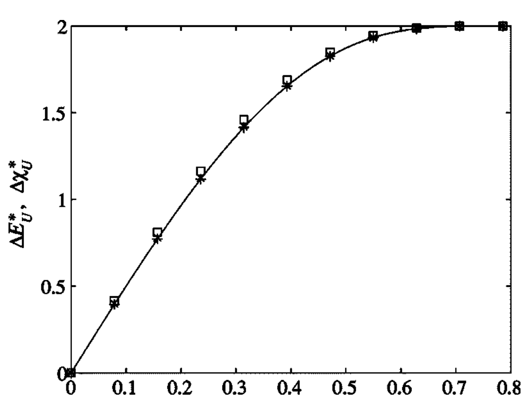


FIG. 9. Capacities with arbitrary initial states or ensembles for the operation $U_3$. The values of $\Delta E_U^{(2)}$ are shown as the solid line, and the values of $\Delta\chi_U^{(4,2)}$, $\Delta\chi_U^{(4,3)}$, and $\Delta\chi_U^{(4,4)}$ are shown as the plusses, crosses, and squares, respectively.

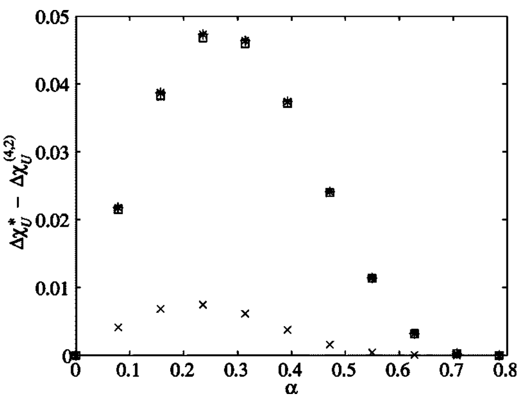


FIG. 10. The differences between $\Delta\chi_U^*$ and $\Delta\chi_U^{(4,2)}$ for the operation $U_3$. The values of $\Delta\chi_U^{(4,3)}-\Delta\chi_U^{(4,2)}$, $\Delta\chi_U^{(4,4)}-\Delta\chi_U^{(4,2)}$, and $\Delta\chi_U^{(4,5)}-\Delta\chi_U^{(4,2)}$ are shown as the crosses, squares, and asterisks, respectively.

tions, rather than simply greater than or equal to, as was shown in Refs. [14,15]. Nevertheless, for the operations we have examined, the values calculated for $\Delta\chi_U$ are quite close to $\Delta E_U$. In addition, our results show that there are no increases in $\Delta E_U^*$ as the ancilla dimension is increased above 2, but there are increases in $\Delta\chi_U^*$. In each case, there were increases in $\Delta\chi_U^*$ with ancilla dimension up to the largest dimension tested. These were small increases, indicating that the asymptotic value $\Delta\chi_U$ was approximated accurately for the larger ancilla dimensions used. Also the calculations indicate that $\Delta\chi_U^*$ is not increased as the ensemble size is increased above 4, so it is not necessary to use arbitrarily large ensemble sizes in estimating $\Delta\chi_U$.

## VII. CONCLUSIONS

We have shown that, for a range of two-qubit unitary operations, the values of the capacities $\chi_U$ and $\Delta\chi_U$ are close to $E_U$ and $\Delta E_U$, respectively. In no case was there a difference larger than 0.05, and in most cases $\chi_U$ was equal to $E_U$. This result supports Conjecture 2 made in the introduction. From these results, it is reasonable to posit an accuracy in the approximation of 5% of log $d$. Here the log $d$ takes account of the fact that the maximum capacity of two-qudit operations scales as log $d$.

We have also shown that, for the capacity $\chi_U$, ancilla dimensions of 2 are not sufficient to accurately estimate the capacity. The results indicate that the capacity is achieved with ancillas of dimension 4. For $\Delta\chi_U$, there were further increases in the capacity with the ancilla dimension above 4, though these differences were very small. In both cases, the results indicate that an ensemble size of 4 is sufficient to calculate the capacity. Also, the results indicate that an ancilla dimension of 2 is sufficient for $\Delta E_U$. These results are summarized in Table I. Thus we find that the results support a modified version of Conjecture 1:

*Conjecture 1′*. For a unitary operation $U$ that acts upon two subsystems of dimension $d$, the Holevo capacities may be estimated accurately using ancillas of dimension $d^2$ and ensembles with $d^2$ states.

TABLE I. The ensemble sizes and ancilla dimensions required for exactly calculating various capacities for two-qubit unitary operations as indicated by the numerical results.

| Capacity | Ensemble size | Ancilla dimension |
|---|---|---|
| $E_U$ | NA | 2 [12] |
| $\chi_U$ | 4 | 4 |
| $\Delta E_U$ | NA | 2 |
| $\Delta\chi_U$ | 4 | $\geqslant 5$ |

Judging from the numerical results, it would be reasonable to posit an accuracy of 1% of log $d$.

In previous work [14,15] it was proven that $\Delta\chi_U \geqslant \Delta E_U$ for two-qubit unitaries; here we have shown that $\chi_U \geqslant E_U$. As part of this derivation we have shown numerically that the maximum final entanglement is obtained for one of two initial states. We have not proven this result, because it is not possible to completely search the entire space of two-qubit operations. However, we have performed a sufficiently thorough search that it is highly unlikely that there is a counterexample.

In the case of capacities where the initial states are unentangled, it is possible to derive further analytic results. We have proven that, in general, $\chi'_U \leqslant E_U$ and $\Delta\chi'_U \leqslant \Delta E_U$, and in the specific case of controlled-$U$ operations $\chi'_U = E_U$ and $\Delta\chi'_U = \Delta E_U$. That is, we have proven that Conjecture 2 holds for these capacities in the case of controlled-$U$ operations. In addition, in the case of $\chi'_U$, Conjecture 1 can be proven to hold. It is possible to obtain the capacity $\chi'_U$ for a two-qudit operation with an ancilla of size $d$ for Bob, no ancilla for Alice and $d^2$ states in the ensemble.

It must be emphasized that there is an inherent uncertainty in the numerical results. It is possible, though unlikely, that there is a significant change in the capacity for larger ensemble sizes or ancilla dimensions than have been tested here. Also, the numerical maximization is not guaranteed to find the global maximum. Nevertheless, it is reasonable to conclude from the numerical results presented here that, for a range of two-qubit unitaries, the capacities for creating entanglement and performing communication are numerically close. It is already known that there are some connections between these capacities [14,15]; the fact that there is numerical agreement suggests that there may be further relations. Further work on analytically deriving relations is desirable but challenging.

## ACKNOWLEDGMENTS

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## APPENDIX: ENSEMBLE SIZE AND ANCILLA DIMENSION LIMITS

Let us consider the ensemble $\mathcal{E}=\{p_i,|\psi_i\rangle_{AB}\}$. We may use this ensemble for any of the capacities $\chi'_U$, $\Delta\chi'_U$, $\chi_U$, or $\Delta\chi_U$.

These capacities differ only in the restriction on the initial ensemble. In each case, the change in the Holevo information is

$$S(\mathrm{Tr}_{A_U} U\bar{\rho}U^\dagger) - S(\mathrm{Tr}_{A_U} \bar{\rho}) - \sum_i p_i[S(\mathrm{Tr}_{A_U} U\rho_i U^\dagger) - S(\mathrm{Tr}_{A_U} \rho_i)], \quad \text{(A1)}$$

where $\rho_i = \mathrm{Tr}_{A_{\mathrm{anc}}} |\psi_i\rangle_{AB}$ and $\bar{\rho} = \Sigma_i p_i \rho_i$.

If the number of states in the ensemble is less than $(d_{A_U} d_B)^2$, then it is possible to find an ensemble that has a smaller number of states and gives a change in the Holevo information that is at least as large. To show this result, from Caratheodory's theorem [22] it is possible to form a convex combination of no more than $(d_{A_U} d_B)^2$ of the $\rho_i$ to obtain $\bar{\rho}$. That is,

$$\bar{\rho} = \sum_{i \in S} q_i \rho_i, \quad \text{(A2)}$$

where $S$ is a set of no more than $(d_{A_U} d_B)^2$ indices. Now let us define $r = \min_{i \in S} p_i / q_i$ and

$$p_i' = \begin{cases} \dfrac{p_i - r q_i}{1 - r} & \text{for } i \in S \\ \dfrac{p_i}{1 - r} & \text{for } i \notin S \end{cases}. \quad \text{(A3)}$$

There must be at least one value of $i$ for which $p_i'$ is zero; we denote the set of indices for which $p_i'$ is nonzero by $S'$. Also, it is clear that

$$\bar{\rho} = \sum_{i \in S'} p_i' \rho_i. \quad \text{(A4)}$$

Therefore there are two ensembles $\mathcal{E}_1 = \{q_i, \rho_i\}$ and $\mathcal{E}_2 = \{p_i', \rho_i\}$, that give the same $\bar{\rho}$, and both of these ensembles have fewer states than the original ensemble $\mathcal{E}$.

The change in Holevo information for the original ensemble may be written as

$$\begin{aligned} \chi(U\mathcal{E}) - \chi(\mathcal{E}) &= S(\mathrm{Tr}_{A_U} U\bar{\rho}U^\dagger) - S(\mathrm{Tr}_{A_U} \bar{\rho}) \\ &\quad - \sum_i p_i[S(\mathrm{Tr}_{A_U} U\rho_i U^\dagger) - S(\mathrm{Tr}_{A_U} \rho_i)] \\ &= S(\mathrm{Tr}_{A_U} U\bar{\rho}U^\dagger) - S(\mathrm{Tr}_{A_U} \bar{\rho}) \\ &\quad - r\sum_{i \in S} q_i[S(\mathrm{Tr}_{A_U} U\rho_i U^\dagger) - S(\mathrm{Tr}_{A_U} \rho_i)] \\ &\quad - (1 - r)\sum_{i \in S'} p_i'[S(\mathrm{Tr}_{A_U} U\rho_i U^\dagger) - S(\mathrm{Tr}_{A_U} \rho_i)] \\ &= r[\chi(U\mathcal{E}_1) - \chi(\mathcal{E}_1)] + (1 - r)[\chi(U\mathcal{E}_2) - \chi(\mathcal{E}_2)]. \end{aligned} \quad \text{(A5)}$$

Thus the change in Holevo information for $\mathcal{E}$ is a weighted average of that for $\mathcal{E}_1$ and $\mathcal{E}_2$. At least one of these must give a change in Holevo information that is as large as that for $\mathcal{E}$. Hence we can find an ensemble that has fewer members, and gives a change in Holevo information that is at least as large. By iterating this procedure, we can obtain an ensemble that has no more than $(d_{A_U} d_B)^2$ states, but gives a change in Holevo information that is at least as large as that for the original ensemble. Therefore it is only necessary to consider ensembles with no more than $(d_{A_U} d_B)^2$ states.

In the case of the capacity $\chi_U'$, the states in the ensemble are $|\psi_i\rangle_{AB} = |\phi_i\rangle_A |\chi\rangle_B$. We use the notation $\bar{\rho}^A = \mathrm{Tr}_B \bar{\rho}$ and $\rho_i^A = \mathrm{Tr}_B \rho_i$. The density $\rho_i^A$ may be expressed as

$$\rho_i^A = \sum_j q_{ij} |\phi_{ij}\rangle_{A_U} \langle \phi_{ij}|. \quad \text{(A6)}$$

The final Holevo information is then

$$\begin{aligned} & S[\mathrm{Tr}_{A_U} U(\bar{\rho}^A \otimes |\chi\rangle_B\langle\chi|)U^\dagger] - \sum_i p_i S[\mathrm{Tr}_{A_U} U(\rho_i^A \\ &\quad \otimes |\chi\rangle_B\langle\chi|)U^\dagger] \\ &\leq S[\mathrm{Tr}_{A_U} U(\bar{\rho}^A \otimes |\chi\rangle_B\langle\chi|)U^\dagger] \\ &\quad - \sum_{ij} p_i q_{ij} S(\mathrm{Tr}_{A_U} U|\phi_{ij}\rangle_{A_U} |\chi\rangle_B). \end{aligned} \quad \text{(A7)}$$

Therefore at least as large a capacity may be obtained using $|\phi_i\rangle_A$ that are not entangled between $\mathcal{H}_{A_U}$ and $\mathcal{H}_{A_{\mathrm{anc}}}$. That is, one may consider states $|\phi_i\rangle_{A_U}$ within $\mathcal{H}_{A_U}$, and omit Alice's ancilla entirely. Also, it is clear that the ancilla for Bob need have dimension no larger than $d_{B_U}$. This is because the Schmidt decomposition of $|\chi\rangle_B$ can have no more than $d_{B_U}$ terms.

Using Caratheodory's theorem, the density $\bar{\rho}^A$ may be expressed as a convex combination of no more than $d_{A_U}^2$ of the $|\phi_i\rangle_{A_U}$. Therefore via exactly the same reasoning as in the general case above, the ensemble in this case need have no more than $d_{A_U}^2$ states.

Similar considerations hold for $\Delta\chi_U'$. The states in the ensemble are $|\psi_i\rangle_{AB} = |\phi_i\rangle_A |\chi_i\rangle_B$, and the change in Holevo information is

$$\begin{aligned} & S(\mathrm{Tr}_{A_U} U\bar{\rho}U^\dagger) - S(\mathrm{Tr}_{A_U} \bar{\rho}) \\ &\quad - \sum_i p_i S[\mathrm{Tr}_{A_U} U(\rho_i^A \otimes |\chi_i\rangle_B\langle\chi_i|)U^\dagger] \\ &\leq S(\mathrm{Tr}_{A_U} U\bar{\rho}U^\dagger) - S(\mathrm{Tr}_{A_U} \bar{\rho}) \\ &\quad - \sum_{ij} p_i q_{ij} S(\mathrm{Tr}_{A_U} U|\phi_{ij}\rangle_{A_U} |\chi_i\rangle_B). \end{aligned} \quad \text{(A8)}$$

Therefore it is again possible to omit the ancilla for Alice. The situation is more complicated for Bob's ancilla, due to the multiple states $|\chi_i\rangle_B$. In this case it does not appear to be possible to place a limit on the dimension required for the ancilla.

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