Non-Additivity of the Entanglement of Purification 
(Beyond Reasonable Doubt)

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We demonstrate the convexity of the difference between the regularized entanglement of purification and the entropy, as a function of the state. This is proved by means of a new asymptotic protocol to prepare a state from pre-shared entanglement and by local operations only.

We go on to employ this convexity property in an investigation of the additivity of the (single-copy) entanglement of purification: using numerical results for two-qubit Werner states we find strong evidence that the entanglement of purification is different from its regularization, hence that entanglement of purification is not additive.

I. INTRODUCTION

It is well understood that entanglement plays a key role in quantum information science. The best known applications of quantum entanglement, like superdense coding\textsuperscript{1} and quantum teleportation\textsuperscript{2}, demonstrate this amply. The theory of quantum entanglement, which aims at quantifying entanglement, has been developed greatly during the past several decades. For a bipartite pure state \(\psi^{AB} = |\psi\rangle\langle\psi|^{AB}\), the von Neumann entropy of the reduced state, \(S(A) = -\text{Tr}\,\psi^{A}\log\psi^{A}\) provides the unique measure of entanglement where \(\psi^{A} = \text{Tr}_{B}|\psi\rangle\langle\psi|^{AB}\). It is denoted \(E(\psi)\), and this number quantifies the asymptotically faithful conversion rate of many copies of \(\psi\) into maximally entangled qubit pairs, and vice versa\textsuperscript{3}. For mixed state, this asymptotic reversibility is lost, in general the so-called distillable entanglement is strictly smaller than the entanglement cost; see the recent survey\textsuperscript{4} for these facts and pointers to the vast literature on entanglement quantification.

Motivated by entanglement theory, Terhal et al.\textsuperscript{5} proposed a measure of total (i.e. encompassing both quantum and classical) correlations in a quantum state, called entanglement of purification.

**Definition 1** Given a bipartite density matrix \(\rho^{AB}\) on \(A\otimes B\), the entanglement of purification (EoP) is

\[
E_P(\rho) := \min E \left( |\psi\rangle\langle\psi|^{AA':BB'} \right)
\]

s.t. \(\psi^{AA'BB'}\) purification of \(\rho^{AB}\),

where \(E \left( |\psi\rangle\langle\psi|^{AA':BB'} \right) = S(\text{Tr}_{B}|\psi\rangle\langle\psi|^{AB})\) is the entanglement of the pure state \(\psi\) across the bipartite cut \(AA' : BB'\).

That the above is really a minimum and not just an infimum follows from the fact that w.l.o.g. the dimensions of \(A'\) and \(B'\) are bounded in terms of \(|A|\) and \(|B|\)\textsuperscript{5}. Indeed, in\textsuperscript{6} it was shown that one may assume

\[|A'|, |B'| \leq \text{rank} \rho^{AB} \leq |A||B|.\]

Entanglement of purification is a genuine measure of total correlation in a bipartite state: it is non-negative, vanishes precisely on the product states \(\rho^{AB} = \rho^{A}\otimes \rho^{B}\) (which are the only states without any correlations), and is non-increasing under local operations. Also, it is known to be asymptotically continuous\textsuperscript{5}. Furthermore, it has an operational interpretation as a cost measure. Namely, it was shown in\textsuperscript{5} that the entanglement cost of preparing many copies of a bipartite state \(\rho^{AB}\), with the restriction that only a vanishing rate of communication is allowed, denoted \(E_{\text{LO}}(\rho)\), equals the regularized entanglement of purification:

\[
E_{\text{LO}}(\rho) = \lim_{n \to \infty} \frac{1}{n}E_P(\rho^{\otimes n}) = : E_P(\rho).
\]

(That a communication \(\Theta(\sqrt{n})\) is sufficient and necessary, even for pure states, was shown by Lo and Popescu\textsuperscript{7} and in\textsuperscript{8,9}.)

Hayashi proved that the optimal visible compression rate for mixed states is equal to \(E_P^\infty\) of a state associated to the ensemble\textsuperscript{10}. More generally, the regularized entanglement of purification characterizes the communication cost of simulating a channel without prior entanglement\textsuperscript{11} (in contrast to the Quantum Reverse Shannon Theorem). Furthermore, in\textsuperscript{12} Theorem 2\textsuperscript{12} entanglement of purification, or rather its regularization, was linked to the maximum advantage a given mixed state yields in dense coding.

However, it is not known how to evaluate the regularized entanglement of purification. As a matter of fact, it is still an open question whether entanglement of purification is additive, i.e.

\[
E_P(\rho^{A_1B_1} \otimes \sigma^{A_2B_2}) \geq E_P(\rho^{A_1B_1}) + E_P(\sigma^{A_2B_2}).
\]

Clearly, a positive answer to this question would imply \(E_P^\infty = E_P\), and thus a single-letter formula for \(E_{\text{LO}}(\rho)\).
Recently, several similar-looking entanglement quantities and capacity-like measures were shown to be non-additive \[13,17\], and so one might speculate that the answer to the above question is negative, too. However, these constructions do not seem to imply anything directly for entanglement of purification.

**Remark 2** \[E_P(\psi^{AB}) = S(\psi)\] for pure states \(\psi = |\psi\rangle|\psi\rangle\), and on product states, \(E_P(\rho^A \otimes \rho^B) = 0\), so additivity holds for these two classes \[3\].

In \[18\] it was shown more generally that \(E_P(\rho^{AB}) = S(\rho^A)\) whenever the (pure or mixed) state \(\rho\) is supported either on the antisymmetric or the symmetric subspace of \(A \otimes B\), with \(|A| = |B|\). So additivity holds for all such states, too.

In the present paper, we prove results which strongly suggest that entanglement of purification may not be additive. In Section II, we will introduce a new property of the regularized entanglement of purification, which can be expressed as the convexity of the difference between regularized entanglement of purification and the entropy of the state, \(E^{\infty}_P(\rho) - S(\rho)\). Then, in section III we investigate numerically the functional \(\rho^A \chi\) where \(E\) for the one-parameter family of Werner states on two qubits: since we find that the latter is not convex, we conclude (except for gross numerical error) that entanglement of purification is different from its regularization. Indeed, our convexity result implies an upper bound on \(E^{\infty}_P\) which is much smaller than our best estimate for \(E_P\) on certain Werner states. Finally, in section IV we conclude, highlighting some open questions.

II. A CONVEXITY PROPERTY OF REGULARIZED ENTANGLEMENT OF PURIFICATION

Here we state our main result, a new property of the regularized entanglement of purification:

**Theorem 3** For a decomposition \(\rho^{AB} = \sum p_i \rho_i^{AB}\) as an ensemble of possibly mixed states \(\rho_i\),

\[
E^{\infty}_P(\rho^{AB}) \leq \sum p_i E^{\infty}_P(\rho_i^{AB}) + \chi(\{p_i; \rho_i\}),
\]

where \(\chi = \chi(\{p_i; \rho_i\}) = S(\sum p_i \rho_i) = \sum p_i S(\rho_i)\) is the Holevo information (cf. \[19\]).

**Proof** We shall describe an asymptotic protocol for creating \(\rho^TN\), using asymptotically optimal ways of generating \(\rho_i^{\delta k}\) (with \(k_i \approx n p_i\)) as subroutines. In the protocol, the term \(\sum p_i E^{\infty}_P(\rho_i^{AB})\) will be naturally visible as the rate of entanglement used, while \(\chi(\{p_i; \rho_i\})\) will emerge as the rate of classical shared randomness (which of course can be obtained from entanglement at rate 1 by measuring).

To be specific, we have

\[
\rho^TN = \sum_{i^n=1,2,\ldots,n} p_i^n \rho_i^n,
\]

with \(p_i^n = p_{i_1} p_{i_2} \cdots p_{i_n}\) and \(\rho_i^n = \rho_{i_1} \otimes \rho_{i_2} \otimes \cdots \otimes \rho_{i_n}\). For a string \(i^n = i_1 i_2 \cdots i_n\) let \(k(i|i^n)\) count the number of occurrences of \(i\). Then, define the set of typical indices,

\[
T := \{i^n : \forall i \; |k(i|i^n) - p_i n| \leq \delta n\}.
\]

Below we outline the argument to show that there exists a family of indices, \(i^n(1), \ldots, i^n(K) \in T, K = 2^{n(\chi + \delta)}\), such that

\[
\rho^TN \approx \sum_{j=1}^K \frac{1}{K} \rho^{i^n(j)},
\]

the approximation being asymptotically perfect in trace norm. Then the protocol to create \(\rho^TN\) goes as follows: The two parties use \(n(\chi + \delta)\) qubits to create the same number of shared random bits; these are used to sample a uniformly random \(i^n(j), j = 1, \ldots, K\). Then for each \(i\), they invoke the given protocols to generate \(k_i = k_i(i^n)\) copies of \(\rho_i\) using \(k_i(E^{\infty}_P(\rho_i) + \delta)\) qubits and \(\text{LO}_{q_i}\), thus creating an approximation to \(\rho^{i^n(j)}\). The total entanglement consumption of this protocol is

\[
\leq n(\chi + \delta) + n \sum_i p_i E^{\infty}_P(\rho_i) + n \delta + n \delta \log |A|,
\]

which is what we want, since \(\delta > 0\) can be made arbitrarily small.

The set \(\{i^n(1), \ldots, i^n(K)\}\) is shown to exist by the probabilistic method: Indeed, we draw the \(i^n(j)\) i.i.d. according to the distribution \(q_i^n := \frac{1}{2^n} p_i^n\) on \(T\), with \(Q = p^n(T)\) the probability of finding a random string \(i^n\) in the set \(T\). The core part of the proof of the main theorem in \[20\] (Theorem 2, specifically p. 163) shows that this works. The same technique was used again in \[21\] Proposition 2, incidentally in a different attempt to quantify total correlations in a quantum state. Here we give only a summary outline.

We need to introduce some more “typicality” notation (cf. \[19\] for more details and properties of these notions): The typical projector \(\Pi^TN\) of \(\rho^TN\) is

\[
\Pi := \left\{ a^{-n S(\rho) - \delta'} n \leq \rho^n n \leq a^{-n S(\rho) + \delta'n} \right\},
\]

the spectral projector corresponding to the typical eigenvalues of \(\rho^TN\). Finally, the conditional typical projectors \(\Pi_{i^n}\) of the states \(\rho_{i^n} = \rho_{i_1} \otimes \rho_{i_2} \otimes \cdots \otimes \rho_{i_n}\),

\[
\Pi_{i^n} := \left\{ a^{-n S - \delta' n} \leq \rho^n \leq a^{-n S + \delta' n} \right\},
\]

where \(S = \sum_i p_i S(\rho_i)\). Consider now the operators

\[
\rho_{i^n} := \Pi \Pi_{i^n} \Pi_{i^n} \Pi,\]

which have the property that for every \(\delta' > 0\) one can choose \(\delta > 0\), such that for large enough \(n\) and all \(i^n \in T\), \(\|\rho_{i^n} - \rho_{i^n}^N\|_1 \leq o(1)\). Thus,

\[
\rho_{i^n}' := \sum_{i^n \in T} q_{i^n} \rho_{i^n},
\]
is supported on the typical subspace and defined such that \(\|\rho^{\otimes n} - \rho^{(n)}\|_1 \leq o(1)\). Define
\[
\Pi' := \left\{ \rho^{(n)I} \geq \frac{\epsilon}{\text{Tr} \, \Pi'} \right\}
\]
as the spectral projector corresponding to the "large" eigenvalues of \(\rho^{(n)I}\).

In other words, this concludes the proof.

Finally let
\[
\tilde{\rho} := \Pi' \rho^{(n)} \Pi' = \sum_{i^n \in T} q_{i^n} \sigma_{i^n},
\]
with \(\sigma_{i^n} = \Pi' \rho^{(n)} \Pi'\).

Now, observe that, restricted to the support of \(\Pi'\), and for \(i^n \in T\),
\[
\tilde{\rho} \geq 2^{-nS(\rho) - S' n} \Pi',
\]

\[
\sigma_{i^n} \leq 2^{-nS + S'} n.
\]

In this situation we can apply the operator sampling lemma in [22] and conclude that with high probability, \(i^n(1), \ldots, i^n(K) \in \mathcal{T}\) are such that for large enough \(n\), \(K \leq 2^{n(x + 3d)}\) and
\[
\left\| \frac{1}{K} \sum_{j=1}^{K} \sigma_{i^n} - \tilde{\rho}^{(n)} \right\|_1 \leq o(1),
\]
hence similarly the same for the distance of the analogous sum over the \(\rho^{(n)}_{i^n}\), from \(\rho^{\otimes n}\). Since \(\delta' > 0\) was arbitrary, this concludes the proof. \(\square\)

For our present purposes, we rearrange the terms in the above theorem:

**Corollary 4** For \(\rho^{AB} = \sum p_i \rho_i^{AB}\),
\[
E^\infty_P (\rho^{AB}) - S(\rho^{AB}) \leq \sum_i p_i \left( E^\infty_P (\rho_i^{AB}) - S(\rho_i^{AB}) \right)
\]

In other words, \(E^\infty_P (\rho) - S(\rho)\) is a convex function of \(\rho\). \(\square\)

Thus if we can find some examples to show \(E_P(\rho) - S(\rho)\) is not convex on quantum states, then \(E^\infty_P\) can not be equal to \(E_P\), which will prove that \(E_P\) is not additive on some states. In the following section, we will present the numerical results for two-qubit Werner states (replicating essentially the study of [3]), which indicate that entanglement of purification is not additive.

### III. TWO-QUBIT WERNER STATES

Here we are considering the two-qubit Werner states, arguably the simplest family of states not covered by the additivity results mentioned in Remark 2.

\[ W(f) := f \Psi_0 + (1 - f) \frac{1}{3} (\mathbb{1} - \Psi_0), \]

with the maximally entangled singlet state \(\Psi_0\) and \(0 \leq f \leq 1\) (the singlet fraction).

Already in the original EoP paper [3], the authors performed a numerical minimization with \(|A'|, |B'| \leq 4\), which thanks to [6] we know to be sufficient to find \(E_P(W(f))\) – see Fig. 1. One way of looking at the minimization that one has to perform is as follows: Diagonalizing the state, \(\rho = \sum_{i=0}^{4} \lambda_i |\Psi_i\rangle \langle \Psi_i|\), where \(|\Psi_i\rangle\) are the four Bell states, starting with the singlet \(|\Psi_0\rangle\), and \(\lambda_0 = \epsilon, \lambda_1 = \lambda_2 = \lambda_3 = \frac{1-\epsilon}{3}\). Then we can write a standard purification
\[
|\varphi\rangle^{ABA'} = \sum_{i=0}^{4} \sqrt{\lambda_i} |\Psi_i\rangle^{AB} |i\rangle^{A'},
\]
and any other purification \(|\psi\rangle \in ABA' B'\) of \(\rho^{AB}\) we can obtain as
\[
|\psi\rangle^{ABA' B'} = (\mathbb{1}^{AB} \otimes V)|\varphi\rangle^{ABA'},
\]
with an isometry \(V : A' \leftrightarrow A'B'\), described by 64 complex numbers (subject to normalization and orthogonality constraints, effectively leaving 30 + 29 + 27 + 25 = 121 independent real parameters). Note that one could extend the isometry to a unitary \(U\) on \(ABA' B'\), with \(U|\phi\rangle^{A0B'} = V|\phi\rangle\) – however, this introduces a large number of spurious variables, in fact more than doubling them to 256, which have no impact on the objective function.

The graph shows an apparent – concave! – kink (discontinuity of the first derivative) at \(f \approx .005\). Note that if the kink was real, we had achieved our goal, since the entropy \(S(W(f))\) is a smooth function on the open interval \((0, 1)\), hence the difference \(\Delta(f) = E_P(W(f)) - S(W(f))\) could not possibly be convex as a function of \(f\).

Motivated by this observation, we did a re-calculation for \(0 \leq f \leq .01\). This revealed that the first regime, where \(E_P(W(f)) \approx 1\), is smaller than it was observed in [3]; the range we determined is about \([0, .004]\) [23], although the deviation is tiny. However, we still see the change from a regime where the function is almost constant 1 to one where it decreases sharply with \(f\). In Fig. 2, we show \(\Delta(f)\) and one can see that indeed it is not convex.

We should point out that by using standard minimization algorithms (local descent with various, usually random, starting points), we cannot calculate the exact value of entanglement of purification: What these methods give us are at best local minima. However, we can treat the local minima from numerics as upper bounds on the entanglement of purifications, since the algorithm finds concrete feasible points with certain values of the objective function to be minimized:
\[
E_P(W(0)) = 1 \quad \text{and} \quad E_P(W(.01)) \leq .9226,
\]
showing via theorem 3 that \(E^\infty_P(W(.005)) \leq .9663\).
Thus on this short interval, $E_P$ is strictly smaller than $\rho_{\infty}$, coming close to the above value of $\rho_{.005}$. A special case of its application is when $\chi((\rho_{AB}, \rho))$. This generalizes a result due to Wyner [24] (cf. [25] for a more modern account) on the creation of a bipartite distribution $P_{XY}$ by local operations (noisy channels) from limited shared randomness:

$$w(P_{XY}) = \min I(V : XY)$$

$s.t. X\rightarrow V\rightarrow Y$ is a Markov chain, where $I(V : XY) = H(XY) - H(XY|V)$ is the Shannon mutual information.

Since the theorem puts a nontrivial bound on the regularized entanglement of purification, expressed conveniently as the convexity of $E_P^{\infty} - S$, we could use it to probe the additivity of entanglement of purification. We find that, apart from the possibility of a gross numerical error, entanglement of purification is non-additive already on certain two-qubit Werner states. Interestingly, we can only say that for some sufficiently large $n$, $\frac{1}{2}E_P(\rho^{\otimes n}) < E_P(\rho)$, but our proof of theorem 3 does not yield directly an estimate for this $n$; in any case, we may expect it to be rather large.

The non-additivity of entanglement of purification also answers a question from [12]: Indeed, our results imply the non-additivity of the “quantum advantage of dense coding” on some states, via their monogamy identity [12, Theorem 2].

To come back to our Werner state example: Of course, it would be most desirable to remove the need for numerical calculation in the argument. We leave a completely rigorous proof of the non-additivity of entanglement of purification to future work; noting only that since our example is concrete, and we have a concrete benchmark,

$$E_P(W(.005)) \approx .9663,$$

this could be accomplished in principle by discretization.
and exhaustive search over the parameter space. The reason we have not done this is that such a brute force approach is too CPU intensive for practical desktop PC calculations.

In a similar vein, we would like to find explicit states $\rho$ and $\sigma$ with

$$E_p(\rho^{A_1B_1} \otimes \sigma^{A_2B_2}) \neq E_p(\rho^{A_1B_1}) + E_p(\sigma^{A_2B_2}).$$

To end, we remark that our study does not impact on the possible non-additivity of $E^\infty_p = E_{LOP}$, which we recommend to the reader as an interesting problem in itself. Even more interesting however is the problem of finding a tractable (or even “single-letter”) expression for $E^\infty_p$, which in a certain sense would generalize Wyner’s beautiful answer for the classical randomness cost of probability distributions $I_{XY}$ [24][25].

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