

Local Purity Distillation in Quantum Systems: Exploring the Complementarity Between Purity and Entanglement

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Quantum thermodynamics and quantum entanglement represent two pivotal quantum resource theories with significant relevance in quantum information science. Despite their importance, the intricate relationship between these two theories is still not fully understood. Here, we investigate the interplay between entanglement and thermodynamics, particularly in the context of local cooling processes. We introduce and develop the framework of Gibbs-preserving local operations and classical communication. Within this framework, we explore strategies enabling remote parties to effectively cool their local systems to the ground state. Our analysis is centered on scenarios where only a single copy of a quantum state is accessible, with the ideal performance defined by the highest possible fidelity to the ground state achievable under these constraints. We focus on systems with fully degenerate local Hamiltonians, where local cooling aligns with the extraction of local purity. In this context, we establish a powerful link between the efficiency of local purity extraction and the degree of entanglement present in the system, a concept we define as *purity-entanglement complementarity*. Moreover, we demonstrate that in many pertinent scenarios, the optimal performance can be precisely determined through semidefinite programming techniques. Our findings open doors to various practical applications, including techniques for entanglement detection and estimation. We demonstrate this by evaluating the amount of entanglement for a class of bound entangled states.

I. INTRODUCTION

Quantum resource theories serve as a fundamental framework for probing quantum phenomena and steering advancements in quantum technologies [1]. Foremost among these theories stand the studies of quantum entanglement [2] and quantum thermodynamics [3, 4]. The resource theory of entanglement investigates the utility of entangled quantum systems within local constraints. Conversely, the resource theory of thermodynamics assesses the potential and limitations of manipulating quantum systems when bound by energy constraints.

In any quantum resource theory, a pivotal challenge is the quantification of resources, which entails gauging the resource content in a specific quantum state. Such resource quantifiers play an integral role in determining a quantum state's aptitude for quantum information processing tasks. In the realm of entanglement quantification, it is essential that the quantifier does not increase under local operations and classical communication (LOCC) [5]. In the bipartite context, a plethora of entanglement quantifiers have been proposed, most of which can be computed efficiently for pure bipartite states [2]. However, when it comes to multipartite scenarios and noisy states, the task becomes substantially more complex, with numerous established entanglement quantifiers proving challenging to compute efficiently, even for pure states.

Concurrently, another salient issue in quantum resource theories is discerning the most efficient methods to create valuable resource states. This concern emerges from the inevitability of noise in practical implementations. Although

the crux of quantum information processing hinges on pure quantum states, the quintessential quantum state encountered in a laboratory setting is invariably noisy, stemming from unavoidable environmental interactions. Hence, it is essential to develop methodologies to convert noisy states into pure resourceful states.

In this article, we introduce the concept of *Gibbs-preserving local operations and classical communication (GLOCC)*. Specifically, these are LOCC protocols that preserve the thermal state of a bipartite or multipartite system. Within this framework, we investigate optimal procedures to cool local systems, corresponding to bringing them to their local ground state. When the local Hamiltonians are fully degenerate, Gibbs-preserving operations give rise to the resource theory of purity [6–8]. Under these conditions, the quest for local cooling mirrors the endeavor to distill pure states at the local level. We establish an intricate relationship between the locally extractable purity and entanglement amount, a phenomenon we coin as *purity-entanglement complementarity*. As a quantifier of entanglement we use geometric entanglement [9, 10], which is useful both for bipartite and multipartite entanglement quantification.

Utilizing semidefinite programming (SDP) techniques, we formulate approaches to estimate the optimal fidelity for establishing local ground states. The delineated relationship between purity and entanglement further allows our techniques to detect and quantify entanglement in numerous relevant settings, if the entanglement is quantified via geometric entanglement. In the bipartite setting, we can estimate the geometric entanglement of any rank-2 state if one of the subsystems is a qutrit, and for any rank-3 state if one of the subsystems is a qubit. Our techniques can also be used to estimate geometric entanglement of PPT entangled states and certain families of

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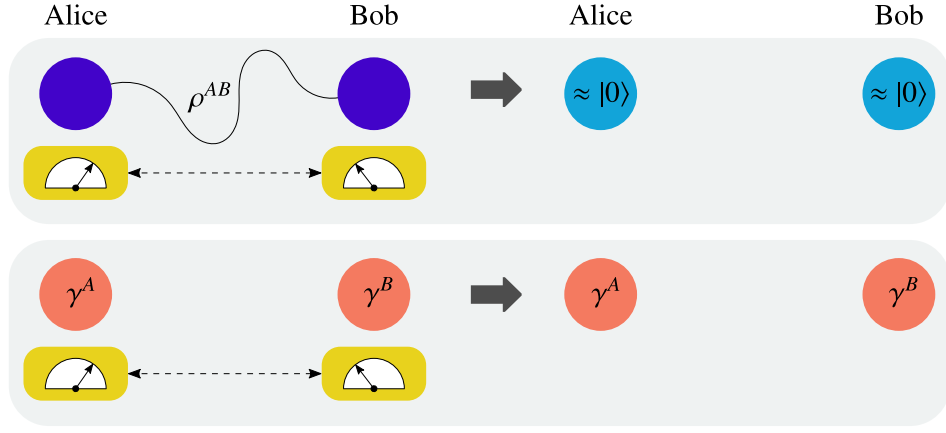


Figure 1. Local cooling of a bipartite system by local Gibbs-preserving operations and classical communication. The goal of the process is to convert an initial bipartite state ρ^{AB} into the ground state $|00\rangle$ with the maximal fidelity (upper part of the figure). The procedure preserves the total Gibbs state $\gamma^A \otimes \gamma^B$ (lower part of the figure).

multipartite pure states.

II. LOCAL COOLING WITH GIBBS-PRESERVING LOCC

In this work, we investigate a context where access is restricted to a single copy of a quantum state. We will first briefly discuss the setting for a single party. Given a quantum state ρ , our objective is to cool the system to the ground state $|0\rangle$ using Gibbs-preserving operations [11]. These are transformations which preserve the Gibbs state $\gamma = e^{-\beta H} / \text{Tr}[e^{-\beta H}]$, where H is the Hamiltonian of the system and $\beta = \frac{1}{kT}$ signifies the inverse temperature. Perfectly attaining the ground state is generally unfeasible; thus, our interest centers on maximizing the fidelity with the ground state. This optimal fidelity is defined as $\max_{\Lambda} \langle 0 | \Lambda[\rho] | 0 \rangle$, and the maximum is taken over all Gibbs-preserving operations Λ . In the presence of a fully degenerate Hamiltonian, the maximal fidelity coincides with the largest eigenvalue of ρ , denoted as $\lambda_{\max}(\rho)$.

Transitioning to a bipartite scenario involving two parties, Alice and Bob, each has local Hamiltonians H_A and H_B respectively. The collective Hamiltonian is represented as $H = H_A + H_B$. The associated Gibbs state is given by $\gamma = \gamma^A \otimes \gamma^B$, where γ^X denotes the local Gibbs state of the party X . Drawing an analogy to Gibbs-preserving operations, an LOCC protocol Λ is termed Gibbs-preserving if $\Lambda[\gamma] = \gamma$. The set of all such transformations will be denoted by GLOCC.

With local energy conceptualized as a resource, two distinct scenarios emerge. In the first scenario, Alice and Bob jointly possess a state ρ^{AB} and their objective is to jointly cool their systems to the ground state $|00\rangle$, see also Fig. 1. The figure of merit in this scenario is given by

$$F_{\max}(\rho^{AB}) = \max_{\Lambda \in \text{GLOCC}} \langle 00 | \Lambda[\rho^{AB}] | 00 \rangle. \quad (1)$$

In the second scenario, Alice teams up with Bob to cool his individual system to the ground state. The figure of merit is

then given by

$$F^{A|B}(\rho^{AB}) = \max_{\Lambda \in \text{GLOCC}} \langle 0 | \text{Tr}_A(\Lambda[\rho^{AB}]) | 0 \rangle. \quad (2)$$

For the second scenario, we will also consider the setting where the classical communication is directed from Alice to Bob only. The corresponding figure of merit will be denoted by $F_{\rightarrow}^{A|B}$.

A noteworthy situation arises when the local Hamiltonians associated with Alice and Bob are fully degenerate. Here, the Gibbs-preservation requirement equates to the LOCC protocol preserving the maximally mixed state. The task of establishing a ground state is then equivalent to extraction of local purity in this setting.

In this article, our emphasis is primarily on the single-copy scenario. However, it is noteworthy that related settings within the asymptotic regime have been explored in previous works, as detailed in references [12–14]. Single-shot purity distillation in the distributed setting has also been considered recently in [15]. For thermal operations, which is a subclass of Gibbs-preserving operations, a related setting has been considered in [16].

III. OPTIMAL EXTRACTION OF LOCAL PURITY

In the subsequent discussion, we investigate techniques to evaluate $F_{\max}$, focusing on the setting where the local Hamiltonians are fully degenerate. Under this premise, $F_{\max}$ can be succinctly represented.

Proposition 1. *When the local Hamiltonians are fully degenerate, we have*

$$F_{\max}(\rho^{AB}) = \max_{U_A, V_B} \langle 00 | U_A \otimes V_B \rho^{AB} U_A^\dagger \otimes V_B^\dagger | 00 \rangle. \quad (3)$$

Hence, to optimize fidelity with the ground state, the best strategy involves implementing local unitaries for both Alice

and Bob. This finding possesses relevance even when extended to setups with more than two parties. For a detailed exposition on this, the reader is directed to the Appendix.

A straightforward examination yields the following upper bound:

$$F_{\max}(\rho^{AB}) = \max_{\sigma^{AB} \in \text{SEP}} \text{Tr}(\rho^{AB} \sigma^{AB}) \leq \max_{\sigma^{AB} \in \text{PPT}} \text{Tr}(\rho^{AB} \sigma^{AB}), \quad (4)$$

where SEP and PPT denote separable states, and states that exhibit positive partial transpose, respectively. Note that the maximization over PPT states is feasible via SDP. If the dimensions of A and B are such that $d_A d_B \leq 6$, the inequality (4) becomes equality, due to the fact that the sets SEP and PPT coincide in these cases [17]. This allows to evaluate $F_{\max}$ in all such settings. In general, when the state $\sigma^* \in \text{PPT}$ that maximizes Eq. (4) is pure, the bound in Eq. (4) is tight.

By performing the maximization over PPT states outlined in Eq. (4) and discerning the largest eigenvalue of the optimal $\sigma^* \in \text{PPT}$, one can approximate $F_{\max}$ with high precision in various settings. Elaborating further, for $\lambda_{\max}(\sigma^*) = 1 - \varepsilon$, we establish the following proposition.

Proposition 2. *It holds that*

$$\text{Tr}(\rho \sigma^*) + \delta \geq F_{\max}(\rho) \geq \text{Tr}(\rho \sigma^*) - 4\sqrt{\varepsilon}, \quad (5)$$

where δ is the precision to which the SDP in Eq. (4) is computed numerically.

Empirically, we found that ε can often be made close to zero, which allows to evaluate $F_{\max}$ with an arbitrary precision in practice. In more detail, for bipartite system of dimension $d_A = d_B = 3$, we sampled 2×10^5 random mixed states¹, finding that in 13 cases ε was above 0.08, and in all other cases ε was below 2×10^{-9} . For systems of dimension $d_A = d_B = 4$ we sampled 2×10^5 random mixed states, finding that in 31 cases ε was above 8×10^{-4} , and in all other states ε was below 3×10^{-8} . For $d_A = d_B = 5$ we sampled 3×10^4 random mixed states, finding that for 23 of them ε was above 0.005, and for all other states ε was below 5×10^{-9} . These results also extend to the multipartite setting, we refer to the Appendix for more details, as well as the proof of the proposition.

Let us now explore the second scenario where Alice aids Bob in cooling his system to its ground state. We initially consider a framework where classical communication flows exclusively from Alice to Bob.

When Alice executes a local measurement characterized by POVM elements $\{M_i^A\}$, the probability of obtaining measurement outcome i manifests as: $p_i = \text{Tr}[M_i^A \otimes \mathbb{1}^B \rho^{AB}]$. Given Alice's measurement outcome, the resultant state of Bob's system is: $\sigma_i^B = \text{Tr}_A[M_i^A \otimes \mathbb{1}^B \rho^{AB}] / p_i$. The maximal fidelity Bob can achieve with the ground state in this setup is represented as:

$$F_{\rightarrow}^{A|B}(\rho^{AB}) = \max \sum_i p_i \lambda_{\max}(\sigma_i^B), \quad (6)$$

with the optimization extending over all ensembles $\{p_i, \sigma_i^B\}$ achievable from ρ^{AB} by Alice's measurements, and $\lambda_{\max}(\sigma)$ denoting the largest eigenvalue of σ . Collating these results, $F_{\rightarrow}^{A|B}$ is expressed as:

$$F_{\rightarrow}^{A|B}(\rho^{AB}) = \max \sum_i \text{Tr}[M_i^A \otimes \mu_i^B \rho^{AB}], \quad (7)$$

where we optimize over all POVMs $\{M_i^A\}$ and quantum states $\{\mu_i^B\}$.

While in the above analysis we assumed that Alice can perform arbitrary POVMs locally, note that Alice can implement a general POVM $\{M_i^A\}$ via a unital operation having the Kraus operators

$$K_i^A = \sqrt{M_i^A}. \quad (8)$$

Thus, optimal performance as in Eq. (7) can also be achieved via GLOCC with one-way communication.

To provide an upper bound for $F_{\rightarrow}^{A|B}$, we can state:

$$F_{\rightarrow}^{A|B}(\rho^{AB}) \leq \max_{X^{AB}} \text{Tr}[X^{AB} \rho^{AB}], \quad (9)$$

where the optimization is over all matrices X^{AB} satisfying:

$$X^{AB} \geq 0, \quad X^{T_B} \geq 0, \quad X^A = \mathbb{1}_A. \quad (10)$$

It is important to note that the right-hand side of Eq. (9) is computationally feasible via SDP. As we will see in the following, for systems of small dimension the inequality (9) is tight.

Theorem 1. *For $d_A d_B \leq 6$ it holds*

$$F_{\rightarrow}^{A|B}(\rho^{AB}) = \max_{X^{AB}} \text{Tr}[X^{AB} \rho^{AB}] \quad (11)$$

with X^{AB} fulfilling Eqs. (10).

We refer to the Appendix for the proof.

We will now turn our attention to the more general setting where classical communication is possible in both directions. For $d = d_A = d_B$ we will show that the problem is symmetric under permutation of Alice and Bob. If Alice assists Bob to extract purity, an optimal GLOCC protocol can always be assumed to produce a state of the form $\mathbb{1}/d \otimes \sigma^B$, where the state σ^B is diagonal in the computational basis. We will now show that by using GLOCC operations it is possible to convert this state into $\sigma^A \otimes \mathbb{1}/d$. Denoting the eigenvalues of σ with p_i , we have $\mathbb{1}/d \otimes \sigma = 1/d \sum_{ij} p_i |ji\rangle\langle ji|$ and $\sigma \otimes \mathbb{1}/d = 1/d \sum_{ij} p_i |ij\rangle\langle ij|$. Alice and Bob can now apply the following GLOCC protocol to convert $\mathbb{1}/d \otimes \sigma$ into $\sigma \otimes \mathbb{1}/d$. For this, Alice and Bob perform local measurements in the computational basis and send the outcome of the measurement to the other party. If Alice obtains outcome j , and Bob obtains outcome i , then Alice applies a local unitary transforming $|j\rangle$ into $|i\rangle$. Correspondingly, Bob applies a local unitary which transforms $|i\rangle$ into $|j\rangle$. It is straightforward to check that the overall transformation is GLOCC, since it preserves the total maximally mixed state. These arguments

¹ To sample a bipartite mixed state of dimension d_{AB} , we sample Haar random pure states of dimension d_{AB}^2 , and trace out a subsystem of dimension d_{AB} .

also demonstrate that two-sided communication is in general useful in the assisted setting, leading to a better performance of the local cooling procedure.

We will now present a method for approximating the optimal fidelity $F^{AB}(\rho^{AB})$, if classical communication is allowed in both directions. In a very similar way as in Eq. (9) we can obtain an upper bound for $F^{AB}(\rho^{AB})$.

Proposition 3. *It holds that*

$$F^{AB}(\rho^{AB}) \leq \max_{X^{AB}} \text{Tr}[X^{AB} \rho^{AB}], \quad (12)$$

where the optimization is over all X^{AB} satisfying

$$\mathbb{I} \geq X^{AB} \geq 0, \quad X^{T_B} \geq 0, \quad \text{Tr}[X^{AB}] = d_A. \quad (13)$$

The proof of this statement is given in the Appendix.

IV. GEOMETRIC ENTANGLEMENT AND PURITY-ENTANGLEMENT COMPLEMENTARITY

In the following, we will review the main properties of geometric entanglement, an entanglement quantifier which is applicable in both, bipartite and multipartite settings [9, 10]. For a pure n -partite state $\psi = |\psi\rangle\langle\psi|$, the multipartite geometric entanglement is defined as [9, 18–20]

$$E_g(\psi) = 1 - \max_{\phi \in \text{SEP}} |\langle\phi|\psi\rangle|^2, \quad (14)$$

where SEP denotes the set of fully separable states. For mixed states, the geometric entanglement is defined as [9]

$$E_g(\rho) = \min_i \sum_i p_i E_g(\psi_i), \quad (15)$$

where the minimum is taken over all pure state decompositions of ρ such that $\sum_i p_i \psi_i = \rho$. As has been shown in [10], E_g can also be expressed as

$$E_g(\rho) = 1 - \max_{\sigma \in \text{SEP}} F(\rho, \sigma) \quad (16)$$

with fidelity $F(\rho, \sigma) = (\text{Tr} \sqrt{\sqrt{\rho} \sigma \sqrt{\rho}})^2$. The geometric entanglement is zero for all separable states, and positive whenever the state is entangled. Moreover, E_g does not increase under LOCC [9]. Several related entanglement quantifiers for mixed states have also been proposed in the literature [21, 22].

We will now demonstrate a powerful complementarity relations, linking the amount of geometric entanglement of a quantum state to the maximal fidelity with the ground state, achievable in an assisted scenario with one-way communication.

Theorem 2. *For any pure state $|\psi\rangle^{ABC}$ it holds that*

$$F_{\rightarrow}^{AB}(\rho^{AB}) + E_g(\rho^{BC}) = 1. \quad (17)$$

The proof of the theorem can be found in the Appendix.

The results presented above provide a strong link between the task of assisted purity extraction and the geometric entanglement, and can also be seen as an operational interpretation of the geometric entanglement in a thermodynamical setting. Furthermore, this relation also holds for infinite dimensional systems.

A similar complementarity relation can also be found for the maximal local purity $F_{\max}(\rho^{AB})$ of a bipartite state and the tripartite geometric entanglement of the purification $|\psi\rangle^{ABC}$. In particular, it holds that $E_g(\psi^{ABC}) + F_{\max}(\rho^{AB}) = 1$, as follows directly from results in [23]. This result extends to any number of parties. For an n -partite state ρ_n let $|\psi_{n+1}\rangle$ be its $n+1$ -partite purification. Then, it holds that [23] $E_g(\psi_{n+1}) + F_{\max}(\rho_n) = 1$.

V. APPLICATIONS

The methods presented in this work have various applications, which we will discuss in the following. One such application concerns evaluation of geometric entanglement. Due to the complementarity relation in Theorem 2, evaluation of geometric entanglement of a mixed state is equivalent to the evaluation of $F_{\rightarrow}$ on a purifying system. Recall that we can evaluate $F_{\rightarrow}^{AB}$ for any system with $d_A d_B \leq 6$ via SDP, see Theorem 1. This means that the geometric entanglement of any state ρ^{AB} can be evaluated via SDP, whenever one of the subsystems is a qutrit and the state has rank at most 2. If one of the subsystems is a qubit, the evaluation of geometric entanglement is possible for all states with rank at most 3. Interestingly, there is no limit on the dimension of the second subsystem. To our knowledge, the geometric entanglement is the first faithful entanglement measure which can be evaluated via SDP for all such states. When it comes to evaluation of geometric entanglement of pure states, our methods imply that $E_g(|\psi\rangle^{ABC})$ can be evaluated via SDP whenever $d_A d_B \leq 6$, i.e., when the joint dimension of any two subsystems is at most 6.

In more general cases, our methods provide a lower bound on the geometric entanglement which is feasible via SDP. This is a consequence of Theorem 2 and the SDP upper bound on $F_{\rightarrow}$ provided in Eq. (9). In fact, this approach also leads to the following lower bound on the geometric entanglement:

$$E_g(\rho^{BC}) \geq 1 - \max_{X^{ABC}} \text{Tr}[X^{ABC} \psi^{ABC}], \quad (18)$$

where $|\psi\rangle^{ABC}$ is a purification of ρ^{BC} and the maximum is taken over all X^{ABC} with the properties

$$X^{ABC} \geq 0, \quad X^{T_A} \geq 0, \quad X^{T_B} \geq 0, \quad X^{T_C} \geq 0, \quad X^A = \mathbb{I}_A. \quad (19)$$

We refer to the Appendix for more details. This lower bound is nonzero even for some bound entangled state, as we demonstrate in Fig. 2 for the 2×4 bound entangled Horodecki states. Surprisingly, our numerical results indicate that the lower bound is tight in this case. In more detail, we find numerically that this lower bound matches with the upper bound on geometric entanglement which we obtained using the algorithm in [24]. The numerical gap between the upper and

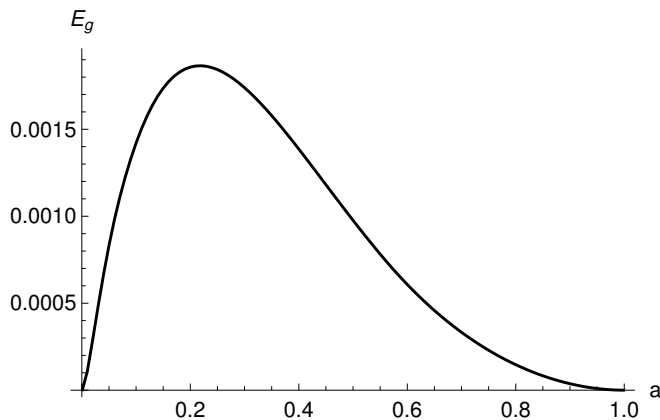


Figure 2. Geometric entanglement for the 2×4 PPT entangled states ρ_a , see Supplemental Material for the definition.

the lower bound is $\Delta E_g \leq 4 \times 10^{-7}$, and the average gap is $\overline{\Delta E_g} \approx 1.2 \times 10^{-8}$, further details can be found in the Appendix. Our results complement earlier research on approximating separable states and evaluating entanglement of bipartite and multipartite states [25–36].

VI. CONCLUSIONS

We have explored the intersection of quantum thermodynamics and quantum entanglement, advancing our understanding of these quantum resource theories. Our development of the Gibbs-preserving local operations and classical communication (GLOCC) framework has enabled us to investigate the intricacies of local cooling processes in quantum systems. This framework has proven to be a powerful tool in analyzing the efficiency and strategies for cooling local systems to their ground states, particularly in settings where only a single copy of the quantum state is available.

In scenarios where local Hamiltonians are fully degenerate, the process of cooling a local system to its ground state corresponds to the extraction of local purity. For this setting, we have established the concept of purity-entanglement complementarity, illustrating a profound connection between the extraction of local purity and the amount of entanglement within a system. This relationship not only offers a practical and operational interpretation of geometric entanglement within the realm of thermodynamics but also simplifies and enhances the

evaluation of geometric entanglement.

Our research has shown that the optimal performance of the cooling process, specifically the maximum fidelity achievable with local ground states, can be efficiently determined through semidefinite programming across a wide range of pertinent scenarios. Leveraging the concept of purity-entanglement complementarity, we have further extended this capability to accurately estimate the geometric entanglement in various families of multipartite pure states as well as bipartite mixed states.

The methodologies introduced in this study hold the potential to tackle a range of pertinent questions in quantum information science, particularly those which can be linked to the evaluation of geometric entanglement. Important examples are verifying the positivity of linear maps and evaluating the maximal output purity of quantum channels [37]. While a comprehensive analysis of these applications is beyond the scope of this article, they present compelling directions for future investigations.

Another compelling question which is left open in this article is related to the effectiveness of the entanglement-detection and estimation method emerging from the purity-entanglement complementarity. While we have successfully shown that this approach can estimate entanglement in specific PPT entangled states with high precision, the performance of this method for other sets of states is currently unclear. Drawing on the findings documented in this work, we hypothesize that the methods developed here could be successfully applied to more general families of noisy states not explicitly addressed in this article.

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Appendix A: Proof of Proposition 1

We will show that $F_{\max}$ as defined in Eq. (1) of the main text can also be expressed as in Eq. (3) of the main text. For this, recall that any LOCC protocol Λ also corresponds to a separable operation $\Lambda(\rho) = \sum_i K_i \rho K_i^\dagger$ with Kraus operators of the form $K_i = A_i \otimes B_i$ [21]. If the operation additionally preserves the maximally mixed state, then $\{K_i^\dagger\}$ also correspond to a valid set of Kraus operators, giving rise to the transformation $\Lambda^\dagger(\rho) = \sum_i K_i^\dagger \rho K_i$. In this case, $\Lambda^\dagger$ is also a separable operation which preserves the maximally mixed state. Denoting with GSEP the set of separable operations which preserve the maximally mixed state we obtain the following:

$$\begin{aligned}
 F_{\max}(\rho^{AB}) &\leq \max_{\Lambda \in \text{GSEP}} \langle 00 | \Lambda[\rho^{AB}] | 00 \rangle \\
 &= \max_{\Lambda^\dagger \in \text{GSEP}} \text{Tr} \left[\rho^{AB} \Lambda^\dagger(|00\rangle\langle 00|) \right] \\
 &\leq \max_{|\psi\rangle, |\phi\rangle} \text{Tr} \left[\rho^{AB} |\psi\rangle\langle\psi|^A \otimes |\phi\rangle\langle\phi|^B \right].
 \end{aligned} \tag{A1}$$

The last inequality follows from the fact that $\Lambda^\dagger(|00\rangle\langle 00|)$ is a separable state. It is further clear that equality can be achieved by choosing $\Lambda^\dagger$ to be a product of two local unitaries, i.e., $\Lambda^\dagger(\rho) = U_A \otimes V_A \rho^{AB} U_A^\dagger \otimes V_A^\dagger$. This completes the proof of Eq. (3) of the main text.

The arguments presented above can be directly extended to n parties, in which case $F_{\max}$ is defined as

$$F_{\max}(\rho_n) = \max_{\Lambda \in \text{GLOCC}} \text{Tr}[\Lambda(\rho_n) |0\rangle\langle 0|^{\otimes n}], \quad (\text{A2})$$

where ρ_n is an n -partite quantum state. Using the same arguments as above, we can express $F_{\max}$ as follows:

$$F_{\max}(\rho_n) = \max_{\{U_i\}} \text{Tr}[U_1 \otimes \cdots \otimes U_n \rho_n U_1^\dagger \otimes \cdots \otimes U_n^\dagger |0\rangle\langle 0|^{\otimes n}], \quad (\text{A3})$$

where the maximum is taken over all local unitaries U_i .

Appendix B: Proof of Proposition 2

First, we note that a pure bipartite pure state ψ is close to a PPT state if and only if it is close to a separable state. This is because

$$\begin{aligned} \|\psi^{T_B}\|_\infty &= \max_{\mu \in \text{SEP}} F(\psi, \mu) \leq \max_{\mu \in \text{PPT}} F(\psi, \mu) \\ &= \max_{\mu \in \text{PPT}} \text{Tr}(\psi \mu) = \max_{\mu \in \text{PPT}} \text{Tr}(\psi^{T_B} \mu) \\ &\leq \max_{\|\mu\|_1 \leq 1} \text{Tr}(\psi^{T_B} \mu) = \|\psi^{T_B}\|_\infty, \end{aligned} \quad (\text{B1})$$

where in the first step, we used the fact that taking the partial transpose in the Schmidt basis of a pure state gives us

$$\begin{aligned} \left(\sum_{ij} \sqrt{p_i p_j} |ii\rangle \langle jj| \right)^{T_B} &= \sum_{ij} \sqrt{p_i p_j} |ij\rangle \langle ji| \\ &= \sum_i p_i |ii\rangle \langle ii| \\ &\quad + \sum_{i < j} \sqrt{p_i p_j} \left(\frac{|ij\rangle + |ji\rangle}{\sqrt{2}} \right) \left(\frac{\langle ij| + \langle ji|}{\sqrt{2}} \right) \\ &\quad - \sum_{i < j} \sqrt{p_i p_j} \left(\frac{|ij\rangle - |ji\rangle}{\sqrt{2}} \right) \left(\frac{\langle ij| - \langle ji|}{\sqrt{2}} \right), \end{aligned} \quad (\text{B2})$$

which means $\|T_B(\phi)\|_\infty$ gives us the square of the largest Schmidt coefficient. An implication of the above results is that for any bipartite pure state $|\psi\rangle$ it holds that

$$\max_{\sigma \in \text{SEP}} F(\psi, \sigma) = \max_{\sigma \in \text{PPT}} F(\psi, \sigma) = \lambda_{\max}(\psi^A). \quad (\text{B3})$$

Consider now a PPT state σ_{PPT} with the property that

$$\lambda_{\max}(\sigma_{\text{PPT}}) = 1 - \varepsilon. \quad (\text{B4})$$

Let $|\phi\rangle$ be the eigenvector corresponding to the largest eigenvalue of σ_{PPT} . It holds that $F(\phi, \sigma_{\text{PPT}}) = \lambda_{\max}(\sigma_{\text{PPT}}) = 1 - \varepsilon$. Moreover, due to Eq. (B3) there is a separable state σ_{SEP} such that $F(\phi, \sigma_{\text{SEP}}) \geq 1 - \varepsilon$.

In the next step, consider a state ρ and let σ_{PPT} be such that

$$\text{Tr}(\rho \sigma_{\text{PPT}}) \geq \max_{\sigma \in \text{PPT}} \text{Tr}(\rho \sigma) - \delta \quad (\text{B5})$$

for a small $\delta > 0$. We note that an arbitrarily small $\delta > 0$ can be achieved via SDP. Moreover, we assume that σ_{PPT} fulfills Eq. (B4) for a small $\varepsilon > 0$. Then there exists a separable state σ_{SEP} and a pure state $|\phi\rangle$ with the properties as discussed below Eq. (B4). We further find that

$$\begin{aligned} |\text{Tr}(\rho \sigma_{\text{PPT}}) - \text{Tr}(\rho \sigma_{\text{SEP}})| &= |\text{Tr}(\rho [\sigma_{\text{PPT}} - \sigma_{\text{SEP}}])| \\ &\leq \sqrt{\text{Tr}(\rho^2) \text{Tr}([\sigma_{\text{PPT}} - \sigma_{\text{SEP}}]^2)} \\ &\leq \sqrt{\text{Tr}(\rho^2)} \|\sigma_{\text{PPT}} - \sigma_{\text{SEP}}\|_1 \\ &\leq \|\sigma_{\text{PPT}} - \sigma_{\text{SEP}}\|_1 \\ &\leq \|\sigma_{\text{PPT}} - \phi\|_1 + \|\phi - \sigma_{\text{SEP}}\|_1 \\ &\leq 2\sqrt{1 - F(\sigma_{\text{PPT}}, \phi)} \\ &\quad + 2\sqrt{1 - F(\phi, \sigma_{\text{SEP}})} \\ &\leq 4\sqrt{\varepsilon}. \end{aligned} \quad (\text{B6})$$

This result implies the following inequality:

$$\begin{aligned} \text{Tr}(\rho \sigma_{\text{PPT}}) &\leq \text{Tr}(\rho \sigma_{\text{SEP}}) + 4\sqrt{\varepsilon} \\ &\leq \max_{\sigma \in \text{SEP}} \text{Tr}(\rho \sigma) + 4\sqrt{\varepsilon}. \end{aligned} \quad (\text{B7})$$

From Eq. (B5) we further obtain

$$\text{Tr}(\rho \sigma_{\text{PPT}}) \geq \max_{\sigma \in \text{SEP}} \text{Tr}(\rho \sigma) - \delta. \quad (\text{B8})$$

In summary, we can bound $\max_{\sigma \in \text{SEP}} \text{Tr}(\rho \sigma)$ from above and from below as follows:

$$\text{Tr}(\rho \sigma_{\text{PPT}}) + \delta \geq \max_{\sigma \in \text{SEP}} \text{Tr}(\rho \sigma) \geq \text{Tr}(\rho \sigma_{\text{PPT}}) - 4\sqrt{\varepsilon}. \quad (\text{B9})$$

The proof of Eq. (5) of the main text is complete by recalling that $F_{\max}(\rho) = \max_{\sigma \in \text{SEP}} \text{Tr}(\rho \sigma)$.

We can extend the argument above to more than two parties. We will now demonstrate this for $n = 3$. Here, PPT means PPT in all bipartitions, and separable means full separability. To get a similar result as in the bipartite case, we need to bound the distance from a pure state that is almost product to a fully separable state. Let ψ_{ABC} be a tripartite pure state and σ_{PPT} is tripartite state which is PPT in all bipartitions such that $F(\psi, \sigma_{\text{PPT}}) = 1 - \varepsilon$ with some $\varepsilon > 0$. Using the same arguments as in the proof of Eq. (5) of the main text, there exist product states $\phi_A^1 \otimes \phi_{BC}^1$ and $\phi_{AB}^2 \otimes \phi_C^2$ such that

$$F(\psi, \phi_A^1 \otimes \phi_{BC}^1) \geq 1 - \varepsilon, \quad (\text{B10})$$

$$F(\psi, \phi_{AB}^2 \otimes \phi_C^2) \geq 1 - \varepsilon. \quad (\text{B11})$$

Using triangle inequality for the trace norm and the Fuchs-van

de Graaf inequality, we have

$$\begin{aligned}
\|\psi_{ABC} - \phi_A^1 \otimes \phi_B^2 \otimes \phi_C^2\|_1 &\leq \|\psi_{ABC} - \phi_A^1 \otimes \phi_{BC}^1\|_1 \quad (\text{B12}) \\
&\quad + \|\phi_A^1 \otimes \phi_{BC}^1 - \phi_A^1 \otimes \phi_B^2 \otimes \phi_C^2\|_1 \\
&= \|\psi_{ABC} - \phi_A^1 \otimes \phi_{BC}^1\|_1 \\
&\quad + \|\phi_{BC}^1 - \phi_B^2 \otimes \phi_C^2\|_1 \\
&\leq \|\psi_{ABC} - \phi_A^1 \otimes \phi_{BC}^1\|_1 \\
&\quad + \|\phi_A^1 \otimes \phi_{BC}^1 - \phi_B^2 \otimes \phi_{AC}^2\|_1 \\
&\leq \|\psi_{ABC} - \phi_A^1 \otimes \phi_{BC}^1\|_1 \\
&\quad + \|\phi_A^1 \otimes \phi_{BC}^1 - \psi_{ABC}\|_1 \\
&\quad + \|\psi_{ABC} - \phi_B^2 \otimes \phi_{AC}^2\|_1 \\
&\leq 2\|\psi_{ABC} - \phi_A^1 \otimes \phi_{BC}^1\|_1 \\
&\quad + \|\psi_{ABC} - \phi_B^2 \otimes \phi_{AC}^2\|_1 \\
&\leq 6\sqrt{\varepsilon}.
\end{aligned}$$

This implies that there exists a separable state σ_{SEP} such that $\|\psi - \sigma_{\text{SEP}}\|_1 \leq 6\sqrt{\varepsilon}$. Using the same arguments as in Eq. (B6) we find

$$\begin{aligned}
|\text{Tr}(\rho\sigma_{\text{PPT}}) - \text{Tr}(\rho\sigma_{\text{SEP}})| &\leq \|\sigma_{\text{PPT}} - \sigma_{\text{SEP}}\|_1 \quad (\text{B13}) \\
&\leq \|\sigma_{\text{PPT}} - \psi\|_1 + \|\psi - \sigma_{\text{SEP}}\|_1 \\
&\leq 8\sqrt{\varepsilon}.
\end{aligned}$$

In summary, this means that for $n = 3$ we can bound F_{max} by maximizing $\text{Tr}(\rho\sigma)$ over all states σ which are PPT in all bipartitions. Note that this maximization is feasible via SDP. If the optimal state σ_{PPT} is such that $\lambda_{\text{max}}(\sigma_{\text{PPT}}) = 1 - \varepsilon$, we obtain the following bound on F_{max} :

$$\text{Tr}(\rho\sigma_{\text{PPT}}) + \delta \geq F_{\text{max}}(\rho) \geq \text{Tr}(\rho\sigma_{\text{PPT}}) - 8\sqrt{\varepsilon}, \quad (\text{B14})$$

where $\delta > 0$ is the error of the SDP.

To demonstrate the efficiency of this approximation, we have sampled 6000 Haar random pure states of three qutrits and evaluated $F_{\text{max}}(\psi^{ABC})$. Note that for any pure tripartite state $|\psi\rangle^{ABC}$ it holds that [23]

$$F_{\text{max}}(\psi^{ABC}) = F_{\text{max}}(\rho^{AB}) = F_{\text{max}}(\rho^{AC}) = F_{\text{max}}(\rho^{BC}), \quad (\text{B15})$$

which means that we can approximate F_{max} either by approximating over bipartite or tripartite states which are PPT in all bipartitions. Evaluating the SDP, we found numerically that $\varepsilon < 1.04 \times 10^{-10}$, which means that F_{max} can be evaluated with a precision of at least 8.2×10^{-5} in these cases. In the same way, we see that the geometric entanglement of Haar random three qutrit states can be evaluated with the same precision.

Appendix C: Proof of Theorem 1

Let us consider a slightly modified maximization problem

$$F'(\rho^{AB}) = \max_{Y^{AB}} \text{Tr}[Y^{AB}\rho^{AB}], \quad (\text{C1})$$

where the maximum is now taken over all matrices Y^{AB} with the properties

$$Y^{AB} \geq 0, \quad Y^{T_B} \geq 0, \quad Y^A = \frac{1}{d_A} \mathbb{1}_A. \quad (\text{C2})$$

It is clear that the maximum on the right-hand side of Eq. (11) of the main text can be expressed as

$$\max_{X^{AB}} \text{Tr}[X^{AB}\rho^{AB}] = d_A F'(\rho^{AB}). \quad (\text{C3})$$

Moreover, Y can be considered as a density matrix since $\text{Tr}(Y) = 1$. For $d_A d_B \leq 6$ Eq. (C2) implies that Y is separable [17], i.e., can be written as $Y = \sum_i p_i Y_i^A \otimes Y_i^B$ with local density matrices $Y_i^{A,B}$ such that $\sum_i p_i Y_i^A = \mathbb{1}_A/d_A$. We thus obtain

$$F'(\rho^{AB}) = \max_i \sum_i \text{Tr}[p_i Y_i^A \otimes Y_i^B \rho^{AB}], \quad (\text{C4})$$

where the maximum is now taken over all local density matrices $Y_i^{A,B}$ and all probability distributions p_i with $\sum_i p_i Y_i^A = \mathbb{1}_A/d_A$. Comparing this expression to Eq. (7) of the main text, we see that $F_{\rightarrow}^{A|B}(\rho^{AB}) = d_A F'(\rho^{AB})$. This completes the proof.

Appendix D: Proof of Proposition 3

We will now show that $F^{A|B}$ can be bounded below by Eq. (12) of the main text, where the maximization is done over all matrices X^{AB} as defined in Eq. (13). For this, we note that $F^{A|B}$ can be upper bounded as follows:

$$\begin{aligned}
F^{A|B}(\rho^{AB}) &= \max_{\Lambda \in \text{GLOCC}} \text{Tr}[\Lambda(\rho^{AB}) \mathbb{1}_A \otimes |0\rangle\langle 0|^B] \quad (\text{D1}) \\
&\leq \max_{\Lambda \in \text{GSEP}} \text{Tr}[\rho^{AB} \Lambda(\mathbb{1}_A \otimes |0\rangle\langle 0|^B)],
\end{aligned}$$

where GSEP denotes the set of separable operations which preserve the maximally mixed state. For any $\Lambda \in \text{GSEP}$ it holds that

$$\mathbb{1}_{AB} \geq \Lambda(\mathbb{1}_A \otimes |0\rangle\langle 0|^B) \geq 0, \quad (\text{D2})$$

$$\text{Tr}[\Lambda(\mathbb{1}_A \otimes |0\rangle\langle 0|^B)] = 2, \quad (\text{D3})$$

and moreover $\Lambda(\mathbb{1}_A \otimes |0\rangle\langle 0|^B)$ has positive partial transpose. This completes the proof.

Appendix E: Proof of Theorem 2

Let $\{M_i^A\}$ be an optimal POVM on Alice's side, maximizing Bob's purity. Recall that the probability p_i of the outcome i as well as the post-measurement state on Bob's side are given by

$$p_i = \text{Tr}[M_i^A \otimes \mathbb{1}^B \rho^{AB}], \quad (\text{E1})$$

$$\sigma_i^B = \frac{1}{p_i} \text{Tr}_A[M_i^A \otimes \mathbb{1}^B \rho^{AB}]. \quad (\text{E2})$$

Denoting by $|v_i\rangle^B$ the eigenstate corresponding to the largest eigenvalue of σ_i^B we can express $F_{\rightarrow}^{AB}$ as follows:

$$F_{\rightarrow}^{AB}(\rho^{AB}) = \sum_i \text{Tr} [M_i^A \otimes v_i^B \rho^{AB}] = \sum_i p_i \lambda_{\max}(\sigma_i^B), \quad (\text{E3})$$

where $\lambda_{\max}(\rho)$ denotes the largest eigenvalue of ρ . Without loss of generality we can further assume that each POVM element M_i^A has rank one.

Let us now consider the action of the POVM $\{M_i^A\}$ on the state $|\psi\rangle^{ABC}$, which is a purification of ρ^{AB} . Conditioned on the measurement outcome i , Bob and Charlie end up with the state

$$\sigma_i^{BC} = \frac{1}{p_i} \text{Tr}_A [M_i^A \otimes \mathbb{1}^{BC} \psi^{ABC}]. \quad (\text{E4})$$

Since M_i^A have rank one, each state σ_i^{BC} is a pure extension of the state σ_i^B . Recall that the geometric entanglement of a pure state σ_i^{BC} is related to the largest eigenvalue of the reduced state σ_i^B as follows [9, 18]:

$$E_g(\sigma_i^{BC}) = 1 - \lambda_{\max}(\sigma_i^B). \quad (\text{E5})$$

Combining these results, we thus obtain:

$$F_{\rightarrow}^{AB}(\rho^{AB}) = 1 - \sum_i p_i E_g(\sigma_i^{BC}). \quad (\text{E6})$$

Using convexity of the geometric entanglement [9] we further arrive at

$$F_{\rightarrow}^{AB}(\rho^{AB}) \leq 1 - E_g(\rho^{BC}). \quad (\text{E7})$$

To complete the proof of the theorem it remains to show that this inequality is actually an equality. To see this, note that there always exist a pure state decomposition $\{q_i, |\phi_i\rangle^{BC}\}$ of the state ρ^{BC} such that

$$E_g(\rho^{BC}) = \sum_i q_i E_g(\phi_i^{BC}) = 1 - \sum_i q_i \lambda_{\max}(\phi_i^B). \quad (\text{E8})$$

Moreover, there always exists a POVM $\{M_i^A\}$ on Alice's side, such that Bob and Charlie end up with this optimal decomposition, i.e., their post-measurement state corresponds to ϕ_i^{BC} with probability q_i [38, 39]. If Alice applies this POVM on her part of ρ^{AB} , then the post-measurement state of Bob is given by ϕ_i^B with probability q_i . Correspondingly, the purity which Bob can obtain is given by $\sum_i q_i \lambda_{\max}(\phi_i^B)$, which is equivalent to $1 - E_g(\rho^{BC})$. This completes the proof.

Appendix F: SDP lower bound on geometric entanglement

We will now demonstrate how the results presented in our article can be used for bounding the geometric entanglement for bipartite quantum states. As stated in the main text, from Theorem 2 we get the following lower bound on the geometric entanglement

$$E_g(\rho^{BC}) \geq 1 - \max_{X^{AB}} \text{Tr} [X^{AB} \rho^{AB}], \quad (\text{F1})$$

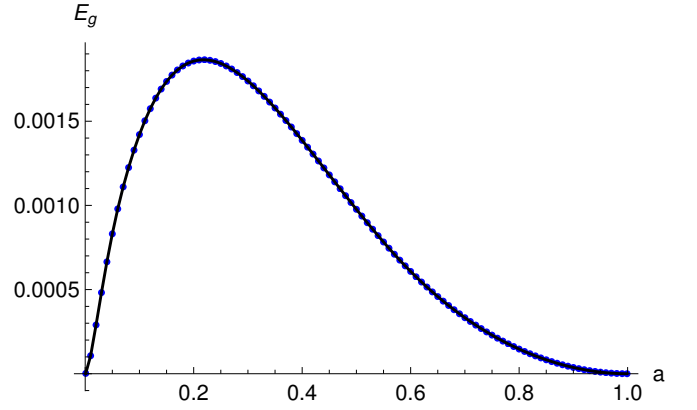


Figure 3. Bounds on geometric entanglement for the 2×4 PPT entangled states ρ_a . Solid curve shows the lower bound on E_g from Eq. (F3), dots represent an upper bound obtained via the algorithm described in [24].

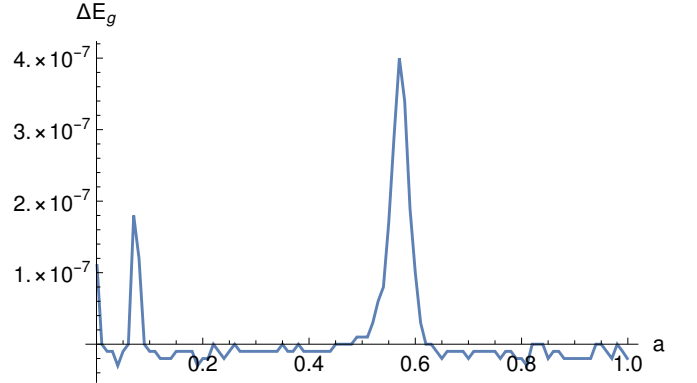


Figure 4. Numerical gap between the upper and the lower bound on the geometric entanglement for the states ρ_a .

where $|\psi\rangle^{ABC}$ is a purification of both states ρ^{AB} and ρ^{BC} , and the maximum is taken over all matrices X^{AB} with the properties

$$X^{AB} \geq 0, \quad X^{TB} \geq 0, \quad X^A = \mathbb{1}_A. \quad (\text{F2})$$

By similar arguments, it is possible to show that E_g can also be bounded from below as follows:

$$E_g(\rho^{BC}) \geq 1 - \max_{X^{ABC}} \text{Tr} [X^{ABC} \psi^{ABC}], \quad (\text{F3})$$

where $|\psi\rangle^{ABC}$ is a purification of ρ^{BC} and the maximum is taken over all X^{ABC} with the properties

$$X^{ABC} \geq 0, \quad X^{TA} \geq 0, \quad X^{TB} \geq 0, \quad X^{TC} \geq 0, \quad X^A = \mathbb{1}_A. \quad (\text{F4})$$

To prove Eq. (F3), note that the geometric entanglement can be expressed as follows [10]:

$$E_g(\rho^{BC}) = 1 - \max \sum_i p_i F_s(\psi_i^{BC}), \quad (\text{F5})$$

where the maximum is taken over all pure state decompositions of ρ^{BC} , and $F_s(\rho) = \max_{\sigma \in \text{SEP}} F(\rho, \sigma)$. From Eq. (F5)

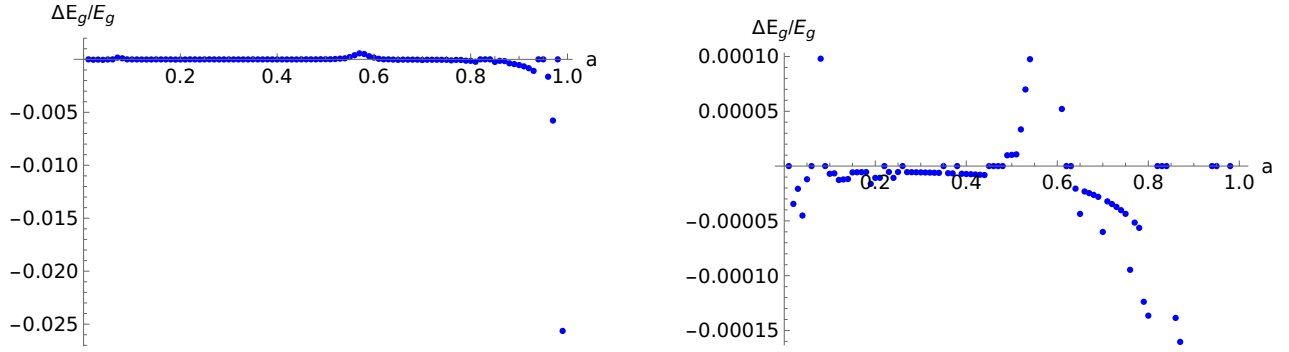


Figure 5. Relative numerical gap $\Delta E_g/E_g$ for the states ρ_a in the ranges $-0.025 \leq \Delta E_g/E_g \leq 0.002$ (left part of the figure) and $-0.00015 \leq \Delta E_g/E_g \leq 0.0001$ (right part of the figure).

it follows that there exist some POVM $\{M_i^A\}$ and pure local states $|\mu_i\rangle^B$ and $|\nu_i\rangle^C$ such that

$$E_g(\rho^{BC}) = 1 - \text{Tr} \left[\sum_i M_i^A \otimes |\mu_i\rangle\langle\mu_i|^B \otimes |\nu_i\rangle\langle\nu_i|^C |\psi\rangle\langle\psi|^{ABC} \right]. \quad (\text{F6})$$

Since the set of matrices X^{ABC} with the properties (F4) contains all matrices of the form $\sum_i M_i^A \otimes |\mu_i\rangle\langle\mu_i|^B \otimes |\nu_i\rangle\langle\nu_i|^C$, we arrive at Eq. (F3). We note that in the same way it is also possible to construct lower bounds on the multipartite geometric entanglement.

An important family of states for which the evaluation of entanglement measures is notoriously difficult are PPT entangled states. Important examples in this context are the 2×4 states [40]

$$\rho_a = \frac{1}{7a+1} \begin{pmatrix} a & 0 & 0 & 0 & 0 & a & 0 & 0 \\ 0 & a & 0 & 0 & 0 & 0 & a & 0 \\ 0 & 0 & a & 0 & 0 & 0 & 0 & a \\ 0 & 0 & 0 & a & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1+a}{2} & 0 & 0 & \frac{\sqrt{1-a^2}}{2} \\ a & 0 & 0 & 0 & 0 & a & 0 & 0 \\ 0 & a & 0 & 0 & 0 & 0 & a & 0 \\ 0 & 0 & a & 0 & \frac{\sqrt{1-a^2}}{2} & 0 & 0 & \frac{1+a}{2} \end{pmatrix}, \quad (\text{F7})$$

which are PPT entangled in the range $0 < a < 1$. Solid curve in Fig. 3 shows the lower bound from Eq. (F3). An upper bound on the geometric entanglement of mixed states can be obtained using the methods described in [24]. We have evaluated the upper bound for $a = n/100$, with the integer n ranging from 0 to 100. The result is shown as dots in Fig. 3. The gap

between the upper and the lower bound is shown in Fig. 4. The numerical gap ΔE_g is never larger than 4×10^{-7} , and the average gap is approximately $\overline{\Delta E_g} \approx 1.2 \times 10^{-8}$. In Fig. 5 we also show the relative numerical gap $\Delta E_g/E_g$. In the vicinity of separable states, i.e., for $a = 0.001$ and $a = 0.999$ we further obtained $\Delta E_g/E_g = 0.06$ and $\Delta E_g/E_g = -2$, respectively. These values are not shown in Fig. 5.

Appendix G: Evaluating geometric entanglement for multipartite pure states

We note that the evaluation of $F_{\max}$ can also be used to evaluate the geometric entanglement for multipartite pure states. We will now discuss this explicitly for 3 and 4 parties. These results follow directly from [23], and we present them here for completeness.

In more detail, for a 3-partite pure state $|\psi\rangle^{ABC}$ it holds that

$$\begin{aligned} E_g(|\psi\rangle^{ABC}) &= 1 - F_{\max}(\rho^{AB}) = 1 - F_{\max}(\rho^{BC}) \\ &= 1 - F_{\max}(\rho^{AC}) = 1 - F_{\max}(\psi^{ABC}), \end{aligned} \quad (\text{G1})$$

where ρ^{XY} denote the reduced states of $|\psi\rangle$. This directly implies that the SDP for evaluating $F_{\max}$ in bipartite states can be used to evaluate E_g for tripartite pure states. For $d_A d_B \leq 6$ it is possible to evaluate $F_{\max}$ via SDP, which means that E_g is also feasible via SDP in all such cases.

For more general sets of 3-partite pure states it is possible to estimate E_g via estimation of $F_{\max}$ of the bipartite subsystems with the precision given in Eq. (5) of the main text. Similarly, geometric entanglement for 4-partite pure states can be estimated by estimating $F_{\max}$ of the reduced 3-partite states, with precision given in Eq. (B14).