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Evaluation of two different entanglement measures on a bound entangled state

Cyril Branciard,[1] Huangjun Zhu,[2,3] Lin Chen,[2] and Valerio Scarani[2,4]
[1]*Centre for Quantum Computer Technology, School of Mathematics and Physics, The University of Queensland, St. Lucia, QLD 4072, Australia*
[2]*Centre for Quantum Technologies, National University of Singapore, Singapore 117543, Singapore*
[3]*NUS Graduate School for Integrative Sciences and Engineering, Singapore 117597, Singapore*
[4]*Department of Physics, National University of Singapore, Singapore 117542, Singapore*
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We consider the mixed three-qubit bound entangled state defined as the normalized projector on the subspace that is complementary to an unextendible product basis [C. H. Bennett *et al.*, Phys. Rev. Lett. **82**, 5385 (1999)]. Using the fact that no product state lies in the support of that state, we compute its entanglement by providing a basis of its subspace formed by "minimally entangled" states. The approach is in principle applicable to any entanglement measure; here we provide explicit values for both the geometric measure of entanglement and a generalized concurrence.

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I. INTRODUCTION

Entanglement measures quantify how much entanglement is contained in a quantum state, which plays a fundamental role in quantum information and computation tasks (for a recent review, see [1]). For example, distillable entanglement quantifies how many Bell states one can asymptotically obtain from target states under local operations and classical communications (LOCC) [2]; in particular, there exist bound entangled states, whose distillable entanglement vanishes under LOCC [3]. Many entanglement measures have been proposed to characterize multipartite states. These measures include the relative entropy of entanglement [4], the geometric measure of entanglement [5], and the generalized concurrence [6]. Multipartite entangled states are a useful resource for promising quantum information tasks, such as one-way quantum computation [7] and multiuser quantum communications [8]: it is therefore essential to be able to characterize their entanglement. In practice, some entanglement measures can be estimated from experimental data [9], or via the efficient method of direct measurements, which can be turned into a verification test in experiments [10].

However, entanglement measures are usually difficult to estimate, especially for multipartite mixed states [11–16]. In this article we study the three-qubit mixed bound entangled state defined as the normalized projector on the subspace complementary to an unextendible product basis (UPB) [17]. This is a typical example of a multipartite mixed state whose entanglement can be detected by entanglement witnesses built from local observables [18]. Recently, a scheme for studying local distinguishability of three-qubit UPB states has also been proposed [19]. Here we use a unified strategy to compute two measures, namely, the geometric measure of entanglement and the generalized concurrence. We find in particular that the optimal decompositions for both measures are different. Our strategy is quite general and could in principle be applied to all entanglement measures.

The article is organized as follows. In Sec. II we introduce the target state and its relation with an UPB, as well as the strategy of computing the two entanglement measures in the following sections. In Sec. III we analytically derive the geometric measure of entanglement. In Sec. IV we give a numerical lower bound and an analytical upper bound on the generalized concurrence. Finally, we conclude in Sec. V.

II. THE STATE AND THE STRATEGY

A. Unextendible product basis and bound entanglement

Consider the following four three-qubit states:

$$\begin{aligned} |\varphi_0\rangle &= |0\rangle_A\,|0\rangle_B\,|0\rangle_C, \\ |\varphi_1\rangle &= |1\rangle_A\,|+\rangle_B\,|-\rangle_C, \\ |\varphi_2\rangle &= |-\rangle_A\,|1\rangle_B\,|+\rangle_C, \\ |\varphi_3\rangle &= |+\rangle_A\,|-\rangle_B\,|1\rangle_C. \end{aligned} \quad (1)$$

They form an UPB [17]: No product state can be found orthogonal to the four states in (1). In other words, if $\mathcal{P}$ is the subspace generated by the four vectors (1), there is no product state in the complementary space $\mathcal{Q} = \mathbb{1} - \mathcal{P}$.

The state defined as the uniform mixture on the space complementary to an UPB is always a bound entangled state [17,20]. In our case, this state reads

$$\rho_{\mathcal{Q}} = \frac{1}{4}\left(\mathbb{1} - \sum_{i=0}^{3} |\varphi_i\rangle\langle\varphi_i|\right), \quad (2)$$

$$\rho_{\mathcal{Q}} = \frac{1}{8}\left\{\mathbb{1} - \frac{1}{2}[\mathbb{1}\otimes\sigma_+\otimes\sigma_- + (\text{cyclic})] - \frac{1}{2\sqrt{2}}(\sigma_+\otimes\sigma_+\otimes\sigma_+ + \sigma_-\otimes\sigma_-\otimes\sigma_-)\right\}, \quad (3)$$

with $\sigma_\pm = (\sigma_z \pm \sigma_x)/\sqrt{2}$ [21]. It is convenient to review rapidly its remarkable properties.

By definition, $\rho_{\mathcal{Q}}$ is entangled: There is no product state in its support, so *a fortiori* it will be impossible to decompose it on product states. It can also be easily verified [17] that one can complete the basis (1) with four vectors such that the first two qubits are entangled and the third one is separable; in other words, $\rho_{\mathcal{Q}}$ can be decomposed in the form

$$\rho_{\mathcal{Q}} = \frac{1}{4}\sum_{i=0}^{3} |\Psi_i\rangle_{AB}\langle\Psi_i| \otimes |\Psi_i'\rangle_C\langle\Psi_i'|. \quad (4)$$

This means that the state is not three-partite entangled. Moreover, from this decomposition it is obvious that the reduced states ρ_{AC} and ρ_{BC} are separable; even more, no measurement of B can prepare an entangled state between A and C, and no measurement of A can prepare an entangled state between B and C. At first sight, one might hope that ρ_{AB} is entangled, or at least that a measurement of C could prepare an entangled state between A and B. However, this is not the case. Indeed, by construction of the basis (1), $\rho_{\mathcal{Q}}$ is invariant under cyclic permutations $A \to B \to C \to A$. Therefore, we can rewrite (4) with states $|\Psi_i\rangle_{BC}|\Psi_i'\rangle_A$ and repeat the preceding reasoning. In conclusion, the entanglement that has to be invested to create $\rho_{\mathcal{Q}}$ is nowhere to be recovered, whichever partition and LOCC strategy is envisaged.

The state $\rho_{\mathcal{Q}}$ is thus a paradigmatic example of bound entanglement. Since it is not symmetric under all permutations, but only the cyclic ones, it does not fall in the family of states for which general studies of entanglement measures have been made [15,16,22,23]. Here we shall show how one can compute the value of entanglement for such a state. The main idea is presented in the next paragraph.

B. Quantifying entanglement

Entanglement measures are normally defined on pure states. For bipartite pure states, there is only one measure, namely the entropy of the reduced density matrix. For multipartite states, the situation is much less well understood and there are several candidates for entanglement measures. Still, they are usually computable on pure states.

The definition of an entanglement measure E on pure states can be extended to any mixed state ρ as follows:

$$E(\rho) = \min_{\{p_i,|\psi_i\rangle\}} \sum_i p_i E(|\psi_i\rangle), \tag{5}$$

where the minimum is to be taken among all possible pure-state decompositions of ρ in the form $\rho = \sum_i p_i|\psi_i\rangle\langle\psi_i|$. There is, however, no general recipe for computing this minimum.

An obvious lower bound is given by

$$E(\rho) \geqslant \min_{|\psi\rangle\in\mathrm{supp}(\rho)} E(|\psi\rangle), \tag{6}$$

where supp(ρ) is the support of ρ. For many mixed states, this lower bound is trivial, because there will be a product state in the support of ρ and therefore the right-hand side is simply 0. However, *for $\rho_{\mathcal{Q}}$ the right-hand side of (6) is not zero*, because we know that there is no product state in its support.

In addition, for the two measures of entanglement considered below, we shall show that one can find a complete orthonormal *basis* $\{|\psi_0\rangle,\ldots,|\psi_3\rangle\}$ of $\mathcal{Q}$ formed by "minimally entangled" states, that is, such that

$$E(|\psi_i\rangle) = \min_{|\psi\rangle\in\mathcal{Q}} E(|\psi\rangle) \tag{7}$$

for all $i = 0,\ldots,3$. As $\rho_{\mathcal{Q}} = \frac{1}{4}\sum|\psi_i\rangle\langle\psi_i|$ for any orthonormal basis $\{|\psi_i\rangle\}$ of $\mathcal{Q}$, this implies that, for these two measures at least,

$$E(\rho_{\mathcal{Q}}) = \min_{|\psi\rangle\in\mathcal{Q}} E(|\psi\rangle). \tag{8}$$

This is the simple but crucial insight that will allow us to compute the entanglement of $\rho_{\mathcal{Q}}$. A similar insight was used for the Smolin state, a permutation invariant four-qubit bound entangled state [11]. In the next two sections, we compute the right-hand side of (8) and exhibit a full basis that reaches this value for two measures of multipartite entanglement, the geometric measure of entanglement [5] in Sec. III and a generalized concurrence [6] in Sec. IV.

III. GEOMETRIC ENTANGLEMENT OF $\rho_{\mathcal{Q}}$

We start by considering the geometric measure of entanglement [5]. For an N-partite pure state $|\psi\rangle$, this measure is defined as

$$E_G(|\psi\rangle) = 1 - \max_{|\phi\rangle\in\Pi} |\langle\psi|\phi\rangle|^2, \tag{9}$$

where Π is the set of all N-partite pure product states $|\phi\rangle = |\phi_1\rangle\otimes\cdots\otimes|\phi_N\rangle$.

Following the strategy defined previously, we compute

$$E_G(\rho_{\mathcal{Q}}) = 1 - \frac{3\sqrt{6}}{8} \simeq 0.081\,44. \tag{10}$$

For comparison, in the case of three qubits, the largest value of geometric measure of entanglement is achieved for the W state and is $E_G(|W\rangle) = \frac{5}{9}$ [13,14].

A. Calculating $\min_{|\psi\rangle\in\mathcal{Q}} E_G(|\psi\rangle)$

From the definition (9) of E_G, we have

$$\begin{aligned}\min_{|\psi\rangle\in\mathcal{Q}} E_G(|\psi\rangle) &= \min_{|\psi\rangle\in\mathcal{Q}} (1 - \max_{|\phi\rangle\in\Pi} |\langle\psi|\phi\rangle|^2)\\ &= 1 - \max_{|\phi\rangle\in\Pi}\max_{|\psi\rangle\in\mathcal{Q}} |\langle\psi|\phi\rangle|^2. \end{aligned}\tag{11}$$

Now, for a given $|\phi\rangle\in\Pi$, the closest state to $|\phi\rangle$ in the subspace $\mathcal{Q}$ is simply the projection of $|\phi\rangle$ onto $\mathcal{Q}$. Denoting with $\tilde{\mathcal{Q}}$ the projector onto the subspace $\mathcal{Q}$, we get

$$\max_{|\psi\rangle\in\mathcal{Q}} |\langle\psi|\phi\rangle|^2 = \langle\phi|\tilde{\mathcal{Q}}|\phi\rangle, \tag{12}$$

so that

$$\begin{aligned}\min_{|\psi\rangle\in\mathcal{Q}} E_G(|\psi\rangle) &= 1 - \max_{|\phi\rangle\in\Pi}\langle\phi|\tilde{\mathcal{Q}}|\phi\rangle\\ &= \min_{|\phi\rangle\in\Pi}\langle\phi|\tilde{\mathcal{P}}|\phi\rangle,\end{aligned}\tag{13}$$

where $\tilde{\mathcal{P}}$ denotes the projector onto the subspace $\mathcal{P}$. We show in Appendix A how to calculate $\min_{|\phi\rangle\in\Pi}\langle\phi|\tilde{\mathcal{P}}|\phi\rangle$ analytically. We obtain

$$\min_{|\psi\rangle\in\mathcal{Q}} E_G(|\psi\rangle) = 1 - \frac{3\sqrt{6}}{8}. \tag{14}$$

B. A whole basis reaching $\min_{|\psi\rangle\in\mathcal{Q}} E_G(|\psi\rangle)$

As also shown in Appendix A, the minimum $\min_{|\phi\rangle\in\Pi}\langle\phi|\tilde{\mathcal{P}}|\phi\rangle$ can be attained by the four states

$|\phi_i\rangle = |a_i\rangle|b_i\rangle|c_i\rangle$ $(i = 0,\ldots,3)$, with

$$|a_i\rangle = \cos\frac{\alpha_i}{2}|0\rangle + \sin\frac{\alpha_i}{2}|1\rangle, \tag{15}$$

$$|b_i\rangle = \cos\frac{\beta_i}{2}|0\rangle + \sin\frac{\beta_i}{2}|1\rangle, \tag{16}$$

$$|c_i\rangle = \cos\frac{\gamma_i}{2}|0\rangle + \sin\frac{\gamma_i}{2}|1\rangle, \tag{17}$$

and for the following values of $\alpha_i,\beta_i,\gamma_i$ [24]:

$$\begin{array}{llll} |\phi_0\rangle: & \alpha_0 = \theta_0, & \beta_0 = \theta_0, & \gamma_0 = \theta_0, \\ |\phi_1\rangle: & \alpha_1 = \pi + \theta_0, & \beta_1 = \frac{\pi}{2} - \theta_0, & \gamma_1 = \frac{3\pi}{2} - \theta_0, \\ |\phi_2\rangle: & \alpha_2 = \frac{3\pi}{2} - \theta_0, & \beta_2 = \pi + \theta_0, & \gamma_2 = \frac{\pi}{2} - \theta_0, \\ |\phi_3\rangle: & \alpha_3 = \frac{\pi}{2} - \theta_0, & \beta_3 = \frac{3\pi}{2} - \theta_0, & \gamma_3 = \pi + \theta_0, \end{array} \tag{18}$$

where $\theta_0 = \arccos(-\frac{\sqrt{6}-2}{2})$.

Let $|\psi_i\rangle$ $(i = 0,\ldots,3)$ be the normalized states corresponding to the projection of $|\phi_i\rangle$ onto $\mathcal{Q}$:

$$|\psi_i\rangle = \frac{1}{\sqrt{\frac{3\sqrt{6}}{8}}}\,\tilde{\mathcal{Q}}|\phi_i\rangle. \tag{19}$$

On the one hand, it can be checked that these four states form an orthonormal basis of $\mathcal{Q}$; they thus provide a decomposition $\rho_{\mathcal{Q}} = \frac{1}{4}\sum_{i=0}^{3}|\psi_i\rangle\langle\psi_i|$. On the other hand, by construction,

$$E_G(|\psi_i\rangle) = 1 - \max_{|\phi\rangle\in\Pi}|\langle\psi_i|\phi\rangle|^2 = 1 - |\langle\psi_i|\phi_i\rangle|^2 = 1 - \frac{3\sqrt{6}}{8}. \tag{20}$$

This concludes the proof of (10).

As a remark: The four states $|\psi_i\rangle$ turn out to be *three-partite* entangled. As we mentioned in Sec. II A, there exist bases of $\mathcal{Q}$ made of bipartite entangled states. It is interesting to note that such bases are not those that minimize the geometric measure of entanglement.

IV. GENERALIZED CONCURRENCE OF $\rho_{\mathcal{Q}}$

The second measure of entanglement that we consider is a generalization of the concurrence defined as [6]

$$E_C(|\psi\rangle) = 2^{1-N/2}\sqrt{2^N - 2 - \sum_j \mathrm{Tr}\,\rho_j^2}, \tag{21}$$

where the multi-index j runs over all $(2^N - 2)$ subsets of the N subsystems and ρ_j is the reduced density matrix of the corresponding subset.

Following the strategy defined earlier, we prove that

$$E_C(\rho_{\mathcal{Q}}) = \frac{\sqrt{897}}{52} \simeq 0.575\,96. \tag{22}$$

In fact, analytically, we prove only $E_C(\rho) \leqslant \frac{\sqrt{897}}{52}$, but we have strong numerical evidence that this is indeed the exact value of $E_C(\rho)$.

In comparison, in the case of three qubits, the largest value of this measure of entanglement is reached for the GHZ state [for which all the reduced states ρ_j in (21) are maximally mixed] and is $E_C(|\mathrm{GHZ}\rangle) = \sqrt{3/2} \simeq 1.2247$.

A. Calculating $\min_{|\psi\rangle\in\mathcal{Q}} E_C(|\psi\rangle)$

Consider first states that lie in the symmetric subspace of $(\mathbb{C}^2)^{\otimes 3}$, denoted $\mathcal{S}$. Among these states, we can find analytically the one that minimizes $E_C(|\psi\rangle)$. The analytical calculations are detailed in Appendix B, and the final result is

$$\min_{|\psi\rangle\in\mathcal{Q}\cap\mathcal{S}} E_C(|\psi\rangle) = \frac{\sqrt{897}}{52}. \tag{23}$$

We have not been able to prove analytically that this value defines the minimum of $E_C(|\psi\rangle)$ over the whole subspace $\mathcal{Q}$; however, a brute-force numerical minimization reaches exactly the same value. Therefore, up to the conjecture that there exists a symmetric state $|\psi_0'\rangle$ that reaches the minimum, backed by numerical evidence, we can assert that

$$\min_{|\psi\rangle\in\mathcal{Q}} E_C(|\psi\rangle) = \frac{\sqrt{897}}{52}. \tag{24}$$

B. A whole basis reaching $\min_{|\psi\rangle\in\mathcal{Q}} E_G(|\psi\rangle)$

We also exhibit in Appendix B three other states $|\psi_1'\rangle, |\psi_2'\rangle$, and $|\psi_3'\rangle$, that form an orthonormal basis of $\mathcal{Q}$ together with $|\psi_0'\rangle$, and that are such that

$$E_C(|\psi_1'\rangle) = E_C(|\psi_2'\rangle) = E_C(|\psi_3'\rangle) = \frac{\sqrt{897}}{52} = E_C(|\psi_0'\rangle). \tag{25}$$

Up to the conjecture mentioned earlier, this concludes the proof of (24).

Note that, as was the case for geometric measure of entanglement, all these four states are three-partite entangled.

V. CONCLUSION

We found a way to estimate the entanglement of the state $\rho_{\mathcal{Q}}$. The entanglement of this state is quantified in terms of geometric measure of entanglement and generalized concurrence [25]; and it is found to be strictly positive, while the state is bound entangled and not fully three-partite entangled.

The remarkable property of $\rho_{\mathcal{Q}}$ that allowed us to estimate its entanglement is the possibility to decompose it into a mixture of minimally entangled states. This was at least possible for both the geometric measure of entanglement and the generalized concurrence; we do not know whether this necessarily holds for all entanglement measures. Nevertheless, our results also illustrate the fact that the two measures of entanglement that we considered are quite different: The optimal decomposition of $\rho_{\mathcal{Q}}$ as a mixture of pure states is not the same for these two measures of entanglement.

Our technique can be applied to other states, whenever such a decomposition into minimally entangled states is possible. As further examples, we give in Appendix C numerical results for the bound entangled state constructed out of the generalized three-qubit "GenShifts" UPB defined in [17,20]. As our technique is scalable, it could as well be extended to higher-dimensional systems, consisting of more than three subsystems. It would also be interesting to apply our approach to different entanglement measures.

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APPENDIX A: CALCULATIONS FOR $E_G(\rho_{\mathcal{Q}})$: ANALYTICAL CALCULATION OF $\min_{|\phi\rangle\in\Pi}\langle\phi|\tilde{\mathcal{P}}|\phi\rangle$

Any state $|\phi\rangle \in \Pi$ can be written as $|\phi\rangle = |a\rangle|b\rangle|c\rangle$, with

$$|a\rangle = \cos\frac{\alpha}{2}|0\rangle + \sin\frac{\alpha}{2}e^{i\varphi_a}|1\rangle, \tag{A1}$$

$$|b\rangle = \cos\frac{\beta}{2}|0\rangle + \sin\frac{\beta}{2}e^{i\varphi_b}|1\rangle, \tag{A2}$$

$$|c\rangle = \cos\frac{\gamma}{2}|0\rangle + \sin\frac{\gamma}{2}e^{i\varphi_c}|1\rangle, \tag{A3}$$

and where $\alpha,\beta,\gamma \in [0,2\pi]$; $\varphi_a,\varphi_b,\varphi_c \in [0,\pi]$. With these notations, we find

$$\begin{aligned}\langle\phi|\tilde{\mathcal{P}}|\phi\rangle = {}& \tfrac{1}{8}(1+\cos\alpha)(1+\cos\beta)(1+\cos\gamma)\\ &+ \tfrac{1}{8}(1-\cos\alpha)(1+\sin\beta\cos\varphi_b)(1-\sin\gamma\cos\varphi_c)\\ &+ \tfrac{1}{8}(1-\sin\alpha\cos\varphi_a)(1-\cos\beta)(1+\sin\gamma\cos\varphi_c)\\ &+ \tfrac{1}{8}(1+\sin\alpha\cos\varphi_a)(1-\sin\beta\cos\varphi_b)(1-\cos\gamma).\end{aligned} \tag{A4}$$

The preceding expression being linear in $\cos\varphi_a$, its minimum can be attained for either $\varphi_a = 0$ or $\varphi_a = \pi$. As the expression is also invariant under the transformation ($\alpha \leftrightarrow 2\pi - \alpha, \varphi_a \leftrightarrow \pi - \varphi_a$), then its minimum can be attained for $\varphi_a = 0$.

Similar arguments can be applied to φ_b and φ_c, which allows us to write

$$\min_{|\phi\rangle\in\Pi}\langle\phi|\tilde{\mathcal{P}}|\phi\rangle = \min_{\alpha,\beta,\gamma\in[0,2\pi]} F(\alpha,\beta,\gamma), \tag{A5}$$

where

$$\begin{aligned}F(\alpha,\beta,\gamma) = {}& \tfrac{1}{8}(1+\cos\alpha)(1+\cos\beta)(1+\cos\gamma)\\ &+ \tfrac{1}{8}(1-\cos\alpha)(1+\sin\beta)(1-\sin\gamma)\\ &+ \tfrac{1}{8}(1-\sin\alpha)(1-\cos\beta)(1+\sin\gamma)\\ &+ \tfrac{1}{8}(1+\sin\alpha)(1-\sin\beta)(1-\cos\gamma)\\ = {}& 1 - \tfrac{1}{16}\det M,\end{aligned} \tag{A6}$$

with

$$M = \begin{pmatrix} \cos\alpha - \sin\alpha & \cos\alpha + \sin\alpha & -2\\ \cos\beta + \sin\beta & -2 & \cos\beta - \sin\beta\\ -2 & \cos\gamma - \sin\gamma & \cos\gamma + \sin\gamma \end{pmatrix}.$$

Now, the Hadamard inequality applied to the row vectors of M gives

$$|\det M| \leqslant 6\sqrt{6}, \tag{A7}$$

from which we conclude that

$$F(\alpha,\beta,\gamma) \geqslant 1 - \frac{3\sqrt{6}}{8}. \tag{A8}$$

The equality is obtained if the three row vectors of M are mutually orthogonal. The following four sets of values for α,β,γ, with $\cos\theta_0 = -\frac{\sqrt{6}-2}{2}$, all satisfy this condition:

$$\begin{array}{llll} |\phi_0\rangle: & \alpha_0 = \theta_0, & \beta_0 = \theta_0, & \gamma_0 = \theta_0,\\ |\phi_1\rangle: & \alpha_1 = \pi + \theta_0, & \beta_1 = \frac{\pi}{2} - \theta_0, & \gamma_1 = \frac{3\pi}{2} - \theta_0,\\ |\phi_2\rangle: & \alpha_2 = \frac{3\pi}{2} - \theta_0, & \beta_2 = \pi + \theta_0, & \gamma_2 = \frac{\pi}{2} - \theta_0,\\ |\phi_3\rangle: & \alpha_3 = \frac{\pi}{2} - \theta_0, & \beta_3 = \frac{3\pi}{2} - \theta_0, & \gamma_3 = \pi + \theta_0. \end{array} \tag{A9}$$

Interestingly, the four states $|\phi_i\rangle$ defined by the corresponding values of $\alpha_i,\beta_i,\gamma_i$ (and with $\varphi_a = \varphi_b = \varphi_c = 0$) also form an UPB of the "GenShifts" type [17,20].

These four states all attain the previous lower bound for $F(\alpha,\beta,\gamma)$, so that for $i = 0,\ldots,3$,

$$\langle\phi_i|\tilde{\mathcal{P}}|\phi_i\rangle = \min_{|\phi\rangle\in\Pi}\langle\phi|\tilde{\mathcal{P}}|\phi\rangle = 1 - \frac{3\sqrt{6}}{8}. \tag{A10}$$

APPENDIX B: CALCULATIONS FOR $E_C(\rho_{\mathcal{Q}})$

1. Calculation of $\min_{|\psi\rangle\in\mathcal{Q}\cap\mathcal{S}} E_C(|\psi\rangle)$

For convenience, let us start by defining a basis for $\mathcal{Q}$. A possible choice is the following:

$$\begin{aligned}|q_0\rangle &= \frac{1}{\sqrt{2}}(|+++\rangle - |---\rangle),\\ |q_1\rangle &= \frac{1}{\sqrt{2}}(|+10\rangle - |-01\rangle),\\ |q_2\rangle &= \frac{1}{\sqrt{2}}(|0+1\rangle - |1-0\rangle),\\ |q_3\rangle &= \frac{1}{\sqrt{2}}(|10+\rangle - |01-\rangle).\end{aligned} \tag{B1}$$

A generic symmetric state in $\mathcal{Q}$ can then be written as

$$|\psi\rangle = \cos\theta|q_0\rangle + \sin\theta e^{i\gamma}\frac{|q_1\rangle + |q_2\rangle + |q_3\rangle}{\sqrt{3}}, \tag{B2}$$

with $\theta,\gamma \in [0,\pi]$.

The sum in the definition (21) of $E_C(|\psi\rangle)$ can be explicitly calculated and is found to be

$$\begin{aligned}\textstyle\sum_j \mathrm{Tr}\,\rho_j^2 = {}& \tfrac{1}{3}(10 + 25\cos^2\theta - 26\cos^4\theta)\\ &- 4\cos^2\theta\sin^2\theta(1-\cos 2\gamma).\end{aligned} \tag{B3}$$

The maximum of this two-variable function is obtained for $\cos^2\theta = \frac{25}{52}$, $\cos 2\gamma = 1$. We get

$$\min_{|\psi\rangle\in\mathcal{Q}\cap\mathcal{S}} E_C(|\psi\rangle) = \frac{\sqrt{897}}{52}, \tag{B4}$$

and the minimum can be reached by two different symmetric states, one of these being

$$|\psi_0'\rangle = \frac{1}{2\sqrt{13}}(5|q_0\rangle + 3|q_1\rangle + 3|q_2\rangle + 3|q_3\rangle). \quad \text{(B5)}$$

2. Three other orthogonal states with the same value of E_C

One can easily check that the following three states,

$$\begin{aligned} |\psi_1'\rangle &= \frac{1}{2\sqrt{13}}(3|q_0\rangle - 5|q_1\rangle + 3|q_2\rangle - 3|q_3\rangle), \\ |\psi_2'\rangle &= \frac{1}{2\sqrt{13}}(3|q_0\rangle - 3|q_1\rangle - 5|q_2\rangle + 3|q_3\rangle), \\ |\psi_3'\rangle &= \frac{1}{2\sqrt{13}}(3|q_0\rangle + 3|q_1\rangle - 3|q_2\rangle - 5|q_3\rangle), \end{aligned} \quad \text{(B6)}$$

all have the same value of E_C as $|\psi_0'\rangle$, and that, together with $|\psi_0'\rangle$, they form an orthonormal basis of $\mathcal{Q}$; they thus provide a decomposition of $\rho_\mathcal{Q}$.

APPENDIX C: ENTANGLEMANT OF THE BOUND ENTANGLED STATE CONSTRUCTED OUT OF THE THREE-QUBIT “GENSHIFTS” UPB

In this appendix we apply our approach to the three-qubit bound entangled state $\rho_\mathcal{Q}(\phi)$ constructed out of the generalized “GenShifts” UPB [17,20], and show numerical results for the values of $E_G[\rho_\mathcal{Q}(\phi)]$ and $E_C[\rho_\mathcal{Q}(\phi)]$.

For a single-qubit state $|\phi\rangle$ and its orthogonal state $|\phi^\perp\rangle$, the “GenShifts” UPB consists of the four states

$$\begin{aligned} |\varphi_0\rangle &= |0, 0, 0\rangle, \\ |\varphi_1\rangle &= |1,\phi,\phi^\perp\rangle, \\ |\varphi_2\rangle &= |\phi^\perp,1,\phi\rangle, \\ |\varphi_3\rangle &= |\phi,\phi^\perp,1\rangle. \end{aligned} \quad \text{(C1)}$$

$\rho_\mathcal{Q}(\phi)$ is then defined as the uniform mixture on the complementary subspace $\mathcal{Q}(\phi)$:

$$\rho_\mathcal{Q}(\phi) = \frac{1}{4}\left(\mathbb{1} - \sum_{i=0}^{3} |\varphi_i\rangle\langle\varphi_i|\right). \quad \text{(C2)}$$

Note that the state $\rho_\mathcal{Q}$ studied in the main text is a particular case of $\rho_\mathcal{Q}(\phi)$, corresponding to $|\phi\rangle = |+\rangle$.

We checked numerically that the critical properties of $\rho_\mathcal{Q}$ that we used to estimate its entanglement are still satisfied by $\rho_\mathcal{Q}(\phi)$: For all choices of $|\phi\rangle$, one can again find two (different) orthonormal bases $\{|\psi_i\rangle\}$ and $\{|\psi_i'\rangle\}$ of $\mathcal{Q}(\phi)$ formed by minimally entangled states, that is, such that

$$E_G(|\psi_i\rangle) = \min_{|\psi\rangle\in\mathcal{Q}(\phi)} E_G(|\psi\rangle), \quad \text{(C3)}$$

$$E_C(|\psi_i'\rangle) = \min_{|\psi\rangle\in\mathcal{Q}(\phi)} E_C(|\psi\rangle), \quad \text{(C4)}$$

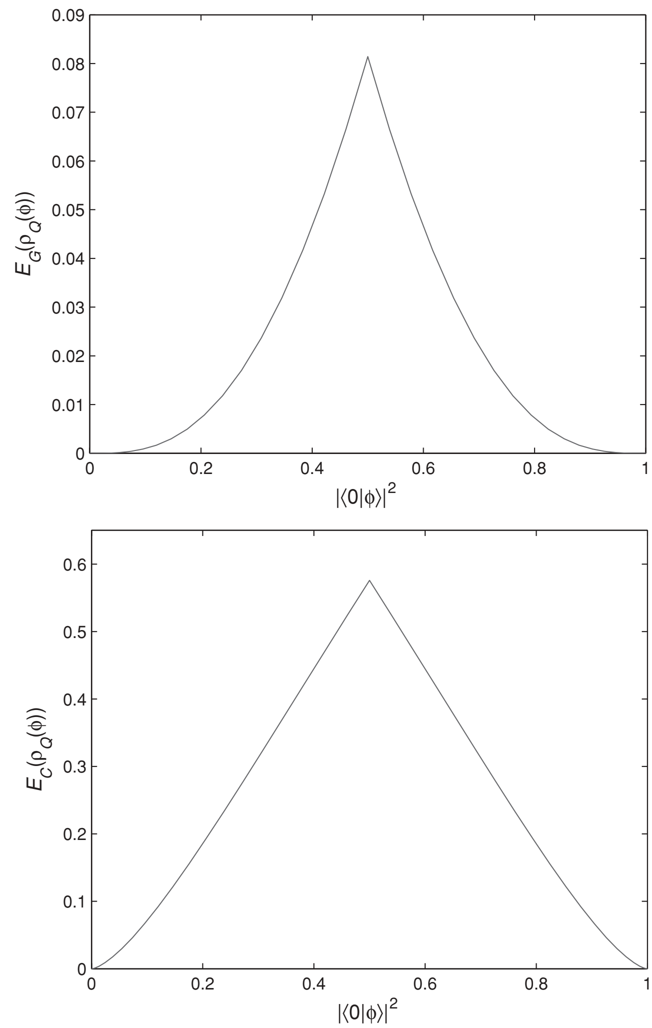

FIG. 1. Numerical calculations of the values of $E_G[\rho_\mathcal{Q}(\phi)]$ (top) and $E_C[\rho_\mathcal{Q}(\phi)]$ (bottom).

for all $i = 0,\ldots,3$. We then conclude that

$$E_G[\rho_\mathcal{Q}(\phi)] = \min_{|\psi\rangle\in\mathcal{Q}(\phi)} E_G(|\psi\rangle), \quad \text{(C5)}$$

$$E_C[\rho_\mathcal{Q}(\phi)] = \min_{|\psi\rangle\in\mathcal{Q}(\phi)} E_C(|\psi\rangle). \quad \text{(C6)}$$

Figure 1 displays the numerical results we obtained for the entanglement of $\rho_\mathcal{Q}(\phi)$ measured by E_G and E_C, as a function of the overlap $|\langle 0|\phi\rangle|^2$. Not surprisingly, the maxima of $E_G[\rho_\mathcal{Q}(\phi)]$ and $E_C[\rho_\mathcal{Q}(\phi)]$ are found when $|\langle 0|\phi\rangle|^2 = |\langle 1|\phi\rangle|^2 = \frac{1}{2}$, which is in particular the case for $\rho_\mathcal{Q} = \rho_\mathcal{Q}(+)$.

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[24] Note already that, as it was the case for the states $|\varphi_i\rangle$, and as it will be the case for all the bases we construct in this article, the states $|\phi_i\rangle$ have the following symmetry: $|\phi_0\rangle$ is symmetric, while $|\phi_1\rangle$, $|\phi_2\rangle$, and $|\phi_3\rangle$ are obtained from one another by cyclic permutations $A \to B \to C \to A$.
[25] The state had only been characterized so far with another entanglement measure, proposed by C. S. Yu and H. S. Song [Phys. Rev. A **73**, 022325 (2006)].