Entanglement Rényi α entropy

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We study the entanglement Rényi α entropy (ERαE) as the measure of entanglement. Instead of a single quantity in standard entanglement quantification for a quantum state by using the von Neumann entropy for the well-accepted entanglement of formation (EoF), the ERαE gives a continuous spectrum parametrized by variable α as the entanglement measure, and it reduces to the standard EoF in the special case $\alpha \to 1$. The ERαE provides more information in entanglement quantification and can be used, for example, to determine the convertibility of entangled states by local operations and classical communication. A series of results is obtained: (i) we show that the ERαE of two states, which can be mixed or pure, may be incomparable, in contrast to the fact that there always exists an order for the EoF of two states; (ii) similar to the case of EoF, we study in a fully analytical way the ERαE for arbitrary two-qubit states, the Werner states, and isotropic states in the general d dimension; and (iii) we provide a proof of the previous conjecture for the analytical functional form of the EoF of isotropic states in the arbitrary d dimension.

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I. INTRODUCTION

Entanglement is a valuable resource for quantum information processing [1]. Quantification of entanglement is a fundamental problem in quantum information science and quantum physics. Various measures of entanglement have been proposed, such as entanglement of formation (EoF), distillable entanglement and entanglement cost [2,3], and relative entropy of entanglement [4]; see reviews [5–7] for more results. These measures have different, yet closely related physical interpretations. In general, they can be associated respectively with different protocols for quantum information processing. Several well-accepted measures of entanglement such as EoF and the relative entropy of entanglement converge to the same quantity for a pure bipartite state, which is the von Neumann entropy of the reduced density operator of this bipartite state. For a given state, entanglement measures are not the same, in general, nor are they a unique quantity even within one kind of measure. A class of measures may constitute the entanglement monotones with physical significance in the framework of local operations and classical communication (LOCC) [8–11]. Rényi α entropy is a natural generalization of von Neumann entropy and it reduces to the latter when α is approaching 1.

In this paper, we shall consider the quantity entanglement Rényi α entropy (ERαE) as the entanglement measure, which is a generalization of the well-known EoF. These entropies parameterized by a continuous variable α can be a spectrum of entanglement monotone. Important applications are found by using Rényi α entropy in describing the entanglement of ground states of many-body systems [12–19], which are pure states.

In contrast to the relatively simple case of pure entangled states, the quantification of mixed-state entanglement is still challenging due to the need for hard optimization procedures [7]. However, for the EoF, analytical results are well known for some special cases, including arbitrary two-qubit states based on the concurrence in the seminal work of Wootters [20], the isotropic states [21], and the Werner states [22] in an arbitrary d dimension. In parallel with those three analytical results, in this paper, we obtain similarly analytical results for the ERαE for those cases. A series of results are obtained, which are different from and complementary to the EoF in quantifying entanglement. We show that two-qubit states may be incomparable, which is in contrast to the expectation by using concurrence that entanglement of two-qubit states can be fully quantified, which is also different from the case of two-qubit pure states. We can show that two mixed states may be incomparable. We find that the optimal pure states' decompositions should not be the same, for example, in the ERαE. Besides, we provide a proof to the conjecture about the analytical functional form of the EoF for isotropic states.

II. DEFINITION

Suppose we have a composite system with subsystems A and B in a pure state $|\psi\rangle$ whose Schmidt decomposition is $|\psi\rangle = \sum_{i=1}^{d} \sqrt{\mu_i}|a_i,b_i\rangle_{AB}$, where $\vec{\mu}$ is the Schmidt vector. For simplicity, we denote the density matrix as $\psi \equiv |\psi\rangle\langle\psi|$, and let $\rho_{B(A)} = \mathrm{tr}_{A(B)}(\psi)$ be the reduced density matrix of subsystem B (or A). The entanglement of the pure state $|\psi\rangle$ can be quantified by the Rényi α entropy of one of the reduced density operators, for example ρ_B, which is defined as

$$\mathcal{R}_\alpha(\psi) \equiv (1-\alpha)^{-1} \log_2 \left(\mathrm{tr}\rho_B^\alpha\right). \quad (1)$$

As pointed out in Sec. I, $\mathcal{R}_\alpha(\psi)$ is reduced to the well-known entanglement measure of von Neumann entropy in the

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$\alpha \to 1$ limit: $\mathcal{R}_{\alpha\to1}(\psi) = -\mathrm{tr}(\rho_B \log_2 \rho_B)$. This measure of entanglement can be easily generalized to mixed states using the so-called convex roof construction [7,11]. For a mixed state with density matrix ρ, the ERαE is defined as

$$\mathcal{R}_\alpha(\rho) \equiv \min_{\{p_k,\psi_k\}} \sum_k p_k \mathcal{R}_\alpha(\psi_k), \tag{2}$$

where the minimization is over all possible pure-state ensembles $\{p_k,\psi_k\}$ satisfying $\rho = \sum_k p_k \psi_k$. As in most cases of a mixed-state entanglement measure, the evaluation of the ERαE of mixed states is much more difficult to carry out due to the complexity involved in the optimization.

Our calculation of the ERαE of symmetric mixed states is closely based on that of two-qubit states; hence, at the outset, we introduce useful concepts and extend existing results concerning ERαE of mixed two-qubit states to a broader range of α.

It is well known that the EoF corresponding to $\alpha \to 1$ for ERαE depends only on concurrence, which has an analytic form for the arbitrary two-qubit state, and EoF itself can act as a measure of entanglement [20]. For $\alpha \in (1,+\infty)$, the ERαE depends similarly only on concurrence [23]. It is then possible that concurrence, in principle, might be the only essential measure of entanglement for a two-qubit state and even the ERαE for $\alpha \in (0,1)$ can act as entanglement monotones [11]. We will show in this paper that this is not the case. We remark that ERαE satisfies monogamy inequality [24,25] for multiqubit states when $\alpha = 2$ [23]. The EoF or concurrence of mixed states in higher-dimensional system are known for classes of states with special symmetry, such as the Werner states [26] and isotropic states [21,22,27].

III. THE CRITICAL VALUE OF α FOR TWO-QUBIT STATE

Suppose we have a composite system of two qubits in a pure state $|\psi\rangle$. Given the spin-flip operation on this state, $|\tilde{\psi}\rangle = \sigma_y|\psi^*\rangle$, its concurrence can be defined as $\mathcal{C}(\psi) = |\langle\tilde{\psi}|\psi\rangle|$. For notation simplicity, we use $\mathcal{C}$ in the following to denote $\mathcal{C}(\psi)$ or $\mathcal{C}(\psi)$ when no confusion arises. It is easy to see that the Schmidt coefficients $\lambda_\pm$ of $|\psi\rangle$, i.e., the eigenvalues of the reduced density matrix ρ_B, are in a one-to-one correspondence with $\mathcal{C}$ via the relation $\lambda_\pm = (1 \pm \sqrt{1-\mathcal{C}^2})/2$. By direct substitution of $\lambda_\pm$ into the definition (1) of the ERαE, we obtain

$$\begin{aligned}\mathcal{R}_\alpha(\psi) &= (1-\alpha)^{-1}\log_2(\lambda_+^\alpha + \lambda_-^\alpha)\\ &\equiv \Omega(\mathcal{C},\alpha),\end{aligned} \tag{3}$$

where we introduce the function $\Omega(\mathcal{C},\alpha)$ for later convenience.

The concurrence of arbitrary mixed state ρ can be similarly defined through the convex roof formula, $\mathcal{C}(\rho) \equiv \min_{\{p_k,\psi_k\}} \sum_k p_k \mathcal{C}(\psi_k)$, where the minimization is again over all possible pure-state decomposition of ρ. An important observation made in [20,28] is that this measure is computable for the two-qubit state. If we generalize the spin-flip operation to any mixed state ρ by $\tilde{\rho} = (\sigma_y \otimes \sigma_y)\rho^*(\sigma_y \otimes \sigma_y)$, and let $\Lambda_i^2(\Lambda_1 \geqslant \Lambda_2 \geqslant \Lambda_3 \geqslant \Lambda_4 \geqslant 0)$ denote the eigenvalues of $\tilde{\rho}\rho$, then the concurrence can be calculated explicitly by $\mathcal{C}(\rho) = \max\{\Lambda_1 - \Lambda_2 - \Lambda_3 - \Lambda_4, 0\}$.

The ERαE of an arbitrary state ρ now becomes

$$\mathcal{R}_\alpha(\rho) = \min_{\{p_k,\psi_k\}} \sum_k p_k \Omega(\mathcal{C}(\psi_k),\alpha). \tag{4}$$

Before we proceed, we first note some existing work on the ERαE. It is proved in [23] that ERαE satisfies monogamy inequality [24,25] for multiqubit states when $\alpha = 2$. Also, the EoF and concurrence of mixed states in a higher-dimensional system are known for classes of states with special symmetry, such as the Werner states [26] and isotropic states [21,22,27].

Going back to the two-qubit system, it is shown in [23,28] that for $\alpha \in [1,+\infty)$, this quantity depends only on $\mathcal{C}(\rho)$ and, in the rest of this section, we investigate its behavior in the range of $\alpha \in (0,1)$. Most of the calculations, albeit complicating, are nonessential to our understanding of the results. Thus we refer the interested readers to Appendices A and B for additional details of the calculation, and only discuss the indications of the results we obtain, which form the basis of our calculation of Werner states. We make use of the convexity of the function $\Omega(\mathcal{C},\alpha)$, which is determined from the inequality

$$\frac{\partial^2\Omega(\mathcal{C},\alpha)}{\partial\mathcal{C}^2}\begin{cases}\leqslant 0, & \alpha \in \left[0,\frac{1}{2}\right]\\ \geqslant 0, & \alpha \in \left[\frac{\sqrt{7}-1}{2},1\right],\end{cases} \tag{5}$$

as well as its monotonicity with respect to $\mathcal{C}$. Thus, when $\alpha \geqslant \alpha_c \equiv \frac{\sqrt{7}-1}{2} \approx 0.82$, the ER$\alpha$E can be calculated analytically based on concurrence by

$$\mathcal{R}_\alpha(\rho) = \Omega(\mathcal{C}(\rho),\alpha). \tag{6}$$

The ERαE for two-qubit states when $\alpha < \alpha_c$ in general is still a challenging problem. However, we may instead consider the Werner state which possesses special symmetry [26].

IV. ERαE OF WERNER STATE

By the use of the permutation operator $\mathbb{F} = \sum_{i,j=1}^d |ij\rangle\langle ji|$, the Werner state ρ_F^W of a bipartite system, consisting of two d-dimensional subsystems, can be defined as

$$\rho_F^W = \frac{1-F}{2}\frac{\mathbb{I}+\mathbb{F}}{d^2+d} + \frac{1+F}{2}\frac{\mathbb{I}-\mathbb{F}}{d^2-d}, \tag{7}$$

where the parameter $F \in [-1,1]$ specifying the state can be given from the relation

$$\mathrm{tr}\left(\mathbb{F}\rho_F^W\right) = -F. \tag{8}$$

Our choice of the parameter F is different from [22] by a minus sign, so that Werner states are separable for $F \leqslant 0$. As we shall show later, the ERαE with $\alpha = 0$ of the qubit-qubit state is, interestingly, equal to F.

We will make use of the result first obtained in [21], but we first introduce some notations to simplify the equations. The convex hull of a function $f(x)$ with $\mathcal{D}$ as its domain is defined as

$$\mathrm{co}(f(x)) \equiv \inf\left\{\sum_k p_k f(x_k)\middle|\sum_k p_k x_k = x, x_k \in \mathcal{D}\right\}, \tag{9}$$

where the coefficients p_k of the convex combinations satisfy $\sum_k p_k = 1$; we also need the function $f_W(\rho) \equiv -\mathrm{tr}(\mathbb{F}\rho)$.

Thus, the ERαE of a Werner state is equal to

$$\mathcal{R}_\alpha\left(\rho_F^W\right) = \mathrm{co}(\omega(F,\alpha,d)), \tag{10}$$

where the function $\omega(F,\alpha,d)$ is defined by $\omega(F,\alpha,d) = \inf\{\mathcal{R}_\alpha(\psi)|f_W(\psi) = F, \mathrm{rank}(\psi) \leqslant d\}$.

To express the value of $f_W(\psi)$, we write the Schmidt decomposition of ψ as

$$|\psi\rangle = \sum_{i=1}^{d} \sqrt{\mu_i}|a_i,b_i\rangle = (U_A \otimes U_B)\sum_{i=1}^{d}\sqrt{\mu_i}|ii\rangle, \tag{11}$$

and let $V \equiv U_A^\dagger U_B, v_{ij} \equiv \langle i|V|j\rangle$; then we arrive at

$$f_W(\psi) = -\sum_{i,j=1}^{d}\sqrt{\mu_i\mu_j}v_{ji}v_{ij}^*. \tag{12}$$

We first note that since the class of Werner state is equivalent to isotropic states for $d = 2$, the calculation for that case can alternatively be done for the set of isotropic states, and the results will be identical. The function $\omega(F,\alpha)$ can be shown to have the explicit formula

$$\omega(F,\alpha) = \begin{cases}\Omega(F,\alpha), & F \in (0,1]\\ 0, & F \in [-1,0].\end{cases} \tag{13}$$

Although this is crucial to our computation of the ERαE of Werner states, the derivation is essentially algebraic and quite tedious. Therefore, here we only present the result and the reader can consult Appendix C for a detailed derivation. Substituting Eq. (13) into Eq. (10), one concludes that

$$\mathcal{R}_\alpha\left(\rho_F^W\right) = \begin{cases}\mathrm{co}(\Omega(\mathrm{F},\alpha)), & F \in (0,1]\\ 0, & F \in [-1,0].\end{cases} \tag{14}$$

Thus as far as the ERαE are concerned, our result implies that the parameter F of Werner states is dimensionless, since Werner states with the same F for given α all have the same value of ERαE regardless of the dimension of the Hilbert space. Also, as in the case of isotropic states, we obtain for the class of Werner states a relation between the parameter F and the ERαE corresponding to $\alpha = 0$,

$$\mathcal{R}_{\alpha=0}\left(\rho_F^W\right) = F. \tag{15}$$

As an example, we can compare the ERαE of a Werner state with $F = 0.8$ and a pure state with $F = 0.5$, as shown in Fig. 1. We note that the pure state here is chosen to be a two-qubit state, in which case if we define F of the said state to be its concurrence, then by Eq. (3) its ERαE coincides in function form with $\omega(F,\alpha)$, which is shown explicitly in Eq. (13). This will simplify the calculation when we perform the comparison, yet the more important reason for choosing such state is as follows: as d increases, the value of the ERαE of a pure state in the $\alpha \to 0$ limit also increases, so the same behavior as in Fig. 1 will always be present as long as we set the EoF of that pure state to be low enough without reducing its d. Thus we essentially only need to verify the existence of a crossing for the case of Werner states and two-qubit pure states, which is indeed true, as demonstrated in Fig. 1: apparently, by the entanglement measure EoF corresponding to $\alpha = 1$, the entanglement of the Werner state is larger than this pure state. This result seems natural and well accepted. Surprisingly, when α is small and is approaching zero, the order of entanglement for those two states is reversed. One can find that the entanglement of the pure state is larger than that of the Werner state.

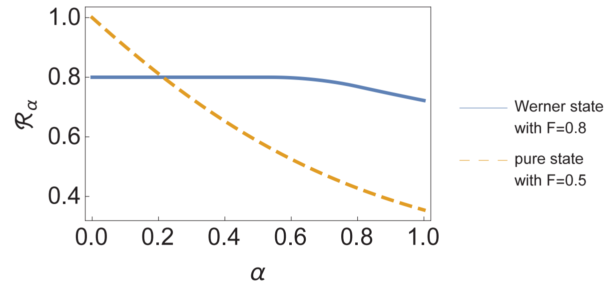

FIG. 1. ERαE of a Werner state and a pure state. The ERαE of the Werner state with $F = 0.8$ and the ERαE of a pure state with $F = 0.5$ are presented depending on parameter α as the x axis. When $\alpha = 1$ which is the case of the standard EoF by von Neumann entropy, the entanglement of the Werner state is larger than that of the pure state. However, the order of the entanglement is reversed when α is close to zero. The specific choice of and definition of F for the pure state are discussed in the main text.

Actually, from Eq. (15), we have that the entanglement of Werner states will always be less than that of an arbitrary pure entangled state in the limit of $\alpha \to 0$. Following the discussions above, we only need to show this for the case of $d = 2$. The optimal pure states' decomposition for a Werner state will include a maximally entangled state with probability F and the identity operator, resulting in that the ERαE equals F, while the ERαE of a generic entangled pure states is 1.

In this sense, we find that the ERαE of Werner states and pure states may be incomparable.

V. ERαE OF ISOTROPIC STATE

The class of isotropic states, specified by a parameter $F \in [0,1]$, consists of convex mixtures of a maximally entangled state and a maximally mixed state,

$$\rho_F^{\mathrm{iso}} = FP_+ + \frac{1-F}{d^2-1}(\mathbb{I} - P_+), \quad F \in [0,1], \tag{16}$$

where P_+ is the projector onto the subspace spanned by the maximally entangled state $|\Psi^+\rangle = \frac{1}{\sqrt{d}}\sum_{i=1}^{d}|ii\rangle$. We can define an isotropic state analog of $f_W(\rho)$ as $f_{\Psi^+}(\rho) = \langle\Psi^+|\rho|\Psi^+\rangle = \mathrm{tr}(P_+\rho)$, which is the fidelity between ρ and Ψ^+.

Again let us start with the formula

$$\mathcal{R}_\alpha\left(\rho_F^{\mathrm{iso}}\right) = \mathrm{co}(\eta(F,\alpha,d)), \tag{17}$$

where the function $\eta(F,\alpha,d)$ is defined as $\eta(F,\alpha,d) = \inf\{\mathcal{R}_\alpha(\psi)|f_{\Psi^+}(\psi) = F, \mathrm{rank}(\psi) \leqslant d\}$. Making use of the Schmidt decomposition in Eq. (11) and defining $W \equiv U_A^T U_B, w_{ij} \equiv \langle i|W|j\rangle$, the straightforward calculation yields

$$f_{\Psi^+}(\psi) = \frac{1}{d}\left|\sum_{i=1}^{d}\sqrt{\mu_i}w_{ii}\right|^2. \tag{18}$$

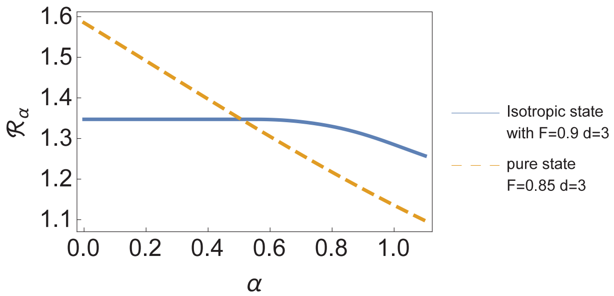

FIG. 2. Comparing the ERαE with $\alpha \in [0,1]$ of an isotropic state and a pure state.

The value of $\eta(F,\alpha,d)$ for $F \in [0,\frac{1}{d}]$ can then be easily deduced by setting $\mu_1 = 1, w_{11} = \sqrt{F}$, which yields $\eta(F,\alpha,d) = 0$. For $F \in (\frac{1}{d},1]$, using the method of Lagrange multipliers, we derive a closed expression of the function $\eta(F,\alpha,d)$ as

$$\eta(F,\alpha,d) = \frac{1}{1-\alpha}\log_2[\gamma^\alpha + (d-1)^{1-\alpha}(1-\gamma)^\alpha], \quad (19)$$

where γ, representing the function $\gamma(F,d)$, is defined as $\gamma(F,d) \equiv \frac{1}{d}[\sqrt{F} + \sqrt{(d-1)(1-F)}]^2$. In the limit of $\alpha \to 1$, $\eta(F,\alpha,d)$ reduces to the function

$$\varepsilon(F,d) = H_2(\gamma) + (1-\gamma)\log_2(d-1), \quad (20)$$

where $H_2(\cdot)$ denotes the binary entropy function. This result, which we have derived here as a special case, is first obtained in [21]; since the calculation of $\eta(F,\alpha,d)$ is just a straightforward generalization, we do not go into the calculation details of Eq. (19). As an application of the results we obtain here, we provide in Appendix D an analytical proof of the conjecture of the EoF of isotropic states in [21], namely,

$$\mathcal{E}\left(\rho_F^{\text{iso}}\right) = \begin{cases} 0, & F \in \left[0,\frac{1}{d}\right] \\ \varepsilon(F,d), & F \in \left[\frac{1}{d},\frac{4(d-1)}{d^2}\right] \\ \frac{d\log_2(d-1)}{d-2}(F-1) + \log_2 d, & F \in \left[\frac{4(d-1)}{d^2},1\right]. \end{cases} \quad (21)$$

Concluding this section, we present in Fig. 2 an example, obtained by numerical evaluation, of a comparison between the Rényi entropy of a certain entangled isotropic state of $F = 0.85$ and a pure state chosen such that its EoF is smaller than that of the former. We further note that the crossing behavior is also possible between two mixed states, although it does not necessarily have to be always present, as indicated in Fig. 3: there is evidently no crossing between the two isotropic states with $d = 3$, yet the two with $F = 0.9, d = 2$ and $F = 0.7$ and $d = 3$, respectively, have crossed the ERαE.

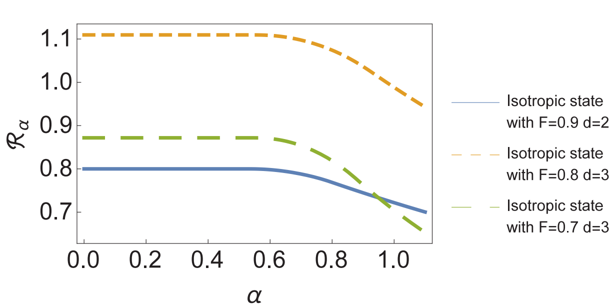

FIG. 3. Comparing the ERαE with $\alpha \in [0,1]$ of mixed states.

We also note that our result provides a nice corollary, namely, the relation between the parameter $F = \text{tr}(P_+\rho)$ specifying the class of isotropic states and its Renyi entropy with $\alpha = 0$,

$$\mathcal{R}_{\alpha=0}\left(\rho_F^{\text{iso}}\right) = \frac{Fd-1}{d-1}\log_2 d. \quad (22)$$

VI. DISCUSSIONS

ERαE quantifies entanglement. For two-qubit states, when $\alpha \geqslant \alpha_c$, ER$\alpha$E can be obtained analytically based on the well-known concurrence. This result implies that the pure states in the optimal decomposition for ERαE when $\alpha \geqslant \alpha_c$ possess the same Schmidt vector similar to that for concurrence. The general analytical formula of ERαE even for the simplest two-qubit states is still a challenging problem, and the pure states' decomposition, in general, will not possess the same Schmidt vector. However, ERαE for Werner states can be obtained. Interestingly, we notice that ERαE for the simplest two-qubit states may be incomparable, implying that they are not local convertible by LOCC. This phenomenon was previously only known for higher-dimensional systems. Analytical results of ERαE for Werner states and isotropic states are obtained. A series of phenomena are found by using ERαE, which may stimulate more interest in studying quantum entanglement quantification.

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APPENDIX A: PROOF OF THE GENERAL FRAMEWORK OF COMPUTING THE ERαE OF STATES WITH LOCAL SYMMETRY

A general approach is derived for systematically calculating the entanglement monotone of states with local symmetry in [22]. Here we present the main steps in the calculations and refer the interested reader to the paper mentioned above for its application in calculating entanglement measures other than ERαE, while the latter is the topic of the main text. Suppose we have a set of states $\rho^{\mathcal{G}}$ invariant under a group, $\mathcal{G}$, of local unitaries, which by definition satisfies the condition

$$[\rho^{\mathcal{G}}, U\otimes V] = 0, \quad \forall (U\otimes V) \in \mathcal{G}. \quad (A1)$$

The twirling operation $\mathcal{P}^{\mathcal{G}}$ is a well-established tool [21], which is defined as

$$\mathcal{P}^{\mathcal{G}}\rho = \int_{(U\otimes V)\in\mathcal{G}} dU (U\otimes V)\rho(U\otimes V)^{\dagger}. \tag{A2}$$

Noting that twirling can be thought of as a probabilistic superposition of unitaries, it thus belongs to the class of local operation and classical communication (LOCC), and by definition an entanglement monotone of a generic state decreases or remains the same under such an operation.

By change of the integration variable, it is easy to show that $[\mathcal{P}^{\mathcal{G}}\rho, U\otimes V] = 0$ for all $(U\otimes V)\in\mathcal{G}$, which means that $\mathcal{P}^{\mathcal{G}}\rho$ also exhibits the symmetry described by group $\mathcal{G}$. Therefore, the result of twirling $\mathcal{P}^{\mathcal{G}}$ depends solely on the fidelities between the twirled state and a certain set of projectors, which are associated with the group of symmetry operations $\mathcal{G}$. This set of quantities (described by a vector in [22]) can also be used as a unique specifier of the states within the class having corresponding symmetry. For isotropic and Werner states, the set of projectors can be simplified to only one operator. Since these are the only sets of states we consider in this paper, we can restrict our discussion to this special case, where we define a function $f_{\mathcal{G}}(\rho)$ with the property that

$$\mathcal{P}^{\mathcal{G}}\rho = \rho^{\mathcal{G}}_{F=f_{\mathcal{G}}(\rho)}, \tag{A3}$$

and the function $f_{\mathcal{G}}(\rho)$ is a one-to-one mapping from the class of symmetrical states to the set of real numbers (or, in general, real vectors).

Now we move on to the calculation of an entanglement monotone: suppose $\mathcal{X}(\psi)$ is defined on the set of pure states, where ψ stands for the corresponding density operator, and we use convex roof construction [7] to generalize this measure to mixed state ρ by

$$\mathcal{X}(\rho) \equiv \inf\left\{\sum_k p_k\mathcal{X}(\psi_k)\middle|\sum_k p_k\psi_k = \rho\right\}. \tag{A4}$$

Then by definition of the infimum, we have

$$\begin{aligned}\mathcal{X}\big(\rho^{\mathcal{G}}_F\big) &= \inf\left\{\sum_k p_k\mathcal{X}(\psi_k)\middle|\sum_k p_k\psi_k = \rho^{\mathcal{G}}_F\right\},\\ &\geqslant \inf\left\{\sum_k p_k\mathcal{X}(\psi_k)\middle|\mathcal{P}^{\mathcal{G}}\left(\sum_k p_k\psi_k\right) = \rho^{\mathcal{G}}_F\right\},\\ \Rightarrow \mathcal{X}\big(\rho^{\mathcal{G}}_F\big) &\geqslant \inf\left\{\sum_k p_k\mathcal{X}(\psi_k)\middle|\sum_k p_k f_{\mathcal{G}}(\psi_k) = F\right\}.\end{aligned} \tag{A5}$$

Let $\{p_k^{(0)},\psi_k^{(0)}\}$ be a pure-state ensemble which is the optimal decomposition achieving the infimum in the right-hand side, namely,

$$\sum_k p_k^{(0)} f_{\mathcal{G}}\big(\psi_k^{(0)}\big) = F, \tag{A6}$$

$$\sum_k p_k^{(0)}\mathcal{X}\big(\psi_k^{(0)}\big) = \inf\left\{\sum_k p_k\mathcal{X}(\psi_k)\middle|\sum_k p_k f_{\mathcal{G}}(\psi_k) = F\right\}. \tag{A7}$$

It follows that the twirling of the new state $\rho' = \sum_k p_k^{(0)}\psi_k^{(0)}$ is just $\rho^{\mathcal{G}}_F$,

$$\begin{aligned}\mathcal{P}^{\mathcal{G}}\rho' &= \mathcal{P}^{\mathcal{G}}\left(\sum_k p_k^{(0)}\psi_k^{(0)}\right)\\ &= \rho^{\mathcal{G}}_{F=f_{\mathcal{G}}(\rho')} = \rho^{\mathcal{G}}_{F=\sum_k p_k^{(0)} f_{\mathcal{G}}(\psi_k^{(0)})} = \rho^{\mathcal{G}}_F,\end{aligned} \tag{A8}$$

and, from the fact that the twirling operation is a LOCC operation, we obtain the inequality

$$\mathcal{X}(\rho') \geqslant \mathcal{X}(\mathcal{P}^{\mathcal{G}}\rho') = \mathcal{X}\big(\rho^{\mathcal{G}}_F\big). \tag{A9}$$

On the other hand, by the property of the convex roof construction in Eq. (A4), we have

$$\sum_k p_k^{(0)}\mathcal{X}\big(\psi_k^{(0)}\big) \geqslant \mathcal{X}\left(\sum_k p_k^{(0)}\psi_k^{(0)}\right) = \mathcal{X}(\rho'), \tag{A10}$$

which, combined with Eqs. (A5), (A7), and (A9), provides a tight bound for $\mathcal{X}(\rho^{\mathcal{G}}_F)$ for the explicit calculation

$$\begin{aligned}\mathcal{X}\big(\rho^{\mathcal{G}}_F\big) &= \mathcal{X}(\rho') = \sum_k p_k^{(0)}\mathcal{X}\big(\psi_k^{(0)}\big)\\ &= \inf\left\{\sum_k p_k\mathcal{X}(\psi_k)\middle|\sum_k p_k f_{\mathcal{G}}(\psi_k) = F\right\}.\end{aligned} \tag{A11}$$

Now we have derived a directly calculable formula of $\mathcal{X}(\rho^{\mathcal{G}}_F)$, which can be computed via a two-step procedure. The first step involves an optimization over pure states with the same value of the function $f_{\mathcal{G}}(\rho)$,

$$\chi(F) = \inf\{\mathcal{X}(\psi)|f_{\mathcal{G}}(\psi) = F\}. \tag{A12}$$

While this function is evaluated in [22] for entanglement of formation of both Werner and isotropic states, we note here that it is not immediately clear how it should be computed for any particular class of states or type of entanglement monotone. The calculation still needs to be done explicitly for specific combinations, given the general framework.

The next step is theoretically easier and more computable in general, but in practice does not always yield elegant or explicit results without numerical calculation. We define the convex hull of a function $f(x)$ defined on $\mathcal{D}$ to be

$$\begin{aligned}&\mathrm{co}(f(x))\\ &= \inf\left\{\sum_k p_k f(x_k)\middle|\sum_k p_k x_k = x, \sum_k p_k = 1, x_k\in\mathcal{D}\right\},\end{aligned} \tag{A13}$$

and the entanglement monotone $\mathcal{X}(\rho_F^{\mathcal{G}})$ of state $\rho_F^{\mathcal{G}}$ can be shown to be

$$\mathcal{X}\big(\rho_F^{\mathcal{G}}\big) = \mathrm{co}(\chi(F)). \tag{A14}$$

It is easy to see that this step is computable in general.

APPENDIX B: PROOF OF CONVEXITY PROPERTY OF THE FUNCTION $\Omega(\mathcal{C},\alpha)$

The function $\Omega(\mathcal{C},\alpha)$ is defined as

$$\Omega(\mathcal{C},\alpha) \equiv (1-\alpha)^{-1}\log_2(\lambda_+^\alpha + \lambda_-^\alpha), \tag{B1}$$

where $\lambda_\pm = (1 \pm \sqrt{1-\mathcal{C}^2})/2$. Let us present the first derivative of $\Omega(\mathcal{C},\alpha)$ with respect to $\mathcal{C}$, $\partial\Omega/\partial\mathcal{C}$, in terms of the Schmidt coefficients $\lambda_\pm$ by using Eq. (B1),

$$\frac{\partial\Omega(\mathcal{C},\alpha)}{\partial\mathcal{C}} = \frac{\alpha}{(1-\alpha)(\lambda_+^\alpha+\lambda_-^\alpha)}\left[\lambda_+^{\alpha-1}\frac{d\lambda_+}{d\mathcal{C}} + \lambda_-^{\alpha-1}\frac{d\lambda_-}{d\mathcal{C}}\right]. \tag{B2}$$

The derivatives of $\lambda_\pm$ are

$$\frac{d\lambda_\pm}{d\mathcal{C}} = \frac{\mathcal{C}}{2(1-2\lambda_\pm)}, \tag{B3a}$$

$$\frac{d^2\lambda_\pm}{d\mathcal{C}^2} = \frac{2}{\mathcal{C}^2(1-2\lambda_\pm)}\frac{d\lambda_\pm}{d\mathcal{C}}. \tag{B3b}$$

Also we know that $d\lambda_+/d\mathcal{C} + d\lambda_-/d\mathcal{C} = 0$, and we introduce the notations $D_1 = |d\lambda_+/d\mathcal{C}| = \mathcal{C}/2\sqrt{1-\mathcal{C}^2}$ and $x \equiv \lambda_-/\lambda_+$. By substituting Eq. (B3) into the derivative in Eq. (B2), we arrive at

$$\frac{\partial\Omega(\mathcal{C},\alpha)}{\partial\mathcal{C}} = \frac{\alpha\lambda_+^{\alpha-1}D_1}{(\alpha-1)(\lambda_+^\alpha+\lambda_-^\alpha)}(1-x^{\alpha-1}) \geqslant 0. \tag{B4}$$

Namely, $\Omega(\mathcal{C},\alpha)$ is a monotonically increasing function with respect to $\mathcal{C}$.

The evaluation of the second derivative of $\Omega(\mathcal{C},\alpha)$ is more complicated,

$$\frac{\partial^2\Omega(\mathcal{C},\alpha)}{\partial\mathcal{C}^2} = -\frac{\alpha\lambda_+^{2\alpha-2}D_1^2}{(1-\alpha)(\lambda_+^\alpha+\lambda_-^\alpha)^2}K, \tag{B5}$$

where

$$K = (1-x^{\alpha-1})^2 + \frac{(1+x)^2}{2x(1-x)}g(x,\alpha), \tag{B6}$$

$$g(x,\alpha) = 1 - x^{2\alpha-1} - (2\alpha-1)(1-x)x^{\alpha-1}, \tag{B7}$$

and $x \in (0,1]$ and $\alpha \in [0,1)$. Observing that

$$\begin{cases} K \geqslant (1-x^{\alpha-1})^2 \geqslant 0, & \alpha \in \left[0,\frac{1}{2}\right] \\ K \leqslant (1-x^{\alpha-1})^2, & \alpha \in \left(\frac{1}{2},1\right), \end{cases} \tag{B8}$$

we thus conclude that the function $\Omega(\mathcal{C},\alpha)$ is concave with respect to $\mathcal{C}$ for $\alpha \in [0,\frac{1}{2}]$,

$$\frac{\partial^2\Omega(\mathcal{C},\alpha)}{\partial\mathcal{C}^2} \leqslant -\frac{\alpha\lambda_+^{2\alpha-2}D_1^2(1-x^{\alpha-1})^2}{(1-\alpha)(\lambda_+^\alpha+\lambda_-^\alpha)^2} \leqslant 0. \tag{B9}$$

This result is actually opposite of the convexity of the function $\Omega(\mathcal{C},\alpha)$ for $\alpha \in (1,+\infty)$. We thus give a negative answer for the holding of the relation

$$\mathcal{R}_\alpha(\rho) = \Omega(\mathcal{C}(\rho),\alpha), \tag{B10}$$

for $\alpha \in [0,\frac{1}{2}]$.

Next, we consider the region $\alpha \in (\frac{1}{2},1)$. For a fixed α, the second derivative of $\Omega(\mathcal{C},\alpha)$ may have a zero corresponding to $\mathcal{C}_0$ in the interval $\mathcal{C}_0 \in [0,1]$. Numerical calculation shows that the value of $\mathcal{C}_0$ increases monotonically with respect to α; see Fig. 4 for the dependence of $\mathcal{C}_0$ on α. So there may exist a critical value of α corresponding to $\mathcal{C}=1$ such that the second derivative of $\Omega(\mathcal{C},\alpha)$ is zero. Such a critical value α_c does exist such that the simplification, meaning the holding of Eq. (6), is still valid for any α larger than this value. In fact, it is not difficult to obtain the value of α_c analytically. One simply considers the limit $\mathcal{C}\to 1$ and the requirement that

$$\lim_{\mathcal{C}\to 1}\frac{\partial^2\Omega(\mathcal{C},\alpha)}{\partial\mathcal{C}^2} \geqslant 0, \tag{B11}$$

which is equivalent to $\lim_{x\to 1} K \leqslant 0$. Referring to the definitions of K and $g(x,\alpha)$ in Eqs. (B6) and (B7), we derive the following inequality:

$$\frac{(\alpha-1)}{3}[3(\alpha-1)+(2\alpha-1)\alpha] \leqslant 0. \tag{B12}$$

The value of α_c can be calculated by considering the condition for equality in the above expression, which gives us

$$\alpha_c = \frac{\sqrt{7}-1}{2} \approx 0.82. \tag{B13}$$

This solution is consistent with our numerical result presented in Fig. 4.

APPENDIX C: DERIVATION OF THE CLOSED FORM OF THE FUNCTION $\omega(F,\alpha,d)$

Here we give a detailed proof of the formula

$$\omega(F,\alpha,d) = \begin{cases}\Omega(F,\alpha), & F \geqslant 0 \\ 0, & F < 0.\end{cases} \tag{C1}$$

The value of $\omega(F,\alpha,d)$ for $F \in [-1,0]$ can be easily obtained by setting $\mu_1 = 1, v_{11} = \sqrt{F}$ in the explicit expression of the function

$$f_W(\psi) = -\sum_{i,j=1}^{d}\sqrt{\mu_i\mu_j}\,v_{ji}v_{ij}^*, \tag{C2}$$

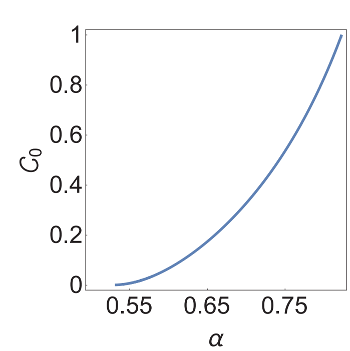

FIG. 4. By using condition $\frac{\partial^2\Omega(\mathcal{C},\alpha)}{\partial\mathcal{C}^2} = 0$, we can find the dependence of $\mathcal{C}_0$, which satisfies this equation, on α.

giving $\omega(F,\alpha,d)=0$, which reproduces the separability condition of the Werner state. While the optimization in the definition of $\omega(F,\alpha,d)=\inf\{\mathcal{R}_\alpha(\psi)|f_W(\psi)=F,\operatorname{rank}(\psi)\leqslant d\}$ for general d cannot be carried out in a straightforward fashion, it is rather simple for the two-qubit state. Setting $d=2$ in Eq. (C2), we have that for $F>0$,

$$\mathcal{C}(\psi)=2\sqrt{\mu_1\mu_2}\geqslant F, \tag{C3}$$

where equality holds if and only if $\mu_{1,2}=\lambda_\pm$. Since the function $\Omega(F,\alpha)$ is monotonically increasing with respect to F, we thus obtain the inequality $\Omega(\mathcal{C}(\psi),\alpha)=\mathcal{R}_\alpha(\psi)\geqslant\Omega(F,\alpha)$. It then follows that

$$\omega(F,\alpha,d)=\begin{cases}\Omega(F,\alpha), & F\geqslant 0\\ 0, & F<0.\end{cases} \tag{C4}$$

When seen as a real vector, $\vec{\mu}=[\mu_i]$ belongs to the convex set of real, at most d-dimensional vectors such that $\sum_{i=1}^d\mu_i=1(\mu_i\geqslant 0)$, which we denote by $\mathcal{K}_d$. It follows that $f_W(\psi)$ can also be seen as a function $f_W(\vec{\mu},V)$ of a real vector $\vec{\mu}$ and a unitary matrix V. For $F\in(0,1]$, we can calculate the quantity defined by

$$\tau(F,\alpha,d)\equiv\inf\left\{\sum_i\mu_i^\alpha|f_W(\vec{\mu},V)=-F,\vec{\mu}\in\mathcal{K}_d\right\}, \tag{C5}$$

from which the function $\omega(F,\alpha,d)$ can be obtained from $\omega(F,\alpha,d)=\log_2[\tau(F,\alpha,d)]$, by the monotonicity of the logarithm function. Noting that the minimization in Eq. (C5), with d larger than 2, always covers all possible combinations of $\{\mu_i,v_{ij}\}$ with $d=2$, we have

$$\tau(F,\alpha,d)\leqslant\tau(F,\alpha,2). \tag{C6}$$

Physically, this implies that the amount of entanglement contained in Werner states is upper bounded by that of a maximally entangled pair of qubits (for example, the Bell states). A consequence of this constraint is that when equality in the infimum in Eq. (C5) is achieved, the largest μ_i, which we denote by $\mu_{\max}$, must be bigger or equal to $\frac{1}{2}$. In fact, if $\mu_{\max}$ is smaller than $\frac{1}{2}$, we will derive a contradiction of Eq. (C6),

$$\mu_{\max}<\frac{1}{2}\Rightarrow\tau(F,\alpha,2)\leqslant\tau(1,\alpha,2)<\sum_i\mu_i^\alpha. \tag{C7}$$

Thus we have a constraint on $\mu_{\max}$ that reads

$$\mu_{\max}\geqslant\tfrac{1}{2}. \tag{C8}$$

Our next step is to seek an upper bound of $\mu_{\max}$, which combined with Eq. (C8) will further constrain the possible values that $\omega(F,\alpha,d)$ may take. First we derive some inequalities that the set of variables $\{\mu_i,v_{ij}\}$ must satisfy. Noting that $\sum_{i=1}^d\mu_i=1$, we have

$$\begin{aligned}1&=\sum_{i=1}^d\mu_i=\sum_{i,j}\mu_i|v_{ji}|^2\\&=\mu_{i_m}+\sum_{j\neq i_m}\mu_j\left|v_{i_mj}\right|^2+\sum_{i,j\neq i_m}\mu_i|v_{ji}|^2=1,\end{aligned} \tag{C9}$$

where i_m is one of the indices such that $\mu_{i_m}=\mu_{\max}$. With the use of the Cauchy-Schwarz inequality, it follows that

$$\left|\sum_{\substack{i\neq j\\ i,j\neq i_m}}^d\sqrt{\mu_i\mu_j}v_{ji}v_{ij}^*\right|^2\leqslant\left(\sum_{\substack{i\neq j\\ i,j\neq i_m}}^d|\sqrt{\mu_i}v_{ji}|^2\right)\left(\sum_{\substack{i\neq j\\ i,j\neq i_m}}^d|\sqrt{\mu_j}v_{ij}^*|^2\right)=\left(\sum_{\substack{i\neq j\\ i,j\neq i_m}}^d\mu_i|v_{ji}|^2\right)^2, \tag{C10}$$

$$\left|\sum_{j\neq i_m}^d\sqrt{\mu_{i_m}\mu_j}v_{ji_m}v_{i_mj}^*\right|^2\leqslant\left(\sum_{j\neq i_m}^d\mu_{i_m}\left|v_{ji_m}\right|^2\right)\left(\sum_{j\neq i_m}^d\mu_j\left|v_{i_mj}^*\right|^2\right). \tag{C11}$$

Thus the following inequalities can be easily derived:

$$\left|\sum_{\substack{i\neq j\\ i,j\neq i_m}}\sqrt{\mu_i\mu_j}v_{ji}v_{ij}^*\right|\leqslant\sum_{\substack{i\neq j\\ i,j\neq i_m}}\mu_i|v_{ji}|^2, \tag{C12}$$

$$\left|\sum_{j\neq i_m}\sqrt{\mu_{i_m}\mu_j}v_{ji_m}v_{i_mj}^*\right|\leqslant\sqrt{st}, \tag{C13}$$

where for later convenience we set

$$s=\sum_{j\neq i_m}\mu_{i_m}\left|v_{ji_m}\right|^2, \tag{C14}$$

$$t=\sum_{j\neq i_m}\mu_j\left|v_{i_mj}^*\right|^2. \tag{C15}$$

Making use of the condition in the infimum given by Eq. (C5), namely $f_W(\vec{\mu},V)=\sum_{i=1}^d\mu_i|v_{ii}|^2+\sum_{i\neq j}\sqrt{\mu_i\mu_j}v_{ji}v_{ij}^*=-F$, we have for $F\in[0,1]$ that

$$\begin{aligned}F&+\sum_{i=1}^d\mu_i|v_{ii}|^2\\&=\left|\sum_{i\neq j}^d\sqrt{\mu_i\mu_j}v_{ji}v_{ij}^*\right|\leqslant 2\left|\sum_{j\neq i_m}^d\sqrt{\mu_{i_m}\mu_j}v_{ji_m}v_{i_mj}^*\right|\\&\quad+\left|\sum_{\substack{i\neq j\\ i,j\neq i_m}}^d\sqrt{\mu_i\mu_j}v_{ji}v_{ij}^*\right|\end{aligned} \tag{C16}$$

$$\leqslant 2\left|\sum_{j\neq i_m}^{d}\sqrt{\mu_{i_m}\mu_j}v_{ji_m}v_{i_mj}^*\right| + \sum_{\substack{i\neq j\\ i,j\neq i_m}}^{d}\mu_i|v_{ji}|^2$$

$$= 1-\mu_{i_m} - \sum_{j\neq i_m}\mu_j\left|v_{i_mj}\right|^2 + 2\left|\sum_{j\neq i_m}^{d}\sqrt{\mu_{i_m}\mu_j}v_{ji_m}v_{i_mj}^*\right|$$

$$\leqslant 1-\mu_{i_m} - \left(\sum_{j\neq i_m}^{d}\mu_j\left|v_{i_mj}^*\right|^2\right) + 2\sqrt{st}$$

$$= 1-\mu_{i_m} - t + 2\sqrt{t\left(\sum_{j\neq i_m}^{d}\mu_{i_m}\left|v_{ji_m}\right|^2\right)}. \tag{C17}$$

To further evaluate the expression in Eq. (C17), we note that this is essentially a quadratic function, with the argument $\sqrt{t}$ satisfying the inequality

$$t = \sum_{j\neq i_m}\mu_j\left|v_{i_mj}^*\right|^2 \leqslant \sum_{j\neq i_m}\mu_j = 1-\mu_{i_m}, \tag{C18}$$

and we consider two possible cases of $\sqrt{t}$ to derive a uniform bound. First, if

$$\sum_{j\neq i_m}\mu_{i_m}\left|v_{ji_m}\right|^2 = \mu_{i_m} - \mu_{i_m}\left|v_{i_mi_m}\right|^2 \geqslant 1-\mu_{i_m}, \tag{C19}$$

then we have $\sum_{j\neq i_m}\mu_j|v_{i_mj}^*|^2 \leqslant 1-\mu_{i_m} \leqslant \mu_{i_m} - \mu_{i_m}|v_{i_mi_m}|^2$ such that

$$F + \sum_{i=1}^{d}\mu_i|v_{ii}|^2 \leqslant 2\sqrt{\mu_{\max}(1-\mu_{\max})}. \tag{C20}$$

If instead the variables $\{\mu_i, v_{ij}\}$ satisfy

$$\sum_{j\neq i_m}^{d}\mu_{i_m}\left|v_{ji_m}\right|^2 = \mu_{i_m} - \mu_{i_m}\left|v_{i_mi_m}\right|^2 < 1-\mu_{i_m}, \tag{C21}$$

then we obtain, similarly,

$$1-\mu_{i_m}\left|v_{i_mi_m}\right|^2 < 2\left(1-\mu_{i_m}\right), \tag{C22}$$

$$\Rightarrow \sum_{j\neq i_m}^{d}\mu_j\left|v_{i_mj}^*\right|^2 \leqslant \mu_{i_m} - \mu_{i_m}\left|v_{i_mi_m}\right|^2 < 1-\mu_{i_m}, \tag{C23}$$

$$\Rightarrow F + \sum_{i=1}^{d}\mu_i|v_{ii}|^2 \leqslant 1-\mu_{i_m}\left|v_{i_mi_m}\right|^2 < 2\left(1-\mu_{i_m}\right), \tag{C24}$$

$$\Rightarrow F + \sum_{i=1}^{d}\mu_i|v_{ii}|^2 \leqslant 2\sqrt{\mu_{\max}(1-\mu_{\max})}. \tag{C25}$$

Combining the two cases, and noting that $\mu_{i_m} = \mu_{\max}$, we derive a constraint of $\mu_{\max}$ in terms of F,

$$F \leqslant F + \sum_{i=1}^{d}\mu_i|v_{ii}|^2 \leqslant 2\sqrt{\mu_{\max}(1-\mu_{\max})}. \tag{C26}$$

Let $\mu(F) = \frac{1+\sqrt{1-F^2}}{2}$ (which, for simplicity, we will denote by μ when no confusion arises), and Eqs. (C8) and (C26) give $\mu_{\max} \leqslant \mu(F)$. Making use of the Schur concavity of the function $\tau(F,\alpha,d)$, we have

$$\tau(F,\alpha,d) = \sum_i \mu_i^\alpha \geqslant \mu_{\max}^\alpha + (1-\mu_{\max})^\alpha \geqslant \tau(F,\alpha,2). \tag{C27}$$

On the other hand, we have already obtained the inequality (C6), and together the two bounds yield

$$\tau(F,\alpha,d) = \sum_i \mu_i^\alpha \geqslant \tau(F,\alpha,2) \geqslant \tau(F,\alpha,d), \tag{C28}$$

indicating that the bound given in Eq. (C6) is indeed tight. We have now succeeded in calculating the functions $\tau(F,\alpha,d)$ and $\omega(F,\alpha,d)$,

$$\tau(F,\alpha,d) = \tau(F,\alpha,2), \tag{C29}$$

$$\omega(F,\alpha,d) = \begin{cases}\Omega(F,\alpha), & F\geqslant 0\\ 0, & F<0.\end{cases} \tag{C30}$$

APPENDIX D: PROOF OF THE CONJECTURE ON THE EoF OF ISOTROPIC STATE

We first state the rigorous result on entanglement of the formation of isotropic state ρ_F^{iso} in d-dimensional Hilbert space, which we denote by $\mathcal{E}(\rho_F^{\text{iso}})$,

$$\mathcal{E}\left(\rho_F^{\text{iso}}\right) = \text{co}\,(\varepsilon(F,d)), \tag{D1}$$

where $\text{co}\,(\cdot)$ denotes the convex hull of a function, and the function $\varepsilon(F,d)$ is found to be

$$\varepsilon(F,d) = H_2(\gamma(F,d)) + [1-\gamma(F,d)]\log_2(d-1), \tag{D2}$$

$$\gamma(F,d) = \frac{1}{d}\left[\sqrt{F} + \sqrt{(d-1)(1-F)}\right]^2, \tag{D3}$$

and $H_2(x)$ is the binary entropy function.

In Vollbrecht and Terhal's work [21], a closed expression of the EoF of isotropic states is conjectured, whose validity the authors argue can always be verified for any given d, by directly plotting the function $\varepsilon(F,d)$ and examining its behavior. The rigorous proof of the $d=3$ case is provided. It is now generally accepted that the conjecture is true for arbitrary d, but it seems that a proof is still necessary. Alternatively, here we seek to prove this conjecture in an analytical fashion, without any presumption about the value of d.

The proof consists of two steps: we first prove a general statement about $\varepsilon(F,d)$, when treating F as the argument and d as a parameter, and the next step simply involves the verification of a criterion of the point $F = \frac{4(d-1)}{d^2}$. First we wish to show that the concavity of $\varepsilon(F,d)$ with respect to F on the interval $F \in [1,0]$ is, in general, analogous to that of the special case with $d=3$, i.e., first concave upwards and then concave downwards. We will prove this statement by directly evaluating the value of the second derivative of $\varepsilon(F,d)$ with respect to F. To keep the equations as simple as possible, we use ε and γ to denote, respectively, the functions

$$\varepsilon(F,d) = H_2(\gamma) + (1-\gamma)\log_2(d-1), \tag{D4}$$

$$\gamma(F,d) = \frac{1}{d}\left[\sqrt{F} + \sqrt{(d-1)(1-F)}\right]^2. \tag{D5}$$

A bit of algebra gives us

$$\frac{d\gamma}{dF} = -\frac{\sqrt{\gamma(1-\gamma)}}{\sqrt{F(1-F)}}, \tag{D6}$$

$$\frac{d^2\gamma}{dF^2} = -\frac{\sqrt{d-1}}{2d\gamma(1-\gamma)\sqrt{F(1-F)}}\left(\frac{d\gamma}{dF}\right)^2. \tag{D7}$$

Substituting the derivatives of γ with respect to F into the relation

$$\frac{\partial^2\varepsilon}{\partial F^2} = \frac{\partial^2\varepsilon}{\partial\gamma^2}\left(\frac{d\gamma}{dF}\right)^2 + \frac{d^2\gamma}{dF^2}\frac{\partial\varepsilon}{\partial\gamma}, \tag{D8}$$

we obtain

$$\frac{\partial^2\varepsilon}{\partial F^2} = \frac{\sqrt{d-1}}{2d[F(1-F)]^{\frac{3}{2}}}\left[\ln\frac{\gamma(d-1)}{1-\gamma} - \frac{2d\sqrt{F(1-F)}}{\sqrt{d-1}}\right]. \tag{D9}$$

Now we only need to examine the sign of the term in the square bracket of the above equation, which is the same as that of $\frac{\partial^2\varepsilon}{\partial F^2}$. In a change of variable, we let $x = \sqrt{\frac{1-F}{F(d-1)}}$, so that $x \in [0,1]$ decreases monotonically with respect to F in the interval $F \in [\frac{1}{d},1]$. Letting the term in the square bracket of Eq. (D9) be a function $f(x)$ of x, we have

$$f(x) = \ln\left(\frac{dx}{1-x}+1\right) - \frac{dx}{1+(d-1)x^2}, \tag{D10}$$

whose behavior at the two ends of the interval $x \in [0,1]$ is easily found to be

$$F \to \frac{1}{d}, \quad x \to 1, \quad \frac{\partial^2\varepsilon}{\partial F^2} \to +\infty; \tag{D11}$$

$$F \to 1, \quad x \to 0, \quad \frac{\partial^2\varepsilon}{\partial F^2} \to -\infty. \tag{D12}$$

Differentiate $f(x)$ with respect to x, and we obtain

$$f'(x) = \frac{(d-1)(d-2)dx\,g(x)}{(1-x)(dx-x+1)[1+(d-1)x^2]^2}, \tag{D13}$$

whose denominator is non-negative, and the function $g(x)$ is equal to

$$g(x) = \left(x+\frac{2}{d-2}\right)^2 - \frac{d^2}{(d-1)(d-2)^2}. \tag{D14}$$

Noting that $g(x)$ is a quadratic function of x, it has two zeros which are easily found to be

$$x_\pm = \frac{-2\sqrt{d-1}\pm d}{(d-2)\sqrt{d-1}}. \tag{D15}$$

The zero $x_- < 0$ is not in the interval $x \in [0,1]$ of our interest, while it can be shown that $x_+ \in (0,1)$ if $d > 2$. Furthermore, by evaluating the value of $g(x)$ in Eq. (D14) to determine the sign of $f'(x)$, we have

$$f'(x)\begin{cases} < 0, & x \in (0,x_+) \\ \geqslant 0, & x \in [x_+,1). \end{cases} \tag{D16}$$

Thus, we conclude that the minimum of the function $f(x)$ on the interval $x \in (0,1)$ is $f(x_+)$,

$$f(x_+) = \ln\sqrt{d-1} - \frac{d-2}{2\sqrt{d-1}} = h(\sqrt{d-1}), \tag{D17}$$

where the function $h(x)$ is defined as

$$h(x) \equiv \ln x - \frac{x}{2} + \frac{1}{2x}. \tag{D18}$$

For $d > 2$, we have $h'(x) = -\frac{(x-1)^2}{2x^2} < 0$, and it follows that

$$f(x_+) < 0. \tag{D19}$$

Combining this with the special case $f(0) = 0$, we have $f(x) < 0$ and $\frac{\partial^2\varepsilon}{\partial F^2} < 0$ for $x \in (0,x_+)$. On the other hand, the function $f(x)$ increases monotonically for $x \in [x_+,1)$, and it can be easily shown that $f(1) \to +\infty$ as $x \to 1$, which ensures that the function $f(x)$ has only one zero in the interval $x \in (0,1)$. Also taking into account Eqs. (D11) and (D12), which gives the limit of $\frac{\partial^2\varepsilon}{\partial F^2}$ as $F \to \frac{1}{d}$ and 1, we conclude that the second derivative $\frac{\partial^2\varepsilon}{\partial F^2}$ has only one zero on the interval $F \in [\frac{1}{d},1]$.

Now that we have proved that the function $\varepsilon(F,d)$ on the interval $F \in [1,0]$ is first concave upwards and then concave downwards as F increases, the next step is simply to find a line that is both tangent to $\varepsilon(F,d)$ and passes the point $F = 1$; in other words, we want to find a solution $F_0 \in (\frac{1}{d},1)$ to the following equation:

$$\log_2 d - \varepsilon = (1-F)\frac{\partial\varepsilon}{\partial F}. \tag{D20}$$

Taking the convexity of the function $\varepsilon(F,d)$ into account, one can deduce that such solution does exist and is unique. In addition, direct calculation shows that the conjecture $F = \frac{4(d-1)}{d^2}$ is indeed the solution to Eq. (D20). Since $\varepsilon(F,d)$ can be easily shown to be monotonously increasing with respect to F, we now have adequate information to determine explicitly the value of $\mathcal{E}(\rho_F^{\mathrm{iso}}) = \lim_{\alpha\to 1}\mathcal{R}_\alpha(\rho_F^{\mathrm{iso}})$,

$$\mathcal{E}\left(\rho_F^{\mathrm{iso}}\right) = \begin{cases} 0, & F \in \left[0,\frac{1}{d}\right] \\ \varepsilon(F,d), & F \in \left[\frac{1}{d},\frac{4(d-1)}{d^2}\right] \\ \frac{d\log_2(d-1)}{d-2}(F-1)+\log_2 d, & F \in \left[\frac{4(d-1)}{d^2},1\right]. \end{cases} \tag{D21}$$

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