Computation of the geometric measure of entanglement for pure multiqubit states

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We provide methods for computing the geometric measure of entanglement for two families of pure states with both experimental and theoretical interests: symmetric multiqubit states with non-negative amplitudes in the Dicke basis and symmetric three-qubit states. In addition, we study the geometric measure of pure three-qubit states systematically in virtue of a canonical form of their two-qubit reduced states and derive analytical formulas for a three-parameter family of three-qubit states. Based on this result, we further show that the W state is the maximally entangled three-qubit state with respect to the geometric measure.

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I. INTRODUCTION

Quantum entanglement, which was first noted by Einstein and Schrödinger [1,2], has been extensively studied in the past 20 years [3]. In particular, multipartite entanglement has attracted increasing attention due to its intriguing properties and potential applications in quantum-information processing.

The importance of multipartite entanglement can be illustrated in two aspects. In respect of application, graph states, prominent examples of entangled multiqubit states, are a useful resource for one-way quantum computation [4] and fault-tolerant topological quantum computation [5]. Multipartite entangled states, such as GHZ states, are essential resources for quantum secret sharing [6,7]. In addition, multipartite entangled states can serve as multiparty quantum channels in virtue of teleportation [8]. In respect of theoretical interests, multipartite states display stronger nonlocality, one of the key features of quantum physics [9–11]. Quantum cryptography beyond pure entanglement distillation has been generalized to multipartite bound entangled states [12]. What's more, recent progress in experiments has made accessible more multipartite entangled states, such as the GHZ states [13], W states [14], six-photon Dicke states [15–17], and so on. Methods for detecting such states have also been developed [18].

Given an entangled state, a natural question to ask is how much entanglement is contained in this state. In quantum-information theory, entanglement is usually quantified by entanglement measures [19]. An entanglement measure is an entanglement monotone, which cannot increase under local operations and classical communications (LOCC), and equal to zero for only classically correlated (separable) states [20]. Hitherto, the most well-known entanglement measures are defined for bipartite states, such as entanglement cost and distillable entanglement [20,21]. For pure bipartite states, there is essentially a unique entanglement measure, the von Neumann entropy of each reduced density matrix, which is easily computable [22].

For multipartite states, while a lot of entanglement measures have been proposed [3,23,24], the characterization of multipartite entanglement is far from being complete. It is generally difficult to calculate such measures even numerically. Moreover, the existence of many types of inequivalent entanglement defies a unique definition. Different entanglement measures often induce different orders and even lead to different maximally entangled states. For example, the Bell state $|\Psi\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ is the maximally entangled state of a two-qubit system for all measures, since it violates the Bell inequality most strongly. However, its multipartite analog, the GHZ state $|\mathrm{GHZ}\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$, is maximally entangled only under some specific entanglement measures, such as three-tangle [25,26]. It is not a maximally entangled state under the definition in Ref. [27], and the geometric measure of entanglement, which is one focus of the present article.

On the other hand, some geometrically motivated multipartite entanglement measures have been providing us insights on quantum entanglement. One prominent example is the geometric measure of entanglement (GM), [24] which quantifies the minimum distance between a given state and the set of product states. In addition to providing a simple geometric picture, GM has significant operational meanings. It is closely related to optimal entanglement witnesses [24,28] and has been shown to quantify the difficulty of multipartite state discrimination under LOCC [29]. Recently, GM has also been applied to show that most entangled states are too entangled to be useful as computational resources [30]. In condensed matter physics, GM has been utilized to study the ground-state properties and to characterize quantum phase transitions [31–34].

There have been extensive literatures on the quantitative calculation of GM for both pure and mixed states [24,28,35–39]. The qualitative analysis on GM has also received much attention [40,41]. In addition, a few numerical methods have been developed for computing the GM of multipartite states, such as the algorithms presented in Refs. [42,43], which allow repeated analytical maximization according to a subset of the parameters with a high efficiency. However, our knowledge about GM is still quite limited. Even for pure three-qubit states, there is no complete analytical solution. In addition, it is still

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uncertain which state is the maximally entangled with respect to GM, although the authors of Ref. [26] conjectured that the W state is such a candidate. Thus it is desirable to compute GM analytically for more entangled states, which is another focus of the present article.

In this article, we would like to compute the GM for several families of multipartite pure states and determine the maximally entangled three-qubit states with respect to GM. Throughout the article, by symmetric states, we mean those states which are supported on the symmetric subspace of the whole Hilbert space.

First, we present an analytical method for computing the GM of symmetric multiqubit states composed of Dicke states with non-negative amplitudes by virtue of a recent simplification on GM of symmetric states [41]. Next, we analytically compute the GM for symmetric three-qubit states. Combining with the results in Ref. [35], we provide a complete analytical solution for GM of any symmetric pure three-qubit states. Recall that many important multiqubit states accessible to experiments so far are symmetric, e.g., GHZ states [13], W states [14], and Dicke states [16,17], and so on. Our results may hopefully help analyze these states in experiments.

Second, we introduce a canonical form of pure three-qubit states based on the canonical form of two-qubit rank-two states developed in Ref. [44]. In virtue of this canonical form, we study the GM of pure three-qubit states systematically and derive explicit analytical formulas of GM for a three-parameter family of three-qubit states. Starting from these results, we prove that, up to local unitary transformations, the W state is the unique maximally entangled pure three-qubit state with respect to GM, confirming the conjecture made in Ref. [26].

The rest of the article is organized as follows. In Sec. II, we propose an analytical method for computing the GM of symmetric multiqubit states with non-negative amplitudes, as well as symmetric three-qubit states. In Sec. III, we derive analytical formulas of GM for a three-parameter family of pure three-qubit states and prove that the W state is the maximally entangled state under GM. We conclude in Sec. IV.

II. ANALYTICAL METHOD FOR COMPUTING GEOMETRIC MEASURE (I): SYMMETRIC STATES

The definition of GM of bipartite or multipartite pure states is motivated by the following simple geometric idea of entanglement quantification: the farther away from the set of separable states, the more entangled a state is [24]. Given a pure state $|\psi\rangle$ of a joint system composed of subsystems $A, B, C, \ldots$, define $G(|\psi\rangle)$ as the maximum overlap between $|\psi\rangle$ and the set of product states, that is,

$$G(|\psi\rangle) := \max_{|\varphi\rangle = |a\rangle|b\rangle|c\rangle\ldots} |\langle\varphi|\psi\rangle|, \qquad (1)$$

where the normalized one-particle states $|a\rangle, |b\rangle, |c\rangle, \ldots$ belong to subsystems $A, B, C, \ldots$, respectively. $G(|\psi\rangle)$ is manifestly invariant under local unitary transformations. It obtains the maximum value 1 only for product states and is thus an inverted

entanglement measure. The GM of a pure state is defined as follows:

$$E_G(|\psi\rangle) := 1 - G(|\psi\rangle)^2, \qquad (2)$$

or in another version $-2\log_2 G(|\psi\rangle)$ sometimes. In this article we will follow the definition in Eq. (2). It can be extended to the GM of mixed states by convex roof construction [24] according to the same idea as in the definition of entanglement of formation [20]:

$$E_G(\rho) := \min_{\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|} \sum_i p_i E_G(|\psi_i\rangle). \qquad (3)$$

$E_G(\rho)$ has been shown to be an entanglement monotone by T.-C. Wei and P. M. Goldbart [24]. An alternative definition of GM for mixed states will be introduced in Sec. III in a different context.

Clearly, $E_G(|\psi\rangle)$ in Eq. (2) is determined by $G(|\psi\rangle)$ in Eq. (1). From now on we focus on $G(|\psi\rangle)$ of pure states $|\psi\rangle$ and call it GM too, if there is no confusion. For a pure bipartite state, the GM is equal to its largest Schmidt coefficient. The problem becomes difficult for pure multipartite states, since there is no Schmidt decomposition in general. The difficulty lies in the linearly increasing number of optimization variables parametrizing the product states $|a\rangle|b\rangle|c\rangle\cdots$ in Eq. (1), as the number of parties increases. In fact, only a few partial results are available on this problem [24,26,35,36].

Recently, the authors of Ref. [41] proved that, for a symmetric pure state $|\psi^{sy}\rangle$, it suffices to consider symmetric product states in the maximization in Eq. (1), that is,

$$G(|\psi^{sy}\rangle) = \max_{|\varphi\rangle = |a\rangle|a\rangle|a\rangle\ldots} |\langle\varphi|\psi^{sy}\rangle|. \qquad (4)$$

This result can greatly simplify the calculation of GM for symmetric states. In the rest of this section, we derive analytical solutions for two families of states, respectively, in virtue of this result. In Sec. II A, we analytically derive GM for symmetric multiqubit states with non-negative amplitudes in the Dicke basis. In Sec. II B, we derive the analytical solution of GM for symmetric pure three-qubit states based on the previous work [35], thus solving this problem completely.

A. Symmetric multiqubit states with non-negative amplitudes

In this subsection, we compute the GM for pure symmetric multiqubit states with non-negative amplitudes in the Dicke basis. More explicitly, we investigate the N-qubit state

$$|\psi^{symq}\rangle := \sum_{m=0}^{N} a_m |m, N\rangle, \qquad (5)$$

where $a_m \geqslant 0$, and $|m, N\rangle$ is the Dicke state [15] defined as

$$|m, N\rangle := \binom{N}{m}^{-1/2} \sum_k P_k |\overbrace{1, \ldots, 1}^{m}, \overbrace{0, \ldots, 0}^{N-m}\rangle, \qquad (6)$$

where P_ks denote the set of all permutations of the spins. By definition, Dicke states are symmetric; so the state

$|\psi^{\text{symq}}\rangle$ is also symmetric, and we can apply Eq. (4) to computing its GM. Let $|a\rangle = \cos\alpha|0\rangle + e^{i\theta}\sin\alpha|1\rangle$ with $\alpha \in [0,\frac{\pi}{2}]$ and $\theta \in [0,2\pi]$; then the GM of the state in Eq. (5) reads

$$
\begin{aligned}
&G(|\psi^{\text{symq}}\rangle) \\
&= \max_{|\varphi\rangle = |a\rangle|a\rangle|a\rangle\dots} \left| \sum_{m=0}^{N} \binom{N}{m}^{1/2} a_m \cos^{N-m}\alpha \sin^m\alpha\, e^{-im\theta} \right|, \\
&\leqslant \max_{|\varphi\rangle = |a\rangle|a\rangle|a\rangle\dots} \sum_{m=0}^{N} \left| \binom{N}{m}^{1/2} a_m \cos^{N-m}\alpha \sin^m\alpha \right|, \\
&= \max_{\alpha\in[0,\frac{\pi}{2}]} \sum_{m=0}^{N} \binom{N}{m}^{1/2} a_m \cos^{N-m}\alpha \sin^m\alpha, \quad (7)
\end{aligned}
$$

where the equality holds when $\theta = 0$. Equation (7) contains only one variable α, so one can easily find out the maximum. For example, let $x = \tan\alpha$, then one can convert $G^2(|\psi^{\text{symq}}\rangle)$ into a rational fraction $A(x)/B(x)$, where $A(x)$ and $B(x)$ are both polynomials on x. By calculating its derivative we can find out the maximum in Eq. (7) explicitly.

A similar idea can be applied to calculating the GM of any symmetric multiqudit state with non-negative amplitudes in the generalized Dicke basis; again, the number of free variables can be reduced by half. Recently, the additivity of GM of states with non-negative amplitudes was proved, i.e., $G(|\alpha\rangle \otimes |\beta\rangle) = G(|\alpha\rangle)G(|\beta\rangle)$ [45]. So we can compute the GM of $|\psi^{\text{symq}}\rangle \otimes |\beta\rangle$ if we know the GM of $|\beta\rangle$ too.

Unfortunately, the present method does not apply to arbitrary symmetric multiqubit states, e.g., those states in Eq. (5) having negative or complex amplitudes. For more complicated states, numerical methods are indispensable for computing their entanglement measures, see, for example, Refs. [42,43].

B. Symmetric three-qubit states

In this subsection, we compute the GM of symmetric pure three-qubit states. Such states can always be converted into the following form with suitable local unitary operations [35]:

$$
|\Phi\rangle = g|000\rangle + t(|011\rangle + |101\rangle + |110\rangle) + e^{i\gamma}h|111\rangle, \quad (8)
$$

where $g,t,h \geqslant 0$, and $\gamma \in [-\frac{\pi}{2},\frac{\pi}{2}]$. So it suffices to calculate the GM for the state $|\Phi\rangle$.

Analytical formula of the GM is already known if at least one of the three parameters g,t,h is vanishing or $\gamma = 0$, $\pm\frac{\pi}{2}$ [24,28,35,36,46]. Hence, we can focus on the family of states with

$$
g,t,h > 0, \quad g^2 + 3t^2 + h^2 = 1, \quad \gamma \in \left(-\frac{\pi}{2},0\right) \cup \left(0,\frac{\pi}{2}\right). \quad (9)
$$

The authors of Ref. [36] have reduced the task of computing the GM of the state $|\Phi\rangle$ to solving the following system of

equations of the three variables φ,θ,λ (see also Appendix A):

$$
\begin{aligned}
&2ht\cos\gamma + 2t(g+t)\sin\theta\cos\varphi - 2ht\cos\gamma\cos\theta \\
&\qquad = \lambda\sin\theta\cos\varphi, \quad (10)
\end{aligned}
$$

$$
\begin{aligned}
&2ht\sin\gamma - 2t(g-t)\sin\theta\sin\varphi - 2ht\sin\gamma\cos\theta \\
&\qquad = \lambda\sin\theta\sin\varphi, \quad (11)
\end{aligned}
$$

$$
\begin{aligned}
&(g^2 - t^2)(1+\cos\theta) - h^2(1-\cos\theta) - 2ht\cos\gamma\sin\theta\cos\varphi \\
&\qquad - 2ht\sin\gamma\sin\theta\sin\varphi = \lambda\cos\theta. \quad (12)
\end{aligned}
$$

For each root (φ_j,θ_j) of Eqs. (10)–(12), we can obtain a GM candidate of the state $|\Phi\rangle$ via the following formula, according to Eq. (A1) in Appendix A,

$$
\begin{aligned}
G_j^2(|\Phi\rangle) = \frac{1}{8}\Big[&3 - 2t^2 + 4(1 - 2h^2 - 4t^2)\cos\theta_j \\
&+ (1 - 6t^2)\cos 2\theta_j + 4gt\cos 2\varphi_j \sin^2\theta_j \\
&+ 32ht\cos(\gamma - \varphi_j)\cos\frac{\theta_j}{2}\sin^3\frac{\theta_j}{2} \Big]; \quad (13)
\end{aligned}
$$

the GM is the maximum over all the GM candidates:

$$
G^2(|\Phi\rangle) = \max_j G_j^2(|\Phi\rangle). \quad (14)
$$

We shall solve Eqs. (10)–(12) in two cases separately; the second case consists of three subcases. In each case we obtain one or a few GM candidates by computing Eq. (13) with the solutions to the system of equations.

Case 1: Suppose $\theta = 0$; then the phase φ does not play any role, and Eqs. (10) and (11) become identities, while Eq. (12) determines λ. In this case we get a GM candidate via Eq. (13) as follows:

$$
G_1^2(|\Phi\rangle) = g^2. \quad (15)
$$

Case 2: To satisfy Eqs. (10)–(12), the roots $\varphi = k\frac{\pi}{2}$ for $k = 0,1,2,3$ lead to $\theta = 0$, which is already discussed. Moreover, $\theta = \pi$ cannot be a legal solution of Eqs. (10) or (11), so this choice is excluded. Hence, it remains to solve Eqs. (10)–(12) under the assumption that

$$
\varphi \in \left(0,\frac{\pi}{2}\right) \cup \left(\frac{\pi}{2},\pi\right) \cup \left(\pi,3\frac{\pi}{2}\right) \cup \left(3\frac{\pi}{2},2\pi\right), \quad \theta \in (0,\pi). \quad (16)
$$

From Eqs. (10)–(12), we can determine λ as a function of θ and φ. Inserting this solution into Eq. (10) and Eq. (11), we can obtain two equations about θ and φ: $E_1(\varphi,\theta) = 0$ and $E_2(\varphi,\theta) = 0$, respectively. This further implies that either

$$
\tan\frac{\theta}{2} = \frac{g}{h\csc 2\varphi \sin(\gamma - \varphi)}, \quad (17)
$$

or

$$
\tan\frac{\theta}{2} = \frac{-t}{h\csc 2\varphi \sin(\gamma + \varphi)}. \quad (18)
$$

Combining either of them and $E_1(\varphi,\theta) = 0$ can lead to a set of solutions.

Case 2.1: There is a simple solution $\tan\varphi = \frac{t+g}{t-g}\tan\gamma$. The variable θ can be determined via either Eq. (17) or (18), which

lead to an identical result in this case. Inserting this solution into Eq. (13), we get another GM candidate:

$$G_2^2(|\Phi\rangle) = g^2 - \frac{(g^2 - t^2)^3}{t^2 - 2t^4 + g^2 - 6g^2t^2 - 2gth^2\cos 2\gamma}. \tag{19}$$

Case 2.2: By combining Eq. (17) and $E_1(\varphi,\theta) = 0$, we can get two polynomial equations:

$$\sum_{i=0}^{4} c_{1i}(g,t,h,\gamma)\cos^i 2\varphi = 0,$$
$$\sum_{i=0}^{4} c_{2i}(g,t,h,\gamma)\cos^i 2\varphi = 0, \tag{20}$$

as well as Case 2.1, which has already been handled. Since Eqs. (20) are quartic equations on $\cos 2\varphi$, we can analytically derive their roots. We may obtain up to 16 different phases $\varphi \in [0,2\pi]$. The variable θ can then be determined via Eq. (17). Hence, we can derive up to 16 GM candidates $G_j(|\Phi\rangle)$ for $j = 3,\ldots,18$ via Eq. (13). This differs a bit from Case 1 and Case 2.1, where only one GM candidate is given respectively.

Case 2.3: Similar to Case 2.2, by combining Eq. (18) and $E_1(\varphi,\theta) = 0$, we can get two quartic polynomial equations on $\cos 2\varphi$, which are analytically solvable. Again we may get up to 16 GM candidates $G_j(|\Phi\rangle)$ for $j = 19,\ldots,34$. This finishes the discussion of Case 2.

Now we have all the GM candidates $G_j(|\Phi\rangle)$ for $j = 1,\ldots,34$. The maximum of them is exactly the GM of the state $|\Phi\rangle$ in Eq. (8). For convenience of the readers, here we repeat the main steps for deriving the GM of the symmetric three-qubit state $|\Phi\rangle$.

Step 1: Compute $G_1(|\Phi\rangle)$ and $G_2(|\Phi\rangle)$ via Eqs. (15) and (19), respectively; two GM candidates can be obtained.

Step 2: Compute $G_j(|\Phi\rangle)$ for $j = 3,\ldots,18$ via Eq. (13) with roots (φ_j,θ_j) of Eqs. (17) and (20); up to 16 GM candidates can be obtained.

Step 3: Similar to Step 2, with the roots (φ_j,θ_j) for $j = 19,\ldots,34$ of Eq. (18) and quartic equations similar to Eq. (20), up to 16 GM candidates can be obtained via Eq. (13).

Step 4: The maximum of all 34 GM candidates is exactly the GM of the state $|\Phi\rangle$.

In conclusion, we have provided a method for analytically deriving the GM of symmetric three-qubit states in Eq. (8) with $\gamma \in (-\frac{\pi}{2},0) \cup (0,\frac{\pi}{2})$. The special cases $\gamma = 0, \pm\frac{\pi}{2}$ have been addressed in Ref. [35]. Calculation shows that our result approaches their result when γ approaches these special values. Hence, we can now compute the GM of any symmetric pure three-qubit states.

III. ANALYTICAL METHOD FOR COMPUTING GEOMETRIC MEASURE (II): MAXIMAL ENTANGLED STATES AMONG PURE THREE-QUBIT STATES

In this section, we introduce a canonical form of pure three-qubit states based on the canonical form of two-qubit rank-two states developed in Ref. [44]. By virtue of this canonical form, the GM of pure three-qubit states is studied systematically. In particular, we derive analytical formulas of GM for the family of pure three-qubit states one of whose rank-two two-qubit reduced states is the convex combination of the maximally entangled state and its orthogonal pure state within the rank-two subspace. Based on these results, we prove that the W state is the maximally entangled three-qubit state with respect to GM, confirming the conjecture in Ref. [26].

Our approach builds on Theorem 1 in Ref. [47], which states that the GM of an n-partite pure state $|\psi\rangle$ is determined by any of its $(n-1)$-partite reduced states ρ, that is,

$$G^2(|\psi\rangle) = g(\rho).$$

Here $g(\rho)$ is an alternative definition of geometric measure and has nothing to do with the parameter g introduced in Eq. (8):

$$g(\rho) = \max_{\rho_1,\ldots,\rho_{n-1}} \mathrm{tr}[\rho(\rho_1 \otimes \cdots \otimes \rho_{n-1})], \tag{21}$$

where $\rho_1,\ldots,\rho_{n-1}$ are pure single-particle states, namely $\rho_i = |a_i\rangle\langle a_i|$. In addition, to any closest product state $\rho_1 \otimes \cdots \otimes \rho_{n-1}$ of ρ, there corresponds a unique closest product state of $|\psi\rangle$ with $\rho_1 \otimes \cdots \otimes \rho_{n-1}$ as a reduced state. A closest product state of ρ is any pure product state $\rho_1 \otimes \cdots \otimes \rho_{n-1}$ which maximizes Eq. (21). From the definition, $g(\rho)$ is a convex function of ρ; this property will be frequently resorted to later.

Note that for a mixed state ρ, $g(\rho)$ is not the standard definition of the GM of ρ (see the first paragraph of Sec. II). Nevertheless, this alternative definition is useful for computing the GM of any purification of ρ [47]. It has also many applications of its own, such as constructing optimal entanglement witnesses [24,28] and quantifying the difficulty of state discrimination under LOCC [28,29].

A. Canonical form of two-qubit rank-two states

In this section we introduce a canonical form of pure three-qubit states based on the canonical form of two-qubit rank-two states developed in Ref. [44] and set the notations useful in later discussions.

For a pure three-qubit state, each two-qubit reduced state lies on a rank-two subspace of the two-qubit Hilbert space. Up to local unitary transformations, the projector Σ_0 onto a general rank-two subspace can be specified by just two parameters γ_1,γ_2 [44]:

$$\Sigma_0 = \frac{1}{2}(1 + u\sigma_3 + v\tau_3 + z_1\sigma_1\tau_1 + z_2\sigma_2\tau_2),$$
$$u = \cos\gamma_1\cos\gamma_2, \quad v = \sin\gamma_1\sin\gamma_2,$$
$$z_1 = \sin\gamma_1\cos\gamma_2, \quad z_2 = \cos\gamma_1\sin\gamma_2,$$
$$\text{with} \quad \frac{1}{2}\pi \geqslant \gamma_1 \geqslant \gamma_2 \geqslant 0, \tag{22}$$

where $\sigma_1,\sigma_2,\sigma_3$ are the Pauli operators for the first qubit and τ_1,τ_2,τ_3 are that for the second qubit. Interchange of the two qubits leads to $\gamma_1 \to \frac{\pi}{2} - \gamma_2$, $\gamma_2 \to \frac{\pi}{2} - \gamma_1$. So without loss of generality, we can assume $\gamma_1 + \gamma_2 \leqslant \frac{\pi}{2}$, $\gamma_2 \leqslant \frac{\pi}{4}$.

Any rank-two state supported on Σ_0 can be written as follows:

$$\rho_{\mathrm{rk2}} = \tfrac{1}{2}(\Sigma_0 + x_1\Sigma_1 + x_2\Sigma_2 + x_3\Sigma_3), \qquad (23)$$

where $\Sigma_1, \Sigma_2, \Sigma_3$ are the Pauli operators for the rank-two subspace [44]:

$$\Sigma_1 = \tfrac{1}{2}(\sin\gamma_1\sigma_1 + \cos\gamma_2\tau_1 + \sin\gamma_2\sigma_1\tau_3 + \cos\gamma_1\sigma_3\tau_1),$$
$$\Sigma_2 = \tfrac{1}{2}(\sin\gamma_2\sigma_2 + \cos\gamma_1\tau_2 + \sin\gamma_1\sigma_2\tau_3 + \cos\gamma_2\sigma_3\tau_2),$$
$$\Sigma_3 = \tfrac{1}{2}(v\sigma_3 + u\tau_3 - z_2\sigma_1\tau_1 - z_1\sigma_2\tau_2 + \sigma_3\tau_3), \qquad (24)$$

and (x_1, x_2, x_3) (satisfying $x_1^2 + x_2^2 + x_3^2 \leqslant 1$) is the Bloch vector of ρ_{rk2}.

Local unitary symmetry and complex conjugation symmetry play an important role in determining the behavior of $g(\rho_{\mathrm{rk2}})$ and in simplifying its calculation. According to Eqs. (22) and (24), simultaneous local unitary transformation $\sigma_3 \otimes \tau_3$ flips the sign of Σ_1, Σ_2, while leaving Σ_0, Σ_3 invariant, that is,

$$\sigma_3 \otimes \tau_3\Sigma_{0,3}\sigma_3 \otimes \tau_3 = \Sigma_{0,3},$$
$$\sigma_3 \otimes \tau_3\Sigma_{1,2}\sigma_3 \otimes \tau_3 = -\Sigma_{1,2}; \qquad (25)$$

under this transformation, the Bloch vector of ρ_{rk2} changes as follows: $(x_1, x_2, x_3) \rightarrow (-x_1, -x_2, x_3)$. Complex conjugation flips the sign of Σ_2, that is

$$\Sigma_j^* = (-1)^{\delta_{j,2}}\Sigma_j, \qquad (26)$$

where $\delta_{j,2}$ is the Kronecker δ function; under this transformation, the Bloch vector of ρ_{rk2} changes as follows: $(x_1, x_2, x_3) \rightarrow (x_1, -x_2, x_3)$. As a consequence of these symmetries, any reasonable entanglement measure is equal for the four states ρ_{rk2} with Bloch vectors $(\pm x_1, \pm x_2, x_3)$, respectively. Without loss of generality, we can assume $x_1, x_2 \geqslant 0$.

If $\gamma_1 = \gamma_2$, the simultaneous local unitary transformation $e^{-i\theta\sigma_3 \otimes \tau_3}$ rotates the Bloch vector of ρ_{rk2} around the x_3 axis, so $g(\rho_{\mathrm{rk2}})$ is rotationally invariant about the x_3 axis. If $\gamma_2 = 0$, the local unitary transformation $e^{-i\theta\tau_1}$ rotates the Bloch vector around the x_1 axis, so $g(\rho_{\mathrm{rk2}})$ is rotationally invariant about the x_1 axis.

Up to local unitary transformations, there is a one-to-one correspondence between pure three-qubit states and rank-two two-qubit states. Hence, the canonical form of rank-two two-qubit states provides a canonical form of pure three-qubit states. Moreover, due to Theorem 1 in Ref. [47] and the arguments given above, computing the GM of pure three-qubit states can be reduced to computing $g(\rho_{\mathrm{rk2}})$ of the family of canonical rank-two two-qubit states in Eq. (23) with $0 \leqslant \gamma_2 \leqslant \gamma_1 \leqslant \frac{\pi}{2}, \gamma_2 + \gamma_1 \leqslant \frac{\pi}{2}, 0 \leqslant x_1, x_2 \leqslant 1$, and $-1 \leqslant x_3 \leqslant 1$. With this background, we can now study the GM of pure three-qubit states systematically.

B. $g(\rho_{\mathrm{rk2}})$ of general two-qubit rank-two states

In this subsection we reduce the task of computing $g(\rho_{\mathrm{rk2}})$ for general two-qubit rank-two states to a maximization problem which involves only two free variables. The number of free variables is further reduced to one for states ρ_{rk2} with $x_2 = 0$.

Let $\rho_1 = \tfrac{1}{2}(1 + \boldsymbol{s}_1 \cdot \boldsymbol{\sigma})$ and $\rho_2 = \tfrac{1}{2}(1 + \boldsymbol{s}_2 \cdot \boldsymbol{\tau})$ be two pure qubit states with Bloch vectors $\boldsymbol{s}_1 = (a, b, c)$ and $\boldsymbol{s}_2 = (a_2, b_2, c_2)$, respectively. Straightforward calculation shows that

$$\mathrm{tr}(\rho_{\mathrm{rk2}}\rho_1 \otimes \rho_2) = \tfrac{1}{4}(1 + ax_1\sin\gamma_1 + bx_2\sin\gamma_2 + c\cos\gamma_1$$
$$\times \cos\gamma_2 + cx_3\sin\gamma_1\sin\gamma_2 + \boldsymbol{w} \cdot \boldsymbol{s}_2), \quad (27)$$

where

$$\boldsymbol{w} = \begin{pmatrix} a(\cos\gamma_2\sin\gamma_1 - x_3\cos\gamma_1\sin\gamma_2) \\ b(-x_3\cos\gamma_2\sin\gamma_1 + \cos\gamma_1\sin\gamma_2) \\ bx_2\sin\gamma_1 + ax_1\sin\gamma_2 \end{pmatrix}^T$$
$$+ \begin{pmatrix} cx_1\cos\gamma_1 + x_1\cos\gamma_2 \\ x_2\cos\gamma_1 + cx_2\cos\gamma_2 \\ cx_3 + x_3\cos\gamma_1\cos\gamma_2 + \sin\gamma_1\sin\gamma_2 \end{pmatrix}^T. \quad (28)$$

Given ρ_{rk2} and ρ_1, the trace in Eq. (27) is maximized when $\boldsymbol{s}_2$ is parallel to $\boldsymbol{w}$. According to Eq. (21), we have

$$g(\rho_{\mathrm{rk2}}) = \max_{\rho_1\rho_2} \mathrm{tr}(\rho_{\mathrm{rk2}}\rho_1 \otimes \rho_2)$$
$$= \tfrac{1}{4}\max_{a^2+b^2+c^2=1} f(a,b,c),$$
$$f(a,b,c) = (1 + ax_1\sin\gamma_1 + bx_2\sin\gamma_2 \qquad (29)$$
$$+ c\cos\gamma_1\cos\gamma_2 + cx_3\sin\gamma_1\sin\gamma_2 + |\boldsymbol{w}|),$$

where $|\boldsymbol{w}|$ denotes the Euclidian norm of $\boldsymbol{w}$. Thus we have reduced the task of computing $g(\rho_{\mathrm{rk2}})$ to that of maximizing the function $f(a,b,c)$ on the unit sphere determined by $a^2 + b^2 + c^2 = 1$, which involves only two free variables. The contours of f are in general some quadratic surfaces. At the maximum of f over the unit sphere, the contour is generally tangent to the sphere. This geometric picture is useful in visualizing the closest product states.

Further simplification is possible for states ρ_{rk2} with $x_2 = 0$. Assuming $x_2 = 0$ and $x_1 \geqslant 0$ (recall that we only need to consider the case $0 \leqslant x_1, x_2 \leqslant 1$ due to consideration on symmetry, see Sec. III A); then $f(a,b,c)$ is an even function of b according to Eq. (29). In addition, $f(|a|, b, c) \geqslant f(-a, b, c)$, and $f(a, \sqrt{1-a^2}, c)$ is nondecreasing with a for $a \geqslant 0$. So the maximum of $f(a,b,c)$ can be obtained in the parameter subspace satisfying $a \geqslant 0, b = 0$. Moreover, the maximum can only be found in this subspace if $x_1 > 0$. Thus the calculation of $g(\rho_{\mathrm{rk2}})$ can be reduced to the optimization problem over the single variable c.

For rank-two subspace with $\gamma_1 = \gamma_2$ or $\gamma_2 = 0$, this simplification is applicable to all states ρ_{rk2}, since it is enough to calculate $g(\rho_{\mathrm{rk2}})$ for states with $x_2 = 0$ due to the symmetry discussed in Sec. III A.

C. The W state is the maximally entangled state with respect to the geometric measure

According to the discussion in Sec. III A, to determine the maximally entangled states of three-qubit with respect to GM, it is enough to determine the global minimum of $g(\rho_{\mathrm{rk2}})$ over the set of canonical two-qubit rank-two states. Due to the convexity [cf. Eq. (21)] and the symmetry of $g(\rho_{\mathrm{rk2}})$, given γ_1, γ_2, x_3, the minimum of $g(\rho_{\mathrm{rk2}})$ (as a function of x_1 and x_2) is obtained at $x_1 = x_2 = 0$. So the global minimum of $g(\rho_{\mathrm{rk2}})$ can be obtained at states with this property. Recall that the state

ρ_{rk2} with $x_1 = x_2 = 0$, $x_3 = -1$ is the maximally entangled state in the rank-two subspace [44]. Hence, these states are convex combination of the maximally entangled state and its orthogonal pure state within the rank-two subspace. They are interesting for a couple of reasons. First, the two-qubit reduced states of many important pure three-qubit states, such as the W state, GHZ state, are among this family of states. Second, from the result on this family of states and that on pure states, both an upper bound and a lower bound of $g(\rho_{\text{rk2}})$ of any state in each rank-two subspace can be obtained by virtue of the convexity and symmetry properties of $g(\rho_{\text{rk2}})$.

Hence, in order to find the maximally entangled three-qubit state with respect to GM, it suffices to investigate $g(\rho_{\text{rk2}})$ of the states ρ_{rk2} with $x_1 = x_2 = 0$. After some elementary algebra (see Appendix B), we derive a simple analytical formula of $g(\rho_{\text{rk2}})$ of this family of states. To emphasize its explicit dependence on the three parameters x_3, γ_1, γ_2, we write $g(x_3, \gamma_1, \gamma_2)$ for $g(\rho_{\text{rk2}})$.

$$g(x_3, \gamma_1, \gamma_2)$$
$$= \begin{cases} \frac{(1-x_3)[1+\cos(\gamma_1+\gamma_2)]}{4}, & \text{I} \\ \frac{(1-x_3^2)\sin\gamma_1\cos\gamma_2(\cos\gamma_2\sin\gamma_1-x_3\cos\gamma_1\sin\gamma_2)}{-2[x_3^2-(\cos\gamma_2\sin\gamma_1-x_3\cos\gamma_1\sin\gamma_2)^2]}, & \text{II} \\ \frac{(1+x_3)[1+\cos(\gamma_1-\gamma_2)]}{4}, & \text{III} \end{cases} \quad (30)$$

where I, II, III denote three intervals, I : $-1 \leqslant x_3 \leqslant x_3^{(3)}$, II : $x_3^{(3)} < x_3 < x_3^{(4)}$, III : $x_3^{(4)} \leqslant x_3 \leqslant 1$. Here $x_3^{(3)}$ and $x_3^{(4)}$ are given by

$$x_3^{(3,4)}(\gamma_1, \gamma_2)$$
$$:= \frac{-\sin\gamma_1\{\pm\sin\gamma_1 + [\cos\gamma_1\cos\gamma_2 + (\sin\gamma_1)^2]\sin\gamma_2\}}{1 + \cos\gamma_1\{\cos\gamma_2 - \sin\gamma_2[\cos\gamma_1\sin\gamma_2 + (\sin\gamma_1)^2\tan\gamma_2]\}}, \quad (31)$$

and obey the inequalities: $-1 \leqslant x_3^{(3)} \leqslant 0 \leqslant x_3^{(4)} \leqslant 1$.

Figure 1 shows $g(x_3, \gamma_1, \gamma_2)$ as a function of x_3 for several different values of γ_1, γ_2. $g(x_3, \gamma_1, \gamma_2)$ is equal to $\frac{1}{2}[1 + \cos(\gamma_1 \mp \gamma_2)]$ at $x_3 = \pm 1$. This is consistent with the well-known result on GM of two-qubit pure states, which is a function of the concurrence; recall that the concurrence is equal to $\sin(\gamma_1 \mp \gamma_2)$ for the two states with $x_3 = \pm 1$ [44]. $g(x_3, \gamma_1, \gamma_2)$ is equal to $\frac{1}{2}$ at $x_3 = 0$, which is independent of the other two parameters. This observation implies that
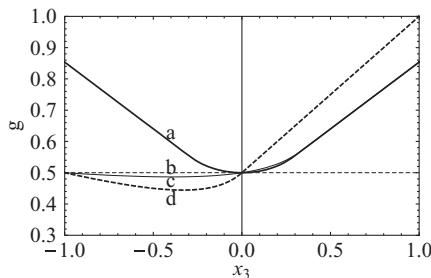

FIG. 2. The minimum of $g(x_3, \gamma_1, \gamma_2)$ over x_3 in each rank-two subspace; the global minimum is obtained at $\gamma_1 = \gamma_2 = \frac{\pi}{4}$.

$G^2(|\psi\rangle) = \frac{1}{2}$ for any pure three-qubit state which is maximally entangled under some bipartite partition; a perfect example is the GHZ state. Once the value of $g(x_3, \gamma_1, \gamma_2)$ is specified at the three points $x_3 = \pm 1, 0$, the value of $g(x_3, \gamma_1, \gamma_2)$ at a generic point can roughly be estimated by interpolation, keeping the convexity of $g(x_3, \gamma_1, \gamma_2)$ with respect to x_3 in mind. This simple picture is very useful in understanding the dependence of $g(x_3, \gamma_1, \gamma_2)$ on various parameters, and why the W state is the maximally entangled state with respect to GM, as we shall see shortly.

It is interesting to note that if $x_3 > x_3^{(4)}$ or $x_3 < x_3^{(3)}$, $g(x_3, \gamma_1, \gamma_2)$ is a linear function of x_3, with positive and negative derivative, respectively. Hence, for given γ_1, γ_2, the minimum of $g(x_3, \gamma_1, \gamma_2)$ is obtained in the interval $x_3^{(3)} \leqslant x_3 \leqslant x_3^{(4)}$. If $\gamma_2 = 0$, $g(x_3, \gamma_1, \gamma_2)$ is an even function of x_3; its minimum for given γ_1 is obtained at $x_3 = 0$, and is equal to $\frac{1}{2}$. Otherwise, the partial derivative of $g(x_3, \gamma_1, \gamma_2)$ with respect to x_3 is positive at $x_3 = 0$; the minimum of $g(x_3, \gamma_1, \gamma_2)$ for given γ_1, γ_2 is obtained in the interval $x_3^{(3)} \leqslant x_3 < 0$ and is smaller than $\frac{1}{2}$. Setting the derivative of $g(x_3, \gamma_1, \gamma_2)$ with respect to x_3 to zero leads to a fourth-order equation about x_3; the minimum can be found after solving this equation. In particular, $-1 < x_3 < 0$ at the global minimum of $g(x_3, \gamma_1, \gamma_2)$. Figure 2 shows the dependence of the minimum of $g(x_3, \gamma_1, \gamma_2)$ over x_3 on γ_1, γ_2; the minimum is also the minimum of $g(\rho_{\text{rk2}})$ in the rank-two subspace. According to the figure, the global minimum of $g(x_3, \gamma_1, \gamma_2)$ is obtained in the rank-two subspace with $\gamma_1 = \gamma_2 = \frac{\pi}{4}$.

To determine the maximally entangled multipartite states is a highly nontrivial task, since it usually involves a massive optimization process over a large parameter space. Even for three qubits, the maximally entangled state with respect to GM is not known for sure, although it has been conjectured with strong evidence that the W state is such a candidate [26]. As an immediate application of the above results, we prove this conjecture rigorously in Appendix C.

Theorem 1. Up to local unitary transformations, the W state is the unique maximally entangled pure three-qubit state with respect to GM.

Theorem 1 can be generalized to mixed states according to the convex roof definition in Eq. (3).

Theorem 2. The W state is the maximally entangled state among all three-qubit states with respect to GM.

FIG. 1. $g(x_3, \gamma_1, \gamma_2)$ as a function of x_3 for several different two-qubit rank-two subspaces. (a) $\gamma_1 = \frac{\pi}{4}$, $\gamma_2 = 0$, (b) $\gamma_1 = \frac{\pi}{2}$, $\gamma_2 = 0$, (c) $\gamma_1 = \frac{3\pi}{8}$, $\gamma_2 = \frac{\pi}{8}$, and (d) $\gamma_1 = \gamma_2 = \frac{\pi}{4}$. Curve (a) and curve (c) coincide in a large interval, because $\gamma_1 - \gamma_2 = \frac{\pi}{4}$ for both the rank-two subspaces, see Eq. (30).
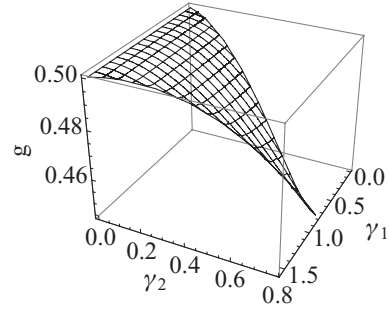
IV. CONCLUSIONS

We have provided analytical methods for deriving the GM of symmetric pure multiqubit states with non-negative amplitudes in the Dicke basis and symmetric pure three-qubit states. Also, we have introduced a systematical method for studying the GM of pure three-qubit states in virtue of a canonical form of their bipartite reduced states. In particular, we have derived explicit analytical formulas of GM for the family of pure three-qubit states one of whose rank-two two-qubit reduced states is a convex combination of the maximally entangled state and its orthogonal pure state within the rank-two subspace. Based on these results, we further proved that the W state is the maximally entangled three-qubit state with respect to GM. Our studies can simplify the calculation of GM and provide a better understanding of multipartite entanglement, especially the entanglement in three-qubit states. Our results also facilitate the comparison of GM with other entanglement measures, like relative entropy of entanglement [28,45]. Moreover, they may help investigate the physical phenomena in multipartite entangled systems emerging in condensed matter physics.

APPENDIX A: DERIVATION OF EQS. (10)–(12)

We will use the technique in Refs. [35,36] to simplify the problem. According to the definition in Eq. (1),

$$
\begin{aligned}
G^2(|\Phi\rangle) &= \max_{|a\rangle|b\rangle|c\rangle} \mathrm{Tr}[|\Phi\rangle\langle\Phi|(|a\rangle\langle a| \otimes |b\rangle\langle b| \otimes |c\rangle\langle c|)] \\
&= \max_{|a\rangle|b\rangle} \mathrm{Tr}[(\mathrm{Tr}_C|\Phi\rangle\langle\Phi|)(|a\rangle\langle a| \otimes |b\rangle\langle b|)], \quad \text{(A1)}
\end{aligned}
$$

where $|a\rangle, |b\rangle$ are normalized qubit states. The second equality follows from Theorem 1 of E. Jung *et al.* [47], which states that any $(n-1)$-qudit reduced state uniquely determines the GM of the original n-qudit pure state, as we have mentioned in the second paragraph of Sec. III.

To reduce Eq. (A1), we use the Bloch sphere representation of qubit [22]:

$$
\rho := \tfrac{1}{2}(I + \boldsymbol{s}_\rho \cdot \boldsymbol{\sigma}), \quad \text{(A2)}
$$

where the components of $\boldsymbol{\sigma}$ are three Pauli matrices and $\boldsymbol{s}_\rho$ is the Bloch vector.

Suppose the states $|a\rangle, |b\rangle$ have Bloch vectors $\boldsymbol{s}_1, \boldsymbol{s}_2$, respectively. Then Eq. (A1) gives rise to two sets of equations:

$$
\boldsymbol{r}_1 + G\boldsymbol{s}_2 = \lambda_1 \boldsymbol{s}_1, \quad \boldsymbol{r}_2 + G\boldsymbol{s}_1 = \lambda_2 \boldsymbol{s}_2,
$$
$$
\boldsymbol{r}_1 = \mathrm{Tr}[\mathrm{Tr}_{BC}(|\Phi\rangle\langle\Phi|)\boldsymbol{\sigma}], \quad \boldsymbol{r}_2 = \mathrm{Tr}[\mathrm{Tr}_{AC}(|\Phi\rangle\langle\Phi|)\boldsymbol{\sigma}],
$$
(A3)

where λ_1, λ_2 are Lagrange multipliers, and the 3×3 matrix G has elements $G_{ij} = \mathrm{Tr}[(\mathrm{Tr}_C|\Phi\rangle\langle\Phi|)(\sigma_i \otimes \sigma_j)]$. Since the reduced density operators $\mathrm{Tr}_{BC}|\Phi\rangle\langle\Phi|$ and $\mathrm{Tr}_{AC}|\Phi\rangle\langle\Phi|$ are identical, one can show that $\boldsymbol{r}_1 = \boldsymbol{r}_2 = \boldsymbol{r}$ after some algebra. It follows that $\boldsymbol{s}_1 = \boldsymbol{s}_2 = \boldsymbol{s}, \lambda_1 = \lambda_2 = \lambda$, and Eq. (A3) reduces to

$$
\boldsymbol{r} + G\boldsymbol{s} = \lambda\boldsymbol{s}. \quad \text{(A4)}
$$

The solutions to Eq. (A4) determine the GM of the state $|\Phi\rangle$ in Eq. (8).

Define $\boldsymbol{s} = (\sin\theta \cos\varphi, \sin\theta \sin\varphi, \cos\theta)$ with $\theta \in [0,\pi]$ and $\varphi \in [0,2\pi]$; then Eq. (A4) reduces to Eqs. (10)–(12).

APPENDIX B: DERIVATION OF EQ. (30)

In this Appendix, we derive Eq. (30). Recall that the relevant parameter range is $0 \leqslant \gamma_2 \leqslant \gamma_1 \leqslant \frac{\pi}{2}, \gamma_2 + \gamma_1 \leqslant \frac{\pi}{2}$, and $-1 \leqslant x_3 \leqslant 1$, see Sec. III A. To simplify the following discussion, we also assume $0 < \gamma_1 < \frac{\pi}{2}$ and $|x_3| < 1$; but it turns out that the final result is applicable without this restriction.

When $x_1 = x_2 = 0$, according to Eqs. (28) and (29),

$$
f(a,b,c) = 1 + c\cos\gamma_1 \cos\gamma_2 + cx_3 \sin\gamma_1 \sin\gamma_2 + |\boldsymbol{w}|,
$$
$$
\boldsymbol{w} = \begin{pmatrix} a(\cos\gamma_2 \sin\gamma_1 - x_3 \cos\gamma_1 \sin\gamma_2) \\ b(-x_3 \cos\gamma_2 \sin\gamma_1 + \cos\gamma_1 \sin\gamma_2) \\ cx_3 + x_3 \cos\gamma_1 \cos\gamma_2 + \sin\gamma_1 \sin\gamma_2 \end{pmatrix}^T;
$$
(B1)

According to Sec. III B, to compute $g(x_3, \gamma_1, \gamma_2)$, or equivalently, the maximum of $f(a,b,c)$ over the unit sphere, we need only to maximize $f_2(c) = f(\sqrt{1-c^2}, 0, c)$ over the single variable c for $-1 \leqslant c \leqslant 1$. Here $f_2(c)$ can be expressed as follows,

$$
\begin{aligned}
f_2(c) &= 1 + u_0 c + \sqrt{u_1 c^2 + 2u_2 c + u_3}, \\
u_0 &= \cos\gamma_1 \cos\gamma_2 + x_3 \sin\gamma_1 \sin\gamma_2 > 0, \\
u_1 &= x_3^2 - (\cos\gamma_2 \sin\gamma_1 - x_3 \cos\gamma_1 \sin\gamma_2)^2, \quad \text{(B2)} \\
u_2 &= (x_3 \cos\gamma_1 \cos\gamma_2 + \sin\gamma_1 \sin\gamma_2)x_3, \\
u_3 &= (\sin\gamma_1)^2 + x_3^2(\cos\gamma_1)^2 > 0.
\end{aligned}
$$

The four coefficients u_0, u_1, u_2, u_3 in Eq. (B2) satisfy the following relations,

$$
u_2 > u_1, \quad u_2^2 - u_1 u_3 > 0, \quad u_0^2 - u_1 > 0; \quad \text{(B3)}
$$

these relations are useful in the following discussion.

To determine the maximum of $f_2(c)$ for $-1 \leqslant c \leqslant 1$, we shall differentiate three cases according to the sign of u_1. Note that u_1 is a quadratic function of x_3 with a positive quadratic coefficient, and that it has the following two zeros:

$$
x_3^{(1,2)} = \frac{\cos\gamma_2 \sin\gamma_1}{\pm 1 + \cos\gamma_1 \sin\gamma_2}, \quad \text{(B4)}
$$

which satisfy the inequalities: $-1 \leqslant x_3^{(2)} < 0 < x_3^{(1)} < 1$; $x_3^{(2)}$ is equal to -1 only if $\gamma_1 + \gamma_2 = 1$.

Case 1: $x_3 = x_3^{(1)}$ or $x_3 = x_3^{(2)}$. In this case $u_1 = 0, u_0, u_2 > 0$,

$$
f_2(c) = 1 + u_0 c + \sqrt{2u_2 c + u_3}, \quad \text{(B5)}
$$

so the maximum of $f_2(c)$ can only be obtained at $c = 1$.

Case 2: $x_3 < x_3^{(2)}$ or $x_3 > x_3^{(1)}$. In this case, $u_0, u_1, u_2 > 0$, the discriminant of the quadratic function $u_1 c^2 + 2u_2 c + u_3$ about c is $4(u_2^2 - u_1 u_3) > 0$, so the quadratic function has two zeros with mean $-u_2/u_1 < 0$. Since the quadratic function must be non-negative in the interval $[-1,1]$ by definition, both zeros must be smaller than or equal to -1. In the interval $[-1,1]$, this quadratic function and $f_2(c)$ are both strictly increasing, so the maximum of $f_2(c)$ can only be obtained at $c = 1$.

Case 3: $x_3^{(2)} < x_3 < x_3^{(1)}$. In this case $u_1 < 0$, the quadratic function $u_1 c^2 + 2u_2 c + u_3$ is positive between its two zeros. One zero is smaller than or equal to -1, and the other larger than or equal to 1. To determine the maximum of $f_2(c)$, we take the first and the second derivatives of $f_2(c)$:

$$f_2'(c) = u_0 + \frac{u_1 c + u_2}{\sqrt{u_1 c^2 + 2u_2 c + u_3}},$$

$$f_2''(c) = \frac{u_1 u_3 - u_2^2}{(u_1 c^2 + 2u_2 c + u_3)^{3/2}} < 0, \tag{B6}$$

where the last inequality follows from Eq. (B3). There is only one solution to the equation $f_2'(c) = 0$,

$$\begin{aligned}
\bar{c} = &-\left[x_3^2 - (\cos\gamma_2 \sin\gamma_1 - x_3 \cos\gamma_1 \sin\gamma_2)^2\right]^{-1} \\
&\times \left[x_3(x_3 \cos\gamma_1 \cos\gamma_2 + \sin\gamma_1 \sin\gamma_2)\right. \\
&+ \sin\gamma_1(\cos\gamma_1 \cos\gamma_2 + x_3 \sin\gamma_1 \sin\gamma_2) \\
&\left.\times (\sin\gamma_1 - x_3 \cos\gamma_1 \tan\gamma_2)\right] \geqslant 0. \tag{B7}
\end{aligned}$$

Since the second derivative of $f_2(c)$ is always negative, $\bar{c}$ is the global maximum of the function $f_2(c)$ in the interval where it is real valued. Restricted to the interval $[-1,1]$, the maximum of $f_2(c)$ is obtained at $\bar{c}$ if $\bar{c} < 1$ and at $c = 1$ otherwise. In both cases, the maximum point is unique. Hence, it remains to determine when $\bar{c} \geqslant 1$ and when $\bar{c} < 1$.

After some algebra, one can show that $x_3^{(1,2)}$ defined in Eq. (B4) and $x_3^{(3,4)}$ defined in Eq. (31) satisfy the following inequalities,

$$-1 \leqslant x_3^{(2)} \leqslant x_3^{(3)} < 0 \leqslant x_3^{(4)} < x_3^{(1)} < 1. \tag{B8}$$

If $\gamma_1 + \gamma_2 = \frac{\pi}{2}$, then $x_3^{(3)} = x_3^{(2)} = -1$, and $\bar{c}$ satisfies the following relation,

$$\begin{cases} \bar{c} < 1 & -1 < x_3 < x_3^{(4)}, \\ \bar{c} \geqslant 1 & x_3^{(4)} \leqslant x_3 < x_3^{(1)}. \end{cases} \tag{B9}$$

If $\gamma_1 + \gamma_2 < \frac{\pi}{2}$, then $-1 < x_3^{(2)} < x_3^{(3)}$, and $\bar{c}$ satisfies the following relation,

$$\begin{cases} \bar{c} < 1 & x_3^{(3)} < x_3 < x_3^{(4)}, \\ \bar{c} \geqslant 1 & x_3^{(2)} < x_3 \leqslant x_3^{(3)} \quad \text{or} \quad x_3^{(4)} \leqslant x_3 < x_3^{(1)}. \end{cases} \tag{B10}$$

According to the observations in the above three cases, if $-1 < x_3 \leqslant x_3^{(3)}$ or $x_3^{(4)} \leqslant x_3 < 1$, the maximum of $f_2(c)$ is obtained at 1; if $-x_3^{(3)} < x_3 < x_3^{(4)}$, the maximum is obtained at $\bar{c}$. The maximum point is unique in both cases. The values

of $f_2(c)$ at 1 and $\bar{c}$ are respectively given by

$$
\begin{aligned}
&f_2(\bar{c}) \\
&= \frac{2(1 - x_3^2)\sin\gamma_1 \cos\gamma_2(\cos\gamma_2 \sin\gamma_1 - x_3 \cos\gamma_1 \sin\gamma_2)}{-\left[x_3^2 - (\cos\gamma_2 \sin\gamma_1 - x_3 \cos\gamma_1 \sin\gamma_2)^2\right]}, \\
&f_2(1) = 1 + \cos\gamma_1 \cos\gamma_2 + x_3 \sin\gamma_1 \sin\gamma_2 \\
&\qquad + |x_3 + x_3 \cos\gamma_1 \cos\gamma_2 + \sin\gamma_1 \sin\gamma_2| \qquad \text{(B11)} \\
&= \begin{cases} (1 - x_3)[1 + \cos(\gamma_1 + \gamma_2)], & x_3 \leqslant x_3^{(3)}, \\ (1 + x_3)[1 + \cos(\gamma_1 - \gamma_2)], & x_3 \geqslant x_3^{(4)}, \end{cases}
\end{aligned}
$$

where in deriving the last equality, we have noticed that

$$\begin{cases} x_3 + x_3 \cos\gamma_1 \cos\gamma_2 + \sin\gamma_1 \sin\gamma_2 \leqslant 0, & x_3 \leqslant x_3^{(3)}, \\ x_3 + x_3 \cos\gamma_1 \cos\gamma_2 + \sin\gamma_1 \sin\gamma_2 \geqslant 0, & x_3 \geqslant x_3^{(4)}. \end{cases}$$

Now Eq. (30) follows immediately when $0 < \gamma_1 < \frac{\pi}{2}$ and $|x_3| < 1$; recall that $g(x_3, \gamma_1, \gamma_2) = \frac{1}{4} \max_{-1 \leqslant c \leqslant 1} f_2(c)$. It is straightforward to verify that the formula is also valid in the special cases $|x_3| = 1$ or $\gamma_1 = 0, \frac{\pi}{2}$, hence the derivation is complete.

APPENDIX C: PROOF OF THEOREM 1

To prove Theorem 1 in Sec. III C, it suffices to show that the global minimum of $g(\rho_{rk2})$ is obtained at the two-qubit reduced state of the W state.

In the relevant parameter range $0 \leqslant \gamma_2 \leqslant \gamma_1 \leqslant \frac{\pi}{2}$, $\gamma_1 + \gamma_2 \leqslant \frac{\pi}{2}$, by taking its derivative with respect to γ_2 in Eq. (30), one can show that, for given γ_1, x_3, $g(x_3, \gamma_1, \gamma_2)$ is monotonically decreasing with γ_2 for $x_3 < 0$ and monotonically increasing with γ_2 for $x_3 > 0$. Assuming $x_3 < 0$, where the global minimum point should satisfy according to Sec. III C; then $g(x_3, \gamma_1, \gamma_2)$ is monotonically decreasing with γ_2. Hence, either $\gamma_1 = \gamma_2$ or $\gamma_1 + \gamma_2 = \frac{\pi}{2}$ at the global minimum of $g(x_3, \gamma_1, \gamma_2)$. We shall show that the unique minimum is obtained at the two-qubit reduced state of the W state in both cases.

1. Special case: $\gamma_1 + \gamma_2 = \frac{\pi}{2}$

If $\gamma_2 = \frac{\pi}{2} - \gamma_1$ ($\frac{\pi}{4} \leqslant \gamma_1 \leqslant \frac{\pi}{2}$), ρ_{rk2} is supported on the symmetrical subspace, according to Eqs. (22)–(24). In this case, Eq. (30) reduces to

$$
g\left(x_3, \gamma_1, \frac{\pi}{2} - \gamma_1\right) \\
= \begin{cases} \frac{1}{2} - \frac{(1 + x_3)x_3(\cos\gamma_1)^2}{-1 + 3x_3 + (1 + x_3)\cos(2\gamma_1)}, & -1 \leqslant x_3 < x_3^{(4)}, \\ \frac{(1 + x_3)[1 + \sin(2\gamma_1)]}{4}, & x_3^{(4)} \leqslant x_3 \leqslant 1, \end{cases} \tag{C1}
$$

where

$$x_3^{(4)} = \frac{1 - \sqrt{2}\sin\left(2\gamma_1 + \frac{\pi}{4}\right)}{3 + \sqrt{2}\sin\left(2\gamma_1 + \frac{\pi}{4}\right)}. \tag{C2}$$

$g(x_3, \gamma_1, \frac{\pi}{2} - \gamma_1)$ is equal to $\frac{1}{2}$ at $x_3 = 0, -1$, independent of γ_1; $g(x_3, \gamma_1, \frac{\pi}{2} - \gamma_1)$ is monotonically increasing with γ_1 for $-1 < x_3 < 0$, and monotonically decreasing for $0 < x_3 \leqslant 1$ (see also Fig. 1).

To determine the maximum of $g(x_3, \gamma_1, \frac{\pi}{2} - \gamma_1)$ for given γ_1, we can set its derivative with respect to x_3 to 0 (in the interval $-1 \leqslant x_3 < x_3^{(4)}$), which leads to the following quadratic equation over x_3,

$$[3 + \cos(2\gamma_1)]x_3^2 + [-2 + 2\cos(2\gamma_1)]x_3 + \cos(2\gamma_1) = 1. \tag{C3}$$

Given $\frac{\pi}{4} \leqslant \gamma_1 \leqslant \frac{\pi}{2}$, the only solution with modulus less than or equal to 1 is

$$x_3^{(5)} = \frac{2\sin\gamma_1(\sin\gamma_1 - \sqrt{2})}{3 + \cos(2\gamma_1)}. \tag{C4}$$

The minimum of $g(x_3, \gamma_1, \frac{\pi}{2} - \gamma_1)$ for given γ_1 is

$$g\left(x_3^{(5)}, \gamma_1, \frac{\pi}{2} - \gamma_1\right) = \frac{[1 + \cos(2\gamma_1) + \sqrt{2}\sin\gamma_1]^2}{[3 + \cos(2\gamma_1)]^2}. \tag{C5}$$

One can show that $g(x_3^{(5)}, \gamma_1, \frac{\pi}{2} - \gamma_1)$ is monotonically increasing with respect to γ_1 by taking its derivative with respect to γ_1; hence, its minimum is obtained at $\gamma_1 = \frac{\pi}{4}$. At this minimum point, $\gamma_1 = \gamma_2 = \frac{\pi}{4}$, $x_3 = x_3^{(5)} = -\frac{1}{3}$, and $g(-\frac{1}{3}, \frac{\pi}{4}, \frac{\pi}{4}) = \frac{4}{9}$. This minimum is also the global minimum of $g(\rho_{\text{rk2}})$.

The rank-two state corresponding to this minimum is exactly the two-qubit reduced state of the W state; moreover, up to local unitary transformations, the W state is the only pure three-qubit state with this rank-two state as a two-qubit reduced state. To see this, recall that the two-qubit reduced state of $|W\rangle = \frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle)$ is

$$\rho_{\text{rk2}}(W) = \frac{1}{3}|00\rangle\langle00| + \frac{2}{3}|\psi^+\rangle\langle\psi^+| \tag{C6}$$

with $|\psi^+\rangle = \frac{1}{\sqrt{2}}(|01\rangle + |10\rangle)$, which is a convex combination of a pure product state and a orthogonal Bell state, thus $\gamma_1 = \gamma_2 = \frac{\pi}{4}$, according to Ref. [44]. In this rank-two subspace, the Bloch vectors of the two states $|00\rangle$ and $|\psi^+\rangle$ are $(0,0,1)$ and $(0,0,-1)$, respectively, and the Bloch vector of the state $\rho_{\text{rk2}}(W)$ is exactly $(0,0,-\frac{1}{3})$.

2. *Special case: $\gamma_2 = \gamma_1 \leqslant \frac{\pi}{4}$*

In this case, Eq. (30) reduces to

$$g(x_3, \gamma_1, \gamma_1)$$
$$= \begin{cases} \frac{(1-x_3)}{2}(\cos\gamma_1)^2, & -1 \leqslant x_3 \leqslant x_3^{(3)}, \\ \frac{-(1-x_3)^2(1+x_3)[\sin(2\gamma_1)]^2}{-1+x_3(2+7x_3)+(1-x_3)^2\cos(4\gamma_1)}, & x_3^{(3)} < x_3 < 0, \\ \frac{(1+x_3)}{2}, & 0 \leqslant x_3 \leqslant 1, \end{cases} \tag{C7}$$

where

$$x_3^{(3)} = -(\tan\gamma_1)^2. \tag{C8}$$

It is interesting to note that $g(x_3, \gamma_1, \gamma_1)$ is independent of γ_1 when $0 \leqslant x_3 \leqslant 1$. If $x_3 < 0$, $g(x_3, \gamma_1, \gamma_1)$ is monotonically decreasing with γ_1. Hence, $\gamma_1 = \frac{\pi}{4}$ at its minimum, the corresponding rank-two subspace is then symmetric. According to the result on symmetric states in the previous subsection, the unique minimum of $g(x_3, \gamma_1, \gamma_1)$ is also obtained at $\gamma_1 = \gamma_2 = \frac{\pi}{4}$, $x_3 = -\frac{1}{3}$.

We have shown that the unique minimum of $g(x_3, \gamma_1, \gamma_2)$ is obtained at $\gamma_1 = \gamma_2 = \frac{\pi}{4}$, $x_3 = -\frac{1}{3}$, and that the corresponding state is the two-qubit reduced state of the W state. This minimum is also the global minimum of $g(\rho_{\text{rk2}})$. To prove that the minimum is unique among all two-qubit rank-two states, it remains to show that it is unique in the rank-two subspace with $\gamma_1 = \gamma_2 = \frac{\pi}{4}$. It suffices to verify that $g(x_1, x_2, -\frac{1}{3}, \frac{\pi}{4}, \frac{\pi}{4}) > g(0, 0, -\frac{1}{3}, \frac{\pi}{4}, \frac{\pi}{4})$ for $x_1^2 + x_2^2 > 0$ [here we write $g(x_1, x_2, x_3, \gamma_1, \gamma_2)$ for $g(\rho_{\text{rk2}})$]. Due to the rotational symmetry of $g(x_1, x_2, x_3, \gamma_1, \gamma_2)$ about the x_3 axis discussed in Sec. III A, this is true if $g(x_1, 0, -\frac{1}{3}, \frac{\pi}{4}, \frac{\pi}{4}) > g(0, 0, -\frac{1}{3}, \frac{\pi}{4}, \frac{\pi}{4})$ for $x_1 > 0$. According to Eq. (29), when $\gamma_1 = \gamma_2 = \frac{\pi}{4}$, $x_2 = 0$, $x_3 = -\frac{1}{3}$,

$$f\left(\frac{2\sqrt{2}}{3}, 0, \frac{1}{3}\right) = \frac{2}{9}[5 + 3x_1 + \sqrt{9 + 3x_1(10 + 9x_1)}]; \tag{C9}$$

hence,

$$\begin{aligned} g\left(x_1, 0, -\frac{1}{3}, \frac{\pi}{4}, \frac{\pi}{4}\right) &\geqslant \frac{1}{4}f\left(\frac{2\sqrt{2}}{3}, 0, \frac{1}{3}\right), \\ &> \frac{4}{9} = g\left(0, 0, -\frac{1}{3}, \frac{\pi}{4}, \frac{\pi}{4}\right). \end{aligned} \tag{C10}$$

This completes the proof of Theorem 1.

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