Analytic expressions for geometric measure of three-qubit states

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A method is developed to derive algebraic equations for the geometric measure of entanglement of three-qubit pure states. The equations are derived explicitly and solved in the cases of most interest. These equations allow one to derive analytic expressions of the geometric entanglement measure in a wide range of three-qubit systems, including the general class of W states and states which are symmetric under the permutation of two qubits. The nearest separable states are not necessarily unique, and highly entangled states are surrounded by a one-parametric set of equally distant separable states. A possibility for physical applications of the various three-qubit states to quantum teleportation and superdense coding is suggested from the aspect of entanglement.

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I. INTRODUCTION

Entangled states have different remarkable applications, and among them are quantum cryptography [1,2], superdense coding [3,4], teleportation [5,6], and the potential speedup of quantum algorithms [7–9]. The entanglement of bipartite systems is well understood [10–13], while the entanglement of multipartite systems offers a real challenge to physicists. In contrast to a bipartite setting, there is no unique treatment of the maximally entangled states for multipartite systems. For this reason it is highly difficult to formulate a theory of multipartite entanglement. Another point which makes it difficult to understand the entanglement for the multiqubit systems is mainly due to the fact that analytic expressions for the various entanglement measures are extremely hard to derive.

We consider pure three-qubit systems [14–17], although the entanglement of mixed states has attracted considerable attention. For example, in a recent experiment [18] the tangle for general mixed states was evaluated, which had never been done before. The three-qubit system is important in the sense that it is the simplest system which gives a nontrivial effect in the entanglement. Thus, we should understand the general properties of the entanglement in this system as much as possible to go further to more complicated higher-qubit systems. The three-qubit system can be entangled in two inequivalent ways—Greenberger-Horne-Zeilinger (GHZ) [19] and W—and neither form can be transformed into the other with any probability of success [20]. This picture is complete: any fully entangled state is SLOCC equivalent to either the GHZ or W method.

Only very few analytical results for tripartite entanglement have been obtained so far [21], and we need more light on the subject. This is our main objective, and we choose the geometric measure of entanglement E_g [22–25]. It is an axiomatic measure [22,26–28], is connected with other measures [29,30], and has an operational treatment. Namely, for the case of pure states it is closely related to the Groverian measure of entanglement [31] and the latter is associated with the success probability of Grover's search algorithm [32] when a given state is used as the initial state.

The geometric measure depends on the entanglement eigenvalue $\Lambda^2_{\max}$ and is given by the formula $E_g(\psi)=1-\Lambda^2_{\max}$. For pure states the entanglement eigenvalue is equal to the maximal overlap of a given state with any complete product state. The maximization over product states gives a *nonlinear eigenproblem* [25] which, except in rare cases, does not allow complete analytical solutions.

Recently the idea was suggested that the nonlinear eigenproblem can be reduced to the linear eigenproblem for the case of three-qubit pure states [33]. The idea is based on a theorem stating that any reduced $(n-1)$-qubit state uniquely determines the geometric measure of the original n-qubit pure state. This means that two qubit mixed states can be used to calculate the geometric measure of three-qubit pure states and this will be fully addressed in this work.

The method gives two algebraic equations of degree 6 defining the geometric measure of entanglement. Thus the difficult problem of geometric measure calculations is reduced to algebraic equation root finding. The equations contain valuable information, are good bases for the numerical calculations, and may test numerical calculations based on other numerical techniques [9].

Furthermore, the method allows one to find the nearest separable states for three-qubit states of most interest and obtain analytic expressions for their geometric measures. It turn out that highly entangled states have their own features.

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Each highly entangled state has a vicinity with no product state, and all nearest product states are on the boundary of the vicinity and form an one-parametric set.

In Sec. II we derive algebraic equations defining the geometric entanglement measure of pure three-qubit states and present the general solution. In Sec. III we examine W-type states and deduce analytic expressions for their geometric measures. States symmetric under the permutation of two qubits are considered in Sec. IV, where the overlap of the state functions with the product states is maximized directly. In Sec. V we give concluding remarks.

II. ALGEBRAIC EQUATIONS

We consider three qubits A, B, and C with state function $|\psi\rangle$. The entanglement eigenvalue is given by

$$\Lambda_{\max} = \max_{q^1q^2q^3} |\langle q^1 q^2 q^3 | \psi\rangle|, \tag{1}$$

and the maximization runs over all normalized complete product states $|q^1\rangle \otimes |q^2\rangle \otimes |q^3\rangle$. Superscripts label single-qubit states, and spin indices are omitted for simplicity. Since in the following we will use density matrices rather than state functions, our first aim is to rewrite Eq. (1) in terms of density matrices. Let us denote by $\rho^{ABC}=|\psi\rangle\langle\psi|$ the density matrix of the three-qubit state and by $\varrho^k=|q^k\rangle\langle q^k|$ the density matrices of the single-qubit states. The equation for the square of the entanglement eigenvalue takes the form

$$\Lambda^2_{\max}(\psi) = \max_{\varrho^1\varrho^2\varrho^3} \mathrm{tr}(\rho^{ABC}\varrho^1 \otimes \varrho^2 \otimes \varrho^3). \tag{2}$$

An important equality

$$\max_{\varrho^3} \mathrm{tr}(\rho^{ABC}\varrho^1 \otimes \varrho^2 \otimes \varrho^3) = \mathrm{tr}(\rho^{ABC}\varrho^1 \otimes \varrho^2 \otimes \mathbb{1}^3) \tag{3}$$

was derived in Ref. [33] where $\mathbb{1}$ is a unit matrix. It has a clear meaning. The matrix $\mathrm{tr}(\rho^{ABC}\varrho^1 \otimes \varrho^2)$ is a $2\otimes 2$ Hermitian matrix and has two eigenvalues. One of the eigenvalues is always zero and the other is always positive, and therefore the maximization of the matrix simply takes a nonzero eigenvalue. Note that its minimization gives zero as the minimization takes the zero eigenvalue.

We use Eq. (3) to reexpress the entanglement eigenvalue by the reduced density matrix ρ^{AB} of qubits A and B in the form

$$\Lambda^2_{\max}(\psi) = \max_{\varrho^1\varrho^2} \mathrm{tr}(\rho^{AB}\varrho^1 \otimes \varrho^2). \tag{4}$$

We denote by $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$ the unit Bloch vectors of the density matrices ϱ^1 and ϱ^2, respectively, and adopt the usual summation convention on repeated indices i and j. Then,

$$\Lambda^2_{\max} = \frac{1}{4}\max_{s_1^2=s_2^2=1} (1 + \boldsymbol{s}_1 \cdot \boldsymbol{r}_1 + \boldsymbol{s}_2 \cdot \boldsymbol{r}_2 + g_{ij}s_{1i}s_{2j}), \tag{5}$$

where

$$\boldsymbol{r}_1 = \mathrm{tr}(\rho^A \boldsymbol{\sigma}),$$

$$\boldsymbol{r}_2 = \mathrm{tr}(\rho^B \boldsymbol{\sigma}),$$

$$g_{ij} = \mathrm{tr}(\rho^{AB}\sigma_i \otimes \sigma_j) \tag{6}$$

and σ_i's are Pauli matrices. The matrix g_{ij} is not necessarily symmetric, but must have only real entries. The maximization gives a pair of equations

$$\boldsymbol{r}_1 + g\boldsymbol{s}_2 = \lambda_1 \boldsymbol{s}_1, \quad \boldsymbol{r}_2 + g^T\boldsymbol{s}_1 = \lambda_2 \boldsymbol{s}_2, \tag{7}$$

where the Lagrange multipliers λ_1 and λ_2 enforce the unit nature of the Bloch vectors. The solution of Eq. (7) is

$$\boldsymbol{s}_1 = (\lambda_1\lambda_2\mathbb{1} - gg^T)^{-1}(\lambda_2\boldsymbol{r}_1 + g\boldsymbol{r}_2), \tag{8a}$$

$$\boldsymbol{s}_2 = (\lambda_1\lambda_2\mathbb{1} - g^Tg)^{-1}(\lambda_1\boldsymbol{r}_2 + g^T\boldsymbol{r}_1). \tag{8b}$$

Now, the only unknowns are Lagrange multipliers, which should be determined by the equations

$$|\boldsymbol{s}_1|^2 = 1, \quad |\boldsymbol{s}_2|^2 = 1. \tag{9}$$

In general, Eqs. (9) give two algebraic equations of degree 6. However, the solution (8a) and (8b) is valid if Eq. (7) supports a unique solution and this is by no means always the case. If the solution of Eq. (7) contains a free parameter, then $\det(\lambda_1\lambda_2\mathbb{1} - gg^T)=0$ and, as a result, Eqs. (8a) and (8b) cannot be applicable. The example presented in Sec. III will demonstrate this situation.

In order to test Eqs. (8a) and (8b) let us consider an arbitrary superposition of W,

$$|W\rangle = \frac{1}{\sqrt{3}}(|100\rangle + |010\rangle + |001\rangle) \tag{10}$$

and flipped W,

$$|\widetilde{W}\rangle = \frac{1}{\sqrt{3}}(|011\rangle + |101\rangle + |110\rangle) \tag{11}$$

states—i.e., the state

$$|\psi\rangle = \cos\,\theta|W\rangle + \sin\,\theta|\widetilde{W}\rangle. \tag{12}$$

Straightforward calculation yields

$$\boldsymbol{r}_1 = \boldsymbol{r}_2 = \frac{1}{3}(2\,\sin\,2\theta\boldsymbol{i} + \cos\,2\theta\boldsymbol{n}), \tag{13a}$$

$$g = \frac{1}{3}\begin{pmatrix} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \tag{13b}$$

where the unit vectors $\boldsymbol{i}$ and $\boldsymbol{n}$ are aligned with the axes x and z, respectively. Both vectors $\boldsymbol{i}$ and $\boldsymbol{n}$ are eigenvectors of matrices g and g^T. Therefore $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$ are linear combinations of $\boldsymbol{i}$ and $\boldsymbol{n}$. Also from $\boldsymbol{r}_1=\boldsymbol{r}_2$ and $g=g^T$ it follows that $\boldsymbol{s}_1=\boldsymbol{s}_2$ and $\lambda_1=\lambda_2$. Then Eqs. (8a) and (8b) for a general solution gives

$$\boldsymbol{s}_1 = \boldsymbol{s}_2 = \sin\,2\varphi\boldsymbol{i} + \cos\,2\varphi\boldsymbol{n} \tag{14}$$

where

$$\sin\,2\varphi = \frac{2\,\sin\,2\theta}{3\lambda - 2}, \quad \cos\,2\varphi = \frac{\cos\,2\theta}{3\lambda + 1}. \tag{15}$$

Elimination of the Lagrange multiplier λ from Eq. (15) gives

$$3 \sin 2\varphi \cos 2\varphi = \cos 2\theta \sin 2\varphi - 2 \sin 2\theta \cos 2\varphi. \tag{16}$$

Let us denote $t=\tan \varphi$. After the separation of the irrelevant root $t=-\tan \theta$, Eq. (16) takes the form

$$\sin \theta t^3 + 2 \cos \theta t^2 - 2 \sin \theta t - \cos \theta = 0. \tag{17}$$

This equation exactly coincides with that derived in Ref. [25]. Since a detailed analysis was given in Ref. [25], we do not want to repeat the same calculation here. Instead we would like to consider the three-qubit states that allow analytic expressions for the geometric entanglement measure by making use of Eq. (7).

III. W-TYPE STATES

Consider the W-type state

$$|\psi\rangle = a|100\rangle + b|010\rangle + c|001\rangle, \quad a^2 + b^2 + c^2 = 1. \tag{18}$$

Without loss of generality we consider only the case of positive parameters a, b, and c. Direct calculation yields

$$\boldsymbol{r}_1 = r_1\boldsymbol{n}, \quad \boldsymbol{r}_2 = r_2\boldsymbol{n}, \quad g = \begin{pmatrix} \omega & 0 & 0 \\ 0 & \omega & 0 \\ 0 & 0 & -r_3 \end{pmatrix}, \tag{19}$$

where

$$r_1 = b^2 + c^2 - a^2, \quad r_2 = a^2 + c^2 - b^2, \quad r_3 = a^2 + b^2 - c^2, \tag{20}$$

and $\omega=2ab$. The unit vector $\boldsymbol{n}$ is aligned with the z axis. Any vector perpendicular to $\boldsymbol{n}$ is an eigenvector of g with eigenvalue ω. Then from Eq. (7) it follows that the components of vectors $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$ perpendicular to $\boldsymbol{n}$ are collinear. We denote by $\boldsymbol{m}$ the unit vector along that direction and parametrize the vectors $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$ as follows:

$$\boldsymbol{s}_1 = \cos \alpha \boldsymbol{n} + \sin \alpha \boldsymbol{m}, \quad \boldsymbol{s}_2 = \cos \beta \boldsymbol{n} + \sin \beta \boldsymbol{m}. \tag{21}$$

Then Eq. (7) reduces to the four equations

$$r_1 - r_3 \cos \beta = \lambda_1 \cos \alpha, \quad r_2 - r_3 \cos \alpha = \lambda_2 \cos \beta, \tag{22a}$$

$$\omega \sin \beta = \lambda_1 \sin \alpha, \quad \omega \sin \alpha = \lambda_2 \sin \beta, \tag{22b}$$

which are used to solve the four unknown constants λ_1, λ_2, α, and β. Equation (22b) imposes either

$$\lambda_1\lambda_2 - \omega^2 = 0 \tag{23}$$

or

$$\sin \alpha \sin \beta = 0. \tag{24}$$

First consider the case $r_1>0$, $r_2>0$, and $r_3>0$ and coefficients a, b, and c form an acute triangle. Equation (24) does not give a true maximum, and this can be understood as follows. If both vectors $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$ are aligned with the z axis, then the last term in Eq. (5) is negative. If the vectors $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$ are antiparallel, then one of scalar products in Eq. (5) is negative. For this reason $\Lambda^2_{\max}$ cannot be maximal. Then Eq. (23) gives the true maximum and we have to choose positive values for λ_1 and λ_2 to get the maximum.

First we use Eq. (22a) to connect the angles α and β with the Lagrange multipliers λ_1 and λ_2:

$$\cos \alpha = \frac{\lambda_2 r_1 - r_2 r_3}{\omega^2 - r_3^2}, \quad \cos \beta = \frac{\lambda_1 r_2 - r_1 r_3}{\omega^2 - r_3^2}. \tag{25}$$

Then Eqs. (22b) and (23) give the following expressions for Lagrange multipliers λ_1 and λ_2:

$$\lambda_1 = \omega\left(\frac{\omega^2 + r_1^2 - r_3^2}{\omega^2 + r_2^2 - r_3^2}\right)^{1/2}, \tag{26a}$$

$$\lambda_2 = \omega\left(\frac{\omega^2 + r_2^2 - r_3^2}{\omega^2 + r_1^2 - r_3^2}\right)^{1/2}. \tag{26b}$$

Equation (7) allows one to write a shorter expression for the entanglement eigenvalue:

$$\Lambda^2_{\max} = \frac{1}{4}(1 + \lambda_2 + r_1 \cos \alpha). \tag{27}$$

Now we insert the values of λ_2 and $\cos \alpha$ into Eq. (27) and obtain

$$4\Lambda^2_{\max} = 1 + \frac{\omega\sqrt{(\omega^2 + r_1^2 - r_3^2)(\omega^2 + r_2^2 - r_3^2)} - r_1 r_2 r_3}{\omega^2 - r_3^2}. \tag{28}$$

The denominator in the above expression is a multiple of the area S of the triangle a,b,c:

$$\omega^2 - r_3^2 = 16S^2. \tag{29}$$

A little algebra yields for the numerator

$$\omega\sqrt{(\omega^2 + r_1^2 - r_3^2) + (\omega^2 + r_2^2 - r_3^2)} - r_1 r_2 r_3 = 16a^2b^2c^2 - \omega^2 + r_3^2. \tag{30}$$

Combining together the numerator and denominator, we obtain the final expression for the entanglement eigenvalue:

$$\Lambda^2_{\max} = 4R^2, \tag{31}$$

where R is the circumradius of the triangle a,b,c. The entanglement value is minimal when the triangle is regular—i.e., for the W state and $\Lambda^2_{\max}(W)=4/9$ [25,34].

Now consider the case $r_3<0$. Since $r_3+r_1=2b^2\geq 0$, we have $r_1>0$ and similarly $r_2>0$. Equation (24) gives the true maximum in this case, and both vectors are aligned with the z axis,

$$\boldsymbol{s}_1 = \boldsymbol{s}_2 = \boldsymbol{n}, \tag{32}$$

resulting in $\Lambda^2_{\max}=c^2$. In view of symmetry,

$$\Lambda^2_{\max} = \max(a^2,b^2,c^2), \quad \max(a^2,b^2,c^2) > \frac{1}{2}. \tag{33}$$

Since the matrix g and vectors $\boldsymbol{r}_1$ and $\boldsymbol{r}_2$ are invariant under rotations around the z axis, the same properties must have

Bloch vectors $\boldsymbol{s}_1$ and $\boldsymbol{s}_2$. There are two possibilities.

(i) Bloch vectors are unique and aligned with the z axis. The solution given by Eq. (32) corresponds to this situation, and the resulting entanglement eigenvalue, Eq. (33), satisfies the inequality

$$\frac{1}{2} < \Lambda_{\max}^2 \leq 1. \tag{34}$$

(ii) Bloch vectors have nonzero components in the xy plane, and the solution is not unique. Equation (21) corresponds to this situation and contains a free parameter. The free parameter is the angle defining the direction of the vector $\boldsymbol{m}$ in the xy plane. Then Eq. (31) gives the entanglement eigenvalue in the highly entangled region:

$$\frac{4}{9} \leq \Lambda_{\max}^2 < \frac{1}{2}. \tag{35}$$

Equation (31) and (33) have joint curves when the parameters a, b, and c form a right triangle and give $\Lambda_{\max}^2=1/2$. The GHZ states have same entanglement value, and it seems to imply something interesting. The GHZ state can be used for teleportation and superdense coding, but the W state cannot. However, the W-type state with right triangle coefficients can be used for teleportation and superdense coding [35]. In other words, both types of states can be applied provided they have the required entanglement eigenvalue $\Lambda_{\max}^2=1/2$.

IV. SYMMETRIC STATES

Now let us consider the state which is symmetric under permutation of qubits A and B and contains three real independent parameters

$$|\psi\rangle = a|000\rangle + b|111\rangle + c|001\rangle + d|110\rangle, \tag{36}$$

where $a^2+b^2+c^2+d^2=1$. According to generalized Schmidt decomposition [14] the states with different sets of parameters are local-unitary (LU) inequivalent. The relevant quantities are

$$\boldsymbol{r}_1 = \boldsymbol{r}_2 = r\boldsymbol{n}, \quad g = \begin{pmatrix} \omega & 0 & 0 \\ 0 & -\omega & 0 \\ 0 & 0 & 1 \end{pmatrix}, \tag{37}$$

where

$$r = a^2 + c^2 - b^2 - d^2, \quad \omega = 2ad + 2bc, \tag{38}$$

and the unit vector $\boldsymbol{n}$ again is aligned with the z axis.

All three terms on the left-hand side (lhs) of Eq. (5) are bounded above: (i) $\boldsymbol{s}_1\cdot\boldsymbol{r}_1 \leq |r|$, (ii) $\boldsymbol{s}_2\cdot\boldsymbol{r}_2 \leq |r|$, and (iii) owing to inequality $|\omega| \leq 1$, $g_{ij}s_{1i}s_{2j} \leq 1$.

Quite surprisingly all upper limits are reached simultaneously at

$$\boldsymbol{s}_1 = \boldsymbol{s}_2 = \mathrm{sgn}(r)\boldsymbol{n}, \tag{39}$$

which results in

$$\Lambda_{\max}^2 = \frac{1}{2}(1 + |r|). \tag{40}$$

This expression has a clear meaning. To understand it we parametrize the state as

$$|\psi\rangle = k_1|00q_1\rangle + k_2|11q_2\rangle, \tag{41}$$

where q_1 and q_2 are arbitrary single-qubit normalized states and the positive parameters k_1 and k_2 satisfy $k_1^2+k_2^2=1$. Then,

$$\Lambda_{\max}^2 = \max(k_1^2,k_2^2); \tag{42}$$

i.e., the maximization takes a larger coefficient in Eq. (41). In the bipartite case the maximization takes the largest coefficient in Schmidt decomposition [31,36] and in this sense Eq. (41) effectively takes the place of Schmidt decomposition. When $|q_1\rangle=|0\rangle$ and $|q_2\rangle=|1\rangle$, Eq. (42) gives the known answer for a generalized GHZ state [25,34].

The entanglement eigenvalue is minimal $\Lambda_{\max}^2=1/2$ on the condition that $k_1=k_2$. These states can be described as follows:

$$|\psi\rangle = |00q_1\rangle + |11q_2\rangle, \tag{43}$$

where q_1 and q_2 are arbitrary single-qubit normalized states. The entanglement eigenvalue is constant $\Lambda_{\max}^2=1/2$ and does not depend on single-qubit state parameters. Hence one may expect that all these states can be applied for teleportation and superdense coding. It would be interesting to check whether this assumption is correct or not.

It turns out that the GHZ state is not a unique state and is one of two-parametric LU-inequivalent states that have $\Lambda_{\max}^2=1/2$. On the other hand, the W state is unique up to LU transformations and the low bound $\Lambda_{\max}^2=4/9$ is reached if and only if $a=b=c$. However, one cannot make such conclusions in general. Five real parameters are necessary to parametrize the set of inequivalent three-qubit pure states [14]. And there is no explicit argument that the W state is not just one of LU-inequivalent states that have $\Lambda_{\max}^2=4/9$.

V. SUMMARY

We have derived algebraic equations defining the geometric measure of three-qubit pure states. These equations have a degree higher than 4, and explicit solutions for general cases cannot be derived analytically. However, explicit expressions are not important. Remember that explicit expressions for the algebraic equations of degree 3 and 4 have a limited practical significance, but the equations themselves are more important. This is especially true for equations of higher degree; the main results can be derived from the equations rather than from the expressions of their roots.

Equation (7) gives the nearest separable state directly, and this separable state has useful applications. In order to construct an entanglement witness, for example, the crucial point lies in finding the nearest separable state [37]. This will be especially interesting for highly entangled states that have a whole set of nearest separable states and allow one to construct a set of entanglement witnesses.

The expression on the rhs of Eq. (5) can be maximized directly for various three-qubit states. Although it is very hard to solve the higher-degree equation, it turns out that a wide range of three-qubit states has a symmetry and this symmetry reduces the equations of degree 6 to the quadratic equations. For this reason Eq. (5) can be used to derive the analytic expressions of the various entanglement measures for the three-qubit states. Also Eq. (5) can be a starting point to explore the numerical computation of the entanglement measures for higher-qubit systems. We hope to discuss this issue elsewhere.

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