Maximally entangled three-qubit states via geometric measure of entanglement

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Bipartite maximally entangled states have the property that the largest Schmidt coefficient reaches its lower bound. However, for multipartite states, the standard Schmidt decomposition generally does not exist. We use a generalized Schmidt decomposition and the geometric measure of entanglement to characterize three-qubit *pure* states and derive a single-parameter family of maximally entangled three-qubit states. The paradigmatic Greenberger-Horne-Zeilinger (GHZ) and *W* states emerge as extreme members in this family of maximally entangled states. This family of states possesses different trends of entanglement behavior: in going from GHZ to *W* states, the geometric measure, the relative entropy of entanglement, and the bipartite entanglement all increase monotonically whereas the three-tangle and bipartition negativity both decrease monotonically.

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I. INTRODUCTION

Maximally entangled states are in essence the natural units of entanglement with which one would like to compare all quantum states. A well-motivated approach to compare different entangled states and quantify their entanglement is to consider how they can transform to each other under local operations and classical communications (LOCCs) in the asymptotic regime. The main question is then to quantify the optimal rate of conversion between two given states [1]. For bipartite systems, this gives rise to the two basic operational entanglement measures: the entanglement cost (EC) [1,2] and the distillable entanglement (ED) [1,3], with Bell states [4,5] emerging as the standard metric of entanglement. While the latter measure is the rate at which copies of the maximally entangled state can be concentrated from those of a given state, the former is the rate at which copies of the maximally entangled state need to be consumed for the preparation of the given state [2,3,6,7].

In contrast, there is no simple and unique characterization of a maximally entangled state in multipartite settings. It has been a long-standing question whether there exists a finite minimal reversible entanglement generating set (MREGS) [8], as the states in MREGS would provide several distinct metrics of entanglement and hence the generalizations of ED and EC would become possible. In addition to the issue of interconversion in the asymptotic limit, another challenge lies in the fact that multipartite states can be entangled in several inequivalent ways [9,10] and that the number of these likely grows exponentially with the number of parties [10].

Perhaps, to get to certain handle of these problems, it is useful, as an initial stage, to elucidate an important question of which pure states can be regarded as the maximally entangled states [11]. A clear definition of these states and the search of an effective method for deriving them could offer a

step toward understanding multipartite entanglement, including the structure of the Hilbert space and multipartite entanglement measures. Any multipartite entanglement measure is perhaps a likely starting point for such a definition of maximally entangled states, as for each measure there must exist a set of states which is maximally entangled. However, these states may not be maximally entangled using a different measure. Therefore, one then has to choose an entanglement measure that gives rise to a set of maximally entangled states that include the known ones in the set. Furthermore, the selected measure should be suitable for any number of parties with any dimensions in order for the notion of maximal entanglement to be properly quantified.

In the setting of three qubits, the Greenberger-Horne-Zeilinger (GHZ) state $|\text{GHZ}\rangle \equiv (|000\rangle + |111\rangle)/\sqrt{2}$ [12] and the *W* state $|W\rangle \equiv (|001\rangle + |010\rangle + |100\rangle)/\sqrt{3}$ [9] have been realized as two inequivalent entangled states that cannot be transformed to each other via LOCC or even stochastically. GHZ state seems to be the most natural generalization of Bell states and possesses a maximum tripartite entanglement characterized by the three-tangle [13]. On the other hand, *W* state possesses zero three-tangle and yet maximizes the residual bipartite entanglement [9]. In some sense, both states are maximally entangled. However, the exact value of entanglement depends on the choice of entanglement measures and it is likely that different measures may give different ordering of the entanglement quantity. For example, using the relative entropy of entanglement (ER) [14], one has $E_R(\text{GHZ}) = 1$ and $E_R(W) = \log_2(9/4) > 1$ [15]. However, using the negativity N across any bipartition, one obtains $N(\text{GHZ}) = 1 > N(W) = 2\sqrt{2}/3$ [16]. Hence, the notion of being maximally entangled can depend on the choice of entanglement measures. In the setting of two qubits, in contrast, the Bell states emerge as the ones that possess maximal entanglement, independent of the choice of measures. Nonetheless, the dependence does appear when one considers two-

qubit mixed states and the form of maximally entangled two-qubit mixed states [17–19] (e.g., parametrized by entropy) can actually vary [19].

Here we characterize maximal entanglement of three-qubit *pure* states via the geometric measure of entanglement [20]. Under this measure, the W state turns out to possess the maximal entanglement. To see whether the GHZ can fit into our picture, we investigate the maximal entanglement with a single parameter γ, which we call the "gauge" phase (which appears in the generalized Schmidt decomposition [21–23] and to be defined below), in analog to the two-qubit maximally entangled mixed states parametrized by the entropy. We derive the whole family of maximally entangled states (characterized by the gauge phase) and show that both GHZ and W emerge as maximally entangled states at two different gauge phases at the opposite ends of this family. Interestingly, in going from GHZ to W as the gauge phase increases, the geometric measure and the relative entropies of entanglement and the bipartite entanglement all increase monotonically whereas the three-tangle and bipartite negativity both decrease monotonically (see Fig. 6). The two different trends of these entanglement monotones for this family of states imply that no states in the family can be interconverted deterministically to each other via LOCC using a single copy [24]. Furthermore, our analysis of using three-tangle shows that any states can be probabilistically converted to one another via stochastic LOCC in the family except to or from the W state. This is because the whole family of the maximally entangled three-qubit states, except the W state, belongs to the GHZ class, a classification introduced by Vidal and Cirac [6].

The paper is organized as follows. In Sec. II, we use a generalized Schmidt decomposition to parameterize three-qubit states. In Sec. III, we consider the case of vanishing gauge phase and obtain the GHZ state. In Sec. IV, we consider the case of maximal gauge phase and obtain the W state. In Sec. V, we consider the general case and derive a one-parameter family of maximally entangled states. Furthermore, we discuss several entanglement properties and interconversion of states in the family of the maximally entangled states. In Sec. VI, we make concluding remarks.

II. GENERALIZED SCHMIDT DECOMPOSITIONS

In general, one needs 14 real parameters to describe a three-qubit pure state. Carteret *et al.* [21] and Acín *et al.* [22] independently proposed generalizations of the Schmidt decomposition in multipartite settings (three qubits, in particular) to reduce the number of necessary parameters. The generalized Schmidt decomposition (GSD) that we shall use is a variant [23] that is closely related to the geometric measure and hence it is more appropriate to our discussions here. Let us briefly discuss this decomposition. For any multiqubit pure state, one can always search a closest product state to it and the local states of the closest product state and their orthonormal states uniquely (up to phases) determine the local bases one uses to express the multiqubit state. One can also relabel the closest product as $|000\rangle$ and the local state orthonormal to $|0\rangle$ by $|1\rangle$ and arrive at the following expression [23]:

$$|\psi\rangle = g|000\rangle + t_1|011\rangle + t_2|101\rangle + t_3|110\rangle + e^{i\gamma}h|111\rangle, \quad (1)$$

where the labels within each ket refer to qubits A, B, and C (or 1, 2, and 3) in that order and will be suppressed whenever no confusion occurs. Furthermore, the parameters in the decomposition satisfy

$$g \geq t_i, h \geq 0, -\pi/2 \leq \gamma \leq \pi/2 \quad \text{and}$$
$$g^2 + h^2 + t_1^2 + t_2^2 + t_3^2 = 1. \quad (2)$$

The reason why we do not have $|001\rangle$, $|010\rangle$, and $|100\rangle$ is that the component $|000\rangle$ is the closest product state and if there were any of the three other components, one could have absorbed them and increased the maximal overlap g. We shall refer to γ as the "gauge phase," as such a factor will necessarily appear in any such decomposition but it may be associated with $|111\rangle$ or with $|100\rangle$ as in Ref. [22]. In what follows, we shall analyze only positive values of the gauge phase since the maximal overlap g is an even function on γ.

Why do we choose to parametrize the family of maximally entangled states by γ (or equivalently the phase in Ref. [22])? Consider the unitary three-qubit gate, control-control-phase (CCP) gate, that multiplies the computational state $|111\rangle$ by a phase factor $e^{i\phi}$ but leaves unchanged the remaining seven basis states $|000\rangle, |001\rangle, \ldots, |110\rangle$. This gate can be used to generate entanglement (one says that it is an entangling gate). If we start with the (unnormalized) product state $(|0\rangle + |1\rangle)(|0\rangle + |1\rangle)(|0\rangle + |1\rangle)$ and apply to it the CCP gate, one obtains $|000\rangle + |001\rangle + |010\rangle + |100\rangle + |110\rangle + |101\rangle + |011\rangle + e^{i\phi}|111\rangle$. It can be shown that this state is entangled and has a three-tangle $\tau = |\sin \phi|/8$ and, moreover, the reduced two-qubit state can also be entangled depending on ϕ. The states in the generalized Schmidt form (1) with fixed g, t_1, t_2, t_3, h but different γ's can be connected by the entangling CCP gate with an appropriate value of phase ϕ. In contrast, any local-unitary transformation that changes any of the five magnitude parameters will generally change the values of the others and most likely take the state out of the generalized Schmidt form. Since any three-qubit pure state can be made into this form by local-unitary transformations, it seems natural to take the gauge phase γ as the parameter to search for the family of maximally entangled states.

The decomposition into the form (1) captures all the three-qubit pure states up to local-unitary transformations. It is thus a convenient starting point for searching maximally entangled three-qubit states. When $|000\rangle$ is the closest product state and the parameters satisfy condition (2), we shall refer to the decomposition as being in the canonical form. In this canonical form, the nearest product state $|000\rangle$ is a stationary point for ψ and should satisfy the stationarity equations [20,21], which represent a nonlinear eigenvalue problem

$$\langle i_1 i_2|\psi\rangle = \mu_i|i_3\rangle, \quad \langle i_1 i_3|\psi\rangle = \mu_i|i_2\rangle, \quad \langle i_2 i_3|\psi\rangle = \mu_i|i_1\rangle, \quad (3)$$

where we can always restrict ourselves to $\mu_i \geq 0$ by adjusting phases of local states $|i\rangle$. The above stationary conditions arise from the requirement that the overlap with product states be extremal under the constraint that product states be

normalized (for derivation, see Refs. [20,29]). The resulting equations generalize the linear eigenvalue problem to a nonlinear form, which has many features different from the linear scenario [29]. (When the number of parties is 2, the generally nonlinear eigenvalue equation becomes linear.) The largest Schmidt coefficient is the maximal nonlinear eigenvalue, i.e., $g = \max_i(\mu_i)$, and thus the nearest product state is the dominant eigenvector of stationarity equations. As mentioned earlier, it uniquely defines the factorizable basis of GSD consisting of $|000\rangle$ and its complimentary orthogonal product states [23].

Our goal is to find a family of maximally entangled states, parameterized by the gauge phase γ. First, we observe that the coefficient g in the canonical decomposition measures the overlap (or the angle) from ψ to the closest unentangled state [20,25] and cannot decrease under LOCC [14,26]. Hence it should be minimal for the maximally entangled states for all other possible parameters (t and h) given fixed gauge phase γ. The crucial point then lies in finding the lower bound on g [27]. In the case of generic three-qubit states, stationarity equations have six solutions. Let μ_1 be the largest eigenvalue and hence $g = \mu_1$. Then clearly we have

$$g \geq \mu = \max(\mu_2, \mu_3, \ldots, \mu_6). \quad (4)$$

This is a strong lower bound on g. If one can compute all the eigenvalues μ_i, then one can find the lowest value of g directly. We shall first do this for special cases $\gamma = 0$ and $\gamma = \pi/2$ and the celebrated GHZ and W states emerge as the maximally entangled states, respectively.

In general, the derivation of eigenvalues μ_i gives rise to unsolvable equations [28,29]. Fortunately, there is a realizable method that gives the desired lower bound. The essence of the method is the following. If the three-qubit state is maximally entangled, then the above inequality would be saturated. Consequently, g must coincide with μ and thus the largest eigenvalue of stationarity equations should be degenerated. This requirement imposes a condition (i.e., *degeneracy condition*) on state parameters, which can then be deduced from stationarity equations. An example is the GHZ state $(|000\rangle + |111\rangle)/\sqrt{2}$, where $|000\rangle$ and $|111\rangle$ are two such "degenerate" states with $\mu = 1/\sqrt{2}$. Following the above procedure, we derive the degeneracy condition for three-qubit states and single out states satisfying this condition. Next we find among these states the one with the minimal g (over the remaining free parameters) for a given value of the gauge phase.

We have seen that the GHZ and W states emerge as maximally entangled states in different contexts, such as via three-tangle and residual bipartite entanglement, respectively, and they are invariant under permuting parties. It is thus natural to assume that maximally entangled states can be made symmetric. This ansatz will be verified against numerical experiments (see Fig. 5). Thus, we shall work with the assumption that $t_1 = t_2 = t_3 \equiv t$ and consider from now on states of the form

$$|\psi\rangle = g|000\rangle + t|011\rangle + t|101\rangle + t|110\rangle + e^{i\gamma}h|111\rangle. \quad (5)$$

Eigenvalues μ_i of the state Eq. (5) satisfy a polynomial equation of degree 12 and are roots of the characteristic poly-

nomial [29]. Local states $|i\rangle$ satisfy the analogous polynomial equation and the general case remains to some extent intractable. However, at extreme values of the gauge phase $\gamma = 0$ and $\gamma = \pi/2$, this polynomial equation can be factorized to cubic equations. Another major step toward analytic solutions is the following. Each of these cubic equations can be further factorized to a linear and quadratic equations. This observation allows us to find all roots of the characteristic polynomial. Some of them have no associated eigenvectors and hence are irrelevant. Some others never maximize the overlap since their value is smaller than $\max(h, t)$ in whole state parameter space [30]. Remaining solutions are listed in the Appendix.

III. GHZ STATE

Consider first the case $\gamma = 0$. All of these states are symmetric and have real coefficients

$$|\psi_0\rangle = g|000\rangle + t(|011\rangle + |101\rangle + |110\rangle) + h|111\rangle. \quad (6)$$

Owing to these properties, the eigenvector with eigenvalue μ is symmetric, i.e., has a form $|qqq\rangle$, and its constituents $|q\rangle$ have real coefficients. In this reason, we will derive here only symmetric solutions as the asymmetric ones give strictly $\mu < g$.

We parameterize the pure one-qubit state $|q\rangle$ by a single angle $|q\rangle = \cos\theta|0\rangle + \sin\theta|1\rangle$ and insert it into Eq. (3). The result is a pair of equations for unknowns θ and μ,

$$g\cos^2\theta + t\sin^2\theta = \mu\cos\theta, \quad h\sin^2\theta + t\sin 2\theta = \mu\sin\theta. \quad (7)$$

These equations have an obvious solution $\mu_1 = g$, $\cos\theta = 1$, reflecting the fact that the state is already written in Schmidt normal form. The second solution is given by solving $\tan\theta$ from dividing the first equation by the latter on both sides. We then arrive at

$$\tan\theta = \frac{r_0}{2t}, \quad \mu_2 = \frac{hr_0 + 4t^2}{\sqrt{r_0^2 + 4t^2}}, \quad (8)$$

where $r_0 = h + \sqrt{h^2 + 8t^2 - 4gt}$. This solution gives rise to a basis $\{|q\rangle, |p\rangle\}$ defined as follows:

$$|q\rangle = \frac{2t|0\rangle + r_0|1\rangle}{\sqrt{r_0^2 + 4t^2}}, \quad |p\rangle = \frac{r_0|0\rangle - 2t|1\rangle}{\sqrt{r_0^2 + 4t^2}}. \quad (9)$$

To obtain the maximal entanglement, we require that $\mu_1 = \mu_2$. Because $|qqq\rangle$ is another equally good dominant eigenvector, one can construct a new Schmidt decomposition of $|\psi_0\rangle$ whose factorizable basis consists of $\{|q\rangle, |p\rangle\}$ instead of $\{|0\rangle, |1\rangle\}$. This new decomposition must not differ from the original one, since coefficients of the canonical form are uniquely defined by state parameters. This in turn means that the basis defined by $\{|q\rangle, |p\rangle\}$ results in a Schmidt form equivalent to Eq. (6)

$$|\psi_0\rangle = g|qqq\rangle + t(|qpp\rangle + |pqp\rangle + |ppq\rangle) + h|ppp\rangle. \quad (10)$$

By expanding the left-hand side of this equality in the computation basis $\{0,1\}$ and identifying the corresponding coef-

ficients with those in Eq. (6), we arrive at the following three conditions on state parameters:

$$\frac{hr_0 + 4t^2}{\sqrt{r_0^2 + 4t^2}} = g, \quad \frac{2t(g-t)}{\sqrt{r_0^2 + 4t^2}} = t, \quad \frac{4t^2(r_0 - h)}{\sqrt{r_0^2 + 4t^2}} = t(2h - r_0).$$

(11)

By taking the ratios of the first two equations and the latter two equations and then eliminating r_0, we obtain the following single condition on state parameters:

$$gh^2 = (g+t)^2(g-2t).$$

(12)

We remark that Eq. (12) uniquely solves Eq. (11) and is in fact the degeneracy condition that forces the correct Schmidt decomposition.

Let us rewrite the degeneracy condition in the following form: $g(g^2 - h^2 - 3t^2) = 2t^3$. Since $t \geq 0$, it follows that $g^2 \geq h^2 + 3t^2$. Then from the normalization condition $g^2 + h^2 + 3t^2 = 1$, it further gives that $g^2 \geq 1/2$ and the lower bound $g^2 = 1/2$ is reached at $t = 0$, $g = h$. The resulting maximal entangled state is the celebrated GHZ state

$$|\text{GHZ}\rangle = \frac{|000\rangle + |111\rangle}{\sqrt{2}}.$$

(13)

IV. W STATE

Consider now the case $\gamma = \pi/2$. This case includes all W-class states. Indeed, the three-tangle of a generic state Eq. (1) is given by

$$\tau = 4g\sqrt{g^2h^4 + 16t_1^2t_2^2t_3^2 + 8gh^2t_1t_2t_3 \cos 2\gamma}.$$

(14)

It vanishes if either

$$gh^2 = 0 \quad \text{and} \quad t_1t_2t_3 = 0$$

(15)

or

$$gh^2 = 4t_1t_2t_3 \neq 0 \quad \text{and} \quad \gamma = \pm \pi/2.$$

(16)

The states satisfying Eq. (15) are biseparable, namely, separable with respect to $A:BC$, $B:AC$, or $C:AB$ bipartition [6,23], and the maximally entangled states are Bell states between BC, AC, or AB.

In Eq. (16), the case of $\gamma = -\pi/2$ is equivalent to that of $\gamma = \pi/2$ because the period of the angle γ is π and the point $-\pi/2$ should be identified with $\pi/2$. All states satisfying Eq. (16) are W-class states [6] and conversely any W-class state has a Schmidt decomposition with coefficients Eq. (16). Thus generic pure three-qubit states have five independent real parameters, whiles W-class states have three of them.

Stationarity equations give four relevant solutions and one of them is symmetric (under qubit permutations) while the remaining three others are not. The easiest way for finding the symmetric solution $|qqq\rangle$ is to set $|q\rangle = e^{i\pi/3}(\cos\theta|0\rangle + i\sin\theta|1\rangle)$ and solve the stationarity Eq. (3), just like what we did for the GHZ case. The solution is

$$\tan\theta = \frac{r_\pi}{2t}, \quad \mu = \frac{hr_\pi + 4t^2}{\sqrt{r_\pi^2 + 4t^2}},$$

(17)

where $r_\pi = h + \sqrt{h^2 + 8t^2 + 4gt}$. Since r_π and r_0 differ only by the sign of t, the degeneracy condition forcing $g = \mu$ can be obtained by taking t to $-t$ in Eq. (12),

$$gh^2 = (g-t)^2(g+2t).$$

(18)

In the case of GHZ, the degeneracy condition is sufficient for finding the maximally entangled state, but in the present case, we need one more condition by examining three other relevant solutions of stationarity equations. The first solution is symmetric under the permutation of qubits A and B, but asymmetric under other permutations and has a form $|qqq'\rangle$. Other two solutions, with symmetric qubit pairs (A,C) and (B,C), respectively, give the same eigenvalue. Thus, it suffices to consider the first solution of these in addition to that in Eq. (17). Its constituent state $|q\rangle$, up to an irrelevant phase factor, can be parameterized by two angles, which are $|q\rangle = \cos\theta|0\rangle + e^{i\varphi}\sin\theta|1\rangle$. (Similar parametrization can be used for $|q'\rangle$.) Straightforward but tedious algebra from solving the stationarity conditions (3) gives rise to the equations obeyed by angles θ and φ,

$$\cos 2\theta = \frac{h^2 + gt - g^2}{h^2 + g^2 - 3gt}, \quad \sin\varphi = \frac{h}{2g}\tan\theta,$$

(19)

as well as the corresponding eigenvalue μ' being

$$\mu'^2 = \frac{g^2h^2 - 4gt^3}{g^2 + h^2 - 3gt}.$$

(20)

We shall present in the Appendix a simpler derivation using another approach outlined in the next section.

Thus far we have obtained two different eigenvalues, namely, μ and μ', and consequently g has two different lower bounds. As argued previously, for the maximally entangled state, both lower bounds should be saturated and this in turn uniquely defines state parameters. Indeed, by using $\mu' = g$, it follows that $(g+t)(g-2t)^2 = 0$ and hence $g = 2t$ (as $g, t \geq 0$). Then the degeneracy condition (18) forces $h^2 = 2t^2$. These two conditions together with the normalization condition give $g = 2/3$, $t = 1/3$, and $h = \sqrt{2}/3$ and thus yield the following maximally entangled state for $\gamma = \pi/2$:

$$|\psi_{\pi/2}\rangle = \frac{2}{3}|000\rangle + \frac{1}{3}(|011\rangle + |101\rangle + |110\rangle) + i\frac{\sqrt{2}}{3}|111\rangle.$$

(21)

This form turns out to be the generalized Schmidt normal form for the W state. Indeed, one can easily verify that $U \otimes U \otimes U|\psi_{\pi/2}\rangle = |W\rangle$, where

$$|W\rangle = \frac{|100\rangle + |010\rangle + |001\rangle}{\sqrt{3}}, \quad U = \frac{1}{\sqrt{3}}\begin{pmatrix} \sqrt{2} & -i \\ 1 & i\sqrt{2} \end{pmatrix}.$$

(22)

Thus, W state is the maximally entangled state for $\gamma = \pi/2$. It should be remarked that at $g = 2t$ and $h^2 = 2t^2$, the fraction defining the angle θ in Eq. (19) is indefinite since both ex-

pressions in denominator and numerator vanish. The reason is that the state $|\psi_{\pi/2}\rangle$ (as well as the W state) is an exceptional state [31] and has countless nearest product states defined solely by the condition $\tan\theta = 2\sqrt{2}\sin\varphi$ [32]. All of these product states are equally distant from $|\psi_{\pi/2}\rangle$ (i.e., infinitely degenerate) and form a circle around it. This infinite degeneracy is best captured when viewed in the computational basis. To be more precise, the closest product states to W state were previously shown [15] to be of the form

$$\left(e^{i\chi/2}\sqrt{\frac{2}{3}}|0\rangle + e^{-i\chi}\sqrt{\frac{1}{3}}|1\rangle \right)^{\otimes 3}, \tag{23}$$

where the arbitrariness of the phase χ clearly shows the infinite degeneracy.

The eigenvalue μ' also exhibits interesting features. If $g = 2t$, then $\mu' = g$ and thus the solution Eq. (19) maximizes the overlap. On the other hand, if $gh^2 = 4t^3$ but $g \neq 2t$, then the solution minimizes the overlap, i.e., resulting in $\mu' = 0$. In order to obtain further insight into this, we relate μ' to the three-tangle τ. For the states in question, $\tau = 4g(gh^2 - 4t^3)$ and μ' can be written as

$$\mu'^2 = \frac{g^2\tau}{\tau + 4g(g+t)(g-2t)^2}. \tag{24}$$

This shows clearly when the asymmetric eigenvalue μ' takes the maximal value and the minimal value.

V. GENERAL CASE

Having warmed up by the previous two examples, we consider now the general case. The GHZ and W are two special cases of the following treatment.

A. Derivation of the degeneracy condition

For symmetric states, any solution of stationarity equations is symmetric under the permutation of either the qubit pair AB, AC, or BC [33]. Without loss of generality, we consider a solution that contains a symmetric pair A and B, i.e., the product state has a form $|qqq'\rangle$ which, of course, does not exclude the possibility $|q'\rangle = |q\rangle$. Furthermore, theorem 1 of Ref. [34] states that the maximal overlap is uniquely determined even if one party of the global pure state is traced out. This enables us to express the maximal overlap in terms of the reduced density matrix ρ^{AB} as follows:

$$g^2 = \max_{\varrho^1, \varrho^2} \mathrm{Tr}(\rho^{AB}\varrho^1 \otimes \varrho^2), \tag{25}$$

where ϱ^1 and ϱ^2 are single-system pure state densities. The density matrix ρ^{AB} can be expanded in terms of identity operator and the Pauli matrices σ's,

$$\rho^{AB} = \frac{1}{4}(\mathbb{1}\otimes\mathbb{1} + \boldsymbol{r}\cdot\boldsymbol{\sigma}\otimes\mathbb{1} + \boldsymbol{r}\cdot\mathbb{1}\otimes\boldsymbol{\sigma} + \boldsymbol{\sigma}\cdot G\cdot\boldsymbol{\sigma}), \tag{26}$$

where $\boldsymbol{r}$ is the Bloch vector of the qubit $A(B)$ and the correlation matrix G is defined by the formula $G_{ij} = \mathrm{Tr}(\rho^{AB}\sigma_i \otimes \sigma_j)$. Explicitly,

$$\boldsymbol{r} = (2ht\cos\gamma, 2ht\sin\gamma, g^2 - h^2 - t^2) \tag{27}$$

and

$$G = \begin{pmatrix} 2t^2 + 2gt & 0 & -2ht\cos\gamma \\ 0 & 2t^2 - 2gt & -2ht\sin\gamma \\ -2ht\cos\gamma & -2ht\sin\gamma & g^2 + h^2 - t^2 \end{pmatrix}. \tag{28}$$

As ρ^{AB} is symmetric under permuting parties, one can set $\varrho^1 = \varrho^2 = \varrho$ [35]. Denote by $\boldsymbol{u}$ the Bloch vector of the density matrix ϱ that gives rise to the maximum of g^2, then Eq. (25) can be rewritten as

$$g^2 = \frac{1}{4}(1 + 2\boldsymbol{u}\cdot\boldsymbol{r} + \boldsymbol{u}\cdot G\boldsymbol{u}). \tag{29}$$

By introducing a Lagrange multiplier λ that constraints $\boldsymbol{u}\cdot\boldsymbol{u} = 1$, the vector $\boldsymbol{u}$ satisfies the following equation:

$$\boldsymbol{r} + G\boldsymbol{u} = \lambda\boldsymbol{u}. \tag{30}$$

Since λ uniquely defines $\boldsymbol{u}$ and g, two solutions have the same eigenvalue if and only if they have the same Lagrange multiplier. By direct substitution, it is easy to see that for the solution $u_z = 1$, we have $\lambda_0 = 2(g^2 - t^2)$ and therefore the largest eigenvalue of Eq. (30) is degenerate if there are two solutions at $\lambda = \lambda_0$. Inserting this value into Eq. (30), one sees that the necessary and sufficient condition for the existence of the second solution corresponding to $\lambda = \lambda_0$ is $\det(G - \lambda_0\mathbb{1}) = 0$, which can be rewritten as

$$(g^2 - t^2)^2(g^2 - 4t^2) = gh^2(g^3 - 3gt^2 + 2t^3\cos 2\gamma). \tag{31}$$

This is the degeneracy condition for arbitrary symmetric states and the solutions contain all three-qubit states that can be regarded as maximally entangled. When $\gamma = 0$, Eq. (31) reduces to Eq. (12) and when $\gamma = \pi/2$, it reduces either to Eq. (18) or $g = 2t$. The latter is equivalent to Eq. (20).

B. Maximally entangled three-qubit states

The degeneracy condition Eq. (31) can be considered as an algebraic equation of degree six for g, where t and γ are free parameters and h^2 can be further eliminated by the normalization condition $h^2 = 1 - g^2 - 3t^2$. It has six roots $g(t, \gamma)$ and as far as we are looking for the largest eigenvalue, we should always take the largest root. In what follows, we will use the notations g_1 for the largest root and g_2 for the second largest root. Equation (31) gives different types of lower bounds depending on whether or not $\cos 2\gamma$ is positive and below we consider these two cases.

Consider first states for which $0 \le \gamma \le \pi/4$. The degeneracy condition can be rewritten as follows:

$$g^2(g^2 - 3t^2)(g^2 - 3t^2 - h^2) = 4t^6 + 2gh^2t^3\cos 2\gamma. \tag{32}$$

The right-hand side of this equation is positive and either $g^2 \le 3t^2$ or $g^2 \ge 3t^2 + h^2$ holds. To find the maximal overlap, we should take the latter case $g^2 \ge 3t^2 + h^2$ and then from the normalization condition, it follows that g is minimal when $t = 0$ and $g = h$. Thus the only maximally entangled state in this class is the GHZ state: $(|000\rangle + e^{i\gamma}|111\rangle)/\sqrt{2}$. It can be understood by reference to Fig. 1, where γ is taken to be $\pi/6$
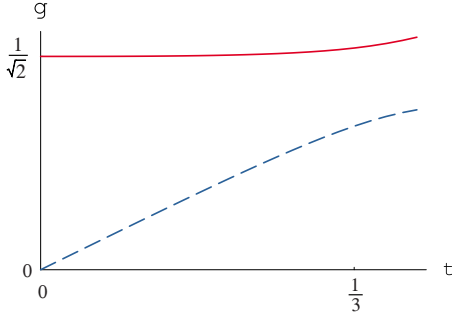
FIG. 1. (Color online) Plots of t dependencies of the largest $g_1(t)$ (solid line) and next $g_2(t)$ (dashed line) roots of the degeneracy condition for $\gamma = \pi/6$. $g_1(t)$ is the largest Schmidt coefficient and has a minimum at $t=0$ which gives the GHZ state.

for illustration. The solid line represents the largest root $g_1(t)$ and the dashed line represents the next root $g_2(t)$ as functions on t. It should be stressed that the largest root $g_1(t)$ never intersects with other roots and therefore it is the largest Schmidt coefficient for all values of t. Moreover, $g_1(t)$ is a monotonically increasing function and our goal is to find its infimum (and hence the supremum of the geometric measure), which is reached at $t=0$, giving rise to the GHZ state [36].

Consider now the interval $\pi/4 < \gamma < \pi/2$. Now the situation is different since g_1 and g_2 are not monotonic functions. In Fig. 2, $g_1(t)$ (solid line) and $g_2(t)$ (dashed line) are plotted at $\gamma = 2\pi/5$. The largest root $g_1(t)$ has a minimum while the next root $g_2(t)$ has a maximum at $t = 0.319\,43$. These two roots never intersect unless $\gamma = \pi/2$. Therefore the minimum of the function $g_1(t)$ is the lower bound of the largest Schmidt coefficient. When γ increases, the minimum of g_1 moves toward larger γ and decreases. Concurrently, the maximum of g_2 moves toward larger γ and increases. Thus, in the range $\pi/4 < \gamma < \pi/2$, one needs to search for the minimum value of $g_1(t)$ over the allowable range of t in order to find the maximal entangled states.

When $\gamma = \pi/2$, minimum of g_1 and maximum of g_2 coincide at $t = 1/3$ and this minimum value of g_1 yields the W state. This is illustrated in Fig. 3.

We remark that the inequality $\min_t g_1(t) > \max_t g_2(t)$ holds for fixed $\gamma \neq \pi/2$. This feature is verified numerically for all values $0 \leq \gamma < \pi/2$. This means that, given a fixed γ,
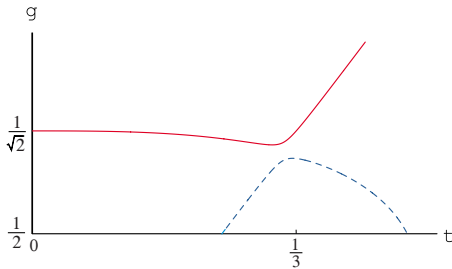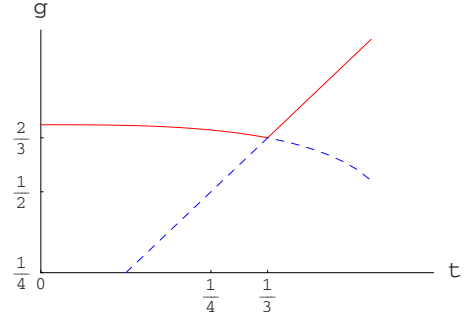

FIG. 2. (Color online) Plots of t dependencies of the largest $g_1(t)$ (solid line) and next $g_2(t)$ (dashed line) roots of the degeneracy condition for $\gamma = 2\pi/5$. $g_1(t)$ has a minimum while $g_2(t)$ has a maximum at $t = 0.319\,43$. These roots never intersect unless $\gamma = \pm \pi/2$.

FIG. 3. (Color online) Plots of t dependencies of the largest $g_1(t)$ (solid line) and next $g_2(t)$ (dashed line) roots of the degeneracy condition for $\gamma = \pi/2$. The two curves touch at $(1/3, 2/3)$.

the minimum of the function $g_1(t)$ is the lower bound on g and also provides justification for the parametrization of maximally entangled states by the gauge phase. The minimum of g_1 gives the value of the maximal overlap g for the maximally entangled state at a given γ. Together with the value of t where the minimum of g_1 is achieved, the complete description of the maximally entangled state is obtained (as h is determined via the normalization condition).

In Fig. 4 we show the dependences of g and h on the gauge phase γ. The dependence of t on γ can be inferred from the normalization $g^2 + 3t^2 + h^2 = 1$. This then defines the family of the maximally entangled three-qubit states. The parameters g and h are both constant and equal to $1/\sqrt{2}$ within the interval $0 \leq \gamma \leq \pi/4$, then decrease with γ, with g reaching $2/3$ and h reaching $\sqrt{2}/3$ at $\gamma = \pi/2$. We remark that we have assumed the maximally entangled states have the permutation invariant form (5) and this is supported by our numerical test that states generated randomly do not achieve g below (or entanglement above) those of the maximally entangled states (see Fig. 5).

C. Survey of maximally entangled states

Once the maximally entangled three-qubit states (and hence their maximal overlap) have been obtained as a func-
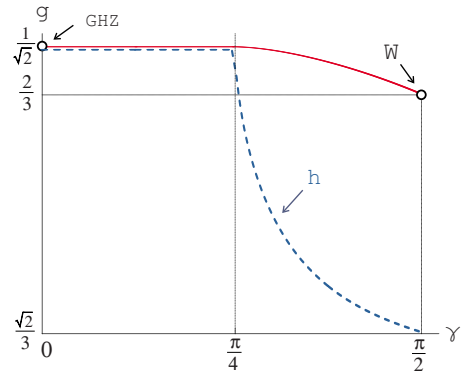

FIG. 4. (Color online) The gauge phase γ dependence of the largest Schmidt coefficient g as well as h of maximally entangled states. g is constant and equal to $1/\sqrt{2}$ within $0 \leq \gamma \leq \pi/4$, then it decreases monotonically and becomes $2/3$ at $\gamma = \pi/2$. Similarly, h is constant and equal to $1/\sqrt{2}$ within $0 \leq \gamma \leq \pi/4$, then it decreases monotonically and becomes $\sqrt{2}/3$ at $\gamma = \pi/2$. The parameter t is obtained from the normalization $g^2 + 3t^2 + h^2 = 1$.
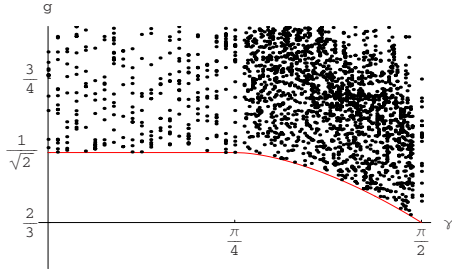
FIG. 5. (Color online) The maximal overlap g vs the gauge phase γ for the family of maximally entangled three-qubit states (red solid curve) as well as randomly generated states (dots). This shows that the family of states we have derived is indeed maximally entangled (with minimal overlap g).

tion of the gauge phase γ, it is of interest to compare the results with other measures. Two other quantities of relevance are the aforementioned three-tangle τ [13] and the residual bipartite entanglement E_r [9]. We show the γ dependences of τ and E_r for the maximally entangled three-qubit states in Fig. 6. We also compare the γ dependences of yet two other measures, the bipartition negativity (N) and the relative entropy of entanglement (E_R), in Fig. 7. The three-tangle τ and the negativity N decrease monotonically for $\gamma \in [\pi/4, \pi/2]$, whereas the residual bipartite entanglement E_r and the relative entropy of entanglement E_R increase and achieve $E_r = 4/3$ and $E_R = \log_2(9/4)$ at $\gamma = \pi/2$ for the W state. The geometric measure for the maximally entangled states is equal to $1 - g^2$ and, hence, as can be inferred from Fig. 4, it increases monotonically. To summarize the behaviors of three different measures, we have that, in going from GHZ to W as γ increases, the geometric measure and the relative entropy of entanglement and the bipartite entanglement all increase monotonically whereas the three-tangle and the negativity both decrease monotonically.

Instead of the geometric measure, one may well use other entanglement measures to derive the maximally entangled states. Conversely, having at one's disposal the set of maximally entangled states, one can analyze and compare different entanglement measures. In this view, the behaviors of the different measures can be understood as follows. The three-tangle quantifies genuine tripartite, i.e., GHZ-type entanglement, but does not detect W-type entanglement at all [37].
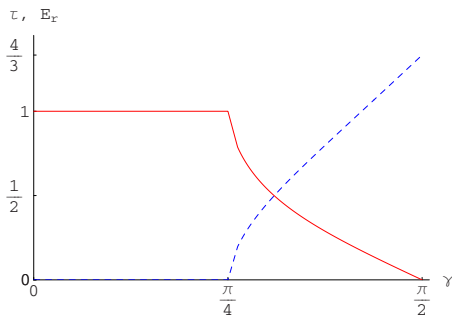

FIG. 6. (Color online) The phase dependence of three-tangle τ (red solid curve) and the residual bipartite entanglement E_r (blue dashed curve) vs γ for the family of maximally entangled three-qubit states.
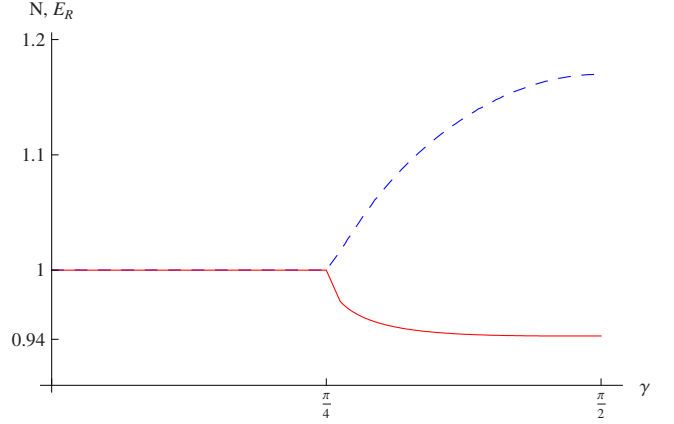

FIG. 7. (Color online) The phase dependence of the negativity N (red solid curve) and the relative entropy of entanglement E_R (blue dashed curve) vs γ for the family of maximally entangled three-qubit states.

Then all states within the interval $-\pi/4 \leq \gamma \leq \pi/4$ possess only GHZ-type entanglement and in going away from these states, the three-tangle detects the residual of GHZ-type entanglement. In this regard, it decreases with γ from $\tau = 1$ at GHZ state and vanishes at W state. On the contrary, the residual bipartite entanglement quantifies the W-type entanglement and does not detect the GHZ-type entanglement at all. Hence, its behavior is opposite to that of the three-tangle. The negativity quantifies entanglement across bipartition. As the GHZ state is equivalent to a Bell state if one makes the bipartition $A:BC$, it possesses the largest negativity $N = 1$. The W state possesses less negativity $N = 2\sqrt{2}/3$, and the family becomes less and less similar to GHZ as one increases the gauge phase; one expects a gradual interpolation of the negativity between these values. The situation of the geometric measure is very different from these measures. It quantifies whole entanglement present in the state and, owing to this, detects a one-parameter set of maximally entangled states. The behavior of the relative entropy of entanglement for this family is qualitatively similar to that of the geometric measure and this is expected as the geometric measure can be used to provide lower bounds on the relative entropy of entanglement [15], with GHZ and W states saturating the bounds.

It is interesting to note that the manifold of GHZ-class maximally entangled states is an open manifold in a sense that there is no state within GHZ-class states that has the global maximal geometric measure of entanglement (which is actually possessed by the W state). Indeed, let us analyze $\gamma = \pi/2$ case once again. The three-tangle τ of these states is given by the formula $\tau = 4g(gh^2 - 4t^3)$ and the degeneracy condition Eq. (18) can be rewritten as follows:

$$4g(g+t)^2(g-2t) = \tau. \tag{33}$$

All of these states are GHZ-class state unless the limit $\tau = 0$ (and hence $g = 2t$, which means that the asymmetric solution comes into action) is reached. Near this limit, g depends on τ by the asymptotic formula $g = 2/3 + \sqrt{3\tau/8} + O(\tau)$ which can be derived from Eq. (33). On the other hand, if $0 \leq \gamma$

$< \pi/2$, then $g > 2/3$. Thus, the largest Schmidt coefficient of the GHZ-class states comes arbitrarily close to 2/3 but never reaches it as the lower bound is only achieved by the W state.

What about the interconversion between states in the family of the maximally entangled states? We have seen that in going from GHZ to W, the geometric measures of entanglement and the bipartite entanglement both increase monotonically whereas the three-tangle decreases monotonically (see Fig. 6). The two different trends of these entanglement monotones for this family of states imply that deterministic interconversion via LOCC among these maximally entangled three-qubit states is not possible. The results of the three-tangle τ and the Dür-Vidal-Cirac classification of entangled states [6] show that under stochastic LOCC, any pure states can be probabilistically converted to one another within the same class and that there are five classes of three-qubit pure states: one class of completely separable states, three classes of biseparable states, and GHZ-class and W-class states. But states in one class cannot be converted to any other in a different class even with SLOCC. In our case, the whole family of the maximally entangled three-qubit states, except the W state (which has $\tau=0$), belongs to the GHZ class (with $\tau>0$). Therefore, under SLOCC, any states in the family of maximally entangled three-qubit states can be probabilistically converted to one another in the family except to or from the W state.

VI. CONCLUDING REMARKS

We use a generalized Schmidt decomposition and the geometric measure of entanglement to characterize three-qubit pure states and derive a single-parameter (characterized by the gauge phase) family of maximally entangled three-qubit states. The resulting family of maximally entangled states connects continuously from GHZ to W state. The paradigmatic GHZ and W states emerge as extreme members in this family of maximally entangled states.

This family of maximally entangled states turns out to possess interesting features of entanglement. In going from GHZ to W, the geometric measure and the relative entropy of entanglement and the bipartite entanglement all increase monotonically whereas the three-tangle and the negativity both decrease monotonically. This clearly exemplifies the ordering issue in the multipartite entanglement. It also implies that deterministic interconversion via LOCC among these maximally entangled three-qubit states is not possible. However, the results of the three-tangle τ and the Dür-Vidal-Cirac classification of entangled states show that under *stochastic* LOCC, any states in the family of maximally entangled three-qubit states can be probabilistically converted to one another in the family (except to or from the W state).

In general, three-qubit pure states require 14 real independent parameters to completely characterize. The use of local-unitary equivalence helps to reduce the number of parameters necessary for the characterization of entangled states. Via the generalized Schmidt decomposition, we have navigated through the remaining vast space and identified the one-parameter maximally entangled states via the geometric measure. But one may as well use other entanglement measures. Will other measures give rise to such a nontrivial family of states? For example, using the gauge phase as the parametrization and the three-tangle as the characterization of entanglement, one obtains that the maximally entangled states being $(|000\rangle + e^{i\gamma}|111\rangle)/\sqrt{2}$, which are essentially the same GHZ state. Such featureless family of states also arises when the characterization of entanglement is replaced by negativity. On the other hand, when using the relative entropy of entanglement, one expects that the resulting family of maximally entangled states will have similar feature to those via the geometric measure, albeit not identical. (It is because that the geometric measure serves as a lower bound of the relative entropy of entanglement.) Perhaps the procedure that we have gone through to identify the maximally entangled states can serve two purposes: (1) to explore certain cross section of Hilbert space via suitable parametrization and choice of entanglement measures and (2) to investigate and compare the behavior of entanglement measures via the resulting family of maximally entangled states, whether they are interesting or featureless. In doing so, one may identify certain distinct states or classify various measures of entanglement. In the former respect, it remains to be seen whether the derived family of entangled states can be of any use in quantum information processing tasks previously unexplored. In the latter respect, one thus has that the various entanglement measures discussed in the present paper can be divided into two different groups: (a) the geometric measure of entanglement, the relative entropy of entanglement, and the residual bipartite entanglement and (b) the three-tangle and the negativity.

While the nonlinear eigenvalues of the W state are infinitely degenerate, eigenvalues of the GHZ-class states are doubly degenerate and thus no invertible local operations can match them. As a remark, it is interesting to see that the whole W-class states have only a single representative in the above one-parameter family of maximally entangled states, namely, the W state, which can be regarded geometrically as the center of the largest full sphere with no unentangled states.

The W-class states form a boundary set for pure three-qubit states and the boundary is the limit $\gamma \to \pi/2$, $gh^2 \to 4t_1t_2t_3$. Accordingly, the W state is the end point of maximally entangled pure states [11]. The boundary behavior of entanglement is different and owing to this, the set of GHZ states is noncompact. Hence GHZ-class states should have noncountably infinite collection of maximally entangled states approaching to the W state.

Several outstanding questions remain: does the minimal reversible entanglement generating set exist? If so, what does it consist of? Can the family of states derived in the present paper constitute in part the generating set? As the consideration of such questions involves reversible conversion of states in the asymptotic limit, few progresses have been made. Unfortunately, in the present paper, such questions are not answered and remain open.

APPENDIX: SOLUTIONS OF STATIONARITY EQUATIONS

As indicated above, we have found all six solutions of stationarity equations for $\gamma=0$ and $\gamma=\pi/2$. In general, these equations have two types of solutions: the nearest separable states for highly and slightly entangled three-qubit states, respectively. There are no slightly entangled states within the subclass of symmetric states and corresponding solutions are irrelevant since $\mu<g$ and the equality $\mu=g$ is never saturated.

At $\gamma=0$, the stationarity Eq. (30) along the y axis reduces to

$$(2gt-2t^2)u_y=\lambda u_y. \tag{A1}$$

Either $u_y=0$ or $\lambda=2t^2-2gt$. The second case does not give a true maximum since $\lambda<0$.

Similar situation occurs at $\gamma=\pi/2$. The stationarity Eq. (30) along the x axis reduces to

$$(2t^2+2gt)u_x=\lambda u_x. \tag{A2}$$

The case $u_x=0$ gives three symmetric solutions, while the remaining case $\lambda=2t^2+2gt$ gives three asymmetric solutions.

Thus, at extreme values of the gauge phase stationarity, equations are factorized to cubic equations. One of the roots of these cubic equations is either $\sin\theta_k=0$ or $\tan\theta_k=\pm(g\pm t)/h$, where the angle θ_k defines the weights of computational basis vectors in the local state as follows: $|i_k\rangle\sim\cos\theta_k|0\rangle+e^{i\varphi}\sin\theta_k|1\rangle$. Hence we know one root of each cubic equation and we can find the other two by solving a quadratic equation. In this way, we find all roots of the characteristic polynomial.

1. Solutions in the case of $\gamma=0$

We list them as follows:
Solution 1 (symmetric, standard)

$$|q_1q_2q_3\rangle=|000\rangle, \quad \mu=g.$$

Solution 2 (symmetric, relevant)

$$|q_1q_2q_3\rangle=|qqq\rangle, \quad |q\rangle=\frac{2t|0\rangle+r_+|1\rangle}{\sqrt{r_+^2+4t^2}}, \quad \mu=\frac{hr_++4t^2}{\sqrt{r_+^2+4t^2}},$$

$$r_+=h+\sqrt{h^2+8t^2-4gt}.$$

Solution 3 (symmetric, irrelevant)

$$|q_1q_2q_3\rangle=|qqq\rangle, \quad |q\rangle=\frac{2t|0\rangle+r_-|1\rangle}{\sqrt{r_-^2+4t^2}}, \quad \mu=\frac{hr_-+4t^2}{\sqrt{r_-^2+4t^2}},$$

$$r_-=h-\sqrt{h^2+8t^2-4gt}.$$

Solution 4 (asymmetric, irrelevant)

$$|q_1q_2q_3\rangle=|qqq'\rangle, \quad |q\rangle=\frac{h|0\rangle-(g+t)|1\rangle}{\sqrt{h^2+(g+t)^2}},$$

$$\mu^2=\frac{g^2h^2+t^2(g+t)^2}{h^2+(g+t)^2}, \quad |q'\rangle=\frac{\langle qq|\psi_0\rangle}{\mu}.$$

Solution 5 (asymmetric, irrelevant, permutation of fourth solution)

$$|q_1q_2q_3\rangle=|qq'q\rangle.$$

Solution 6 (asymmetric, irrelevant, permutation of fourth solution)

$$|q_1q_2q_3\rangle=|q'qq\rangle.$$

2. Solutions in the case of $\gamma=\pi/2$

Solutions for $\gamma=\pi/2$ are:
Solution 1 (symmetric, standard)

$$|q_1q_2q_3\rangle=|000\rangle, \quad \mu=g.$$

Solution 2 (symmetric, relevant)

$$|q_1q_2q_3\rangle=|qqq\rangle, \quad |q\rangle=e^{i\pi/3}\frac{2t|0\rangle+ir_\pi|1\rangle}{\sqrt{r_\pi^2+4t^2}},$$

$$\mu=\frac{hr_\pi+4t^2}{\sqrt{r_\pi^2+4t^2}}, \quad r_\pi=\sqrt{h^2+4gt+8t^2}+h.$$

Solution 3 (symmetric, irrelevant)

$$|q_1q_2q_3\rangle=|qqq\rangle, \quad |q\rangle=e^{i\pi/3}\frac{2t|0\rangle-is_\pi|1\rangle}{\sqrt{s_\pi^2+4t^2}},$$

$$\mu=\frac{hs_\pi-4t^2}{\sqrt{s_\pi^2+4t^2}}, \quad s_\pi=\sqrt{h^2+4gt+8t^2}-h.$$

Solution 4 (asymmetric, relevant)

$$|q_1q_2q_3\rangle=|qqq'\rangle, \quad |q\rangle=\cos\theta|0\rangle+e^{i\varphi}\sin\theta|1\rangle,$$

$$\mu'^2=\frac{g^2h^2-4gt^3}{g^2+h^2-3gt},$$

$$\cos 2\theta=\frac{h^2+gt-g^2}{h^2+g^2-3gt}, \quad \sin\varphi=\frac{h}{2g}\tan\theta.$$

Solution 5 (asymmetric, relevant, permutation of fourth solution)

$$|q_1q_2q_3\rangle=|qq'q\rangle.$$

Solution 6 (asymmetric, relevant, permutation of fourth solution)

$$|q_1q_2q_3\rangle=|q'qq\rangle.$$

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