Three-tangle for mixtures of generalized GHZ and generalized W states

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**Abstract.** We give a complete solution for the three-tangle of mixed three-qubit states composed of a generalized Greenberger–Horne–Zeilinger (GHZ) state, $a|000\rangle + b|111\rangle$, and a generalized W state, $c|001\rangle + d|010\rangle + f|100\rangle$. Using the methods introduced by Lohmayer et al (2006 *Phys. Rev. Lett.* 97 260502), we provide explicit expressions for the mixed-state three-tangle and the corresponding optimal decompositions for this more general case. Moreover, as a special case, we obtain a general solution for a family of states consisting of a generalized GHZ state and an orthogonal product state.
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1. Introduction

The occurrence of entanglement in multipartite systems is one of the most important and distinctive features in quantum theory [1, 2]. With the ever-increasing number of applications of entanglement, its quantification has become one of the foremost topics in contemporary quantum information research. Nowadays multipartite entangled states of up to eight trapped photons can be generated in a controlled way [3, 4] awaiting quantitative and qualitative analysis, e.g. for quantum information processing. But also in the field of condensed matter physics, the study of entanglement has gathered interest in the context of quantum many-body phenomena and there is strong evidence that multipartite entanglement plays an important role [5]. However, these conclusions are of qualitative nature and are based on the presence of what is called the residual entanglement [6, 7]. Its decomposition into the various multipartite entanglement classes is still missing, and it is not even clear whether such a fragmentation is possible.

A key aspect of this problem is that only the entanglement of pure and mixed states of two qubits is well understood [8]–[12], but to date there is no generally accepted theory for classification and quantification of entanglement in multipartite qubit systems. For three-qubit systems, numerous interesting results have been found [6], [13]–[23]. A complete characterization in terms of stochastic local operations and classical communication of three-qubit entanglement has been achieved only for pure states [6, 14]. It leads to a schematic characterization for mixed states [18]. A crucial concept for this is the so-called three-tangle, a polynomial invariant for three-qubit states that quantifies the three-partite entanglement contained in a pure three-qubit state (the three-tangle is equal to the modulus of the hyperdeterminant [24, 25]). It is the first milestone towards a systematic approach to describing multipartite entanglement. However, even for the simplest case of rank-2 mixed states, no general expression is known for its three-tangle. Note that rank-2 mixed states occur naturally when one qubit is traced out in a pure multipartite entangled state. An important example is three-qubit mixed states that emerge from various classes of genuinely entangled pure four-qubit states [26].

Recently, Lohmayer et al [22] have provided an analytic quantification of the three-tangle for a representative family of rank-2 three-qubit states, namely for mixtures of a symmetric GHZ state and an orthogonal symmetric W state. But the family of states analyzed there does not cover all possible mixed states relevant for a study of the three-tangle in certain important four-qubit states, e.g. the cluster states. In this paper, we achieve this goal by showing that the methods of [22, 27] can be extended to rank-2 mixtures of a generalized GHZ state and an
orthogonal generalized W state. This generalized family of states includes admixtures of a wide class of complete product states or factorized states containing bipartite entanglement, with the generalized GHZ state. In the latter case, the exact convex roof can be extended to the entire Bloch ball, and the result shows a striking similarity to the concurrence of mixtures between a two-qubit entangled state and an orthogonal product state.

Since the set of states for which we provide analytical solutions crosses all classes of mixtures between a generalized GHZ state and an orthogonal state of zero three-tangle, it can also be useful as an extensive ‘test ground’ for any forthcoming proposal of a general expression for the mixed-state three tangle. Furthermore, it provides the tools for a systematic investigation of extended monogamy relations.

This paper is organized as follows: in section 2, we introduce some basic terminology and give a precise formulation of the problem whose general solution we outline in section 3. In section 4, we discuss special cases of this solution, in particular we find the three-tangle for rank-2 mixtures of generalized GHZ states and certain orthogonal product states.

2. Notation and formulation of the problem

Consider the state $|\psi\rangle$ in a three-qubit Hilbert space $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_C$. Its coefficients with respect to a basis of product states (the ‘computational basis’) are $\psi_{jkl} = \langle jkl|\psi\rangle$, $j, k, l \in \{0, 1\}$. An important measure for the entanglement in pure three-qubit states is the three-tangle (or residual tangle) introduced in [6]. The three-tangle of $|\psi\rangle$ is a so-called polynomial invariant [28, 29] and can be written in terms of the coefficients $\psi_{ijk}$ as

$$
\tau_3(\psi) = 4|d_1 - 2d_2 + 4d_3|,
$$

(1)

$$
d_1 = \psi_{000}^2 \psi_{111}^2 + \psi_{001}^2 \psi_{110}^2 + \psi_{010}^2 \psi_{101}^2 + \psi_{100}^2 \psi_{011}^2,
$$

$$
d_2 = \psi_{000} \psi_{111} \psi_{011} \psi_{100} + \psi_{000} \psi_{111} \psi_{101} \psi_{010} + \psi_{000} \psi_{111} \psi_{110} \psi_{001} + \psi_{011} \psi_{100} \psi_{101} \psi_{010} + \psi_{011} \psi_{100} \psi_{110} \psi_{001} + \psi_{101} \psi_{100} \psi_{110} \psi_{001},
$$

$$
d_3 = \psi_{000} \psi_{110} \psi_{011} \psi_{100} + \psi_{111} \psi_{001} \psi_{010} \psi_{100}.
$$

The three-tangle of a mixed state

$$
\rho = \sum_j p_j \pi_j, \quad \pi_j = \frac{|\phi_j\rangle\langle \phi_j|}{\langle \phi_j|\phi_j\rangle}
$$

(2)

can be defined as convex-roof extension [30] of the pure state three-tangle,

$$
\tau_3(\rho) = \min_{\text{decompositions}} \sum_j p_j \tau_3(\pi_j).
$$

(3)

A given decomposition $\{q_k, \pi_k : \rho = \sum_k q_k \pi_k\}$ with $\tau_3(\rho) = \sum_k q_k \tau_3(\pi_k)$ is called optimal. We note that $\tau_3(\rho)$ is a convex function on the convex (and compact) set $\Omega$ of density matrices $\rho$.

In this paper, we determine three-tangle and optimal decompositions for the family of mixed three-qubit states

$$
\rho(p) = p|g\text{GHZ}_{a,b}\rangle\langle g\text{GHZ}_{a,b}| + (1-p)|g\text{W}_{c,d,f}\rangle\langle g\text{W}_{c,d,f}|
$$

(4)

composed of a generalized GHZ state

$$
|g\text{GHZ}_{a,b}\rangle = a|000\rangle + b|111\rangle, \quad |a|^2 + |b|^2 = 1
$$

(5)

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and a generalized W state

$$|gW_{c,d,f}⟩ = c|001⟩ + d|010⟩ + f|100⟩, \quad |c|^2 + |d|^2 + |f|^2 = 1.$$  \hspace{1cm} (6)

We note that $τ_3(gW_{c,d,f}) = 0$ and $τ_3^{GHZ} := τ_3(gGHZ_{a,b}) = 4|a^2b^2|$. For the symmetric GHZ and W states $(a = b = 1/\sqrt{2}$ and $c = d = f = 1/\sqrt{3}$) the problem and results of [22] are recovered.

3. The generic case

In this section, it is assumed that none of the coefficients is zero, i.e. $a, b, c, d, f \neq 0$. The opposite case corresponds to either a rank-2 mixture of a generalized GHZ and a biseparable state, or to a mixture of a generalized W and a completely factorized state. This will be studied in the next section.

In the following, we will apply the methods developed in [22, 27]. There, it was shown that in order to find the convex roof of an entanglement measure for rank-2 mixed states, it is useful to study the pure states that are superpositions of the eigenstates of $ρ_gGHZ\!a, b⟩ - \sqrt{1 - p} e^{iϕ} |gW_{c,d,f}⟩$.

The three-tangle of these states is

$$τ_3(p, ϕ) = 4|p^2a^2b^2 - \sqrt{p(1 - p)^3} e^{3iϕ} cdf|.$$  \hspace{1cm} (8)

The phases of the coefficients in $|gGHZ_{a,b}⟩$ and $|gW_{c,d,f}⟩$ merely produce different offsets for the relative phase $ϕ$ in the expression for the three-tangle, equation (8). Therefore, it suffices to consider the case where all coefficients are positive real numbers.

In the following, it will be beneficial to introduce the definition

$$s = \frac{4cdf}{a^2b} > 0.$$  \hspace{1cm} (9)

If we factor out the three-tangle $τ_3^{GHZ}$ of the generalized GHZ state, the three-tangle of the superposition (7) can be written as

$$τ_3(p, ϕ) = τ_3^{GHZ} \left| p^2 - \sqrt{p(1 - p)^3} e^{3iϕ} s \right|.$$  \hspace{1cm} (10)

Since $τ_3^{GHZ}$ is just a constant factor, the behaviour of this function of $p$ and $ϕ$ is completely determined by the value of the parameter $s$.

As a first step, we identify the zero-simplex containing all mixed states $ρ(p)$ with $τ_3(ρ(p)) = 0$. Its corner states are obtained as the zeros of equation (10). One obvious solution is $p = 0$, which corresponds to a pure generalized W state. Therefore, in the calculation of the other solutions we can assume $p > 0$ and the zeros are determined by

$$\sqrt{p^3} = \sqrt{(1 - p)^3} e^{3iϕ} s.$$  \hspace{1cm} (11)

Since $p$ and $s$ are real and positive, this implies

$$ϕ = n\frac{2π}{3}, \quad n \in \mathbb{N}.$$  \hspace{1cm} (12)

Note that the $2\pi/3$-periodicity is due to the fact that this relative phase is induced by the local transformation $\text{diag}(\exp(i2\pi/3), 1)$ on each qubit.
For $p$, we then get the solution

$$p_0 = \frac{s^{2/3}}{1 + s^{2/3}} = \frac{\sqrt{16c^2d^2f^2}}{\sqrt{a^4b^2} + \sqrt{16c^2d^2f^2}}$$

This means that in addition to the state $|gW_{c,d,f}\rangle$ the three-tangle vanishes for $|p_0, n \cdot 2\pi/3\rangle$, $n = 0, 1$ and 2. All mixed states whose density matrices are convex combinations of those four states have zero three-tangle. On the Bloch sphere with gGHZ and gW at its poles, this corresponds to a simplex with those four states at the corners. All $\rho(p)$ with $p < p_0$ are inside this set, and therefore $\tau_3(\rho(p)) = 0$ for $0 \leq p \leq p_0$.

In order to determine the mixed three-tangle of $\rho(p)$ for $p > p_0$, we note that for any fixed $p$, $\tau_3(p, \varphi)$ takes a minimum at $\varphi_0 = 0$ which due to the symmetry of $\tau_3$ is repeated at $\varphi_1 = 2\pi/3$ and $\varphi_2 = 4\pi/3$. Consequently, for any value of $p$ the state $\rho(p)$ can be decomposed into the three states $|p, \varphi_i\rangle$, $i = 0, 1$ and 2. Therefore, the characteristic curve $\tau_3(p, 0)$ is an upper bound to $\tau_3(\rho(p))$. Moreover it is known to give the correct values for the three-tangle at $p = p_0$ (at the top face of the zero simplex) and $p = 1$ ($\rho(1) = |gGHZ_{a,b}\rangle\langle gGHZ_{a,b}|$). However, if there is a range of values where $\tau_3(p, 0)$ is a concave function, there are decompositions for $\rho(p)$ with a lower average three-tangle \[22\]. Therefore, it is important to examine where the function $\tau_3(p, 0)$ is concave for $p \geq p_0$.

For $\varphi = 0$ and $p \geq p_0$, the term inside the absolute value bars in (10) is real and positive, and the characteristic curve $\tau_3(p, 0)$ is equal to

$$t(p) = \tau_3^{gGHZ} \cdot \left( p^2 - \sqrt{p(1 - p)}^3 \right).$$

Concavity of $t(p)$ is indicated by a negative sign of its second derivative

$$t''(p) = \tau_3^{gGHZ} \cdot \left( 2 - \frac{8p^2 - 4p - 1}{4p\sqrt{p(1 - p)}} \right).$$

The limit $p \to 1$ ($p = 1 - \varepsilon$) in (15) gives

$$t''(1 - \varepsilon) = -\frac{3\tau_3^{gGHZ}}{4\sqrt{\varepsilon}} + 2\tau_3^{gGHZ} + O(\varepsilon^{1/2}),$$

that is, $t(p)$ is concave close to $p = 1$. On the other hand, for small $p$

$$t''(p) = \frac{\tau_3^{gGHZ}}{4p^{3/2}} + O(p^{-1/2}).$$

That is, close to $p = 0$ we find that $t(p)$ is convex (note that due to the absolute value, $\tau_3(p, 0)$ is actually concave close to $p = 0$). Due to continuity, there must be at least one zero of $t''(p)$ in between. Moreover, we note that the third derivative

$$t'''(p) = \frac{-3\tau_3^{gGHZ}}{8p^2\sqrt{p(1 - p)^3}} \leq 0$$

is negative for all values of $p$. Thus $t''(p)$ is strictly monotonic and has precisely one zero, implying that $t(p)$ is convex before and concave after that point. As the mixed state three-tangle is convex, the characteristic curve needs to be convexified where it is concave in the interval $[p_0, 1]$. Since the concavity extends up to $p = 1$, corresponding to the state $|gGHZ_{a,b}\rangle$, that state has to be part of the optimal decomposition \[27\] in this interval.
The symmetry and the results in [22] suggest that a good ansatz for the optimal decomposition is

$$\rho(p) = \alpha |g_{GHZ_{a,b}}\rangle \langle g_{GHZ_{a,b}}| + \frac{1 - \alpha}{3} \sum_{k=0}^{2} p_{1,k} \cdot \frac{2\pi}{3} \begin{pmatrix} p_{1}, k \cdot \frac{2\pi}{3} \end{pmatrix},$$

(19)

where \( p_{1} \) is chosen such that the mixed-state three-tangle becomes minimal. The value of \( \alpha \) is fixed by \( p \) and \( p_{1} \):

$$\alpha = \frac{p - p_{1}}{1 - p_{1}}.$$  

(20)

The average three-tangle for this decomposition is \((p > p_{0})\)

$$\tau_{3}^{\text{conv}}(p, p_{1}) = \frac{p - p_{1}}{1 - p_{1}} \cdot \tau_{3}^{g_{GHZ}} + \frac{1 - p}{1 - p_{1}} \cdot t(p_{1}).$$

(21)

This describes a linear interpolation between \( \tau_{3}(p_{1}, 0) \) and \( \tau_{3}^{g_{GHZ}} \). Note that for \( p < p_{1}, \) \( (19) \) ceases to be a valid decomposition because \( \alpha \) becomes negative.

To find the minimum in \( p_{1} \) for given \( p \), we look for the zeros of the derivative \( \partial \tau_{3}^{\text{conv}}/\partial p_{1} \). The resulting equation has the solution

$$p_{1}^{\text{noabs}} = \frac{1}{2} + \frac{1}{2\sqrt{1 + s^{2}}}.$$  

(22)

Note that for \( s > 2\sqrt{2} \) we get \( p_{1}^{\text{noabs}} < p_{0} \). In that case the minimum is reached at the border \( p_{1} = p_{0} \) of the considered interval \([p_{0}, 1]\), and therefore

$$p_{1} = \max \left\{ p_{0}, \frac{1}{2} + \frac{1}{2\sqrt{1 + s^{2}}} \right\}.$$  

(23)

Putting it all together, we present the central result of this paper

$$\tau_{3}(\rho(p)) = \begin{cases} 0, & \text{for } 0 \leq p \leq p_{0}, \\ \tau_{3}(p, 0), & \text{for } p_{0} \leq p \leq p_{1}, \\ \tau_{3}^{\text{conv}}(p, p_{1}), & \text{for } p_{1} \leq p \leq 1, \end{cases}$$

(24)

where \( p_{0} \) is given by \((13)\), \( p_{1} \) by \((23)\), \( \tau_{3}(p, 0) \) by \((8)\) and \( \tau_{3}^{\text{conv}}(p, p_{1}) \) by \((21)\). The corresponding optimal decompositions are

$$\rho(p) = \begin{cases} \frac{p_{0}}{p_{0}} \rho_{\Delta}(p_{0}) + \frac{p_{0} - p}{p_{0}} \pi_{gW}, & \text{for } 0 \leq p \leq p_{0}, \\ \rho_{\Delta}(p), & \text{for } p_{0} \leq p \leq p_{1}, \\ \frac{1 - p}{1 - p_{1}} \rho_{\Delta}(p_{1}) + \frac{p - p_{1}}{1 - p_{1}} \pi_{gGHZ}, & \text{for } p_{1} \leq p \leq 1, \end{cases}$$

(25)

where

$$\rho_{\Delta}(p) = \frac{1}{3} \sum_{k=0}^{2} p_{1,k} \cdot \frac{2\pi}{3} \begin{pmatrix} p_{1}, k \cdot \frac{2\pi}{3} \end{pmatrix}.$$  

(26)

and \( \pi_{f} \) as defined in \((2)\).

The curve \((24)\) is convex, and for all \( p \) and \( \varphi \): \( \tau_{3}(\rho(p)) \leq \tau_{3}(p, \varphi) \). Therefore it is a lower bound to the three-tangle of \( \rho(p) \). On the other hand, for each \( p \) we have given an explicit decomposition realizing this lower bound. Thus, it also represents an upper bound and hence coincides with the three-tangle of \( \rho(p) \).

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4. Special cases

In this section, we will discuss various special cases of our general solution (24).

First, we briefly demonstrate that the results for the symmetric GHZ state and the symmetric W state in [22] are reproduced. Indeed, the general behavior described in section 3 (i.e. analytic properties of the three-tangle, optimal decompositions) matches that found in [22], so we only have to check the values of $p_0$ and $p_1$. In the symmetric case, we have $a = b = 1/\sqrt{2}$ and $c = d = f = 1/\sqrt{3}$, resulting in

$$s = \frac{2^{7/2}}{3^{3/2}}.$$  \hfill (27)

Inserting this in (13) and (23) leads to

$$p_0 = \frac{2^{7/3}/3}{1 + 2^{7/3}/3} = \frac{4\sqrt{2}}{3 + 4\sqrt{2}},$$  \hfill (28)

$$p_1 = \frac{1}{2} + \frac{1}{2\sqrt{1 + 2^{7/3}}} = \frac{1}{2} + \frac{3}{2}\sqrt{\frac{3}{155}},$$  \hfill (29)

as found in [22].

Next, we consider the limiting cases where at least one of the coefficients is 0. Those require extra care as the calculations above have been done under the assumption of non-vanishing coefficients. However, since we are dealing with continuous functions, one should expect that the results still apply, although possibly in a degenerate form.

The first case we consider is when the generalized GHZ state degenerates into a pure three-party product state. This corresponds to the limit $s \to \infty$. However, note that at the same time $\tau_{3}^{g\text{GHZ}} \to 0$ such that (10) remains regular. This can be seen by looking at the explicit form (8). It is clear that in this case $\tau_{3}(\rho(p)) = 0$ for all $p$.

There are two non-equivalent ways to achieve this. One possibility is $b = 0$ which reduces the generalized GHZ state to $|000\rangle$. In this case, the three-tangle (8) vanishes for all superpositions (7), and therefore also all mixed states anywhere inside the Bloch sphere have vanishing three-tangle.

The other way to get $s \to \infty$ is $a = 0$ where the generalized GHZ state is reduced to $|111\rangle$. While $\rho(p)$ as a mixture of product and gW state again has no three-tangle, unlike in the case $b = 0$ the three-tangle does not vanish everywhere on the Bloch sphere. Equation (8) reduces to

$$\tau_{3}(p, \varphi) = 16\sqrt{p(1 - p)^3} c d f,$$  \hfill (30)

which is independent of $\varphi$ and is concave for all $p \in [0, 1]$. Thus, the zero simplex degenerates into a zero axis. As long as $c d f > 0$, outside this axis the three-tangle never vanishes. If both $a = 0$ and $c d f = 0$, the three-tangle is zero everywhere inside the Bloch sphere.

The opposite limiting case is $s = 0$, that is, when at least one of the coefficients $c$, $d$ or $f$ vanishes. Note that for the three-tangle it does not matter whether only one of them vanishes, resulting in a product of a single-qubit state with a generalized Bell state, or two of them, resulting in a product of three single-qubit states: in all cases (10) reduces to

$$\tau_{3}(p, \varphi) = \tau_{3}^{g\text{GHZ}} \cdot p^2,$$  \hfill (31)
Figure 1. Three-tangle for \( s = 7 > 2\sqrt{2} \) (a) and \( s = 2.3 < 2\sqrt{2} \) (b). In both cases \( \tau_3^{\text{GHZ}} = 0.0396 \). The solid line is the minimal pure state tangle, \( \tau_3(p, 0) \) (10). The short-dashed line is \( t(p) \) (14). The dotted vertical lines show the positions of \( p_0 \) (13), \( p_1^{\text{noabs}} \) (22) and \( p_1 \) (23), and the thick dashed line gives the resulting mixed three-tangle \( \tau_3(\rho(p)) \) (24). In addition, the first figure shows with a dotted line the curve which would result from using \( p_1^{\text{noabs}} \) instead of \( p_1 \) in (21).

which is convex for all \( p \in [0, 1] \); indeed, (13) and (23) yield \( p_0 = 0 \) and \( p_1 = 1 \) at \( s = 0 \). Consequently,

\[
\tau_3(\rho(p)) = \tau_3^{\text{GHZ}} \cdot p^2, \tag{32}
\]

for all \( p \). Even more, \( \tau_3(\rho) = \tau_3^{\text{GHZ}} \cdot p^2 \) for any mixed state \( \rho \) inside the Bloch sphere with \( \langle g_{\text{GHZ},a,b} | \rho | g_{\text{GHZ},a,b} \rangle = p \). We would like to point out that this result is reminiscent of the situation both for two-qubit superpositions [31] and for two-qubit mixtures of an arbitrary entangled state and an orthogonal product state.
5. Conclusion

In this paper, we have given explicit expressions for the three-tangle of mixtures $\rho(p)$ according to (4) of arbitrary generalized GHZ and orthogonal generalized W states, including the limiting cases where those states are reduced to product states. We have found that the qualitative pattern described in [22] for mixtures of symmetric GHZ and W states is more general. Up to a certain value $p_0$ given by (13), the mixed three-tangle vanishes. The optimal decomposition for those states consists of the pure states (7) for which the three-tangle is zero. One is always the generalized W state at the bottom of the Bloch sphere; the other three form an equilateral horizontal triangle at the height of $p_0$.

For $p > p_0$, there may follow a region up to some value $p_1$ given by equation (23), where the mixed state three-tangle follows the minimal pure state three-tangle (10) with the same value for $p$ (which for positive real coefficients is achieved at $\varphi = 0$). In this region, the optimal decomposition consists of the three states with this property, which form a horizontal equilateral triangle with corners on the Bloch sphere and $\rho(p)$ in the center. At $s \geq 2\sqrt{2}$, $p_1$ and $p_0$ coincide and for $s$ exceeding this threshold, the region with ‘leaves’ of constant three-tangle in the convex roof (cf [22], figure 1) is absent. This can be viewed as contraction of this middle region into a single point.

For $p > p_1$, the three-tangle grows linearly up to its maximum value at $p = 1$. The optimal decomposition in this case consists of the three pure superposition states for $p = p_1$ with minimal three-tangle and the generalized GHZ state. That is, the convex roof in the Bloch sphere is affine for an entire simplex whose corners are given by the four pure states that form the optimal decomposition. Moreover, we have demonstrated how the results of this work connect to the findings for the special case of mixtures of a symmetric GHZ and a symmetric W state [22].

In principle, the scheme of three regions for $p$ values as outlined above holds also in the limiting cases when some of the coefficients in the states vanish, except that in this situation the ‘outer regions’ may shrink away. A common feature of these limits is a $\varphi$-independent characteristic curve. If the generalized GHZ state degenerates into a product state, $\tau_3(\rho(p)) = 0$ for all $p$. On the other hand, for $s = 0$ (i.e. at least one of the coefficients in the generalized W states vanishes), both ‘outer’ affine regions disappear and the whole range of $p$ is covered by the ‘middle region’ with a strictly convex characteristic curve. This case corresponds to a mixture of a generalized GHZ state and an orthogonal product state and the exact convex roof of the three-tangle is obtained for the entire Bloch ball.

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