Geometric measure of entanglement for multipartite quantum states

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The degree to which a pure quantum state is entangled can be characterized by the distance or angle to the nearest unentangled state. This geometric measure of entanglement, already present in a number of settings [A. Shimony, Ann. NY. Acad. Sci. 755, p.675 (1995) and H. Barnum and N. Linden, J. Phys. A: Math. Gen. 34, p.6787 (2001)], is explored for bipartite and multipartite pure and mixed states. It is determined for arbitrary two-qubit mixed states and for generalized Werner and isotropic states, and is also applied to certain multipartite mixed states.

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Introduction: Only recently, after more than half a century of existence, has the notion of entanglement become recognized as central to quantum information processing. As a result, the task of characterizing and quantifying entanglement has emerged as one of the prominent themes of quantum information theory. There have been many achievements in this direction, primarily in the setting of bipartite systems. Among these, one highlight is Wootters’ formula for the entanglement of formation for two-qubit mixed states; others include corresponding results for highly symmetrical states of higher-dimensional systems. The issue of entanglement for multipartite states poses an even greater challenge, and there have been correspondingly fewer achievements: notable examples include applications of the relative entropy, negativity, and Schmidt measure.

In this Letter, we present an attempt to face this challenge by developing and investigating a certain geometric measure of entanglement, first introduced by Shimony in the setting of bipartite pure states and generalized to the multipartite setting (via projection operators of various ranks) by Barnum and Linden. We begin by examining this geometric measure in pure-state settings, and then extend it to mixed states, showing that it satisfies certain criteria for good entanglement measures. We demonstrate that this measure is no harder to compute than the entanglement of formation $E_F$, and exemplify this fact by giving formulas corresponding to $E_F$ for (i) arbitrary two-qubit mixed, (ii) generalized Werner, and (iii) isotropic states. We conclude by applying the geometric entanglement measure to certain families of multipartite mixed states, for which we provide a practical method for computing entanglement, and illustrate this method via two examples.

It is not our aim to cast aspersions on existing approaches to entanglement; rather we simply wish to add one further aspect to the discussion.

Basic geometric ideas; application to pure states: We begin with an examination of entangled pure states, and how one might quantify their entanglement by making use of simple ideas of Hilbert space geometry. Let us start by developing a quite general formulation, appropriate for multipartite systems comprising $n$ parts, each of which can have a distinct Hilbert space. Consider a general $n$-partite pure state $|\psi\rangle = \sum_{p_1 \cdots p_n} \chi_{p_1 p_2 \cdots p_n} |c_{p_1}^{(1)} \cdots c_{p_n}^{(n)}\rangle$.

One can envisage a geometric definition of its entanglement content via the distance $d = \min_{|\phi\rangle} \| |\psi\rangle - |\phi\rangle \|$ between $|\psi\rangle$ and the nearest separable state $|\phi\rangle$ (or equivalently the angle between them). Here, $|\phi\rangle \equiv \otimes_{i=1}^{n} |\phi_i^{(i)}\rangle$ is an arbitrary separable (i.e., Hartree) $n$-partite pure state, the index $i = 1 \ldots n$ labels the parts, and $|\phi_i^{(i)}\rangle \equiv \sum_{p_i} c_{p_i}^{(i)} |\psi_{p_i}\rangle$. Naturally, the more entangled a state is, the further away it will be from its best unentangled approximant and the wider will be the angle between them.

To actually find the nearest separable state, it is convenient to minimize, instead of $d$, the quantity $\| |\psi\rangle - |\phi\rangle \|^2$, subject to the constraint $\langle \phi | \phi \rangle = 1$. In fact, in solving the resulting stationarity condition one may restrict one’s attention to the subset of solutions $|\phi\rangle$ that obey the further condition that for each factor $|\phi_i^{(i)}\rangle$ one has $\langle \phi_i^{(i)} | \phi_i^{(i)} \rangle = 1$. Thus, one arrives at the nonlinear eigenproblem for the stationary $|\phi\rangle$:

$$\sum_{p_1 \cdots p_n} \chi_{p_1 p_2 \cdots p_n}^* c_{p_1}^{(1)} \cdots c_{p_n}^{(n)} = \Lambda c_{p_i}^{(i)}^*, \quad (1a)$$

$$\sum_{p_1 \cdots p_n} \chi_{p_1 p_2 \cdots p_n} c_{p_1}^{(1)} \cdots c_{p_n}^{(n)} = \Lambda c_{p_i}^{(i)}, \quad (1b)$$

where the eigenvalue $\Lambda$ is associated with the Lagrange multiplier enforcing the constraint $\langle \phi | \phi \rangle = 1$, and $^*$ denotes exclusion. In basis-independent form, Eqs. (1) read

$$\langle \psi | \bigotimes_{j \neq i} |\phi_j^{(j)}\rangle \rangle = \Lambda \langle \phi_i^{(i)} |, \quad \left( \bigotimes_{j \neq i} \langle \phi_j^{(j)} | \right) |\psi\rangle = \Lambda |\phi_i^{(i)}\rangle. \quad (2)$$

From Eqs. (1) or (2) one readily sees that the eigenvalues $\Lambda$ are real, in $[-1, 1]$, and independent of the choice of the local basis $\{ |\psi_{p_i}\rangle\}$. Hence, the spectrum $\Lambda$ can be interpreted as the cosine of the angle between $|\psi\rangle$ and $|\phi_i^{(i)}\rangle$: the largest, $\Lambda_{\text{max}}$, which we call the entanglement eigenvalue, corresponds to the closest separable state.
Although, in determining the closest separable state, we have used the squared distance between the states, there are alternative (basis-independent) candidates for entanglement measures: the distance, the sine, or the sine squared of the angle \( \theta \) between them (with \( \cos \theta \equiv \text{Re} \langle \psi | \phi \rangle \)). We shall adopt \( E_{\text{sin}^2} = 1 - \Lambda_{\text{max}} \) as our entanglement measure because, as we shall see, when generalizing \( E_{\text{sin}^2} \) to mixed states we have been able to show that it satisfies a set of criteria for entanglement measures. We remark that determining the entanglement of \( |\psi\rangle \) is equivalent to finding the Hartree approximation to the ground-state of the auxiliary Hamiltonian \( \mathcal{H} \equiv -|\psi\rangle\langle\psi| + g \).

In bipartite applications, the eigenproblem \( \mathcal{H} \) is in fact linear, and solving it is actually equivalent to finding the Schmidt decomposition \( \mathcal{H} \). Moreover, the entanglement eigenvalue is equal to the square of the maximal Schmidt coefficient. By constrast, for the case of three or more parts, the eigenproblem is a nonlinear one, for which one can, in general, only address the problem directly, i.e., by determining the eigenvalues and eigenvectors simultaneously, presumably numerically. Yet, as we shall illustrate shortly, there do exist certain types of states whose entanglement eigenvalues can be determined analytically.

**Illustrative examples:** Suppose we are already in possession of the Schmidt decomposition of some two-qubit pure state: \( |\psi\rangle = \sqrt{p} |00\rangle + \sqrt{1-p} |11\rangle \). Then we can read off the entanglement eigenvalue: \( \Lambda_{\text{max}} = \max\{ \sqrt{p}, \sqrt{1-p} \} \). Now, recall \( \Lambda_{\text{max}} \) that the concurrence \( C \) for this state is \( 2\sqrt{p(1-p)} \). Hence, one has

\[
\Lambda_{\text{max}}^2 = 1/2 \left( 1 + \sqrt{1 - C^2} \right),
\]

which holds for arbitrary two-qubit pure states.

The possession of symmetry by a state can alleviate the difficulty associated with solving the nonlinear eigenproblem. To see this, consider a state \( |\psi\rangle = \sum_{\sigma_1, \sigma_2, \ldots, \sigma_n} \chi_{\sigma_1 \sigma_2 \cdots \sigma_n} |e^{(1)}_{\sigma_1} e^{(2)}_{\sigma_2} \cdots e^{(n)}_{\sigma_n}\rangle \) that obeys the symmetry that the nonzero amplitudes \( \chi \) are invariant under permutations. What we mean by this is that, regardless of the dimensions of the factor Hilbert spaces, the amplitudes are only nonzero when the indices take on the first \( \nu \) values (or can be arranged to do so by appropriate relabeling of the basis in each factor) and, moreover, that these amplitudes are invariant under permutations of the parties, i.e., \( \chi_{\sigma_1 \sigma_2 \cdots \sigma_n} = \chi_{\tau_1 \tau_2 \cdots \tau_n} \), where the \( \sigma\)'s are any permutation of the \( \tau\)'s. (This symmetry may be obscured by arbitrary local unitary transformations.) For such states, it seems reasonable to anticipate that the closest Hartree approximant retains this permutation symmetry. Assuming this to be the case—and numerical experiments of ours support this assumption— in the task of determining the entanglement eigenvalue one can start with the Ansatz that the closest separable state has the form \( |\phi\rangle \equiv \otimes_{i=1}^n (\sum_j c_j^{(i)} |e_j^{(i)}\rangle) \), i.e., is expressed in terms of copies of a single factor state, for which \( c_j^{(i)} = c_j \). To obtain the entanglement eigenvalue it is thus only necessary to maximize \( \text{Re} \langle \phi | \phi \rangle \) with respect to \( \{ c_j^{(i)} \}_{j=1}^p \), a simpler task than maximization over the \( \sum_{i=1}^n d_i \) amplitudes of a generic product state.

To illustrate this, we consider several examples involving permutation-invariant states, restricting attention to \( \nu = 2 \). The most natural realizations are \( n \)-qubit systems. One can classify these symmetric states, as follows:

\[
|S(n,k)\rangle \equiv \sqrt{k!(n-k)!} \sum_{\text{permutations}} |0\cdots01\cdots1\rangle.
\]

As the amplitudes are all positive, one can assume that the closest Hartree state is of the form \( |\phi\rangle = (\sqrt{p} |0\rangle + \sqrt{1-p} |1\rangle)^\otimes n \), for which the maximal overlap (w.r.t. \( p \)) gives the entanglement eigenvalue for \( |S(n,k)\rangle \):

\[
\Lambda_{\text{max}}(n,k) = \sqrt{\frac{n!}{k!(n-k)!} \left( \frac{k}{n} \right)^k \left( \frac{n-k}{n} \right)^{n-k}}.
\]

For fixed \( n \), the minimum \( \Lambda_{\text{max}} \) (and hence the maximum entanglement) among the \( |S(n,k)\rangle \)'s occurs for \( k = n/2 \) (for \( n \) even) and \( k = (n \pm 1)/2 \) (for \( n \) odd). In fact, for fixed \( n \) the general permutation-invariant state can be expressed as \( \sum_k \alpha_k |S(n,k)\rangle \) with \( \sum_k |\alpha_k|^2 = 1 \). The entanglement of such states can be addressed via the strategy that we have been discussing, i.e., via the maximization of a function of (at most) three real parameters. The simplest example is provided by the \( n \)-GHZ state: \( |n\text{GHZ}\rangle \equiv (|S(n,0)\rangle + |S(n,n)\rangle) / \sqrt{2} \). It is easy to show that (for all \( n \)) \( \Lambda_{\text{max}}(n\text{GHZ}) = 1/\sqrt{2} \) and \( E_{\text{sin}^2} = 1/2 \).

We now focus our attention on three-qubit settings. Of these, the states \( |S(3,0)\rangle = |000\rangle \) and \( |S(3,3)\rangle = |111\rangle \) are not entangled and are, respectively, the components of the the 3-GHZ state: \( |\text{GHZ}\rangle \equiv (|000\rangle + |111\rangle) / \sqrt{2} \). The states \( |S(3,2)\rangle \) and \( |S(3,1)\rangle \), denoted \( \mathcal{W} \equiv |S(3,2)\rangle = (|001\rangle + |010\rangle + |100\rangle) / \sqrt{3} \) and \( \tilde{\mathcal{W}} \equiv |S(3,1)\rangle = (|110\rangle + |101\rangle + |011\rangle) / \sqrt{3} \), are equally entangled, having \( \Lambda_{\text{max}} = 2/3 \) and \( E_{\text{sin}^2} = 5/9 \).

Next, consider a superposition of the \( \mathcal{W} \) and \( \tilde{\mathcal{W}} \) states: \( |\text{WW}(s,\phi)\rangle \equiv \sqrt{s} |\mathcal{W}\rangle + \sqrt{1-s} e^{i\phi} |\tilde{\mathcal{W}}\rangle \). It is easy to see.

![FIG. 1: Entanglement of the pure state](image-url)
that its entanglement is independent of $\phi$: the transformation $\{ (0), |1\rangle \} \rightarrow \{ (0), e^{-i\phi}|1\rangle \}$ induces $|WW(s, \phi)\rangle \rightarrow e^{-i\phi}|WW(s, 0)\rangle$. To calculate $\Lambda_{\text{max}}$, assume that the separable state is $(\cos \theta |0\rangle + \sin \theta |1\rangle) \otimes |\Phi^{+}\rangle$, and maximize its overlap with $|WW(s, 0)\rangle$. Then we find that the tangent $t \equiv \tan \theta$ is the particular root of the polynomial $\sqrt{1-s^2} + 2\sqrt{s}t - 2\sqrt{1-s}t - \sqrt{s} = 0$ that lies in the range $t \in [\sqrt{1/2}, \sqrt{2}]$. Via $\theta(s)$, $\Lambda_{\text{max}}$ (and $E_{\sin^2} = 1 - \Lambda_{\text{max}}$) can be expressed as

$$\Lambda_{\text{max}}(s) = \frac{1}{2}\left(\sqrt{s} \cos \theta(s) + \sqrt{1-s} \sin \theta(s)\right) \sin 2\theta(s).$$

In Fig. 1, we show $E_{\sin^2}(|WW(s, \phi)\rangle)$ vs. $s$. In fact, $\Lambda_{\text{max}}$ of the more general superposition

$$|SS_{n,k_1,k_2}(r, \phi)\rangle = \sqrt{r} |S(n, k_1)\rangle + \sqrt{1-r} e^{i\phi} |S(n, k_2)\rangle$$

($k_1 \neq k_2$) turns out to be independent of $\phi$, as in the case of $|WW(s, 0)\rangle$, and can be computed in the same way. We note that although the curve in Fig. 1 is convex, concavity does not hold uniformly over $k_1$ and $k_2$.

For our last pure-state example, we consider superpositions of $W$ and GHZ states: $|WG(s, \phi)\rangle = \sqrt{s}|W\rangle + \sqrt{1-s} e^{i\phi} |GHZ\rangle$. For these, the phase $\phi$ cannot be “gauged” away and, hence, $E_{\sin^2}$ depends on $\phi$. In Fig. 2 we show $E_{\sin^2}$ vs. $s$ at $\phi=0$ and $\pi$ (bounding curves), as well as $E_{\sin^2}$ for randomly generated values of $s \in [0, 1]$ and $\phi \in [0, 2\pi]$ (dots). It is interesting to observe that the ‘$\pi$’ state has higher entanglement than the ‘0’ does. As the numerical results suggest, the ($\phi$-parametrized) $E_{\sin^2}$ vs. $s$ curves of $|WG(s, \phi)\rangle$ lie between the ‘$\pi$’ and ‘0’ curves.

Extension to mixed states: The extension to mixed states $\rho$ can be made via the use of the convex roof (or hull) construction [indicated by “co”], as was done for the entanglement of formation (see, e.g., Ref. [3]). The essence is a minimization over all decompositions $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$, into pure states, i.e.,

$$E(\rho) = (\text{co } E_{\text{pure}})(\rho) = \min_{\{p_i, |\psi_i\rangle\}} \sum_i p_i E_{\text{pure}}(|\psi_i\rangle).$$

Now, any good entanglement measure $E$ should, at least, satisfy the following criteria (c.f. Refs. 3, 2, 3):

C1. (a) $E(\rho) \geq 0$; (b) $E(\rho) = 0$ if $\rho$ is not entangled.
C2. Local unitary transformations do not change $E$.
C3. Local operations and classical communication (LOCC) (as well as post-selection, if one wishes) do not increase the expectation value of $E$.
C4. Entanglement is convex under the discarding of information, i.e., $\sum_i p_i E(\rho_i) \geq E(\sum_i p_i \rho_i)$.

The issue of the desirability of additional features, such as continuity and additivity, requires further investigation, but C1-C4 are regarded as the minimal set, if one is to guarantee that one has an entanglement monotone.

Does the geometric measure of entanglement obey C1-4? From the definition (3) it is evident that C1 and C2 are satisfied provided that $E_{\text{pure}}$ satisfies them, as it does for $E_{\text{pure}}$ being any function of $\Lambda_{\text{max}}$ consistent with C1. It is straightforward to check that C4 holds, by the convex hull construction. The consideration of C3 seems to be more delicate. The reason is that our analysis of whether or not it holds depends on the explicit form of $E_{\text{pure}}$. For C3 to hold, it is sufficient to show that the average entanglement is nonincreasing under any trace-preserving, unilocal operation: $\rho \rightarrow \sum_k V_k \rho V_k^\dagger$, where $V_k$ is the Kraus operator of the form $V_k = I \otimes \cdots \otimes I \otimes V_k^1 \otimes \cdots \otimes I$ and $V_k^1 V_k = I$. Furthermore, it suffices to show that C3 holds for the case of a pure initial state, i.e., $\rho = |\psi\rangle\langle\psi|$. We now prove that for the particular (and by no means unnatural) choice $E_{\text{pure}} = E_{\sin^2}$, C3 holds. To be precise, for any quantum operation on a pure initial state, i.e., $|\psi\rangle\langle\psi| \rightarrow \sum_k V_k |\psi\rangle\langle\psi| V_k^\dagger$, we aim to show that $\sum_k p_k E_{\sin^2}(V_k |\psi\rangle\langle\psi| V_k^\dagger) \leq E_{\sin^2}(|\psi\rangle\langle\psi|)$, where $p_k \equiv \text{Tr} V_k |\psi\rangle\langle\psi| V_k^\dagger = |\langle V_k^1| V_k \rangle|^2$. Then, we find that the operation $V_k$ is state-to-state or state-to-ensemble. Let us respectively denote by $\Lambda$ and $\Lambda_k$ the entanglement eigenvalues corresponding to $|\psi\rangle$ and the (normalized) pure state $V_k |\psi\rangle/\sqrt{\text{Tr} V_k}$.

Before moving on to the terra incognita of mixed multipartite entanglement, we test the geometric approach in the setting of mixed bipartite states, by computing $E_{\sin^2}$ for three classes of states for which $E_{\text{p}}$ is known. Arbitrary two-qubit mixed states: For these we show that

$$E_{\sin^2}(\rho) = \frac{1}{2} \left(1 - \sqrt{1 - C(\rho)^2}\right),$$

where $C(\rho)$ is the concurrence.

FIG. 2: Entanglement of $|WG(s, \phi)\rangle$ versus $s$. The upper curve is for $\phi = \pi$ whereas the lower one is for $\phi = 0$. Dots represent states with randomly generated $s$ and $\phi$. 
where $C(\rho)$ is the Wootters concurrence of the state $\rho$. Recall that in his proof of the formula for $E_{F}$, Wootters showed that there exists an optimal decomposition $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ in which every $|\psi_i\rangle$ has the concurrence of $\rho$ itself. (More explicitly, every $|\psi_i\rangle$ has the identical concurrence, that concurrence being the infimum over all decompositions.) By using Eq. 5 one can, via Eq. 6, relate $E_{\sin^2}$ to $C$ for any two-qubit pure states. As $E_{\sin^2}$ is a monotonically increasing function of $C \in [0, 1]$, the optimal decomposition for $E_{\sin^2}$ is identical to that for the entanglement of formation $E_{F}$. Thus, we see that Eq. 6 holds for any two-qubit mixed state. The fact that $E_{\sin^2}$ is related to $E_{F}$ via the concurrence $C$ is inevitable for two-qubit systems, as both are determined by the one independent Schmidt coefficient.

Generalized Werner states: Any state $\rho_{W}$ of a $C^d \otimes C^d$ system is called a generalized Werner state if it is invariant under $\mathbf{P}_1 : \rho \rightarrow \int dU (U \otimes U^\dagger) \rho (U^\dagger \otimes U)$, where $U$ is any element of the unitary group $U(d)$ and $dU$ is the corresponding normalized Haar measure. Such states can be expressed as a linear combination of two operators: the identity $\mathbb{1}$, and the swap $\hat{F} \equiv \sum_{ij} |ij\rangle\langle ji|$, i.e., $\rho_{W} \equiv a \mathbb{1} + b \hat{F}$, where $a$ and $b$ are real parameters related via the constraint $Tr_{W} \rho_{W} = 1$. This one-parameter family of states can be conveniently expressed in terms of the single parameter $f = Tr(\rho_{W} \hat{F})$. By employing the technique by developed by Vollbrecht and Werner [6] [as applied to $E_{F}(\rho_{W})$] to $E_{\sin^2}$, one arrives at the geometric entanglement function for Werner states:

$$E_{\sin^2}(\rho_{W}(f)) = \frac{1}{4}(1 - \sqrt{1 - f^2}) \quad \text{for} \quad f \leq 0,$$

and zero otherwise.

Isotropic states: These are states invariant under $\mathbf{P}_2 : \rho \rightarrow \int dU (U \otimes U^* \rho (U^* \otimes U)$, and can be expressed as

$$\rho_{iso}(F) \equiv \frac{1 - F}{d^2 - 1} (\mathbb{1} - |\Phi^+\rangle\langle\Phi^+|) + F|\Phi^+\rangle\langle\Phi^+|,$$

where $|\Phi^+\rangle \equiv \frac{1}{\sqrt{d}} \sum_{i=1}^{d} |ii\rangle$ and $F \in [0, 1]$. For $F \in [0, 1/d]$, this state is known to be separable [14]. By using the Vollbrecht-Werner technique and following arguments similar to those of Terhal and Vollbrecht [6], applied to $E_{F}(\rho_{iso})$, one arrives (for $F \geq 1/d$) at

$$E_{\sin^2}(\rho_{iso}(F)) = 1 - \frac{1}{d}(\sqrt{F} + \sqrt{(1-F)(d-1)})^2. \quad (12)$$

Mixtures of multipartite symmetric states: As a final example we consider mixed states of the form $(k_1 \neq k_2)$

$$\rho_{n; k_1k_2}(r) = \frac{1}{2} \left[ S(n, k_1) \right]' S(n, k_1) + (1-r) \left[ S(n, k_2) \right]' S(n, k_2).$$

From the independence of $E_{\sin^2}$ with respect to $r$, one can show that $E_{\sin^2}(\rho_{n; k_1k_2}(r))$ vs. $r$ can be constructed from the convex hull of the entanglement function of $\rho_{n; k_1k_2}(r, 0)$ vs. $r$. An example is shown in Fig. 1. If the dependence of $E_{\sin^2}$ on $r$ is already convex for the pure state, its mixed-state counterpart has precisely the same dependence. Figure 1 for which $(n, k_1, k_2) = (3, 1, 2)$, exemplifies such behavior.

Concluding remarks: We have considered a general, geometrically motivated measure of entanglement, applicable to pure and mixed quantum states involving arbitrary numbers and structures of parties. We have illustrated this measure via several examples. In bipartite settings, this approach provides an—in general, inequivalent—alternative to the entanglement of formation; it is, moreover, naturally extendable to multipartite settings.

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