Geometric measures of entanglement and the Schmidt decomposition

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Abstract
In the standard geometric approach, the entanglement of a pure state is \( \sin^2 \theta \), where \( \theta \) is the angle between the entangled state and the closest separable state of products of normalized qubit states. We consider here a generalization of this notion by considering separable states that consist of products of unnormalized states of different dimensions. The distance between the target-entangled state and the closest unnormalized product state can be interpreted as a measure of the entanglement of the target state. The components of the closest product state and its norm have an interpretation in terms of, respectively, the eigenvectors and eigenvalues of the reduced density matrices arising in the Schmidt decomposition of the state vector. For several cases where the target state has a large degree of symmetry, we solve the system of equations analytically and look specifically at the limit where the number of qubits is large.

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1. Introduction

With recognition of its role as a resource in quantum computing \cite{1}, the nature of entanglement in quantum systems is a problem of much current interest \cite{2–4}. Of particular importance is a quantitative measure of entanglement \cite{5}. Two of the more commonly used measures are the von Neumann entropy, which is based on reduced density matrices \cite{2}, and a geometric measure, which is based on the distance to the nearest product state \cite{6–10}. In this paper we...
introduce a geometric measure of entanglement based on the distance between an unnormalized product state and a target-entangled state. The norm of the closest product state can be related to both the distance and angle between the product and target states. This result motivates the interpretation of the distance to the closest product state as a measure of the entanglement of the initial state.

We begin by defining our notation. We consider a system of \( q \) qubits. The dimension of the corresponding Hilbert space is \( n = 2^q \). We will decompose the system into a set of subsystems. The subsystems are labelled as \( A, B, C, \ldots \) such that \( n = u \cdot v \cdot w \cdot \ldots \). An arbitrary set of basis states of system \( A \) is labelled \(|i⟩\), the basis states of \( B \) are \(|j⟩\), the basis states of \( C \) are \(|k⟩\), etc. Using this notation we write

\[
|A⟩ = \sum_{i=0}^{u-1} a_i|i⟩, \quad |B⟩ = \sum_{j=0}^{v-1} b_j|j⟩, \quad |C⟩ = \sum_{k=0}^{w-1} c_k|k⟩, \ldots
\]

We consider an arbitrary normalized entangled pure state and write its wavefunction as

\[
|ψ⟩ = \sum_{i=0}^{u-1} \sum_{j=0}^{v-1} \sum_{k=0}^{w-1} \cdots \chi_{ijk} \cdots |i⟩ \otimes |j⟩ \otimes |k⟩ \cdots, \quad ⟨ψ|ψ⟩ = 1.
\]

In this paper we introduce a new geometric measure of the entanglement of this state. The paper is organized as follows. In section 2 we introduce our geometric measure of entanglement. In section 3 we show that, for a given entangled state, a connection can be established between the components and norm of the closest product state, and the basis states and eigenvalues of the Schmidt decomposition of the entangled state. In section 4 we study some general symmetries of our measure. In section 5 we derive some exact solutions for cases where the target state \(|ψ⟩\) has a large degree of symmetry, and in section 6 we present our conclusions.

### 2. Optimum Euclidean distance

In this section we introduce a new geometric measure of entanglement. We look at the distance between the pure entangled state (2) and an arbitrary unnormalized product state. Extremizing this distance allows us to identify the closest product state. The distance between the state \(|ψ⟩\) and this closest product state is our geometric measure of the entanglement of \(|ψ⟩\).

We consider the product state

\[
|φ⟩ = |A⟩ \otimes |B⟩ \otimes |C⟩ \otimes \cdots = \sum_{i=0}^{u-1} a_i|i⟩ \otimes \sum_{j=0}^{v-1} b_j|j⟩ \otimes \sum_{k=0}^{w-1} c_k|k⟩ \otimes \cdots \quad (3)
\]

The state \(|φ⟩\) is not assumed to be normalized:

\[
⟨φ|φ⟩ = N_A N_B N_C \cdots; \quad N_A = ⟨A|A⟩ = \sum_{i=0}^{u-1} a_i^∗ a_i, \quad N_B = ⟨B|B⟩ = \sum_{j=0}^{v-1} b_j^∗ b_j, \ldots
\]

The distance between the states \(|ψ⟩\) and \(|φ⟩\) is

\[
D^2 = ⟨ψ − φ|ψ − φ⟩ = 1 − ⟨ψ|ψ⟩ − ⟨φ|φ⟩ + N_A N_B N_C \cdots
\]

\[
= \left( \sum_{i=0}^{u-1} \sum_{j=0}^{v-1} \sum_{k=0}^{w-1} \cdots \right) (a_i^∗ b_j^∗ c_k^* \cdots − \chi_{ijk}^* \cdots)(a_i b_j c_k \cdots − \chi_{ijk} \cdots).
\]
We extremize this distance with respect to the coordinates of $|A\rangle$, $|B\rangle$, \ldots:

$$\frac{\partial D^2}{\partial a_i} = 0 \Rightarrow a_i^* N_B N_C \ldots = \left( \sum_{i=0}^{w-1} \sum_{j=0}^{w-1} \cdots \right) b_j c_k \ldots \chi_{ijk}^* \ldots$$  

$$\frac{\partial D^2}{\partial b_j} = 0 \Rightarrow b_j^* N_A N_C \ldots = \left( \sum_{i=0}^{w-1} \sum_{j=0}^{w-1} \cdots \right) a_i c_k \ldots \chi_{ijk}^* \ldots$$  

$$\frac{\partial D^2}{\partial c_k} = 0 \Rightarrow c_k^* N_A N_B \ldots = \left( \sum_{i=0}^{w-1} \sum_{j=0}^{w-1} \cdots \right) a_i b_j \ldots \chi_{ijk}^* \ldots$$  

\[\text{(6)}\]

Rewriting equation (6), we have

$$N_A N_B N_C \ldots = \left( \sum_{i=0}^{w-1} \sum_{j=0}^{w-1} \sum_{k=0}^{w-1} \cdots \right) a_i b_j c_k \ldots \chi_{ijk}^* \ldots = \langle \psi | \phi \rangle.$$  

\[\text{(7)}\]

In exactly the same way we could extremize the distance in equation (5) with respect to the coordinates of $|A\rangle$, $|B\rangle$, \ldots and obtain $N_A N_B N_C \ldots = \langle \phi | \psi \rangle$. Substituting these results into (5) we find that at the extrema the distance between $|\psi\rangle$ and $|\phi\rangle$ is

$$D_C^2 = 1 - N_A N_B N_C \ldots = 1 - \cos^2 \theta_C,$$  

\[\text{(8)}\]

where we have defined the critical angle $\theta_C$ as the angle between $|\psi\rangle$ and $|\phi\rangle$ at the extrema

$$\cos \theta_C = \frac{\langle \psi | \phi \rangle}{\sqrt{\langle \phi | \phi \rangle \langle \psi | \psi \rangle}} \bigg|_{\text{critical}} = \sqrt{N_A N_B N_C \ldots}.$$  

\[\text{(9)}\]

In order to demonstrate the consistency of these results, we look at the Cauchy–Schwartz inequality which requires

$$\langle \phi - \psi | \phi - \psi \rangle \langle \phi | \phi \rangle \geq |\langle \phi - \psi | \phi \rangle|^2.$$  

\[\text{(10)}\]

Using (4) and (5) we have

$$D^2 \cdot (N_A N_B N_C \cdots) \geq (N_A N_B N_C \cdots) - \langle \psi | \phi \rangle^2.$$  

\[\text{(11)}\]

Using (7) and (8) we find that at the extrema,

$$1 - N_A N_B N_C \cdots \geq 0 \Rightarrow N_A N_B N_C \cdots \leq 1.$$  

\[\text{(12)}\]

This inequality guarantees that the cosine of the critical angle (equation (9)) is a real number which satisfies $1 > \cos \theta_C > -1$, and that the square of the critical distance (equation (8)) is real and positive.

We can compare the results in equations (8), (9) with those that would be obtained using a product of normalized states. We use $\langle A | A \rangle = \langle B | B \rangle = \cdots = 1$. We take the derivative of $D^2$ with respect to $a_i$ as before, but now we insert a Lagrange multiplier term of the form $\lambda \langle A | A \rangle$. This approach produces the same critical angle as before (equation (9)). The corresponding minimal distance is

$$D_N^2 = \langle \phi_N | \phi_N - \psi \rangle = D^2 + (1 - \sqrt{\langle \phi | \phi \rangle})^2 = 2(1 - \cos \theta_C),$$  

\[\text{(13)}\]

which can be compared with the result for unnormalized product states (equation (8)). A geometric representation of this comparison appears in figure 1.
3. Relationship between the distance measure and the Schmidt decomposition

The equations in (6) which determine the extremal points of the distance to the closest product state are nonlinear and must be solved numerically, except in special cases. One of the special cases for which a closed-form solution exists occurs when the \( n \)-dimensional system is decomposed into two subsystems. We consider a \( u \)-dimensional subsystem \( A \), and a \( v \)-dimensional subsystem \( B \), such that \( n = uv \). In this case equations (6) decouple to yield

\[
\begin{align*}
\alpha_i N_A N_B &= \sum_{i=0}^{u-1} \sum_{j=0}^{v-1} \chi_{ij} \chi_{ij}^* a_i, \\
\beta_j N_A N_B &= \sum_{j=0}^{v-1} \sum_{i=0}^{u-1} \chi_{ij} \chi_{ij}^* b_j.
\end{align*}
\]

(14)

Each of these equations can be solved for the product \( N_A N_B \) and give, respectively,

\[
\begin{align*}
\det \begin{vmatrix} N_A N_B \delta_{ii'} - \sum_{j=0}^{v-1} \chi_{ij} \chi_{ij}^* \end{vmatrix} &= 0, \\
\det \begin{vmatrix} N_A N_B \delta_{jj'} - \sum_{i=0}^{u-1} \chi_{ij} \chi_{ij}^* \end{vmatrix} &= 0.
\end{align*}
\]

(15)

These solutions can be related to the eigenvalues of the reduced density matrix. We consider the \( n \)-dimensional state in equation (2) and write its wavefunction and density matrix in the computational basis:

\[
|\psi\rangle = \sum_{z=0}^{n-1} \chi_z |z\rangle, \quad \rho = \sum_{z=0}^{n-1} \sum_{z'=0}^{n-1} \chi_z \chi_{z'}^* |z\rangle \langle z'|.
\]

(16)

Decomposing the system into a \( u \)-dimensional subsystem \( A \) and a \( v \)-dimensional subsystem \( B \), we obtain

\[
|\psi\rangle = \sum_{i=0}^{u-1} \sum_{j=0}^{v-1} \chi_{ij} |i\rangle \langle j|, \quad \rho = \sum_{i=0}^{u-1} \sum_{i'=0}^{u-1} \sum_{j=0}^{v-1} \sum_{j'=0}^{v-1} \chi_{ij} \chi_{i'j'}^* |i\rangle \langle i'| \otimes |j\rangle \langle j'|.
\]

(17)
Next we calculate the reduced density matrices. The reduced density matrix \( \rho_A \) is obtained by tracing over the subsystem \( B \), and the reduced density matrix \( \rho_B \) is obtained by tracing over the subsystem \( A \). The definitions are

\[
\begin{align*}
\text{Tr}_A(\rho) &= \sum_{t=0}^{u-1} (|t\rangle \otimes \mathbb{1}_B) \rho (|t\rangle \otimes \mathbb{1}_B), \\
\text{Tr}_B(\rho) &= \sum_{t=0}^{v-1} (\mathbb{1}_A \otimes |t\rangle) \rho (\mathbb{1}_A \otimes |t\rangle),
\end{align*}
\]

where \( \mathbb{1}_A \) and \( \mathbb{1}_B \) are the identity matrices in the subspaces of \( A \) and \( B \), respectively. We obtain

\[
\rho_A = \text{Tr}_B(\rho) = \sum_{t=0}^{v-1} \sum_{i'=0}^{u-1} \sum_{j'=0}^{v-1} \chi_{ij} \chi_{i'j'}^* |t\rangle |j\rangle |i\rangle |i'\rangle = \sum_{j=0}^{v-1} \sum_{i'=0}^{u-1} \chi_{ij} \chi_{i'j'}^* |t\rangle |j\rangle |i\rangle |i'\rangle,
\]

or, in terms of components,

\[
(\rho_A)_{ii'} = \sum_{j=0}^{v-1} \chi_{ij} \chi_{i'j'}^*.
\]

Similarly, the reduced density matrix \( \rho_B = \text{Tr}_A(\rho) \) is obtained by tracing over the subsystem \( A \) and can be written as

\[
(\rho_B)_{jj'} = \sum_{i=0}^{u-1} \chi_{ij} \chi_{ij'}^*.
\]

Using equations (20) and (21) we can rewrite the extremal conditions of equations (14) in the form

\[
\sum_{i=0}^{u-1} (\rho_A)_{ii'} a_{i'} = N_A N_B a_i, \quad \sum_{j=0}^{v-1} (\rho_B)_{jj'} b_{j'} = N_A N_B b_j.
\]

Equation (22) shows that \( N_A N_B \) are the eigenvalues corresponding to the eigenvectors \( a_i \) and \( b_j \) of the reduced density matrices \( \rho_A \) and \( \rho_B \).

This result can be interpreted in terms of the Schmidt decomposition as follows [1, 11–15]. Let us write the extrema conditions of equation (6) as

\[
\begin{align*}
\hat{a}_i \sigma &= \sum_{j=0}^{v-1} \chi_{ij} \hat{b}_j^* \\
\hat{b}_j \sigma &= \sum_{i=0}^{u-1} \chi_{ij} \hat{a}_i^*,
\end{align*}
\]

where \( \hat{a}_i = a_i / \sqrt{N_A} \) and \( \hat{b}_j = b_j / \sqrt{N_B} \) are, respectively, the left-singular and right-singular vectors corresponding to the singular values \( \sigma = \sqrt{N_A N_B} \) of the matrix \( \chi \). The singular value decomposition of the matrix \( \chi \) can then be written as

\[
\chi = A \Sigma B^\dagger,
\]

where the columns of the (unitary) matrices \( A \) and \( B \) are, respectively, the vectors \( \hat{a}_i \) and \( \hat{b}_j \), and \( \Sigma \) is a diagonal matrix whose elements are the singular values \( \sigma \). This can be used to rewrite the state \(|\psi\rangle\) in (17) in terms of the Schmidt decomposition involving a single summation:

\[
|\psi\rangle = \sum_{k=0}^{\min(u-1,v-1)} \sqrt{p_k} |\alpha_k\rangle \otimes |\beta_k\rangle,
\]
where the Schmidt coefficients \( p_k \), which are identified with the singular values \( \sigma \), satisfy \( \sum_k p_k = 1 \), and the states \( |\alpha_k\rangle \) and \( |\beta_k\rangle \) are identified with, respectively, the left-singular and right-singular vectors \( \tilde{a}_i \) and \( \tilde{b}_j \). Calculating the corresponding reduced density matrices using (18), we obtain

\[
\rho_A = \text{Tr}_B(\rho) = \sum_k p_k |\alpha_k\rangle \langle \alpha_k|, \quad \rho_B = \text{Tr}_A(\rho) = \sum_k p_k |\beta_k\rangle \langle \beta_k|,
\]

from which one can see that \( |\alpha_k\rangle \) are the eigenvectors of \( \rho_A = \text{Tr}_B(\rho) \) and \( |\beta_k\rangle \) are the eigenvectors of \( \rho_B = \text{Tr}_A(\rho) \) with corresponding eigenvalues \( p_k \).

We remark that the Schmidt decomposition gives rise to several other measurements of entanglement. The reduced density matrices \( \rho_A \) and \( \rho_B \) in (26) have the same non-zero eigenvalues and, for a product state, only one non-zero eigenvalue is present. As a result, for a non-product state, the eigenvalues of the reduced density matrix can be used to quantify the degree of entanglement. One commonly used measure of entanglement is the von Neumann entropy:

\[
S = -\text{Tr}(\rho_A \ln \rho_A) = -\text{Tr}(\rho_B \ln \rho_B) = -\sum_k p_k \log_2 p_k.
\]

It is interesting to consider the particular case that the \( n \)-dimensional space is split into the product of a single qubit space and another space of dimension \( u = n/2 \). In this case, one of the equations in (15) will become a quadratic equation for the product \( N_A N_B \) with solutions

\[
N_A N_B \equiv \mu_{\pm} = \frac{1}{2} [1 \pm \sqrt{1 - 4C}] , \quad C = \sum_{j=1}^{u-1} \sum_{k=0}^{j-1} |\chi_{0j} \chi_{1k} - \chi_{1j} \chi_{0k}|^2.
\]

The Schmidt decomposition (equation (25)) becomes

\[
|\psi\rangle = \sqrt{\mu_+} |\alpha_+\rangle \otimes |\beta_+\rangle + \sqrt{\mu_-} |\alpha_-\rangle \otimes |\beta_-\rangle.
\]

Using equation (9) we can relate the eigenvalues \( N_A N_B = \mu_{\pm} \) to the cosine of the angle between \( |\psi\rangle \) and the closest product state \( |\phi\rangle \). Since \( \mu_+ \) is the larger of the two eigenvalues we write \( \cos \theta_{\max} = \mu_+ \) and equation (29) becomes

\[
|\psi\rangle = \cos \theta_{\max} |\alpha_+\rangle \otimes |\beta_+\rangle + \sin \theta_{\max} |\alpha_-\rangle \otimes |\beta_-\rangle.
\]

If \( |\psi\rangle \) was a product state, the reduced density matrix would have only one non-zero eigenvalue and we would have \( \mu_- = \sin^2 \theta_{\max} = 0 \). This result is consistent with our geometric approach: from equation (8), \( \sin^2 \theta_{\max} = 0 \) corresponds to a zero minimal distance between the state \( |\psi\rangle \) and the nearest product state, which means that \( |\psi\rangle \) is itself a product state.

The Schmidt decomposition can also be applied to multipartite pure states [14]. One starts with a state \( |\psi\rangle \) and decomposes it into two subsystems: a single qubit system \( A \), and a subsystem \( (BC \ldots Z) \) containing all other qubits. Using a Schmidt decomposition, we can write

\[
|\psi\rangle = \sum_{l_A} \sqrt{p_{l_A}^A} |\psi_{l_A}^A\rangle \otimes |\psi_{l_A}^{BC\ldots Z}\rangle.
\]

One then decomposes \( |\psi_{l_A}^{BC\ldots Z}\rangle \) into two subsystems: another single qubit system \( B \), and a subsystem \( (CD \ldots Z) \) containing all other qubits. Using a Schmidt decomposition we can write

\[
|\psi_{l_A}^{BC\ldots Z}\rangle = \sum_{l_B} \sqrt{p_{l_B}^B} |\psi_{l_B}^B\rangle \otimes |\psi_{l_B}^{CD\ldots Z}\rangle.
\]
This process is continued until the last two qubit spaces \( Y \) and \( Z \) are reached, with the result

\[
|\psi\rangle = \sum_{i_a \ldots j_z} \sqrt{p_{i_a}^{A} p_{i_b}^{B} \ldots p_{i_v}^{Y} p_{i_u}^{Z}} |\psi_{i_a}^{A}\rangle \otimes |\psi_{i_b}^{B}\rangle \otimes \cdots \otimes |\psi_{i_v}^{Y}\rangle \otimes |\psi_{i_u}^{Z}\rangle.
\]  

(33)

Now we consider the geometric interpretation of this result. Consider the distance between \( |\psi\rangle \) and a state \( |\phi^{A;BC\ldots Z}\rangle = |\phi^{A}\rangle \otimes |\phi^{BC\ldots Z}\rangle \), where \( |\phi^{A}\rangle \) is a single qubit state and \( |\phi^{BC\ldots Z}\rangle \) is the state of the remaining qubits. This distance is

\[
D_{A;BC\ldots Z}^2 = \langle |\psi\rangle - [\phi^{A} \otimes \phi^{BC\ldots Z}] |\psi\rangle - [\phi^{A} \otimes \phi^{BC\ldots Z}] \rangle.
\]  

(34)

Finding the extremal points of this distance will result in a system of (linear) equations, as in equation (15), which determine the components of the state \( |\phi^{A;BC\ldots Z}\rangle \). There is a direct correspondence between the coefficients of the closest product state and the basis states of the Schmidt decomposition (equation (31)), and the norm of the closest product state is related to the corresponding Schmidt coefficients.

We can then consider the distance between the state \( |\phi^{BC\ldots Z}\rangle \) and a state \( |\phi^{B;CD\ldots Z}\rangle = |\phi^{B}\rangle \otimes |\phi^{CD\ldots Z}\rangle \):

\[
D_{B;CD\ldots Z}^2 = \langle |\phi^{BC\ldots Z}\rangle - [\phi^{B} \otimes \phi^{CD\ldots Z}] |\phi^{BC\ldots Z}\rangle - [\phi^{B} \otimes \phi^{CD\ldots Z}] \rangle,
\]  

(35)

where \( |\phi^{B}\rangle \) is a single qubit state and \( |\phi^{CD\ldots Z}\rangle \) is the state of the remaining qubits. Extremizing this distance will again result in a system of linear equations determining the components of the state \( |\phi^{B;CD\ldots Z}\rangle \). Once again, there is a direct correspondence between the coefficients of the closest product state and the basis states of the Schmidt decomposition (equation (32)), and the norm of the closest product state is related to the corresponding Schmidt coefficients.

This process may be continued until the last two qubit states \( |\phi^{Y}\rangle \) and \( |\phi^{Z}\rangle \) are reached.

In analogy with equation (9), we can define the cosine of the critical angle \( \theta_{C} \):

\[
\cos \theta_{C} = \frac{\langle \psi | \phi \rangle}{\sqrt{\langle \phi | \phi \rangle \langle \psi | \psi \rangle}} \bigg|_{\text{critical}} \ldots |\phi\rangle = |\phi^{A}\rangle \otimes |\phi^{B}\rangle \otimes \cdots |\phi^{Z}\rangle.
\]  

(36)

The quantity \( \sin^2 \theta_{C} = 1 - \cos^2 \theta_{C} \) is a measure of the entanglement of the original multipartite state.

The advantage of this procedure is that it involves solving a series of linear equations, as compared to the approach of section 2 which produces the nonlinear equations of equation (6). The disadvantage is that the result depends on the order that the series of decompositions are made: the sequence \( A\ B\ C \ldots Y\ Z \) described above will differ from the sequence \( B\ C \ldots Z\ A \). In [14], the entanglement is given by the minimal value obtained by looking at all permutations of the possible orders of the decompositions.

4. Symmetries

The equation that gives the distance between the target-entangled state and the nearest product state (equation (8)) is invariant under certain transformations of the parameters \( \{a_{i}, b_{i}, \ldots \} \). In order to see these symmetries explicitly, we can reparameterize each set of coefficients. For the coefficients \( a_{i} \), we write

\[
a_{i} = A_{i} e^{\omega_{i}}.
\]  

(37)
with similar equations for the coefficients \(b_i, c_i, \ldots\). Using generalized spherical coordinates in \(n\) dimensions we can rewrite the set of real variables \(A_i\) in terms of magnitude \(A\) and \((n-1)\) angles \(\theta_i\):

\[
\begin{bmatrix}
A_1 \\
A_2 \\
A_3 \\
\vdots \\
A_k \\
\vdots \\
A_{n-1} \\
A_n
\end{bmatrix}
= A
\begin{bmatrix}
\cos \theta_1 \\
\sin \theta_1 \cos \theta_2 \\
\sin \theta_1 \sin \theta_2 \cos \theta_3 \\
\vdots \\
(\Pi_{i=1}^{k-1} \sin \theta_i) \cos \theta_k \\
\vdots \\
\sin \theta_1 \cdots \sin \theta_{n-2} \cos \theta_{n-1} \\
\sin \theta_1 \cdots \sin \theta_{n-2} \sin \theta_{n-1}
\end{bmatrix}
\equiv Af_i(\theta^a).
\tag{38}
\]

We can also parameterize the phase angles \(\alpha_i^a\) as

\[
e^{i\alpha_i^a}
\begin{bmatrix}
e^{i\alpha_1} \\
e^{i\alpha_2} \\
\vdots \\
e^{i\alpha_n}
\end{bmatrix}
= e^{i\alpha_1}
\begin{bmatrix}
e^{i(\alpha_2-\alpha_1)} \\
\vdots \\
e^{i(\alpha_n-\alpha_1)}
\end{bmatrix}
\equiv e^{i\alpha_1}
\begin{bmatrix}
e^{i\beta_2} \\
\vdots \\
e^{i\beta_n}
\end{bmatrix}
\equiv e^{i\alpha_1} e^{i\beta_i}.
\tag{39}
\]

where \(\beta_1 \equiv 0\). Using this notation we write

\[
a_i = A e^{i\alpha_i} f_i(\theta^a) e^{i\phi_i} \\
b_i = B e^{i\alpha_i} f_i(\theta^b) e^{i\phi_i}
\]

\[
\vdots
\]

We can use this parameterization to rewrite the distance function (8). We make the definitions

\[
\langle \phi | \phi \rangle \equiv N^2, \\
|\phi\rangle \equiv N|\hat{\phi}\rangle, \langle \hat{\phi} | \psi \rangle = 1.
\tag{41}
\]

Note that the first line in (41) gives

\[
\langle \phi | \phi \rangle = A^2 B^2 C^2 \cdots = N_A N_B N_C \cdots = N^2.
\tag{42}
\]

Using these definitions the distance in equation (5) becomes

\[
D^2 = N^2 - N[\langle \psi | \hat{\phi} \rangle + \langle \hat{\phi} | \psi \rangle] + 1.
\tag{43}
\]

Extremizing we obtain

\[
\frac{\partial D^2}{\partial N} = 0 \Rightarrow 2N - [\langle \psi | \hat{\phi} \rangle + \langle \hat{\phi} | \psi \rangle] = 0,
\]

\[
\Rightarrow N = \text{Re}[\langle \psi | \hat{\phi} \rangle],
\tag{44}
\]

which means that at the extrema,

\[
D^2_C = N^2 - N(2N) + 1 = 1 - N^2.
\tag{45}
\]

We note that equations (42) and (45) are consistent with (8).

To make this result more clear, we can look explicitly at the dependence of the distance function on the overall phase of the coefficients of the product state. We define the overall
phase angle $\delta = \alpha^a_1 + \alpha^b_1 + \cdots$ and obtain
\[
\langle \phi | \psi \rangle = N \langle \hat{\phi} | \hat{\psi} \rangle = N e^{i \delta} \sum_{i=1}^{u} \sum_{j=1}^{v} \sum_{k=1}^{\cdots} f_i(\theta^a) e^{-i \theta^b_j} f_j(\theta^b) e^{-i \theta^a_k} \chi_{ij} \cdots .
\]
(46)

which gives
\[
\frac{\partial}{\partial \delta} \langle \psi | \phi \rangle = N \frac{\partial}{\partial \delta} \langle \hat{\psi} | \hat{\phi} \rangle = iN \langle \psi | \hat{\phi} \rangle,
\]
\[
\frac{\partial}{\partial \delta} \langle \phi | \psi \rangle = N \frac{\partial}{\partial \delta} \langle \hat{\phi} | \hat{\psi} \rangle = -iN \langle \psi | \hat{\phi} \rangle.
\]
(47)

From equation (43) we have
\[
\frac{\partial}{\partial \delta} \frac{D^2}{\partial \delta^2} = -N \frac{\partial}{\partial \delta} \left( \langle \psi | \hat{\phi} \rangle + \langle \hat{\phi} | \psi \rangle \right) = -iN \left[ \langle \psi | \hat{\phi} \rangle - \langle \hat{\phi} | \psi \rangle \right] = 2N \text{Im} \langle \psi | \hat{\phi} \rangle.
\]
(48)

which means that at the extrema, $\text{Im} \langle \psi | \hat{\phi} \rangle = 0$. From equation (44) we obtain that at the extrema,
\[
N = \langle \psi | \hat{\phi} \rangle = \langle \hat{\phi} | \psi \rangle.
\]
(49)

This means that the critical angle defined by
\[
\cos \theta_C = \left. \frac{\langle \psi | \hat{\phi} \rangle}{\sqrt{\langle \phi | \phi \rangle \langle \psi | \psi \rangle}} \right|_{\text{critical}} = N
\]
(50)
is the same critical angle as in equation (9).

5. Exact solutions

In this section we look at some states with a large degree of symmetry for which equations (6) can be solved exactly. We consider a system of $q$ qubits and divide the Hilbert space of dimension $n = 2^q$ into $q$ spaces, each of dimension 2. Using the notation of section 1, we have $n = u \cdot v \cdot w \cdots$ with $u = v = w = \cdots = 2$. The basis states in each single qubit system are
\[
|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.
\]
(51)
The product state in equation (3) becomes
\[
|\phi\rangle = (a_0|0\rangle + a_1|1\rangle)(b_0|0\rangle + b_1|1\rangle)(c_0|0\rangle + c_1|1\rangle) \cdots \\
= (a_0b_0c_0 \cdots |0, 0, 0, \cdots \rangle + (a_0b_0c_1 \cdots |0, 0, 1, \cdots \rangle + (a_0b_1c_0 \cdots |0, 1, 0, \cdots \rangle + (a_0b_1c_1 \cdots |0, 1, 1, \cdots \rangle + \cdots .
\]
(52)

For ease of calculation we will be considering initial target states $|\psi\rangle$ with a high degree of symmetry. It therefore makes sense to look for solutions that also have a high degree of symmetry. In particular, cases 1, 2 and 4 below start with $|\psi\rangle$ that do not distinguish between individual qubits. Although case 3 has less symmetry, we will nonetheless in all cases look for nearest product states that are invariant under the interchange of any two qubits, so that
\[
a_0 = b_0 = \cdots = a_0, \\
a_1 = b_1 = \cdots = a_1,
\]
(53)
which means $N_A = N_B = \cdots = N$. 

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As we will see, such solutions do exist for all cases considered. However, since we cannot determine whether the solutions that we find represent global minima of the distance function, it is possible that the true minimum breaks the symmetry of the target entangled state. That is, the closest product state may have less symmetry than the entangled state. This is a very interesting question that will be pursued elsewhere.

5.1. Analytic expressions

5.1.1. Case 1.

Consider
\[ |\psi\rangle = \sqrt{p} |00\ldots0\rangle + \sqrt{1-p} |11\ldots1\rangle. \]
(54)

The only two non-zero components of \(\psi_{ijk\ldots}\) are
\[ \psi_{00\ldots0} = \sqrt{p}, \quad \psi_{11\ldots1} = \sqrt{1-p}, \]
and equation (6) becomes
\[ a_0 N_B N_C \cdots = \sqrt{p} b_0 c_0 \cdots \]
\[ a_1 N_B N_C \cdots = \sqrt{1-p} b_1 c_1 \cdots. \]
(56)

Using equation (53), equation (56) becomes
\[ \alpha_0 N^q - 1 = \sqrt{p} \alpha_0^q - 1, \quad \alpha_1 N^q - 1 = \sqrt{1-p} \alpha_1^q - 1. \]
(57)

Solving this set of equations, we obtain
\[ \alpha_2 = \frac{N^{2(q-1)/(q-2)}}{(1-p)^{1/(q-2)}}, \quad \alpha_0 = \frac{(1-p)^{1/(q-2)}}{p^{1/(q-2)}} - \alpha_2, \]
(58)

which gives
\[ N = \alpha_0^2 + \alpha_2^2 = \frac{N^{2(q-1)/(q-2)}}{(1-p)^{1/(q-2)}} \left[ 1 + \frac{(1-p)^{1/(q-2)}}{p^{1/(q-2)}} \right]. \]
(59)

Rearranging we obtain
\[ N^q = \frac{p(1-p)}{ \left[ p^{1/(q-2)} + (1-p)^{1/(q-2)} \right]^{q-2}}. \]
(60)

We can look at the large \(q\) limit. Defining \(A = [p^{1/(q-2)} + (1-p)^{1/(q-2)}]^{q-2}\) we have
\[ \log A = (q-2) \log(p^{1/(q-2)}) + (q-2) \log \left[ 1 + \left( \frac{1-p}{p} \right)^{1/(q-2)} \right], \]
\[ \approx \log p + (q-2) \log 2 + \frac{1}{2} \log \left( \frac{1-p}{p} \right), \]
\[ = (q-2) \log 2 + \frac{1}{2} \log[p(1-p)], \]
\[ = \log[2^{q-2} \sqrt{p(1-p)}], \]
(61)

which gives
\[ N^q \approx \frac{\sqrt{p(1-p)}}{2^{q-2}}. \]
(62)

Figure 2 shows the behaviour of \(D^2\) for several values of \(p\).

Note that in the limit of large \(q\), \(D^2 = 1 - N^q \to 1\) which suggests that the entanglement goes to a maximum in this limit. However, since we do not know whether this is a global minimum, it is in principle possible that the state is moving arbitrarily close to different product states.
5.1.2. Case 2. Consider

$$|\psi\rangle = [|10\ldots0\rangle + |01\ldots0\rangle + \cdots + |00\ldots1\rangle]/\sqrt{q}. \quad (63)$$

The only non-zero coefficients $\psi_{ijk\ldots}$ are

$$\psi_{100\ldots0} = \psi_{010\ldots0} = \psi_{001\ldots0} = \cdots = \psi_{000\ldots1} = \frac{1}{\sqrt{q}}, \quad (64)$$

and equation (6) becomes

$$a_0 N_B N_C \cdots = \frac{1}{\sqrt{q}} [b_1 c_0 d_1 d_0 \cdots + b_0 c_1 d_0 \cdots + b_0 c_0 d_1 \cdots + \cdots] \quad (65)$$

Using equation (53), equation (65) becomes

$$a_0 N q^{-1} = \psi a_1 q^{-2} (q - 1), \quad a_1 N q^{-1} = \psi a_0 q^{-1}. \quad (66)$$

Solving the set of equations in (66) we obtain

$$a_1 q^{-2} = \frac{\sqrt{q} N q^{-1}}{(q - 1)(q - 1)/2}, \quad a_0^2 = \alpha_1^2 (q - 1), \quad (67)$$

which gives

$$N = \alpha_0^2 + \alpha_1^2 = \frac{N^{2(q-1)/(q-2)}}{(1 - \frac{1}{q})^{(q-1)/(q-2)}}. \quad (68)$$

Rearranging we obtain

$$N q = \left(1 - \frac{1}{q}\right)^{q-1}. \quad (69)$$

A plot of $D^2$ is given in figure 3.
This is an interesting case, because it can be shown that in the limit \( q \to \infty \), \( N^q \to e^{-1} = 0.37 \), so that \( D^2 \to 0.63 \). Normalization of the target state therefore implies that in this limit it must be the linear combination of our solution product state and at least one other product state. Hence one can conclude that the target state is entangled in the large \( q \) limit.\(^5\)

5.1.3. Case 3. Consider

\[ |\psi\rangle = [|1100\cdots0\rangle + |0110\cdots0\rangle + |0011\cdots0\rangle + \cdots + |00011\cdots0\rangle + |10\cdots01\rangle] / \sqrt{q}. \]

(70)

The only non-zero coefficients \( \psi_{ijk\cdots} \) are

\[ \psi_{1100\cdots0} = \psi_{0110\cdots0} = \psi_{0011\cdots0} = \cdots = \psi_{00011\cdots0} = \psi_{10000\cdots1} = 1 / \sqrt{q}. \]

(71)

Using equation (53), equation (6) gives

\[ N^{q-1} = 2\alpha_1^{q-2} \sqrt{q}, \quad N^{q-1} = \sqrt{q}\alpha_0^2 \alpha_1^{q-4} - \frac{2}{\sqrt{q}} \alpha_0^2 \alpha_1^{q-4}. \]

(72)

Solving the equations in (72) we obtain

\[ \frac{\alpha_0}{\alpha_1} = \frac{\sqrt{2}}{\sqrt{q-2}}, \quad \alpha_1 = \frac{1}{2^{q-2} - q^{q-2}} N^{(q-1)/(q-2)}, \]

(73)

which gives

\[ N = \alpha_0^2 + \alpha_1^2 = \frac{1}{q-2} 2^{1/(2(q-1))} q^{1+1/(q-2)} N^{2(q-1)/(q-2)}. \]

(74)

\(^5\) There is perhaps a small loophole to this argument. It is of course possible to take specific linear combinations of the product state that again yield product states (e.g. \( \frac{1}{\sqrt{2}} (|00\rangle + |01\rangle + |10\rangle + |11\rangle) = \frac{1}{\sqrt{2}} (|00\rangle + |11\rangle) \frac{1}{\sqrt{2}} (|01\rangle + |10\rangle) \)). Under the present circumstances, this seems unlikely.
Rearranging we extract
\[ N^q = 4(q - 2)^{q-2}q^{1-q}. \] (75)

A plot of \( D^2 \) is also given in figure 3.

Considering the \( q \to \infty \) limit, we find
\[ N^q \to \frac{4e^{-1}}{q} \to 0; \] (76)
so in this limit, the distance between the target state and solution state is maximal.

It is interesting to note that this target state is not invariant under arbitrary interchange of qubits. It is only invariant under cyclic permutation of the qubits. It is therefore not completely obvious that a completely symmetric product state would be a local minimum of the geometric distance. Moreover, it would not be surprising in this case if this solution turned out not to be the global minimum.

5.1.4. Case 4. Consider the case where \( |\psi\rangle \) has \( q \) qubits consisting of all possible combinations of \( p \) entries of ’1’ and \( q - p \) entries of ’0’. The normalization is
\[ \psi^{-1} = \sqrt{\frac{q}{p}} = \sqrt{\frac{q!}{p!(q-p)!}}. \] (77)

Using equation (53), equation (6) becomes
\[
\begin{align*}
\alpha_0 N^{q-1} &= \psi_0 \alpha_1^p \alpha_0^{q-p-1} \left( \frac{q-1}{p} \right), \\
\alpha_1 N^{q-1} &= \psi_1 \alpha_0^{p-1} \left( \frac{q-1}{p-1} \right).
\end{align*}
\] (78)

Solving the set of equations in (78) we obtain
\[ \alpha_1^{q-2} = \frac{N^{q-1}}{\psi \left( \frac{q}{p} - 1 \right)^{(q-p)/2} \left( \frac{q-1}{p-1} \right)}, \quad \alpha_0^2 = \alpha_1^2 \left( \frac{q}{p} - 1 \right). \] (79)

which gives
\[ N = \alpha_0^2 + \alpha_1^2 = \left( \frac{q}{p} \right) \frac{(p-1)/(q-2)}{(1 - \frac{p}{q})^{q-p}/(q-2) \left( \frac{q-1}{p-1} \right)^{1/(q-2)}}. \] (80)

Rearranging we obtain
\[ N^q = \left( \frac{p}{q} \right)^{q-p-1} \left( 1 - \frac{p}{q} \right)^{q-p} \left( \frac{q-1}{p-1} \right). \] (81)

In the limit \( q \gg p \), we can approximate
\[
\begin{align*}
\left( \frac{q}{p} - 1 \right) &= \frac{(q-1)!}{(p-1)!(q-p)!} \approx \frac{1}{(p-1)!} q^{p-1} + \mathcal{O} \left( q^{p-2} \right), \\
\left( 1 - \frac{p}{q} \right)^{q-p} &\approx \exp(-p),
\end{align*}
\] (82)

which leads to
\[ N^q \approx \frac{p^{p-1} \exp(-p)}{(p-1)!} + \mathcal{O} \left( \frac{1}{q} \right). \] (83)
The above gives a finite answer between 0 and 1 for all finite $p$, but in the limit that $p \to \infty$, we find that

$$N^q \to \frac{1}{\sqrt{2\pi p}} \to 0.$$ (84)

A plot of $D^2$ for various values of $p$ is given in figure 4.

5.2. Graphical results

We show below a graph of our results for the entanglement measure as a function of the number of qubits for the four cases solved in this section. The range of $q$ in all cases is kept relatively small so that the structure near $q = 0$ can be discerned. We know the asymptotic behaviour in each case, and it is clear that the asymptotic values are approached monotonically. This has been verified numerically.

6. Conclusions

We have considered a generalization of the usual geometric measure of entanglement of pure states using the distance to the nearest unnormalized product state. This definition does not lead to any computational advantages, since the set of equations that determine the measure are still nonlinear in general. However, our definition does provide an interpretation of the standard entanglement measure as the distance to the closest product state. We have also found a relationship between the norm and components of the closest separable state, and the coefficients and basis states of the Schmidt decomposition of the state $|\psi\rangle$.

The question of whether our geometrical definition of entanglement has an operational interpretation is both important and non-trivial. For the bipartite case the relationship between geometrical definitions and other measures is fairly well understood in general (see for example [16]). As explained in section 3, there is a direct connection between our specific geometrical definition, and the von Neumann entropy (cf equation (27)). Thus, for the bipartite case,
operational interpretations for the standard definitions can in all likelihood be carried over to the geometrical ones. Beyond the bipartite case, entanglement is not universally understood. We cannot yet connect our geometric measure to an operational interpretation for a multipartite system. This is currently under investigation.

For several cases where the target state has a large degree of symmetry, we have solved the system of nonlinear equations analytically, and looked specifically at the limit where the number of qubits is large. These results indicate that our new definition of entanglement, while similar to other definitions that can be found in the literature, is worthy of further study.

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