Characterization of separability and entanglement in \((2 \times D)\)- and \((3 \times D)\)-dimensional systems by single-qubit and single-qutrit unitary transformations

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We investigate the geometric characterization of pure state bipartite entanglement of \((2 \times D)\)- and \((3 \times D)\)-dimensional composite quantum systems. To this aim, we analyze the relationship between states and their images under the action of particular classes of local unitary operations. We find that invariance of states under the action of single-qubit and single-qutrit transformations is a necessary and sufficient condition for separability. We demonstrate that in the \((2 \times D)\)-dimensional case the von Neumann entropy of entanglement is a monotonic function of the minimum squared Euclidean distance between states and their images over the set of single qubit unitary transformations. Moreover, both in the \((2 \times D)\)- and in the \((3 \times D)\)-dimensional cases the minimum squared Euclidean distance exactly coincides with the linear entropy (and thus as well with the tangle measure of entanglement in the \((2 \times D)\)-dimensional case). These results provide a geometric characterization of entanglement measures originally established in informational frameworks. Consequences and applications of the formalism to quantum critical phenomena in spin systems are discussed.

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I. INTRODUCTION

The theory of pure state bipartite entanglement, a trait of quantum mechanics first discovered more than half a century ago \(^\text{i}\), is by now well understood in terms of the entropic content, as first lucidly pointed out by Schrödinger \(^\text{ii}\), of the reduced states of a given bipartite quantum system \(^\text{iii}\). \(^\text{iv}\). \(^\text{v}\). \(^\text{vi}\). General inseparability criteria are straightforwardly defined for pure states of composite systems in terms of the factorization of a given state as a tensor product involving the pure states of each subsystem \(^\text{vii}\). \(^\text{viii}\). Besides the direct quantification via the von Neumann entropy of the reduced states, and the extension to mixed states via convex roof constructions \(^\text{ix}\). \(^\text{x}\). \(^\text{xi}\), it is possible to introduce geometric quantifications of entanglement in terms of relative entropies \(^\text{xii}\). \(^\text{xiii}\). \(^\text{xiv}\) or Hilbert space distances defined according to different norms \(^\text{xv}\). \(^\text{xvi}\). \(^\text{xvii}\).

An interesting point worth closer investigation is the nature of the possible relations between entropic and geometric measures of entanglement and, in parallel, the amount of information on the global nature of pure states of a composite quantum systems that can be gained by looking at how states transform under local operations that, by definition, do not change the content of entanglement (local unitaries). In fact, besides playing a central role in quantum computation and quantum information processing, single-subsystem operations provide global informations on the state of the system. They find a natural motivation in the operational approach to the study of physical systems: Looking at the response to a given action is a basic tool to investigate the nature of physical properties.

In the present work we address these questions in the case of \((2 \times D)\)-dimensional and \((3 \times D)\)-dimensional bipartite systems. We investigate the response of pure states to a particular class of local unitaries performed on the two-dimensional subsystem (single-qubit unitary operations) in the \((2 \times D)\)-dimensional case, and on the three-dimensional subsystem in the \((3 \times D)\)-dimensional case (single-qutrit unitary operations). The specific class of single-qubit unitary operations that we consider is the one formed by all the unitary, Hermitian, and traceless single-qubit transformations. The analogous class of single-qutrit unitary operations is the one formed by all the unitary exponentiations of single-qutrit transformations that are Hermitian, traceless, and with non degenerate spectrum. This analysis yields that a necessary and sufficient condition for the separability of pure states is the existence of at least one element of these classes that leaves the state unchanged. In fact, this element turns out to be unique up to a parity flip. Introducing the standard Euclidean distance between a state and its image under a transformation, we find that in the \((2 \times D)\)-dimensional case the entropy of entanglement is a monotonic function of the minimum squared distance and that the latter, both in the \((2 \times D)\)- and \((3 \times D)\)-dimensional cases, coincides exactly with the linear entropy (or equivalently, in the \((2 \times D)\)-dimensional case, with entanglement monotones such as the squared concurrence and the tangle). These results provide a geometric-operational characterization of entropic measures and entanglement

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quantifications that were originally formulated in terms of informational concepts.

The paper is organized as follows: In Section II we introduce the set of single-qubit unitary operations and analyze the different transformations that they induce on the pure states of a $(2 \times D)$-dimensional bipartite quantum system. We find that pure state inseparability, or entanglement qualification, can be completely characterized according to the different ways in which pure states are transformed by single-qubit local unitaries. Concerning the quantification of pure state entanglement, in Section III we show that the von Neumann entropy of entanglement coincides with the linear entropy. We will find that such transformations allow as well to recast the separability properties of all pure states of the bipartite system $A|B$.

Proceeding in steps, let us first consider the situation in which the state $|\Psi\rangle$ is completely factorized with respect to the bipartition $A|B$:

$$|\Psi\rangle = |\Psi_F\rangle = |\Phi_A\rangle \otimes |\Xi_B\rangle,$$  \hspace{1cm} (1)

where $|\Phi_A\rangle \in \mathcal{H}_A$ and $|\Xi_B\rangle \in \mathcal{H}_B$. Because subsystem $A$ is a qubit, one can always write the projection operator $P^A_\phi$ on the state $|\Phi_A\rangle$ as:

$$P^A_\phi \equiv |\Phi_A\rangle\langle\Phi_A| = \frac{1}{2}(1_A + \bar{\sigma}_A),$$  \hspace{1cm} (2)

where $1_A$ is the identity operator acting on $\mathcal{H}_A$ and $\bar{\sigma}_A$, acting on the same Hilbert space, is a Hermitian, unitary, and traceless operator such that $\bar{\sigma}_A|\Phi_A\rangle = |\Phi_A\rangle$, and $\bar{\sigma}_A|\Phi_A\rangle = -|\Phi_A\rangle$, where $|\Phi_A\rangle$ is the vector orthogonal to $|\Phi_A\rangle$. The operator $\bar{\sigma}_A$ is uniquely defined once the state $|\Phi_A\rangle$ is assigned; equivalently, the latter can always be defined as the unique right eigenvector of the former with unit eigenvalue.

Let us now introduce the set of single-qubit unitary operations $U_{(A|B)}$ (SQUOs), defined as those unitary transformations on $\mathcal{H}_A \otimes \mathcal{H}_B$ that act separately as the identity $1_B$ on $\mathcal{H}_B$ and nontrivially on $\mathcal{H}_A$ in the form

$$U_{(A|B)} = \mathcal{O}_A \otimes 1_B,$$  \hspace{1cm} (3)

where the operator $\mathcal{O}_A$ acting on $\mathcal{H}_A$ is such that $\mathcal{O}_A = \mathcal{O}_A^\dagger$, $\mathcal{O}_A^2 = 1_A$, $\text{Tr}\mathcal{O}_A = 0$ (Hermitian, unitary, and traceless). If we choose $\mathcal{O}_A = \bar{\sigma}_A$, then, from Eqs. 2, 3, and 1 we immediately recover that if the state of the composite system is factorized, then the SQUO

$$\bar{U}_{(A|B)} = \bar{\sigma}_A \otimes 1_B$$  \hspace{1cm} (4)

leaves the state unaltered:

$$\bar{U}_{(A|B)}|\Psi_F\rangle = (\bar{\sigma}_A \otimes 1_B)|\Psi_F\rangle = |\Psi_F\rangle.$$  \hspace{1cm} (5)

The SQUO 4 that leaves the separable state $|\Psi_F\rangle$ strictly unchanged will be denoted as the direct preserving SQUO, and it is uniquely defined. If we define the factorized state $|\Psi_F^\perp\rangle$ orthogonal to $|\Psi_F\rangle$ with respect to qubit $A$:

$$|\Psi_F^\perp\rangle = |\Phi_A^\perp\rangle \otimes |\Xi_B\rangle,$$  \hspace{1cm} (6)

then there exists a unique orthogonal SQUO $\bar{U}_{(A|B)}^{\perp}$ that leaves invariant the orthogonal factorized state $|\Psi_F^\perp\rangle$:

$$\bar{U}_{(A|B)}^{\perp}|\Psi_F^\perp\rangle = |\Psi_F^\perp\rangle.$$  \hspace{1cm} (7)

Applied to the factorized state $|\Psi_F\rangle$, the orthogonal preserving SQUO 7 yields

$$\bar{U}_{(A|B)}^{\perp}|\Psi_F\rangle = -|\Psi_F\rangle.$$  \hspace{1cm} (8)

Therefore, the orthogonal preserving SQUO 7, when applied to the separable state $|\Psi_F\rangle$ produces only an unobservable, absolute $\pi$ phase shift. Obviously, the reciprocal holds as well: $\bar{U}_{(A|B)}|\Psi_F\rangle = -|\Psi_F\rangle$.  

II. SINGLE-QUBIT UNITARY OPERATIONS AND SEPARABILITY

Consider a bipartite quantum system $A|B$ whose associated Hilbert space is the $(2 \times D)$-dimensional tensor product $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ of the bidimensional space $\mathcal{H}_A$ and the $D$-dimensional space $\mathcal{H}_B$, with $D \geq 2$ arbitrary integer. A specific, but important, realization is given, for instance, by a system of arbitrary integer. A specific, but important, realization
Summarizing, if the state of a composite \((2 \times D)\)-dimensional bipartite quantum system \(A|B\) is such that the two-level subsystem \(A\) is decoupled from the \(D\)-dimensional subsystem \(B\), then there exist two unitary single-qubit operations defined according to Eqs. (4) and (7) that, respectively, leave the factorized state unchanged, or modify it by an unobservable global phase factor \(\exp(i\pi)\). Viceversa, if the state \(|\Psi\rangle\) is entangled, then there is no SQUO that leaves the state unchanged or modified by an unobservable global phase factor. In fact, if such a SQUO existed, then \(|\Psi\rangle\) would be one of its two eigenvectors corresponding to one of the two possible eigenvalues \(\pm 1\). Hence, it could be put in the form of Eq. (14), leading to a contradiction with the initial hypothesis that the state is entangled. Collecting these results, one has that the existence of a unique SQUO that leaves the state unchanged is a necessary and sufficient condition for the factorizability of all pure states \(|\Psi\rangle\) of arbitrary \((2 \times D)\)-dimensional bipartite quantum systems:

\[
|\Psi\rangle = |\Psi_F\rangle \iff \exists \ U_{(A|B)} \big| \ U_{(A|B)}|\Psi\rangle = \pm |\Psi\rangle . \tag{9}
\]

As a consequence, SQUOs are in principle a useful tool for the qualification of entanglement in pure states of \((2 \times D)\)-dimensional bipartite systems by providing a necessary and sufficient criterion for their separability.

III. SQUOS, HILBERT SPACE DISTANCE, AND ENTANGLEMENT

In this section we demonstrate that the linear entropy, or equivalently the tangle measure of bipartite entanglement, for any pure state \(|\Psi\rangle\) of a \((2 \times D)\)-dimensional system can be rigorously recast in terms of the Euclidean distance in Hilbert space between the state \(|\Psi\rangle\) itself and the state obtained from \(|\Psi\rangle\) by transforming it according to an appropriate SQUO. This result has in turn interesting consequences on the quantification of entanglement via observable quantities associated to SQUOs.

Let us begin by briefly recalling some basic notions. Let \(|\Psi\rangle\) be any arbitrary pure state belonging to \(\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B\), and \(\rho_A = \text{Tr}_B(|\Psi\rangle \langle \Psi|)\) the reduced state of subsystem \(A\). The von Neumann entropy (entropy of entanglement) measuring the bipartite entanglement of state \(|\Psi\rangle\) is defined as \(S(|\Psi\rangle) = -\text{Tr}[\rho_A \ln \rho_A]\). Moreover, for a generic \(l\)-dimensional reduced state \(\rho_A\), the linear entropy \(S_L\) is defined as \(S_L = \frac{1}{l^2} (1 - \text{Tr}[\rho_A^2])\), where the quantity \(\mu = \text{Tr}[\rho_A^2]\) measures the purity of the reduced state \(\rho_A\). In the special case of \(l = 2\), the linear entropy can be written as \(S_L = 4 \text{Det} \rho_A\) and the latter quantity is also known as the tangle \(T\) of the pure states \(|\Psi\rangle\) of \((2 \times D)\)-dimensional systems, one then has:

\[
S_L(|\Psi\rangle) = 4 \text{Det} \rho_A . \tag{10}
\]

The von Neumann entropy Eq. (11) is thus a simple monotonic function of the tangle (linear entropy) Eq. (13). The latter varies in the interval \([0, 1]\), vanishing for separable states and reaching unity for maximally entangled states (or equivalently, maximally mixed reductions with minimal purity \(\mu = 1/2\)). It is an entanglement monotone that plays an essential role in the theory of distributed entanglement and of its ensuing monogamy property due to the trade-off between bipartite and multipartite nonlocal correlations. In a seminal paper Coffman, Kundu, and Wootters [17] showed that the tangle is an upper bound to the sum of all possible pairwise bipartite entanglements, when measured by the concurrences [18] [19], for all states of a system of three qubits. Recently, Osborne and Verstraete [20] extended the result of Coffman, Kundu and Wootters by proving that the tangle bounds from above the sum of all pairwise entanglement in the general case of systems of \(N\) qubits: The distribution of bipartite quantum entanglement, as measured by the tangle \(\tau\) (or equivalently, by the linear entropy \(S_L\)), satisfies a tight monogamy inequality [20]:

\[
\tau(\rho_{A_1|\{A_2A_3\cdots\{A_N\}})) \geq \sum_{i=2}^{N} \tau(\rho_{A_1|A_i}) , \tag{12}
\]

where \(\tau(\rho_{A_1|\{A_2A_3\cdots\{A_N\}}))\) denotes the bipartite quantum entanglement measured by the tangle across the bipartition \(A_1|\{A_2A_3\cdots\{A_N\}}\). As a consequence of the Schmidt decomposition, the monogamy inequality Eq. (12) holds in general if the system under consideration is any bipartition \(A|B\) between a qubit \(A\) and a \(D\)-dimensional qudit \(B\), with \(D \geq 2\).

Let us now consider the Euclidean distance between the state \(|\Psi\rangle\) and the transformed state \(|\Psi_T\rangle\) obtained from \(|\Psi\rangle\) by acting on it with a SQUO: \(|\Psi_T\rangle = U_{(A|B)}|\Psi\rangle\). Denoting such a distance by \(d(|\Psi\rangle, |\Psi_T\rangle)\), we have:

\[
d(|\Psi\rangle, |\Psi_T\rangle) = \sqrt{1 - |\langle \Psi| \Psi_T \rangle|^2} . \tag{13}
\]

Assuming normalized states, the Euclidean distance Eq. (13) varies in the interval \([0, 1]\), vanishing if and only if \(|\Psi_T\rangle = |\Psi\rangle\), and reaching unity if and only if the two states are orthogonal. After introducing the distance Eq. (13) in \(\mathcal{H}\) we can move on to recast in geometric and quantitative forms the separability criterion previously established. As we have shown, subsystem \(A\) (qubit \(A\)) is factorized from the rest of the system (subsystem \(B\)) if and only if there exists a unique, preserving SQUO \(U_{(A|B)}\) that leaves the global state \(|\Psi\rangle\) unchanged: \(|\Psi_T\rangle = U_{(A|B)}|\Psi\rangle = |\Psi\rangle\). Thus, if subsystem \(A\) is factorized, the distance \(d(|\Psi\rangle, U_{(A|B)}|\Psi\rangle)\) vanishes. For any SQUO different from \(U_{(A|B)}\) and \(U_{(A|B)}^+\) the transformed state \(|\Psi_T\rangle = U_{(A|B)}|\Psi\rangle \neq \pm |\Psi\rangle\) and \(d(|\Psi\rangle, U_{(A|B)}|\Psi\rangle) > 0\). On the other hand, as soon as qubit \(A\) is at least partially entangled with the rest of the system (i.e. with at least some part of subsystem \(B\)) we have that any SQUO will always change the state \(|\Psi\rangle\).
and hence, regardless of the choice of the transformation, $d > 0$. So we have that necessary and sufficient condition for the factorizability of a state $|\Psi\rangle$ is that there exists a SQUO for which the distance between the state and its image under its action vanishes.

Keeping in mind these preliminary results we can go on to quantify the content of bipartite entanglement for an entangled pure state $|\Psi\rangle$ by determining the minimum of the distance Eq. (13) between the entangled state $|\Psi\rangle$ and the set of its images under all possible SQUOs. Any pure state $|\Psi\rangle$ of the bipartition $A|B$ can always be put in the form

$$|\Psi\rangle = \sum_n c_n |\uparrow\rangle |n\rangle + c_{n,\downarrow} |\downarrow\rangle |n\rangle,$$  \hspace{1cm} (14)

where $|\uparrow\rangle$ and $|\downarrow\rangle$ stand for the elements of an orthonormal basis in the two-dimensional Hilbert space of qubit $A$, the set $\{|n\rangle\}$ forms an orthonormal basis in the $D$-dimensional Hilbert space of subsystem $B$, and $\sum_n |c_n|_2^2 + |c_{n,\downarrow}|_2^2 = 1$. The most general unitary, Hermitian, and traceless single-qubit operation $O_A$ in the basis formed by $|\uparrow\rangle$ and $|\downarrow\rangle$ can be cast in the form

$$O_A = \begin{pmatrix} \cos \theta & \sin \theta e^{-i\varphi} \\ -\sin \theta e^{i\varphi} & \cos \theta \end{pmatrix} \hspace{1cm} (15)$$

where $\sigma_A^\alpha$ are the Pauli matrices associated to qubit $A$, $\theta$ varies in $[0, \pi]$, and $\varphi$ in $[0, 2\pi]$. Thus the distance Eq. (13) associated to any SQUO is a two-dimensional function $d(\theta, \varphi)$ of the angular variables $\theta, \varphi$ that parameterize the single-qubit rotations $O_A$.

Exploiting relations Eq. (14) and Eq. (15) in Eq. (13), we can evaluate the squared Euclidean distance between the entangled state $|\Psi\rangle$ and its image under any arbitrary SQUO:

$$d^2(\theta, \varphi) = 1 - |\langle \Psi | \Psi_T \rangle|^2 = 1 - |\langle \Psi | U_{(A|B)} \rangle|^2 = 1 - (M_z \cos \theta + M_x \sin \theta \cos \varphi + M_y \sin \theta \sin \varphi)^2, \hspace{1cm} (16)$$

where the expectations $M_\alpha = \langle \Psi | \sigma_A^\alpha |\Psi\rangle$ read

$$M_z = \sum_n |c_n|_2^2 - |c_{n,\downarrow}|_2^2,$$

$$M_x = \sum_n c_n^* c_{n,\downarrow} + c_{n,\downarrow}^* c_n,$$

$$M_y = -i \sum_n c_n^* c_{n,\downarrow} - c_{n,\downarrow}^* c_n. \hspace{1cm} (17)$$

Minimizing the distance Eq. (13) (or, equivalently, the squared distance Eq. (16)) over the entire set of SQUOs, i.e. over the set $\{\theta, \varphi\}$, we find that the unique absolute minimum is reached for two different pairs of values $(\theta, \varphi)$, corresponding, respectively, to the extremal SQUO $U_{(A|B)}^{extr}$ and to its orthogonal SQUO $U_{(A|B)}^{extr}\perp$:

$$\varphi_1 = \arctan\left(\frac{M_y}{M_x}\right),$$

$$\varphi_2 = \pi + \arctan\left(\frac{M_y}{M_x}\right), \hspace{1cm} (18)$$

$$\hat{\theta}_{1,2} = \arctan\left(\frac{M_z \cos \varphi_{1,2} + M_y \sin \varphi_{1,2}}{M_x}\right).$$

It is immediate to observe that the two different extremes correspond to the same absolute minimum for the distance (or equivalently, the squared distance), because these two quantities identify two transformed states that coincide but for a global phase factor. Given the squared Euclidean distance Eq. (16), considering its minimum $\min_{(\theta, \varphi)} d^2(|\Psi\rangle, |\Psi_T\rangle) \equiv d^2(\hat{\theta}_{1,2}, \hat{\varphi}_{1,2})$ yields

$$d^2(\hat{\theta}_{1,2}, \hat{\varphi}_{1,2}) = 1 - (M_z^2 + M_y^2 + M_x^2). \hspace{1cm} (19)$$

This exactly the expression of the linear entropy $S_L$ (or equivalently, the tangle $\tau$) Eq. (11) when cast in terms of the spin expectation values $[21]$. In conclusion, for all pure states of $(2 \times D)$-dimensional quantum systems, one has

$$S_L(|\Psi\rangle) = \tau(|\Psi\rangle) = \min_{(\theta, \varphi)} d^2(|\Psi\rangle, |\Psi_T\rangle). \hspace{1cm} (20)$$

The minimum of the Euclidean squared distance between an entangled pure state and the set of its images under SQUOs, coincides with the linear entropy and with the tangle measure of the total entanglement between qubit $A$ and the rest of the system $[17, 20]$. As an obvious corollary, the von Neumann entropy measure of pure state entanglement is a simple monotonic function of the minimum squared Euclidean distance Eq. (16). These findings provide a geometric characterization and interpretation, in terms of single-qubit unitary transformations and Euclidean distances in Hilbert space, of entropy and entanglement measures such as the linear entropy, the tangle, and the von Neumann entropy.

Before ending this section we illustrate an alternative derivation of the above results that will be useful in the analysis of the $(3 \times D)$-dimensional case. In the minimization procedure we have taken advantage of the fact that SQUOs may be parameterized, see Eq. (15), as functions of the two real parameters $\theta$ and $\varphi$. However, independently of the choice of the parameters, any SQUO is characterized by the fact that it must possess two eigenvalues equal to $\pm 1$, with associated eigenvectors $|+\rangle = \cos(\theta/2) |\uparrow\rangle + e^{i\varphi} \sin(\theta/2) |\downarrow\rangle$ and $|-\rangle = \sin(\theta/2) |\uparrow\rangle - e^{-i\varphi} \cos(\theta/2) |\downarrow\rangle$. Hence, the minimization can be carried out in in two different but equivalent ways: The one illustrated above, in which a given basis is fixed and the SQUO is a function of two real parameters, and a second one in which a given form of the SQUO is fixed, for instance as

$$O_A = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \hspace{1cm} (21)$$
and the orthonormal basis can be varied as a function of the two real parameters \( \theta \) and \( \phi \). Obviously, by virtue of the unitary equivalence of representations, the results that are obtained following the two different procedures coincide. In the basis of the eigenvectors of the SQUO Eq. (21), the state \( |\Psi\rangle \) can be written as 
\[
|\Psi\rangle = \sum_n c_{n, +}|+\rangle|n\rangle + c_{n, -}|-\rangle|n\rangle.
\]
Given this expression for the generic state, and taking into account the action of the SQUO in Eq. (24) we obtain for the squared Euclidean distance between the initial and the transformed state the following expression
\[
d^2(|\Psi\rangle, |\Psi_T\rangle) = 1 - (\rho_{11} - \rho_{22})^2 = 4\rho_{11}\rho_{22},
\]
where \( \rho_{11} = \sum_n |c_{n, +}|^2 \) and \( \rho_{22} = \sum_n |c_{n, -}|^2 \) are the diagonal elements of the reduced density matrix \( \rho_A \). It is straightforward to observe that expression Eq. (22) coincides with the linear entropy \( S_L \) (or the tangle \( T \)) if the state \( |\Psi\rangle \) is expressed in the basis formed by the eigenvectors of the reduced density matrix \( \rho_A \). Therefore what we are left to prove is that the minimum of the expression Eq. (22) over all possible bases in the two-dimensional Hilbert space is actually reached in the basis of the eigenvectors of \( \rho_A \). This is easily seen by recalling the trivial fact that the determinant of a matrix is invariant under a change of basis. Let us denote by \( \rho_{11}, \rho_{22} \) the matrix elements of \( \rho_A \) in the basis of its eigenvectors, and by \( \rho_{\alpha, \beta}' \) the matrix elements of \( \rho_A \) in a different basis, arbitrarily chosen. Comparing the expressions of the determinant of \( \rho_A \) in the two bases, one has
\[
\rho_{11}\rho_{22} = \rho_{11}'\rho_{22}' - |\rho_{12}'|^2 \leq \rho_{11}'\rho_{22}',
\]
and the proof follows.

**IV. LINEAR ENTROPY AND TANGLE AS PROJECTION OPERATORS ON PURE STATES**

In the previous section we have showed that the tangle and the linear entropy coincide with the minimum squared Euclidean distance between a state and the set of its images under the action of SQUOs. The key point in the evaluation of the distance Eq. (14) is the calculation of the real expectation value of \( U_{(A|B)} \) that can be always put in the form
\[
\langle \Psi | U_{(A|B)} | \Psi \rangle = \langle \Psi | U_{(A|B)} | \Psi \rangle = \text{Tr}(\rho U_{(A|B)}) ,
\]
where \( \rho \) is the density matrix (projector) associated to the pure state \( |\Psi\rangle \); \( \rho = |\Psi\rangle \langle \Psi| \). Taking into account that any SQUO acts as the identity for the degrees of freedoms that belong to subsystem \( B \), we may simply trace out all these degrees of freedoms to obtain
\[
\langle \Psi | U_{(A|B)} | \Psi \rangle = \text{Tr}(\rho_A O_A) ,
\]
where \( \rho_A \) is the reduced density matrix of qubit \( A \). The unitary, Hermitian, traceless operator \( O_A \) can always be expressed as a linear combination of Pauli matrices, with eigenvalues ±1 and eigenvectors \( |\pm\rangle \). Thus
\[
O_A = |+\rangle\langle+| - |−\rangle\langle−| .
\]
We can then write
\[
\langle \Psi | U_{(A|B)} | \Psi \rangle = \text{Tr}(\rho_A |+\rangle\langle+|) - \text{Tr}(\rho_A |−\rangle\langle−|) .
\]
Since the states \( |\pm\rangle \) form a complete basis set for the subsystem \( A \), the traces \( \text{Tr}(\rho_A |+\rangle\langle+|) \) and \( \text{Tr}(\rho_A |−\rangle\langle−|) \) are not independent and satisfy the relation
\[
\text{Tr}(\rho_A |+\rangle\langle+|) + \text{Tr}(\rho_A |−\rangle\langle−|) = 1 .
\]
Exploiting Eq. (25), relation Eq. (27) can be rewritten in the form
\[
\langle \Psi | U_{(A|B)} | \Psi \rangle = 2\text{Tr}(\rho_A |+\rangle\langle+|) - 1 = 2\text{Tr}(\rho_A \rho_A^p) - 1 ,
\]
where \( \rho_A^p \) denotes the density matrix associated to a pure state \( |+\rangle \) defined in the qubit \( A \). Reminding the expression of the Euclidean distance Eq. (14), we have that
\[
d^2(|\Psi\rangle, |\Psi_T\rangle) = 1 - (2\text{Tr}(\rho_A \rho_A^p) - 1)^2 .
\]
Eq. (30) shows that minimization of the squared distance in Eq. (30) is equivalent to maximizing the “local factorizability” or “pure state overlap” \( F_A \equiv (2\text{Tr}(\rho_A \rho_A^p) - 1)^2 \), i.e. the projection of the reduced density matrix onto a pure state. The local factorizability varies in the interval \([0, 1]\), vanishing for a maximally entangled state (\( \rho_A \) maximally mixed) and attaining unity for a separable state (\( \rho_A \) pure). Thus, for an entangled state \( |\Psi\rangle \) the nonvanishing minimum attainable by the squared distance \( d^2 \) is equivalent to the non-unity maximum attainable by the local factorizability \( F_A \), and it is finally straightforward to prove that
\[
S_L = \tau = \min_{\{\theta, \phi\}} d^2 = 1 - \max_{\{\theta, \phi\}} F_A .
\]
This expression establishes the reciprocal relations existing between the entanglement of pure states, the minimum squared Euclidean distance of an entangled state from the entire set of its images under all possible SQUOs, and the maximum over the set of all possible SQUOs of the pure-state overlap of single-qubit reductions.

**V. SINGLE-QUTRIT UNITARY OPERATIONS AND ENTANGLEMENT IN \((3 \times D)\)-DIMENSIONAL SYSTEMS**

Let us consider the case of \((3 \times D)\)-dimensional composite quantum systems. Due to the rapidly rising number of parameters with the local dimension of subsystem \( A \) and the involved generalizations of the Bloch sphere construction \([22, 23, 24, 25]\), we will follow the strategy
of minimization outlined in the last part of Section III by keeping a fixed given expression for the single-qutrit transformation and then spanning over all orthonormal bases in the Hilbert space of the qutrit. We first need to define the class of single-qutrit unitary transformations (SQUITOs). We have seen that the SQUOs have three defining properties: Unitarity, Hermiticity, and Tracelessness. The last property obscures the fact that it is equivalent to require that the spectrum of a given, fixed local unitary be, for instance, of the form \( \lambda_k \) for \( k = 1, 2, 3 \) of a local unitary acting on the three-dimensional subsystem \( A \) one necessarily has \( |\lambda_k|^2 = 1 \) and this relation, together with all the other requirements, imposes that the eigenvalues of a given, fixed local unitary be, for instance, of the form \( e^{i\phi}, e^{i(2\pi/3 + \phi)}, \) and \( e^{i(-2\pi/3 + \phi)} \), where \( \phi \) is a global phase factor that can be set to zero without loss of generality.

We can now proceed to define the form of the associated SQUUTO acting on a \((3 \times D)\)-dimensional space, for which the local part of the transformation, acting on the three-dimensional subspace, is unitary, traceless, and with non degenerate spectrum of eigenvalues:

\[
U_{(A|B)} = \exp \left( \frac{2\pi i}{3} \hat{O}_A \otimes \mathbf{1}_B \right),
\]

where \( \hat{O}_A \) is an hermitian and traceless operator whose matrix form, in the basis of its eigenstates, reads

\[
\hat{O}_A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.
\]

This form coincides, in analogy to Eq. (21), to the matrix form of the operator corresponding to the \( z \) component of the spin-1 subsystem.

Having selected a particular form of the SQUITOs, we must look at the action of this operator on a generic state defined in a \((3 \times D)\)-dimensional Hilbert space. As for the case in which party \( A \) was a qubit, any pure state \( |\Psi\rangle \) of the bipartition \( A|B \), with party \( A \) being a qubit, can always be cast in the form

\[
|\Psi\rangle = \sum_n c_{n,+}|+\rangle|n\rangle + c_{n,0}|0\rangle|n\rangle + c_{n,-}|\rangle|n\rangle,
\]

where the set \( \{|n\rangle\} \) forms an orthonormal basis in the \( D \)-dimensional Hilbert space of subsystem \( B \). The set \( \{+\}, \{0\}, \{-\} \) is formed by the eigenstates of \( \hat{O}_A \) associated, respectively, to the eigenvalues 1, 0, -1, and is a basis in the three-dimensional Hilbert space of qutrit \( A \). Finally, \( \sum_n |c_{n,+}|^2 + |c_{n,0}|^2 + |c_{n,-}|^2 = 1 \). The action of the SQUUTO transforms the generic state \( |\Psi\rangle \) in the state \( \Psi_T = U_{(A|B)}|\Psi\rangle \) that reads

\[
|\Psi_T\rangle = \sum_n e^{i\Delta c_n,+}|n\rangle + c_{n,0}|0\rangle|n\rangle + e^{-i\Delta c_n,-}|n\rangle,
\]

where \( \Delta c_n = c_{n,+} - c_{n,-} \) and \( \Delta c_n = c_{n,+} - c_{n,-} \).

Hence

\[
\langle \Psi | \Psi_T \rangle = e^{i\Delta c_n,+} \sum_n c_{n,+}^2 + \sum_n c_{n,0}^2 + e^{-i\Delta c_n,-} \sum_n c_{n,-}^2
\]

\[
= e^{i\Delta c_n,+} \rho_{11} + \rho_{22} + e^{-i\Delta c_n,-} \rho_{33},
\]

where \( \rho_{11} = \sum_n |c_{n,+}|^2, \rho_{22} = \sum_n |c_{n,0}|^2 \), and \( \rho_{33} = \sum_n |c_{n,-}|^2 \) are the diagonal elements of the reduced density matrix \( \rho_A \) obtained by tracing over all the degree of freedom of the \( D \)-dimensional subsystem \( B \). From Eq. (30), after some elementary algebra, it is straightforward to obtain the expression of the squared Euclidean distance between \( |\Psi\rangle \) and the transformed state \( |\Psi_T\rangle = U_{(A|B)}|\Psi\rangle \):

\[
d^2(|\Psi\rangle, |\Psi_T\rangle) = 1 - \frac{1}{2} \left[ (\rho_{11} - \rho_{22})^2 + (\rho_{11} - \rho_{33})^2 + (\rho_{22} - \rho_{33})^2 \right] = \frac{3}{2} \left[ 1 - (\rho_{11}^2 + \rho_{22}^2 + \rho_{33}^2) \right].
\]

In analogy with the \((2 \times D)\)-dimensional case, we are left with the task of minimizing the expression of the squared Euclidean distance Eq. (42). This amounts to maximizing the sum of the squared diagonal elements of the reduced density matrix \( \rho_A \) over all possible bases. It is easy to show that such maximum is achieved in the basis formed by the eigenvectors of the reduced density matrix \( \rho_A \). Observing that the trace of \( \rho_A^2 \) is invariant under changes of basis, we denote by \( \rho_{A,\alpha} \) the matrix elements of \( \rho_A \) in the basis of its eigenvectors and by \( \rho'_{A,\alpha} \) the matrix elements of \( \rho_A \) in a different basis, arbitrarily chosen. Comparing the expressions of \( Tr(\rho_A^2) \) in the two bases, one has

\[
\rho_{11}' + \rho_{22}' + \rho_{33}' = \rho_{11}^2 + \rho_{22}^2 + \rho_{33}^2
\]

so that

\[
\rho_{11}' + \rho_{22}' + \rho_{33}' \geq \rho_{11}^2 + \rho_{22}^2 + \rho_{33}^2,
\]

and the proof follows. Hence the minimum of the squared Euclidean distance reads

\[
\min_{U_{(A|B)}} d^2(|\Psi\rangle, |\Psi_T\rangle) = \frac{3}{2} \left[ 1 - (\gamma_1^2 + \gamma_2^2 + \gamma_3^2) \right],
\]

where the \( \gamma_i \) are the eigenvalues of the reduced density matrix \( \rho_A \) \( (\gamma_i = \rho_{A,\alpha}) \). From the definition of the linear entropy we finally have:

\[
S_L(|\Psi\rangle) = \min_{U_{(A|B)}} d^2(|\Psi\rangle, |\Psi_T\rangle).
\]
The lower boundary line of the interval of values for the linear entropy corresponds to the case of two eigenvalues of the reduced density matrix $\rho_A$ of qutrit $A$ being equal and smaller than the remaining one ($\gamma_1 = \gamma_2 < \gamma_3$). The left upper boundary line corresponds to one vanishing eigenvalue and the remaining two eigenvalues being distinct ($\gamma_1 = 0, \gamma_2 \neq \gamma_3$). The right upper boundary line corresponds to two coinciding eigenvalues greater than the remaining one ($\gamma_2 = \gamma_3 > \gamma_1$). The lower and upper left boundary lines match at separability; the lower and upper right boundary lines match at maximal entanglement; the upper left and upper right boundary lines match when one eigenvalue vanishes and the other two are equal. This point corresponds to the case in which a two-dimensional subsystem (subspace) of qutrit $A$ is perfectly entangled with subsystem $B$. All quantities being plotted are dimensionless.

Thus the minimum of the squared Euclidean distance between pure states of $(3 \times D)$-dimensional composite quantum systems and their images under single-qutrit unitary operations coincides with their linear entropy, in full correspondence with the result obtained in Section III in the case of $(2 \times D)$-dimensional systems. Vanishing of the Euclidean distance, corresponding to the vanishing the linear entropy or, equivalently, to the reduced state $\rho_A$ of the qutrit being pure, is again a necessary and sufficient condition for separability. One interesting difference with the $(2 \times D)$-dimensional case is however that now the linear entropy is not an entanglement monotone as it is not in one-to-one correspondence with the von Neumann entropy (entropy of entanglement).

Comparison between the two measures, plotted in Fig. II reveals that they coincide at the lower and upper extrema of separability and maximal entanglement, while in the intermediate region the linear entropy varies in a restricted range at fixed von Neumann entropy. The lower boundary line of the interval of values for the linear entropy corresponds to the case of two eigenvalues of the reduced density matrix $\rho_A$ of qutrit $A$ being equal and smaller than the remaining one ($\gamma_1 = \gamma_2 < \gamma_3$). The left upper boundary line corresponds to one vanishing eigenvalue and the remaining two eigenvalues being distinct ($\gamma_1 = 0, \gamma_2 \neq \gamma_3$). The right upper boundary line corresponds to two eigenvalues equal and greater than the remaining one ($\gamma_2 = \gamma_3 > \gamma_1$). The two lines match at the cusp point associated to one vanishing and two coinciding eigenvalues. This situation corresponds to the case in which a two-dimensional subsystem (subspace) of qutrit $A$ is perfectly entangled with subsystem $B$. Qualitatively, this behavior of the linear and von Neumann entropies for the pure states of $(3 \times D)$-dimensional bipartite quantum systems is similar to that of the negativity versus the concurrence for the mixed states of two qubits [20], and is a particular case of the general comparison between Rényi entropies of different order for fixed $N$-point discrete probability distributions [27].

One might think to go further along this line to investigate the effects of single-quartet unitary operations on pure states of $(4 \times D)$-dimensional bipartite quantum systems, and so on, but, unfortunately, in these higher-dimensional cases the very definition of the Euclidean distance between a state and its images is not unique, as it becomes dependent on the ordering of the eigenvalues of the local unitary transformation. Such a problem does not arise if subsystem $A$ consists of a qubit or a qutrit. In fact, in these cases, the quantities involved do not depend on the ordering of the eigenvalues.

VI. CONSEQUENCES, APPLICATIONS, AND OUTLOOK

In the present work we have discussed two different questions that in fact turn out to be related. One concerns the possibility of characterizing global entanglement properties of composite quantum systems by suitably defined local unitary transformations (that, by definition, do not change the entanglement of a given state). The other regards the nature of the relationships between entropic and geometric measures of entanglement. By defining a suitable class of local unitaries, the single-qubit transformations that are simultaneously unitary, Hermitian, and traceless, we have found that a simple necessary and sufficient condition for inseparability stems from the invariance properties of pure states under such transformations. This result is straightforwardly generalized to the $(3 \times D)$-dimensional case. We have then showed that single-subsystem unitary operations allow for a simple geometrical reformulation of the von Neumann entropy and other known entropic measures. In particular, both in the $(2 \times D)$- and $(3 \times D)$-dimensional cases, we have demonstrated that the minimum squared Euclidean distance between pure states and their images under single-subsystem unitary transformations coincides exactly with the linear entropy. In turn, this result implies that in the $(2 \times D)$-dimensional case the entropy of entanglement is a unique, single-valued, and monotonic function of the minimal Euclidean distance.

Besides the conceptual interest, these findings can be of use in applications, for instance in measuring and characterizing the separability properties and entanglement content of the ground state $|G\rangle$ of generic,
translationally-invariant models of interacting qubits (two-level systems or spin 1/2) or qutrits (spin 1), both at and away from criticality [28]. In particular, such a characterization can be obtained operationally by introducing an observable, the energy of excitation $\Delta E$ above the ground state, that is associated to single-qubit or single-qutrit unitary transformations and is defined as [28]: $\Delta E = \langle G | O^\dagger H G - (G | H | G) \rangle$, where $O$ is a shorthand for the single-spin unitary operation between an arbitrarily selected spin (subsystem $A$) and the rest of the system (subsystem $B$), and $H$ denotes the Hamiltonian of the system. This excitation energy is positive defined, vanishes if and only if the ground state is factorized, and is a monotonic function of the linear entropy (or equivalently of the tangle in the (2 $\times$ 2)-dimensional case). Aside from the characterization of ground-state properties at the approach of quantum critical points from a quantum informatic standpoint [29], and the relations to single-site entanglement [30], we expect that the method of local unitary operations may be of particular importance as a general technique to ascertain the existence and the location of factorizability points, i.e. values of the Hamiltonian parameters for which the ground state (and, in general, any pure state) factorizes and becomes classical in models of interacting many-body quantum systems [31].

Concerning the extension of the methods discussed in this work to higher-dimensional situations and to mixed states, the present strategy will certainly need to be modified and integrated by developing more sophisticated tools, including the use of multiple operations to yield properly defined distances between states and generalizations to mixed-states fidelities and metrics [32]. However, some important simplifications occur if one restricts the analysis to the case of multimode pure Gaussian states of infinite-dimensional systems, for which the framework introduced in the present work can be successfully applied with only minor modifications [33].

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