A geometric approach to the distribution of quantum states in bipartite physical systems

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(Dated: January 8, 2014)

Abstract

Any set of pure states living in an given Hilbert space possesses a natural and unique metric—the Haar measure—on the group $U(N)$ of unitary matrices. However, there is no specific measure induced on the set of eigenvalues $\Delta$ of any density matrix $\rho$. Therefore, a general approach to the global properties of mixed states depends on the specific metric defined on $\Delta$. In the present work we shall employ a simple measure on $\Delta$ that has the advantage of possessing a clear geometric visualization whenever discussing how arbitrary states are distributed according to some measure of mixedness. The degree of mixture will be that of the participation ratio $R = 1/Tr(\rho^2)$ and the concomitant maximum eigenvalue $\lambda_m$. The cases studied will be the qubit-qubit system and the qubit-qutrit system, whereas some discussion will be made on higher-dimensional bipartite cases in both the $R$-domain and the $\lambda_m$-domain.

PACS numbers: 03.65.Ud; 03.67.Bg; 03.67.Mn; 89.70.Cf

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I. INTRODUCTION

The amount of entanglement and the purity of quantum states of composite systems exhibit a dualistic relationship. As the degree of mixture increases, quantum states tend to have a smaller amount of entanglement. In the case of two-qubits systems, states with a large enough degree of mixture are always separable [1]. A detailed knowledge of the relation between the degree of mixture and the amount of entanglement is essential in order to understand the limitations that mixture imposes on quantum information processes such as quantum teleportation or quantum computing. To study the relationship between entanglement and mixture we need quantitative measures for these two quantities. The entanglement of formation provides a natural quantitative measure of entanglement with a clear physical motivation. As for mixedness, there are several measures of mixture that can be useful within the present context. The von Neumann measure

\[ S = -Tr (\hat{\rho} \ln \hat{\rho}) , \]  

is important because of its relationship with the thermodynamic entropy. On the other hand, the so called participation ratio,

\[ R(\hat{\rho}) = \frac{1}{Tr(\hat{\rho}^2)} , \]  

is particularly convenient for calculations [1, 2]. Another measure for mixedness can be found in the maximum eigenvalue of a density matrix \( \lambda_m \), which is in turn a monotonically increasing function for the Renyi entropy \( SR_\infty \).

Given a particular way to explore the space of both pure and mixed states in bipartite systems, it is possible to provide a clear physical geometric insight into the problem of how states distribute according to their degree of mixture, which is the main subject of the present work.

This paper is organized as follows: in Section II we introduce the nature of the measures defined on the set of eigenvalues and unitary matrices. Section III analyzes 2x2 systems and how their concomitant states are distributed according to \( R \) and \( \lambda_m \). Section IV provides a further analytic approach for 2x3 and additional bipartite systems. In Section V we discuss the implications of the non-uniqueness of a general measure for mixed states and
the corresponding geometric implications into our problem. Finally, some conclusions are
drawn in Section VI.

II. MEASURES ON THE SET OF EIGENVALUES AND UNITARY MATRICES

In order to perform a survey of the properties of arbitrary (pure and mixed) states of the
concomitant state-space $\mathcal{S}$, it is necessary to introduce an appropriate measure $\mu$ on this
space. Such a measure is needed to compute volumes within $\mathcal{S}$, as well as to determine what
is to be understood by a uniform distribution of states on $\mathcal{S}$. The natural measure that we
are going to adopt here was first considered in Refs. [1, 3]. An arbitrary (pure or mixed)
state $\rho$ of a quantum system described by an $N$-dimensional Hilbert space can always be
expressed as the product of three matrices,

$$\rho = UD[\{\lambda_i\}]U^\dagger.$$  \hfill (3)

Here $U$ is an $N \times N$ unitary matrix and $D[\{\lambda_i\}]$ is an $N \times N$ diagonal matrix whose diagonal
elements are $\{\lambda_1, \ldots, \lambda_N\}$, with $0 \leq \lambda_i \leq 1$, and $\sum_i \lambda_i = 1$. The group of unitary matrices
$U(N)$ is endowed with a unique, uniform measure: the Haar measure $\nu$ [4]. On the other
hand, the $N$-simplex $\Delta$, consisting of all the real $N$-uples $\{\lambda_1, \ldots, \lambda_N\}$ appearing in (3), is a
subset of a $(N - 1)$-dimensional hyperplane of $\mathcal{R}^N$. Consequently, the standard normalized
Lebesgue measure $\mathcal{L}_{N-1}$ on $\mathcal{R}^{N-1}$ provides a natural measure for $\Delta$. The aforementioned
measures on $U(N)$ and $\Delta$ lead then to a natural measure $\mu$ on the set $\mathcal{S}$ of all the states of
our quantum system [1, 3, 4], namely,

$$\mu = \nu \times \mathcal{L}_{N-1}.$$ \hfill (4)

All our present considerations are based on the assumption that the uniform distribution of
states of a quantum system is the one determined by the measure (4). Thus, in our numerical
computations, we are going to randomly generate states according to the measure (4). The
quantities $\mu_i$ computed with a Monte Carlo procedure have an associated error which is on
the type $t_{M-1,\alpha/2} \sigma_x/\sqrt{M-1}$, where $M$ is the number of generated states, $t_{M-1,\alpha/2}$ is the value
corresponding to the Student distribution with $M - 1$ degrees of freedom, computed with a
certain desired accuracy $1 - \alpha$, and $\sigma_x$ is the usual computed standard deviation. Therefore,
if we seek a result with an error say less than $10^{-3}$ units, we have to generate a number
of points $M$ around 10 or 100 million. If not stated explicitly, from now on all quantities computed are exact up to the last digit.

The applications that have appeared so far in quantum information theory, in the form of dense coding, teleportation, quantum cryptography and specially in algorithms for quantum computing (quantum error correction codes for instance), deal with finite numbers of qubits. A quantum gate which acts upon these qubits or even the evolution of that system is represented by a unitary matrix $U(N)$, with $N = 2^n$ being the dimension of the associated Hilbert space $\mathcal{H}_N$. The state $\rho$ describing a system of $n$ qubits is given by a hermitian, positive-semidefinite $(N \times N)$ matrix, with unit trace. In view of these facts, it is natural to think that an interest has appeared in the quantification of certain properties of these systems, most of the times in the form of the characterization of a certain state $\rho$, described by $N \times N$ matrices of finite size. Natural applications arise when one tries to simulate certain processes through random matrices, whose probability distribution ought to be described accordingly.

A. The Haar measure

As stated before, in the space of pure states, with $|\Psi\rangle \in \mathcal{H}_N$, there is a natural candidate measure, induced by the Haar measure on the group $\mathcal{U}(N)$ of unitary matrices. In mathematical analysis, the Haar measure \cite{5} is known to assign an “invariant volume” to what is known as subsets of locally compact topological groups. In origin, the main objective was to construct a measure invariant under the action of a topological group \cite{6}. Here we present the formal definition \cite{7}: given a locally compact topological group $G$ (multiplication is the group operation), consider a $\sigma$-algebra $Y$ generated by all compact subsets of $G$. If $a$ is an element of $G$ and $S$ is a set in $Y$, then the set $aS = \{ as : s \in S \}$ also belongs to $Y$. A measure $\mu$ on $Y$ will be left-invariant if $\mu(aS) = \mu(S)$ for all $a$ and $S$. Such an invariant measure is the Haar measure $\mu$ on $G$ (it happens to be both left and right invariant). In other words \cite{8}, the Haar measure defines the unique invariant integration measure for Lie groups. It implies that a volume element $d\mu(g)$ is identified by defining the integral of a function $f$ over $G$ as $\int_G f(g)d\mu(g)$, being left and right invariant

$$\int_G f(g^{-1}x)d\mu(x) = \int_G f(xg^{-1})d\mu(x) = \int_G f(x)d\mu(x).$$ 

(5)
The invariance of the integral follows from the concomitant invariance of the volume element \( \mathrm{d}\mu(g) \). It is plain, then, that once \( \mathrm{d}\mu(g) \) is fixed at a given point, say the unit element \( g = e \), we can move performing a left or right translation. Suppose that the map \( x \rightarrow g(x) \) defines the action of a left translation. We have \( x^i \rightarrow y^i(x^j) \), with \( x^i \) being the coordinates in the vicinity of \( e \). Assume, also, that \( \mathrm{d}x^1...\mathrm{d}x^n \) defines the volume element spanned by the differentials \( \mathrm{d}x^1, \mathrm{d}x^2, ..., \mathrm{d}x^n \) at point \( e \). It follows then that the volume element at point \( g \) is given by \( \mathrm{d}\mu(g) = |J|^{-1}\mathrm{d}x^1...\mathrm{d}x^n \), where \( J \) is the Jacobian of the previous map evaluated at the unit element \( e \): \( J = \frac{\delta(y^1...y^n)}{\delta(x^1...x^n)} \). In a right or left translation, both \( \mathrm{d}x^1...\mathrm{d}x^n \) and \( |J| \) are multiplied by the same Jacobian determinant, preserving invariance of \( \mathrm{d}\mu(g) \). The Lie groups also allow an invariant metric and \( \mathrm{d}\mu(g) \) is just the volume element \( \sqrt{g}\mathrm{d}x^1...\mathrm{d}x^n \).

We do not gain much physical insight with these definitions of the Haar measure and its invariance unless we identify \( G \) with the group of unitary matrices \( U(N) \), the element \( a \) with a unitary matrix \( U \) and \( S \) with subsets of the group of unitary matrices \( U(N) \), so that given a reference state \( |\Psi_0\rangle \) and a unitary matrix \( U \in U(N) \), we can associate a state \( |\Psi_0 = U|\Psi_0\rangle \) to \( |\Psi_0\rangle \). Physically what is required is a probability measure \( \mu \) invariant under unitary changes of basis in the space of pure states, that is,

\[
P_{\text{Haar}}^{(N)}(U|\Psi) = P_{\text{Haar}}^{(N)}(|\Psi\rangle).
\]

These requirements can only be met by the Haar measure, which is rotationally invariant.

**III. ANALYTICAL APPROACH FOR 2X2 SYSTEMS. GENERATION OF STATES**

The two-qubits case \( (N = 2 \times 2) \) is the simplest quantum mechanical system that exhibits the feature of quantum entanglement. The relationship between entanglement and mixedness has been described intensively in the literature. One given aspect is that as we increase the degree of mixture, as measured by the so called participation ratio \( R = 1/\text{Tr}[\rho^2] \), the entanglement diminishes (on average). As a matter of fact, if the state is mixed enough, that state will have no entanglement at all. This is fully consistent with the fact that there exists a special class of mixed states which have maximum entanglement for a given \( R \) \(^2\) (the maximum entangled mixed states MEMS). These states have been recently reported to be achieved in the laboratory \(^9\) using pairs of entangled photons. Thus for practical or purely theoretical purposes, it may happen to be relevant to generate mixed states of two-qubits
with a given participation ratio $R$. It may represent an excellent tool in the simulation of
algorithms in a given quantum circuit: as the input pure states go through the quantum
gates, they interact with the environment, so that they become mixed with some $R$. This
degree of mixture $R$, which varies with the number of iterations, can be used as a probe for
the evolution of the degradation of the entanglement present between any two qubits in the
circuit. Different evolutions of the degree of mixture on the output would shed some light
on the optimal architecture of the circuit that has to perform a given algorithm.

Here we describe a numerical recipe to randomly generate two-qubit states, according
to a definite measure, and with a given, fixed value of $R$. Suppose that the states $\rho$ are
generated according to the product measure $\mu = \nu \times \mathcal{L}_{N-1}$ \cite{[4]}, where $\nu$ is the Haar measure
on the group of unitary matrices $U(N)$ and the Lebesgue measure $\mathcal{L}_{N-1}$ on $\mathbb{R}^{N-1}$ provides a
reasonable measure for the simplex of eigenvalues of $\rho$. In this case, the numerical procedure
we are about to explain owes its efficiency to the following geometrical picture which is valid
only if the states are supposed to be distributed according to measure \cite{[4]}. We shall identify
the simplex $\Delta$ with a regular tetrahedron of side length 1, in $\mathbb{R}^3$, centred at the origin. Let
$r_i$ stand for the vector positions of the tetrahedron’s vertices. The tetrahedron is oriented
in such a way that the vector $r_4$ points towards the positive $z$-axis and the vector $r_2$ is
contained in the $(x,z)$-semiplane corresponding to positive $x$-values. The positions of the
tetrahedron’s vertices correspond to the vectors

\begin{align*}
    r_1 &= \left(-\frac{1}{2\sqrt{3}}, -\frac{1}{2}, -\frac{1}{4}\sqrt{\frac{2}{3}}\right) \\
r_2 &= \left(\frac{1}{\sqrt{3}}, 0, -\frac{1}{4}\sqrt{\frac{2}{3}}\right) \\
r_3 &= \left(-\frac{1}{2\sqrt{3}}, \frac{1}{2}, -\frac{1}{4}\sqrt{\frac{2}{3}}\right) \\
r_4 &= (0, 0, \frac{3}{4}\sqrt{\frac{2}{3}}). \quad (7)
\end{align*}

The mapping connecting the points of the simplex $\Delta$ (with coordinates $(\lambda_1, \ldots, \lambda_4)$) with
the points $r$ within tetrahedron is given by the equations

\[ \lambda_i = 2(r \cdot r_i) + \frac{1}{4} \quad i = 1, \ldots, 4, \]
\[ r = \sum_{i=1}^{4} \lambda_i r_i \] 

(8)

The degree of mixture is characterized by the quantity \( R^{-1} \equiv Tr(\rho^2) = \sum_i \lambda_i^2 \). This quantity is related to the distance \( r = |r| \) to the centre of the tetrahedron \( T_\Delta \) by

\[ r^2 = -\frac{1}{8} + \frac{1}{2} \sum_{i=1}^{4} \lambda_i^2. \] 

(9)

Thus, the states with a given degree of mixture lie on the surface of a sphere \( \Sigma_r \) of radius \( r \) concentric with the tetrahedron \( T_\Delta \). To choose a given \( R \) is tantamount to define a given radius of the sphere. There exist three different possible regions (see Fig. 1):

• region I: \( r \in [0, h_1] \) \( (R \in [4, 3]) \), where \( h_1 \equiv h_c = \frac{1}{4} \sqrt{\frac{2}{3}} \) is the radius of a sphere tangent to the faces of the tetrahedron \( T_\Delta \). In this case the sphere \( \Sigma_r \) lies completely within the tetrahedron \( T_\Delta \). Therefore we only need to generate at random points over its surface. The cartesian coordinates for the sphere are given by

\[
\begin{align*}
x_1 &= r \sin \theta \cos \phi \\
x_2 &= r \sin \theta \sin \phi \\
x_3 &= r \cos \theta,
\end{align*}
\]

(10)

Denoting \( \text{rand}_u() \) a random number uniformly distributed between 0 and 1, the random numbers \( \phi = 2\pi \text{rand}_u() \) and \( \theta = \arccos(2\text{rand}_u() - 1) \) (its probability distribution

FIG. 1. Geometric evolution of a growing sphere inside a tetrahedron, depicting the distribution nature of states \( \rho \) generated according to the measure (??). See text for details.
being \( P(\theta) = \frac{1}{2} \sin(\theta) \) define an arbitrary state \( \rho \) on the surface inside \( T_\Delta \). The angle \( \theta \) is defined between the centre of the tetrahedron (the origin) and the vector \( r_4 \), and any point aligned with the origin. Substitution of \( r = (x_1, x_2, x_3) \) in (8) provides us with the eigenvalues \( \{\lambda_i\} \) of \( \rho \), with the desired \( R \) as prescribed by the relationship (9). With the subsequent application of the unitary matrices \( U \) we obtain a random state \( \rho = U D(\Delta) U^\dagger \) distributed according to the usual measure \( \mu = \nu \times L_{N-1} \).

- region II: \( r \in [h_1, h_2] \) \( (R \in [3, 2]) \), where \( h_2 \equiv \sqrt{h_c^2 + \left(\frac{D}{2}\right)^2} = \frac{\sqrt{2}}{4} \) denotes the radius of a sphere which is tangent to the sides of the tetrahedron \( T_\Delta \). Contrary to the previous case, part of the surface of the sphere lies outside the tetrahedron. This fact means that we are able to still generate the states \( \rho \) as before, provided we reject those ones with negative weights \( \lambda_i \).

- region III: \( r \in [h_2, h_3] \) \( (R \in [2, 1]) \), where \( h_3 \equiv \sqrt{h_c^2 + D^2} = \frac{\sqrt{6}}{4} \) is the radius of a sphere passing through the vertices of \( T_\Delta \). The generation of states is a bit more involved in this case. Again \( \phi = 2\pi \text{rand}_u() \), but the available angles \( \theta \) now range from \( \theta_c(r) \) to \( \pi \). It can be shown that \( w \equiv \cos(\theta_c) \) results from solving the equation \( 3r^2w^2 - \sqrt{\frac{3}{2}}rw + \frac{3}{8} - 2r^2 = 0 \). Thus, \( \theta(r) = \arccos(w(r)) \), with \( w(r) = \cos \theta_c(r) + (1 - \cos \theta_c(r)) \text{rand}_u() \). Some states may be unacceptable \( (\lambda_i < 0) \) still, but the vast majority are accepted.

Combining these three previous regions, we are able to generate arbitrary mixed states \( \rho \) endowed with a given participation ratio \( R \).

### A. \textbf{R-domain}

In this case the degree of mixture is characterized by the quantity \( \omega_2 = \text{Tr}(\hat{\rho}^2) = \sum_i p_i^2 \).

This quantity is related to the distance \( r = |r| \) to the centre of the tetrahedron \( T_\Delta \) by

\[
r^2 = -\frac{1}{8} + \frac{1}{2}\omega_2.
\]

Thus, the states with a given degree of mixture lie on the surface of a sphere of radius \( r \) concentric with the tetrahedron \( T_\Delta \).

The volume associated with states endowed with a value of \( \omega_2 \) lying within a small interval \( dw_2 \) is clearly associated with the volume \( dV \) of the subset of points in \( T_\Delta \) whose distances
to the centre of $T_\Delta$ are between $r$ and $r + dr$, with $rdr = \omega_2 d\omega_2$. Let $\Sigma_r$ denote the sphere of radius $r$ concentric with $T_\Delta$. The volume $dV$ is then proportional to the area $A(r)$ of the part of $\Sigma_r$ which lies within $T_\Delta$. In order to compute the aforementioned area, it is convenient to separately consider three different ranges for the radius $r$.

Let us first consider the range of values $r \in [0, h_1]$, where $h_1 = \frac{1}{4} \sqrt{\frac{2}{3}}$ is the radius of a sphere tangent to the faces of the tetrahedron $T_\Delta$. In this case the sphere $\Sigma_r$ lies completely within the tetrahedron $T_\Delta$. Thus, the area we are interested in is just the area of the sphere,

$$A_I(r) = 4\pi r^2. \quad (12)$$

We now consider a second range of values of the radius, $r \in [h_1, h_2]$, where $h_2 = \frac{\sqrt{2}}{4}$ denotes the radius of a sphere which is tangent to the sides of the tetrahedron $T_\Delta$. In this case, the area of the portion of $\Sigma_r$ which lies within $T_\Delta$ is

$$A_{II}(r) = 4\pi \left[ r^2 - 2r(r - h_1) \right]. \quad (13)$$

Finally, we consider the range of values $r \in [h_2, h_3]$, where $h_3 = \frac{\sqrt{6}}{4}$ is the radius of a sphere passing through the vertices of $T_\Delta$. This case is, by far, the most intricate one, where many methods borrowed from spherical trigonometry are employed. In this case the area $A_{III}$ of the part of the sphere $\Sigma_r$ lying within $T_\Delta$ is

$$A_{III}(r) = 4(S_A - 3S_B), \quad (14)$$

where

$$S_A = r^2(3\beta - \pi),$$

$$S_B = r^2 \left[ h(-\pi + 2\sin^{-1}(C_1C_2)) + 2\sin^{-1} \sqrt{\frac{1 - C_1^2 C_2^2}{1 + C_2^2}} \right]. \quad (15)$$

The quantities appearing in the right hand sides of the above expressions are defined by

$$\beta = \cos^{-1} \left[ \frac{\cos A - \cos^2 A}{\sin^2 A} \right]; \quad A = 2\sin^{-1}(D_1/r); \quad D_1 = \frac{1}{2} \left( \frac{1}{2} - \sqrt{r^2 - \frac{1}{8}} \right), \quad (16)$$

and
\[ h = h_1/r; \quad C_1 = \frac{h}{\sqrt{1 - h^2}}; \quad C_2 = \frac{C_B}{\sqrt{1 - C_B^2}}; \]
\[ C_B = \sqrt{\frac{D_2^2 - D_1^2}{r^2 - D_1^2}}; \quad D_2 = r\sqrt{1 - h^2}. \] (17)

Using the relation between \( r \) and the participation rate \( R = 1/Tr(\rho^2) \),
\[ r^2 = -\frac{1}{8} + \frac{1}{2R}, \] (18)
we analytically obtained the probability \( F(R) \) of finding a quantum state with a participation rate \( R \),
\[ F(R) = f(r) \left| \frac{dr}{dR} \right|, \] (19)
where \( f(r) = A(r) / (\text{Volume}[T\Delta]) \), and \( A(r) \) is given by equations (12-14). The distribution \( F(R) \) was first determined numerically by Zyczkowski et al. in [1]. Here we compute \( F(R) \) analytically [? ] and, as expected, the calculations coincide with the concomitant numerical results and the ones reported in [1].

**B. \( \lambda_m \)-domain**

Coming back to two-qubits, the quantity \( \omega_q \) is not appropriately suited to discuss the limit \( q \to \infty \). However, \( \omega_q^{1/q} \) does exhibit a nice behaviour when \( q \to \infty \). Indeed, we have
\[ \lim_{q \to \infty} (Tr\rho^q)^{1/q} = \lim_{q \to \infty} \left( \sum_i p_i^q \right)^{1/q} = \lambda_m, \] (20)
where
\[ \lambda_m = \max \{ p_i \} \] (21)
is the maximum eigenvalue of the density matrix \( \rho \). Hence, in the limit \( q \to \infty \), the \( q \)-entropies (when properly behaving) depend only on the largest eigenvalue of the density matrix. For example, in the limit \( q \to \infty \), the Rényi entropy reduces to
\[ S_{\infty}^{(R)} = -\ln (\lambda_m). \] (22)
It is worth realizing that the largest eigenvalue itself constitutes a legitimate measure of mixture. Its extreme values correspond to (i) pure states ($\lambda_m = 1$) and (ii) the identity matrix ($\lambda_m = 1/4$). It is also interesting to mention that, for states diagonal in the Bell basis, the entanglement of formation is completely determined by $\lambda_m$ (This is not the case, however, for general states of two-qubits systems).

In terms of the geometric representation of the simplex $\Delta$, the set of states with a given value $\lambda_m$ of their maximum eigenvalue is represented by the tetrahedron determined by the four planes

$$\lambda_m = 2(r \cdot r_i) + \frac{1}{4}, \quad i = 1, \ldots, 4. \quad (23)$$

The four vertices of this tetrahedron are given by the intersection points of each one of the four possible triplets of planes that can be selected among the four alluded to planes.

For $q \to \infty$ the accessible states with a given degree of mixture are on the surface of a small tetrahedron $T_i$ concentric with the tetrahedron $T_{\Delta}$. We are going to characterize each tetrahedron $T_i$ (representing those states with a given value of $\lambda_m$) by the distance $l$ between (i) the common centre of $T_{\Delta}$ and $T_i$ and (ii) each vertex of $T_i$. The volume associated with states with a value of $\lambda_m$ belonging to a given interval $\lambda_m$ is proportional to the area $A(l)$ of the portion of $T_i$ lying within $T_{\Delta}$.

Following a similar line of reasoning as the one pursued in the case $q = 2$, we consider three ranges of values for $l$. The first range of $l$-values is given by $l \in [0, h_1/3]$. The particular value $l = h_1/3$ corresponds to a tetrahedron $T_i$ whose vertices are located at the centres of the faces of $T_{\Delta}$. Within the aforementioned range of $l$-values, $T_i$ is lies completely within $T_{\Delta}$. Consequently, $A(l)$ coincides with the area of $T_i$,

$$A_I(l) = 24\sqrt{3}l^2. \quad (24)$$

The second range of $l$-values corresponds to $l \in [h_1/3, h_1]$. The area of the part of $T_i$ lying within $T_{\Delta}$ is now

$$A_{II}(l) = 3\sqrt{3} \left[ 8l^2 - \frac{3}{2}(3l - h_1)^2 \right] \quad (25)$$

Finally, the third range of $l$-values we are going to consider is $l \in [h_1, 3h_1]$. In this case we have
\[ A_{III}(l) = \frac{3}{2} \sqrt{3} (3h_1 - l)^2 \]  

(26)

In a similar way as in the \( q = 2 \) case, the above expressions for \( A(l) \) lead to the analytical form of the probability (density) \( F(\lambda_m) \) of finding a two-qubits state with a given value of its greatest eigenvalue,

\[
F(\lambda_m) = \frac{A(l)}{\text{Volume}[T\Delta]} \left| \frac{dl}{d\lambda_m} \right|. 
\]  

(27)

Remarkably enough, as \( q \) tends to infinity all discontinuities in the derivative of \( F(\lambda_m) \) disappear. In the \( \lambda_m \)-domain the distribution is completely smooth, as opposed to the \( R \)-domain.

IV. ANALYTICAL APPROACH FOR 2X3 SYSTEMS AND HIGHER SYSTEMS

A. \( R \)-domain

Previously, we obtained the distribution \( F(R) \) vs. \( R \) for two-qubits \((N = 4)\), under the assumption that they are distributed according to measure \([4]\). Through a useful analogy, we have mapped the problem into a geometrical one in \( \mathbb{R}^3 \) regarding interior and common sections of two geometrical bodies. In the previous case we saw that the main difficulty lies in the third region, where the region of the growing sphere inside the tetrahedron is not described by a spherical triangle. The extension to higher dimensions, however, requires a thorough account of the geometrical tools required, but still it is in principle possible. So, one can find the distribution of states according to \( R = 1/Tr(\rho^2) \) basically by computing the surface area of a growing ball of radius \( r \) in \( N - 1 \) dimensions (sphere) that remains inside an outer regular \( N \)-polytope \( T\Delta \) (tetrahedron) of unit length, excluding the common regions. A \((N - 1)\)-dimensional sphere can be parameterized in cartesian coordinates.
\[ x_1 = r \sin(\phi_1) \sin(\phi_2) \sin(\phi_3) ... \sin(\phi_{N-3}) \sin(\phi_{N-2}) \]
\[ x_2 = r \sin(\phi_1) \sin(\phi_2) \sin(\phi_3) ... \sin(\phi_{N-3}) \cos(\phi_{N-2}) \]
\[ x_3 = r \sin(\phi_1) \sin(\phi_2) \sin(\phi_3) ... \cos(\phi_{N-3}) \]
\[ ... \]
\[ x_{N-2} = r \sin(\phi_1) \cos(\phi_2) \]
\[ x_{N-1} = r \cos(\phi_1), \quad (28) \]

with the domains \(0 \leq \phi_j \leq \pi\) for \(1 \leq j \leq N - 3\) and \(0 \leq \phi_{N-2} < 2\pi\). The definition of the \(N\)-polytope \(T_\Delta\) then is required. This problem is not trivial at all, because new geometrical situations appear in the intersection of these two bodies. In point of fact there are \(N - 2\) intermediate regimes between \(R = N\) and \(R = 1\) appearing at integer values of \(R\) (recall the previous two-qubits case), where a change in the growth of interior hyper-surfaces occurs (at the values \(r_i = \sqrt{(N - R_i)/2} r_i N, R_i = 1, ..., N\)). In any case we can always generate random states \(\rho\) in arbitrary dimensions and compute the corresponding \(F_N(R)\) distributions. This is done in Fig. 2 for several cases. The relation (18) is generalized to \(N\) dimensions in the form

\[ r^2 = -\frac{1}{2N} + \frac{1}{2R}. \quad (29) \]

The distribution \(F_N(R), R \in [N - 1, N]\) can be obtained analytically

\[ F_N(R) \sim \frac{1}{R^2} \left[ \frac{1}{R} - \frac{1}{N} \right]^{\frac{N-3}{2}} \quad (30) \]

which has been numerically checked. The particular form of \(F(R)\) for arbitrary \(N\) is difficult to obtain, but nevertheless one can obtain quantitative results for asymptotic values of \(N\).

It may be interesting to know the position of the maximum of \(F(R)\) or the mean value \(\langle R \rangle\), which turns to be \(\simeq N/2\) \([10]\) for states \(\rho\) generated according to (4). There is the so called Borel lemma \([11]\) in discrete mathematics that asserts that (translated to our problem) when you grow a \((N - 1)\)-ball inside \(T_\Delta\), from the moment that it swallows, say, 1/2 of the volume of it, then the area outside drops very quickly with further grow. So the maximum intersection with the sphere should be approximately for the radius \(r^*\) where the volume of the ball \(V_{N-1}\) equals that of the \(T_\Delta\)-polytope \(V_T\). The usual formulas for the volumes of
FIG. 2. Plot of the $F_N(R)$ distributions of mixed states $\rho$ numerically computed in arbitrary dimensions, generated according to (??). As we increase the total dimension $N$, the curves become smoother, in correspondence with our geometric interpretation. See text for details.

$(N - 1)$-dimensional spheres and regular unit $N$-polytopes are $V_{N-1} = \frac{\pi^{(N-1)/2}}{\Gamma\left(\frac{N+1}{2}\right)} r^{N-1}$ and $V_T = \frac{1}{(N-1)!} \sqrt{\frac{N}{2^{N-1}}}$, respectively.

It is then that we can assume that the position of $R(r^*) \simeq R'$ such that $F(R = R')$ is maximal. Substituting $r^*$ in (29), and after some algebra, we obtain the beautiful result

$$\lim_{N \to \infty} \frac{1/R(r^*)}{1/N} = \frac{2\pi + e}{2\pi} \simeq 1.43.$$  \hspace{1cm} (31)

In other words, $F_N(1/R) \sim \delta(1/R - 1/N)$ for large $N$.

We must emphasize that this type of distributions $F_N(R)$ are “degenerated” in some cases, that is, different systems may present identical $F(R)$ distributions (for instance, there
is nothing different from this perspective between $2 \times 6$ and $3 \times 4$ systems). We do not know to what extend these distributions are physically representative of such cases, as far as entanglement is concerned. What is certain is that all states $\rho$ with $R \in [N - 1, N]$ possess a positive partial transpose. In point of fact, they are indeed separable, as shown in [12]. We merely mean by this that a state close enough to the maximally mixed state $\frac{1}{N}I_N$ is always separable. In other words, states lying on $(N - 1)$-spheres with radius $r \leq r_c \equiv 1/\sqrt{2N(N - 1)}$ are always separable.

B. $\lambda_m$-domain

When regarding the maximum eigenvalue $\lambda_m$ as a proper degree of mixture one is able to find a geometrical picture analogue to the one of the growing sphere. In that case a nested inverted tetrahedron grows inside the outer tetrahedron representing the simplex of eigenvalues $\Delta$. The generalization to higher bipartite systems is similar to the $R$-case, but far much easier to implement mathematically. As in that case, we have a high degree of symmetry in the problem. The advantage is that one does not deal with curved figures but perfectly flat and sharp surfaces instead. This fact makes the general problem more approachable.

We have seen that the problem of finding how the states of a bipartite quantum mechanical system are distributed according to their degree of mixedness can be translated to the realm of discrete mathematics. If we consider our measure of mixedness to be the maximum eigenvalue $\lambda_m$ of the density matrix $\hat{\rho}$ and the dimension of our problem to be $N = N_A \times N_B$, we compute the distribution of states in arbitrary dimensions by letting an inner regular $N$-polytope $T_l$ to grow inside an outer unit length $N$-polytope $T_\Delta$, the vertices of the former pointing towards the centre of the faces of the latter. In fact, it can be shown that the radius $l$ of the maximum hypersphere that can be inscribed inside the inner polytope is directly related to $\lambda_m$.

By computing the surface area of $T_l$ strictly inside $T_\Delta$, we basically find the desired probability (density) $F_N(\lambda_m)$ of finding a state $\hat{\rho}$ with maximum eigenvalue $\lambda_m$ in $N$ dimensions.

To fix ideas, it will prove useful first to define the vertices of $T_\Delta$ and $T_l$. In fact it is essential, because we need to deal with elements of cartesian geometry in $N$-dimensions. These vectors are given as
\[ \vec{r}_1 = \left( -\frac{1}{2}, -\frac{1}{2\sqrt{3}}, -\frac{1}{4}\sqrt{\frac{2}{3}}, \ldots, -\frac{1}{N-1}\sqrt{\frac{N-1}{2N}} \right) \]
\[ \vec{r}_2 = \left( \frac{1}{2}, -\frac{1}{2\sqrt{3}}, -\frac{1}{4}\sqrt{\frac{2}{3}}, \ldots, -\frac{1}{N-1}\sqrt{\frac{N-1}{2N}} \right) \]
\[ \vec{r}_3 = \left( 0, \frac{1}{\sqrt{3}}, -\frac{1}{4}\sqrt{\frac{2}{3}}, \ldots, -\frac{1}{N-1}\sqrt{\frac{N-1}{2N}} \right) \]
\[ \vec{r}_4 = \left( 0, 0, \frac{3}{4}\sqrt{\frac{2}{3}}, \ldots, -\frac{1}{N-1}\sqrt{\frac{N-1}{2N}} \right) \]
\[ \ldots \]
\[ \vec{r}_N = \left( 0, 0, 0, \ldots, \sqrt{\frac{N-1}{2N}} \right), \] (32)

with \( \sqrt{\frac{N-1}{2N}} \) being the distance from the center to any vertex of this regular \( N \)-polytope of unit length. One can easily check that \( \sum_i \vec{r}_i = \sum_{i,j} \vec{r}_i \cdot \vec{r}_j = 0 \), as required. This particular choice for the position of the vertices of this \( N \)-simplex is such that it simplifies going from one dimension to the next by adding a new azimuthal axis each time. This vectors comply with the relations

\[ \vec{r}_i \cdot \vec{r}_j = -\frac{1}{2N} + \frac{1}{2}\delta_{ij}, \]
\[ \lambda_m = 2(\vec{r} \cdot \vec{r}_i) + \frac{1}{N}, \quad i = 1 \ldots N, \] (33)

where the last equation is the general form of (23).

Once we have a well defined \( T_\Delta \), to know the coordinates of \( T_i \) is straightforward. In fact, \( T_i \) is the reciprocation (see [13]) of \( T_\Delta \). This means that the coordinates of \( T_i \) are obtained by reversing the sign of the ones of \( T_\Delta \), multiplied by a suitable factor (which can be shown to be \( \sqrt{2N(N-1)}l \), with \( l \) defined as the length between the centre of \( T_i \) to the centre of any of its faces, which in turn points towards the vertices of \( T_\Delta \)). Thus, we can relate \( l \) with \( \lambda_m \) through a general (23)-relation \( \lambda_m = 2l \sqrt{\frac{N-1}{2N}} + \frac{1}{N} \), such that \( \frac{dl}{d\lambda_m} = \sqrt{(2N)/(N-1)/2} \).

Several distributions \( F_N(\lambda_m) \) are obtained numerically by generating random states \( \rho \) according to (4) in Fig. 3. It becomes apparent that as \( N \) grows, the distributions are biased towards \( \lambda \simeq 1/N \), in absolute agreement with the result (31).

As in the \( R \)-case, \( F_N(\lambda_m) \) is distributed into \( N-1 \) regions separated at fixed values of \( \lambda_m^{(i)} = \frac{1}{N-i}, \ i = 1..(N-2) \). The general recipe for obtaining \( F_N(\lambda_m) \) is tedious and long,
FIG. 3. Plot of the $F_N(\lambda_m)$ distributions of mixed states $\rho$ numerically computed in arbitrary dimensions, generated according to (4). As we increase the total dimension $N$, the curves tend to peak around $1/N$. See text for details.

but some nice general results are obtained. The $F_N(\lambda_m)$-distributions for the ranges a) $\lambda_m \in [\frac{1}{N}, \frac{1}{N-1}]$ and b) $\lambda_m \in [\frac{1}{2}, 1]$ are general and read

$$F_I(\lambda_m) = \kappa \frac{N}{(N-2)!} \sqrt{\frac{N-1}{2^{N-2}}} \left[ \sqrt{2N(N-1)} l(\lambda_m) \right]^{N-2},$$

$$F_{Last}(\lambda_m) = \kappa \frac{N}{(N-2)!} \sqrt{\frac{N-1}{2^{N-2}}} \left[ \frac{\sqrt{\frac{N-1}{2N}} - l(\lambda_m)}{\sqrt{\frac{N}{2(N-1)}}} \right]^{N-2},$$

respectively, where $\kappa \equiv \frac{dl}{d\lambda_m} / \text{Volume}[T_{\Delta}]$ is introduced for convenience.

For the qubit-qutrit system, we have ($N = 6$). Defining $r_i \equiv \sqrt{\frac{N-1}{2N}}$ and $y_i \equiv (l(\lambda_m)(N -$
1) \( -\frac{1}{\sqrt{N-1}}r_i \), in addition to the previous regions \([34]\) we obtain

\[
F_{II}(\lambda_m) = \kappa \left[ \frac{F_I(\lambda_m)}{\kappa} - \frac{(N-1)N}{(N-2)!} \sqrt{\frac{N-1}{2N^2-2}} [y_i=1]^{N-2} \right];
\]

\[
F_{III}(\lambda_m) = \kappa \left[ \frac{F_{II}(\lambda_m)}{\kappa} + \frac{2^9 (N-1)N}{54 (N-2)!} \sqrt{\frac{N-1}{2N^2-2}} [y_i=2]^{N-2} \right];
\]

\[
F_{IV}(\lambda_m) = \kappa \left[ \frac{F_{III}(\lambda_m)}{\kappa} - \frac{2^3 (N-1)N}{54 (N-2)!} \sqrt{\frac{N-1}{2N^2-2}} [y_i=3]^{N-2} \right],
\]  

(35)

for \( \lambda_m \in \left[ \frac{1}{5}, \frac{1}{4}, \frac{1}{3} \right], \) and \( \left[ \frac{1}{3}, \frac{1}{2} \right], \) respectively. From the previous formulas one can infer a general induction procedure. Analytical results are in excellent agreement with numerical generations.

V. NON-UNIQUENESS OF A GENERAL MEASURE FOR MIXED STATES. GEOMETRIC IMPLICATIONS

In Refs. [1, 3], a basic question regarding a natural measure \( \mu \) for the set of mixed states \( \rho \) was debated. As described in Secs. (7.1) and (9.1), it is know, the set of all states \( \mathcal{S} \) can be regarded as the cartesian product \( \mathcal{S} = \mathcal{P} \times \Delta \), where \( \mathcal{P} \) stands for the family of all complete sets of orthonormal projectors \( \{\hat{P}_i\}_{i=1}^N \), \( \sum_i \hat{P}_i = I \) (\( I \) being the identity matrix), and \( \Delta \) is the set of all real \( N \)-tuples \( \{\lambda_1, \ldots, \lambda_N\} \), with \( \lambda_i \geq 1 \) and \( \sum_i \lambda_i = 1 \). It is universally accepted to assume the Haar measure \( \nu \) to be the one defined over \( \mathcal{P} \), because of its rotationally-invariant properties. But when it turns to discuss an appropriate measure over the simplex \( \Delta \), some controversy arises. In all previous considerations here, we have regarded the Lebesgue measure \( \mathcal{L}_{N-1} \) as being the “natural” one. But one must mention that Slater has argued [14, 15] that, in analogy to the classical use of the volume element of the Fisher information metric as Jeffreys’ prior [16] in Bayesian theory, a natural measure on the quantum states would be the volume element of the Bures metric. The problem lies on the fact that there is no unique probability distribution defined over the simplex of eigenvalues \( \Delta \) of mixed states \( \rho \). In point of fact, the debate was motivated by the fact that the volume occupied by separable two-qubits states was found in [1] to be greater than 50\% \( (P_{sep} = 0.6312) \) using the measure \( \mu \), something which is surprising.

One such probability distribution that is suitable for general considerations is the Dirichlet distribution [3]
\[ P_\eta(\lambda_1, \ldots, \lambda_N) = C_\eta \lambda_1^{\eta-1} \lambda_2^{\eta-1} \ldots \lambda_N^{\eta-1}, \quad (36) \]

with \( \eta \) being a real parameter and \( C_\eta = \frac{\Gamma[N\eta]}{\Gamma[\eta^N]} \) the normalization constant. This is a particular case of the more general Dirichlet distribution. The concomitant probability density for variables \((\lambda_1, \ldots, \lambda_N)\) with parameters \((\eta_1, \ldots, \eta_N)\) is defined by

\[ P_\eta(\lambda_1, \ldots, \lambda_N) = C_\eta \lambda_1^{\eta_1-1} \lambda_2^{\eta_2-1} \ldots \lambda_N^{\eta_N-1}, \quad (37) \]

with \( \lambda_i \geq 0, \sum_{i=1}^N \lambda_i = 1 \) and \( \eta_1, \ldots, \eta_N > 0 \), and \( C_\eta = \Gamma(\sum_{i=1}^N \eta_i)/\prod_{i=1}^N \Gamma(\eta_i) \). Clearly, distribution (37) generalizes (36). This distribution admits a clear interpretation. As known, the multinomial distribution provides a probability of choosing a given collection of \( M \) items out of a set of \( N \) items with repetitions, the probabilities being \((\lambda_1, \ldots, \lambda_N)\). These probabilities are the parameters of the multinomial distribution. The Dirichlet distribution is the conjugate prior of the parameters of the multinomial distribution.

A new measure then can be defined as \( \mu_\eta = \nu \times \Delta_\eta \), where \( \Delta_\eta \) denotes the simplex of eigenvalues distributed according to (36) (The Haar measure \( \nu \) remains untouched). Thus, one clearly recovers the Lebesgue measure \( L_{N-1} \) for \( \eta = 1 \) (uniform distribution), and Slater’s argumentation reduces to take \( \eta = \frac{1}{2} \) in (36). For \( \eta \to 0 \) one obtains a singular distribution concentrated on the pure states only, while for \( \eta \to \infty \), the distribution peaks on the maximally mixed state \( \frac{1}{N} I \). We will see shortly that changing the continuous parameter \( \eta \) indeed modifies the average purity (as expressed in terms of \( R = 1/\text{Tr}(\rho^2) \)) of the generated mixed states.

In what follows we numerically generate mixed states whose eigenvalues are distributed following (36). This is done in order to tackle the dependence of relevant quantities on the parameter \( \eta \). Let us consider the way mixed states are distributed according to \( R \). We focus our attention on the two-qubits instance, but similar studies can be extended to arbitrary bipartite dimensions. As shown in Fig. 4, the distributions \( P(R) \) vs. \( R \) are shown for \( \eta = \frac{1}{2}, 1, 2 \) (from left to right in this order) while Fig. 5 shows analogous distributions for the maximum eigenvalue \( \lambda_m \) for \( \eta = \frac{1}{2}, 1, 2 \) (from right to left). Notice the different shapes. We can no longer attribute a geometrical description to \( P(R) \) except for \( \eta = 1 \). In \( \text{[3]} \) \( P(R) \) for \( \eta = \frac{1}{2} \) was first derived. Here we can provide different distributions for arbitrary \( \eta \)-values.

A way to devise a certain range of reasonable \( \eta \)-values is to study the average \( R \) induced
FIG. 4. \( P(R) \) vs. \( R \) distributions for two qubit systems, whose eigenvalues are distributed according to (36), for the values \( \eta = \frac{1}{2}, 1, 2 \) (from left to right in this order). It is plain from this figure that the uniform distribution \( (\eta = 1) \) appears more balanced than the others. Also, the particularity of \( R = 2, 3 \) seems to disappear for \( \eta > 1 \). See text for details.

for every \( \eta \)-distribution. This is performed in Fig. 6. The average \( R \)-value \( \langle 1/\text{Tr}(\rho^2) \rangle \) and \( R^* \equiv 1/\langle \text{Tr}(\rho^2) \rangle \) are plotted versus \( \eta \). \( \langle R \rangle \) (solid line) can only be computed numerically, but luckily \( R^* \) (dashed line) is obtained in analytical fashion for all \( N \)

\[
\langle \text{Tr}\rho^2 \rangle_N(\eta) = C_\eta \int_0^{1/\eta} d\lambda_1 \lambda_1^{\eta-1} \int_0^{1-\lambda_1} d\lambda_2 \lambda_2^{\eta-1} \ldots \int_0^{1-\sum_{i=2}^{N-2} \lambda_i} d\lambda_{N-1} \lambda_{N-1}^{\eta-1} (1 - \sum_{i=1}^{N-1} \lambda_i)^{\eta-1} \left[ \sum_{j=1}^N \lambda_j^2 \right] = \left[ N - \frac{N - 1}{\eta + 1} \right]^{-1}. \tag{38}
\]

The fact that \( R^* \) matches exact results validates all our present generations. The actual value
FIG. 5. Probability (density) distributions of the maximum eigenvalue $\lambda_m$ of two qubit systems, whose eigenvalues are distributed according to (36), for the values $\eta = \frac{1}{2}, 1, 2$ (from right to left).

When employing $\lambda_m$ as a degree of mixture, the derivative of these distributions is discontinuous at the special values $\lambda_m = \frac{1}{2}, \frac{1}{3}$ for $\eta < 1$. See text for details.

$\langle R \rangle$ is slightly larger than $R^*$ for all values of $\eta$, but both of them coincide for low and high values of the parameter $\eta$. It is obvious from Fig. 6 that we cannot choose distributions that depart considerably from the uniform one $\eta = 1$, because in that case we induce probability distributions that favor high or low $R$ already.

Perhaps the best way is to go straight to the question that originated the controversy on the $\Delta$-measures: what is the dependency of the a priori probability $P_{\text{sep}}$ of finding a two-qubits mixed state being separable? In Fig. 7 we depict $P_{\text{sep}}$ vs. $\eta$ for states complying with PPT (lower curve) and those which violate the $q = \infty$-entropic inequalities (upper
FIG. 6. Average $R$-value $\langle 1/Tr(\rho^2) \rangle$ (solid line) and $R^* \equiv 1/\langle Tr(\rho^2) \rangle$ (dashed line) for two qubit and one qubit-qutrit systems, plotted versus the Dirichlet parameter $\eta$. See text for details.

curve). It seems reasonable to assume that a permissible range of $\eta$-distributions belong to the interval $[\frac{1}{2}, 2]$, within which $P_{sep}$ remains around the reference point $P_{sep} = 0.5$.

However, in view of the previous outcomes we believe that the results obtained considering the uniform $\eta = 1$-distribution for the simplex $\Delta$ (the one that allow us to exploit a simple geometric analogy) remains the most natural choice possible, independent of any form that one may adopt for a generic probability distribution.

VI. CONCLUSIONS

We have introduced a geometric picture to obtain the probability $F$ of finding quantum states of two-qubits with a given degree of mixture (as measured by an appropriate function
FIG. 7. Probability of finding a state $\rho$ of two-qubits being positive partial transposed (lower curve), and violating the strongest entropic criterion $q = \infty$ (upper curve). This figure illustrates the fact that one can arbitrarily choose any $P_{sep}$ by generating two qubit mixed states with different Dirichlet parameter $\eta$. See text for details.

of $\omega_q$) is analytically found for $q = 2$ and $q \to \infty$. In the latter case, the $q$-entropies become functions of the statistical operator’s largest eigenvalue $\lambda_m$. In point of fact, $\lambda_m$ itself constitutes a legitimate measure of mixture. During the derivation of the probability (density) distributions $F_N$ of finding a bipartite mixed state in arbitrary dimensions $N = N_A \times N_B$ with a given degree of mixture, we saw that it is more convenient to use $\lambda_m$ instead of $R$. Finally, we have derived explicitly the distribution $F_N(\lambda_m)$ vs. $\lambda_m$ for the physical meaningful case of a qubit-qutrit system ($N = 6$).
ACKNOWLEDGEMENTS

J. Batle acknowledges partial support from the Physics Department, UIB. J. Batle acknowledges fruitful discussions with J. Rosselló, Maria del Mar Batle and Regina Batle.

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