Volume of the set of separable states. II

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The problem of how many entangled or, respectively, separable states there are in the set of all quantum states is investigated. We study to what extent the choice of a measure in the space of density matrices ϱ describing N-dimensional quantum systems affects the results obtained. We demonstrate that the link between the purity of the mixed states and the probability of entanglement is not sensitive to the measure chosen. Since the criterion of partial transposition is not sufficient to distinguish all separable states for $N \geqslant 8$, we develop an efficient algorithm to calculate numerically the entanglement of formation of a given mixed quantum state, which allows us to compute the volume of separable states for $N=8$ and to estimate the volume of the bound entangled states in this case. [S1050-2947(99)05110-0]

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I. INTRODUCTION

Entangled states have been known almost from the very beginning of quantum mechanics and their somewhat unusual features have been investigated for many years. However, recent developments in the theory of quantum information and quantum computing have caused a rapid increase in the interest in the study of their properties and possible applications. To illustrate this trend let us quote some data from the Los Alamos quantum physics archives. In 1994 only one paper posted in these archives contained the key word ''entangled'' (or entanglement) in the title, while two such papers were posted in 1995. Since then the number of such papers has increased dramatically, and was equal to 8, 30, and 70 in the consecutive years 1996, 1997, and 1998, respectively.

We do not dare fit some fast growing curves to these data nor speculate when such an increase will eventually saturate. On the other hand, since so many authors have dealt with entangled states, it is legitimate to ask whether such states are ''typical'' in quantum theory or if they are rather rare and unusual. Vaguely speaking, we shall be interested in the relative likelihood of encountering an entangled state [1]. One may also ask a complementary question concerning the set of *separable* states, that can be represented as a sum of product states.

Consider a quantum system described by the density matrix ρ that represents a mixture of the pure states of the N-dimensional Hilbert space. Let us assume that the system consists of two subsystems, of dimension n_A and n_B, where $N=n_A n_B$. To formulate the basic question, ''*What is the probability of finding an entangled state of size N?*,'' one needs to:

(i) Define the probability measure μ, according to which the random density matrices ρ are drawn.

(ii) Find an efficient technique, which would allow one to judge whether a given mixed state ρ is entangled.

Representing any density matrix in the diagonal form $\rho = UdU^\dagger$ we proposed [1] to use a product measure $\mu=\Delta_1 \times \nu$, where Δ_1 describes the uniform measure on the simplex $\Sigma_{i=1}^{N} d_i=1$ and ν stands for the Haar measure in the space of unitary matrices $U(N)$. Based on the partial transposition criterion [2,3], we found that under this measure the volume of the set of separable states is positive and decreases with the system size N [1]. Some more general analytical bounds were also provided by Vidal and Tarrach [4]. Recently, Slater suggested estimating the same quantity using some other measures in the space of the density matrices [5,6]. One may thus expect that the volume of the separable states depends on the measure chosen. We show that this is indeed the case. In this work we investigate which statistical properties describing the set of the entangled states may be universal; e.g., which do not depend on the measure used. In particular, we demonstrate that the relation between the purity of mixed states and the probability of entanglement is not very sensitive to the measure assumed. Based on numerical results we conjecture that the volume of the separable states decreases exponentially with the system size N.

For $N=4$ and $N=6$ a density matrix is separable if and only if its partial transpose is positive [3]. For $N>6$, however, there exist states that are not separable and that do satisfy this criterion [7]. These states cannot be distilled into the singlet form and are called *bound entangled states* [8–11]. Since there are no explicit conditions allowing one to distinguish between separable and bound entangled states, in Ref. [1] only the upper bound for the volume of separable states has been considered for $N>6$. In this paper we present an efficient numerical method of computing the *entanglement of formation E* [12] for any density matrix. This method allows us to estimate the volume of bound entangled states, by taking a reasonably small cutoff entanglement E_c and counting these states, satisfying the partial transposition criterion for which $E>E_c$. Our numerical results are to a large extent independent of the exact value of E_c.

The paper is organized as follows. In Sec. II we review the necessary definitions and study how the upper bound of the volume of the separable states depends on the system size and the measure used. The subsequent section is devoted to an analysis of the simplest case $N=4$, for which the bound entangled states do not exist. In this case the analytical formula for the entanglement of formation is known [13,14] and we study how this quantity changes with the purity of the mixed states. In Sec. IV we study the case N

=8 and estimate the volume of the free entangled states, bound entangled states, and separable states. The paper is concluded by Sec. V, containing a list of open questions. In Appendix A we prove the rotational invariance of the two distinguished measures Δ_o and Δ_u, defined on the $(N-1)$-dimensional simplex, and demonstrate the link to the ensembles of random matrices. The algorithm of computing the entanglement of formation for a given density matrix is presented in Appendix B.

II. VOLUME OF STATES WITH POSITIVE PARTIAL TRANSPOSITION

A. Product measures in the space of mixed density matrices

To discuss the probability of a mixed quantum state possessing a given property, one needs to define a probability measure μ in the space of density matrices ($N\times N$ positive Hermitian matrices with trace equal to unity). Each density matrix can be diagonalized by a unitary rotation. Let B be a diagonal unitary matrix. Since

$$\rho=UdU^{\dagger}=UBdB^{\dagger}U^{\dagger}, \tag{1}$$

the rotation matrix U is determined up to N arbitrary phases entering B. The total number of independent variables used to parametrize in this way any density matrix ρ is equal to N^2-1. Since the literature seemed not to distinguish any natural measure in this space, we approached the problem by defining a product measure [1]

$$\mu_u=\Delta_1\times\nu_H. \tag{2}$$

The measure ν is defined in the space of unitary matrices $U(N)$, while Δ is defined in the $(N-1)$-dimensional simplex determined by the trace condition $\Sigma_{i=1}^{N}d_i=1$. In Ref. [1] we took for ν the Haar measure on $U(N)$, while the uniform measure Δ_1 was used on the simplex. Our choice was motivated by the fact that both component measures are rotationally invariant. For ν_H this follows directly from the definition of the Haar measure, while in Appendix A we prove that the uniform measure Δ_1 corresponds to taking, for the vector d_i, the squared moduli of complex elements of a column or a row (say, the first column) of an auxiliary random unitary matrix V drawn with respect to ν_H,

$$d_i=|V_{i1}|^2. \tag{3}$$

Hereafter we will thus refer to the measure defined by Eq. (2) as the unitary product measure μ_u.

As correctly pointed out by Slater [5,6], our choice of measure is by far not the only possible one. He discussed several possible measures, and proposed picking the measure on the $(N-1)D$ simplex from a certain family of Dirichlet distributions,

$$\Delta_\lambda(d_1,\dots,d_{N-1})=C_\lambda d_1^{\lambda-1}\dots d_{N-1}^{\lambda-1}\times(1-d_1-\cdots-d_{N-1})^{\lambda-1}, \tag{4}$$

where $\lambda>0$ is a free parameter and C_λ stands for a normalization constant. The last component is determined by the trace condition $d_N=1-d_1-\cdots-d_{N-1}$. The uniform measure Δ_1 corresponds to $\lambda=1$. Slater distinguishes also the case $\lambda=1/2$, which is related to the Fisher information metric [15], the Mahalonobis distance [16], and Jeffreys' prior distance [17], and was used for many years in different contexts [18–20]. Since this measure is induced by squared elements of a column (a row) of a random *orthogonal* matrix (see Appendix A), we shall refer to

$$\mu_o:=\Delta_{1/2}\times\nu_H \tag{5}$$

as to the orthogonal product measure in the space of the mixed quantum states. Therefore, both measures may be directly linked to the well-known Gaussian unitary (orthogonal) ensembles of random matrices [21], referred to as GUE (GOE). The measure μ_u is determined by squared components of an eigenvector of a GUE matrix, while the measure μ_o may be defined by components of an eigenvector of GOE matrices [22]. Some properties of the orthogonal measure μ_o have recently been studied in [23]. Let us stress that the name of the product measure (orthogonal or unitary) is related to the distribution Δ on the simplex $\vec{d}$, while the random rotations U are always assumed to be distributed according to the Haar measure ν_H in $U(N)$.

It is interesting to consider the limiting cases of the distribution (4). For $\lambda\to0$ one obtains a singular distribution concentrated on the pure states only [6], while in the opposite limit $\lambda\to\infty$, the distribution peaks on the maximally mixed state ρ_* described by the vector $\vec{d}=\{1/N,\dots,1/N\}$. Changing the continuous parameter λ, one can thus control the average purity of the generated mixed states.

B. Separable states

Consider a composite quantum system described by the density matrix ρ in the N-dimensional Hilbert space $\mathcal{H}=\mathcal{H}_A\otimes\mathcal{H}_B$. The dimension of the system N is equal to the product n_An_B of the dimensions of both subsystems. If the state $\rho\in\mathcal{H}$ can be expressed as $\rho=\rho_A\otimes\rho_B$, with $\rho_A\in\mathcal{H}_A$ and $\rho_B\in\mathcal{H}_B$, it is called the *product* state (or factorizable state). This occurs if and only if $\rho=\mathrm{Tr}_B\rho\otimes\mathrm{Tr}_A\rho$, where Tr_A and Tr_B denote the operations of partial tracing. In other words, for such states the description of the composite state is equivalent to the description in both subsystems.

A given quantum state ρ is called *separable* if it can be represented by a sum of product states [24]

$$\varrho=\sum_{i=1}^{k}p_i\varrho_{Ai}\otimes\tilde{\varrho}_{Bi}, \tag{6}$$

where ϱ_{Ai} and ϱ_{Bi} are the states on $\mathcal{H}_B$ and $\mathcal{H}_B$, respectively. The smallest number k of product states used in the above decomposition is called the *cardinality* of the separable state ρ [25].

In general, no explicit necessary and sufficient conditions are known for a mixed state to be separable. However, Peres found a necessary condition showing that each separable state has the positive partial transpose [2]. Later Horodeccy

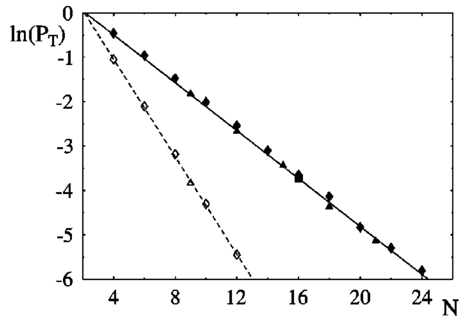

FIG. 1. Probability P_T of finding a state with positive partial transpose as a function of the dimension of the problem N for the unitary product measure (open symbols) and for the orthogonal product measure (full symbols). For $N \leqslant 6$, it is equal to the probability P_S of finding a separable state, while for $N > 6$ it gives an upper bound for this quantity. Different symbols distinguish different sizes of one subsystem: $n_A = 2$ ($\diamond$), 3 ($\triangle$), and 4 ($\square$).

demonstrated that for $N=4$ and $N=6$ this is also a sufficient condition [3]. To represent any state ρ it is convenient to use an arbitrary orthonormal product basis $|e_j\rangle \otimes |e_l\rangle$, $j = 1,\ldots,n_A$, $l = 1,\ldots,n_B$; and to define the matrix $\rho_{jl,j'l'} = \langle e_j| \otimes \langle e_l|\rho|e'_j\rangle \otimes |e'_l\rangle$. The operation of *partial transposition* is then defined [2] as

$$\varrho^{T_2}_{jl,j'l'} \equiv \varrho_{jl',j'l}. \tag{7}$$

Even though the matrix ρ^{T_2} depends on the particular base used, its eigenvalues $\{d'_1 \geqslant d'_2 \geqslant, \ldots, \geqslant d'_N\}$ do not. The matrix ρ^{T_2} is positive if and only if all eigenvalues d'_i are not negative. The practical application of the partial transpose criterion is thus straightforward: for a given state ρ, one computes ρ^{T_2}, diagonalizes it, and checks the signs of all eigenvalues. To characterize quantitatively the violation of positivity we introduced [1] the negativity

$$t := \sum_{i=1}^{N} |d'_i| - 1, \tag{8}$$

which is equal to zero for all of the states with positive partial transpose.

C. Relative volume in the space of the density matrices

In Ref. [1] we presented several analytical lower and upper bounds for the volume of separable states. They were obtained assuming the unitary product measure, but the same reasoning can be repeated for other measures. The key result: an analytical proof that the volume of separable states is positive and less than 1 is obviously valid for any nonsingular measure.

To analyze the influence of the measure chosen for the volume of separable states P_s we picked several random density matrices (ca. 10^6) distributed according to the orthogonal and unitary product measures, and verified that their partial transpose (7) was positive. The results are displayed in Fig. 1 as a function of the system size N. Note that for $N > 6$ we obtained in this way the volume P_T of states with positive partial transposition, which gives an upper bound for the volume of separable states. In fact, $P_T = P_S + P_B$, where the volume P_B of the entangled states with positive partial transpose is studied in Sec. IV.

TABLE I. Probability P_T of finding a mixed state of size N with positive partial transpose and the mean negativity $\langle t\rangle$ for two product measures orthogonal μ_o and unitary μ_u. For $N=4$ and $N=6$ one has $P_T = P_S$.

N	n_A	n_B	$\langle P_T\rangle_{\mu_u}$	$\langle t\rangle_{\mu_u}$	$\langle P_T\rangle_{\mu_o}$	$\langle t\rangle_{\mu_o}$
4	2	2	0.632	0.057	0.352	0.142
6	2	3	0.384	0.076	0.122	0.182
8	2	4	0.229	0.082	0.042	0.204
9	3	3	0.166	0.094	0.022	0.238
10	2	5	0.134	0.097	0.013	0.217
12	2	6	0.079	0.098	0.0043	0.226
12	3	4	0.071	0.098	0.0039	0.266

The symbols are labeled according to the size of the first subsystem n_A. For both measures the symbols seem to lie on one curve, which would imply that $P_T(n_A, n_B) = P_T(n_A \times n_B)$. However, this relation is only approximate, since $P_T(2\times 6) \neq P_T(3\times 4)$, as pointed out by Smolin [26]. Numerical results for P_T and $\langle t\rangle$ for $N \leqslant 12$ are collected in Table I. The difference between $P_T(2\times 6)$ and $P_T(3\times 4)$ is not large, and was smaller than the statistical error of the results reported in [1]. Therefore it is reasonable to neglect for a while these subtle effects, depending on the way the N-dimensional system is composed, and to ask, how, in a first approximation, P_T changes with N.

Figure 1, produced in a semilogarithmical scale, shows that for both measures the probability P_T decreases exponentially with the system size N. Obtained numerical results allow us to conjecture that $\lim_{N\to\infty} P_T(N) = 0$ for any (nonsingular) probability measure used. We observe different slopes of both lines received for different probability measures. The best fit gives $P_{Tu} \sim 1.8e^{-0.26N}$ for the unitary product measure μ_u and $P_{To} \sim 3.0e^{-0.55N}$ for the orthogonal product measure μ_o. The dependence of the probability P_T on the chosen measure is due to the fact that each measure distinguishes states of a different purity. This issue is discussed in detail in the following sections.

III. 2×2 CASE: POSITIVE PARTIAL TRANSPOSE ASSURES SEPARABILITY

A. Purity versus separability

For the $N=4$ case the partial transpose criterion is sufficient to assure the separability [3], so $P_B = 0$ and $P_S = P_T$. Let us investigate how the probability of drawing a separable state changes with its purity, which may be characterized by the von Neumann entropy $H_1(\varrho) = -\operatorname{Tr}(\varrho \ln \varrho)$. Another quantity, called the participation ratio

$$R(\varrho) = \frac{1}{\operatorname{Tr}(\varrho^2)}, \tag{9}$$

is often more convenient for calculations. It varies from unity (for pure states) to N (for the totally mixed state ρ_*

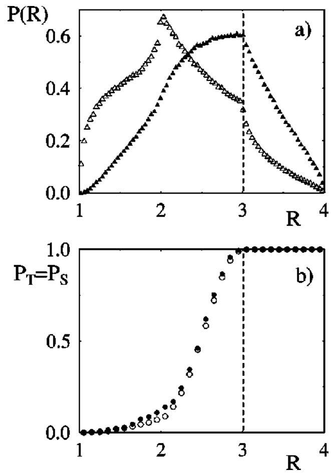

FIG. 2. Purity and separability in $(N=4)$-dimensional Hilbert space. Open symbols represent averaging over the orthogonal product measure μ_o, while closed symbols are obtained with the unitary measure μ_u; (a) probability distributions $P(R)$; (b) conditional probability of finding a separable state as a function of the participation ratio R. All states beyond the dashed vertical line placed at $R=N-1=3$ are separable.

proportional to the identity matrix $\mathbf{I}$) and may be interpreted as an effective number of states in the mixture. This quantity gives a lower bound for the rank r of the matrix ρ, namely, $r \geqslant R$. Moreover, it is related to the von Neumann–Renyi entropy of order 2, $H_2(\varrho)=\ln R(\varrho)$. The latter, also called the purity of the state; together with other quantum Renyi entropies,

$$H_q(\varrho)=\frac{1}{1-q}\ln[\mathrm{Tr}\,\varrho^q] \tag{10}$$

is used, for $q \neq 1$, as a measure of how much a given state is mixed (see, e.g., [27]). Subspaces of a constant R belong to hypersheres centered at ϱ_k of the radius $\sqrt{1/R-1/N}$.

Figure 2 presents the probability distributions $P(R)$ for $N=4$ density matrices generated according to both product measures. As discussed before, the orthogonal measure μ_o is concentrated at the less mixed states (lower values of R) than the unitary measure μ_u. For example, the mean value averaged over the orthogonal product measure $\langle R\rangle_o \approx 2.184$ is much smaller than the corresponding mean with respect to the unitary measure $\langle R\rangle_u \approx 2.653$. Observe a nonsmooth behavior of both distributions at $R=3$ $(R=2)$, for which the manifolds of a constant R start to touch the faces (edges) of the three-dimensional (3D) simplex formed by d_1, d_2, and d_3.

Although the distributions $P(R)$ differ considerably for both measures, the conditional probability of encountering the separable state $P_S(R)$ is almost measure independent, as shown in Fig. 2(b). This is the main result of this section: the different results obtained for the probability P_S of using various product measures μ_λ are due to the different weights attributed to the mixed states. Since the average mixture $\langle R\rangle_{\mu_\lambda}$ grows monotonically with the parameter λ (from 1 for $\lambda \to 0$ to 4 for $\lambda \to \infty$), the probability P_S also increases with this parameter from zero to unity. Note that for both curves the probability P_S achieves unity at $R=3$: all sufficiently mixed states are separable. This fact has already been proved in [1], but see also [28] for complementary, constructive results.

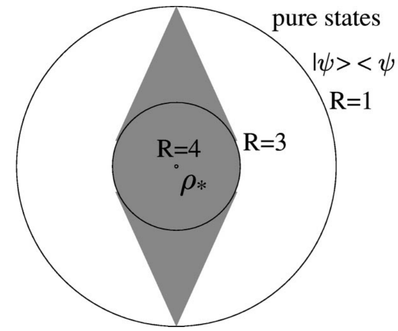

FIG. 3. Sketch of the set of mixed quantum states for $N=4$. The gray color represents the separable states.

The above considerations allow us to sketch the set of entangled states in the case $N=4$. In analogy to the Bloch sphere, corresponding to $N=2$, we take the liberty to depict the set of all quantum states by a ball. Since it is hardly possible to draw a picture precisely representing the complex structure of the 15-dimensional space of the density matrices, Fig. 3 should be treated cautiously. In particular, the structure of the set of density matrices is not as simple, and there exist several points inside the ball that do not correspond to density matrices. Furthermore, the six-dimensional space of the pure states possesses the structure of the complex projective space CP^3, which is much more complicated than a hypersphere. In the sense of the Hilbert–Schmidt metric $(\Delta_{HS}(\rho_1,\rho_2)=\sqrt{\mathrm{Tr}[(\rho_1-\rho_2)^2]})$ the set of pure states forms a six-dimensional subset of the 14-dimensional hypersphere of a radius $\sqrt{3}/2$ centered at $\rho_*=\mathbf{I}/4$. Keeping this fact in mind, we represent this manifold by a circle in our oversimplified two-dimensional sketch.

The set of separable states is visualized in Fig. 3 as the ''needle of a compass:'' it is convex, has a positive measure, and includes the vicinity of the maximally mixed state ρ_*. Moreover, it touches the manifold of pure states (pure separable states do exist), but the measure of this common set is equal to zero. The more mixed the state (localized closer to the center of the ''ball''), the larger the probability of encountering a separable state. All states with $R \geqslant 3$ are separable; this hypershere s^{14} of the radius $1/2\sqrt{3}$ is represented by a smaller circle.

B. Entanglement of formation

After discussing the problem of how the probability of encountering a separable state changes with the degree of mixing R, we may discuss a related issue: how the average the entanglement depends on R. For this purpose we need a quantitative measure of the entanglement of a given mixed state. Several such quantities have recently been proposed and analyzed [12,29–39], and none of them can be considered as the unique, canonical measure. However, the quantity called *entanglement of formation* [12] plays an important role, due to a simple interpretation: it gives the minimal amount of entanglement necessary to create a given density matrix.

For a pure state $|\psi\rangle$, one defines the von Neuman entropy of the reduced state,

$$E(\psi) = -\operatorname{Tr}\rho_A \ln \rho_A = -\operatorname{Tr}\rho_B \ln \rho_B, \tag{11}$$

where ρ_A is the partial trace of $|\psi\rangle\langle\psi|$ over the subsystem B, while ρ_B has the analogous meaning. This quantity vanishes for a product state. The entanglement of formation of the mixed state ρ is then defined [12] as

$$E(\rho) = \min \sum_{i=1}^{k} p_i E(\Psi_i), \tag{12}$$

and the minimum is taken over all possible decompositions of the mixed state ρ into pure states

$$\rho = \sum_{i=1}^{k} p_i |\Psi_i\rangle\langle\Psi_i|, \quad \sum_{i=1}^{k} p_i = 1. \tag{13}$$

The decomposition of ρ into the smallest possible number of k pure states, for which this minimum is achieved, will be called *optimal decomposition*, while the number k will be called the *cardinality* of an entangled state. This definition may be considered as an extension of the concept of the cardinality of separable states introduced in [25], since for any separable state ρ_S one has $E(\rho_S) = 0$.

In Appendix B we present an algorithm allowing one to perform the minimization crucial to the definition (12). It gives an upper estimate of the entanglement of formation for an arbitrary density matrix of size N. The algorithm proposed works fine for N of the order of 10 or smaller. In the case of two quantum bits (qubits), discussed in this section, an analytical solution was found by Hill and Wootters [13,14], who introduced the concept of *concurrence*.

For any 4×4 density matrix ρ one defines the flipped state $\tilde{\rho} = O\rho^* O^T$, where ρ^* denotes the complex conjugation, and the orthogonal flipping matrix O contains only four nonzero elements along the antidiagonal: $O_{14} = O_{41} = 1$ and $O_{23} = O_{32} = -1$. The concurrence $C(\rho)$ is then defined [13]

$$C(\rho) := \max\{0, \alpha_1 - \alpha_2 - \alpha_3 - \alpha_4\}, \tag{14}$$

where α_i's are the eigenvalues, in decreasing order, of the Hermitian matrix $\sqrt{\sqrt{\rho}\tilde{\rho}\sqrt{\rho}}$. Note that this matrix determines the Bures distance [40] between ρ and $\tilde{\rho}$. In other words, α_i's are the non-negative square roots of the moduli of the complex eigenvalues of the non-Hermitian matrix $\rho\tilde{\rho}$.

The concurrence C of a given state ρ determines its entanglement of formation [13,14],

$$E(\rho) = h\left(\frac{1}{2}\left[1 + \sqrt{1 - C^2(\rho)}\right]\right), \tag{15}$$

where

$$h(x) := -x\ln(x) - (1-x)\ln(1-x) \tag{16}$$

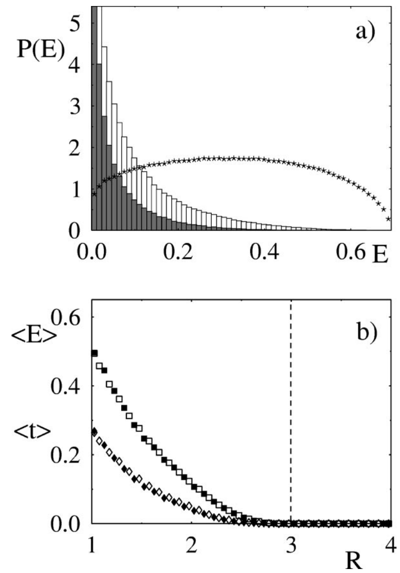

FIG. 4. The 2×2 system. (a) The distributions $P(E)$ of the entanglement of formation obtained for the density matrices generated according to μ_o (white histogram, open symbols) and μ_u (gray histogram, closed symbols), and the rotationally uniform distribution in the set of pure states (*); (b) average entanglement $E(R)$ (squares) and average negativity $t(R)$ (diamonds) for both measures μ.

is the Shannon entropy of the two-element partition $\{x, 1-x\}$.

Note that in the definition of entropy (11) the natural logarithm was used (in contrast to the binary logarithm present in [13]), so the entanglement $E \in [0, \ln 2]$. Two histograms in Fig. 4 present the probability distribution $P(E)$ obtained for $N=4$ random density matrices distributed according to both product measures μ_o and μ_u. The singular peak at $E=0$, corresponding to the separable states, is omitted. Large entanglements of formation are rather unlikely. The mean values are not large: $\langle E\rangle_o \approx 0.055$ and $\langle E\rangle_u \approx 0.018$, since the averages are influenced by a considerable fraction of separable states with $E=0$. The probability of obtaining a given value of E is larger for the orthogonal measure, which favors purer and more likely entangled states.

Both histograms may be compared with the probability distribution $P(E)$ obtained for the ensemble of pure states, represented by stars in Fig. 4(a). This distribution is less peaked; vaguely speaking, different degrees of entanglement are almost equally likely among the pure states. The minimum of probability can be observed for maximally entangled states ($E = \ln 2$), while the mean $\langle E\rangle_{\rm pure} \approx 0.328$ is close to $(\ln 2)/2$. Since the singular distribution concentrated exclusively on pure states corresponds to the case $\lambda \to 0$ in the distribution (4), we observe that the mean entanglement $\langle E\rangle$ decreases with the increase of the parameter λ, as the distributions Δ_λ increasingly favor more mixed states.

Although the mean entanglement $\langle E\rangle$ strongly depends on the measure used, the conditional mean entanglement $E(R)$, averaged over all states of the same degree of mixing R, is not sensitive to the choice of measure, as demonstrated in Fig. 4(b). This allows us to formulate a general quantitative conclusion, valid for nonsingular measures in the space of density matrices: *the larger the average degree of mixing R*,

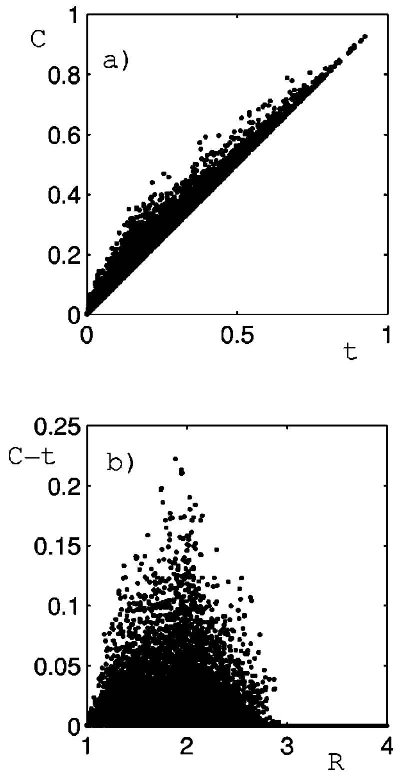

FIG. 5. Ten thousand random density matrices of size $N=4$ distributed according to the orthogonal product measure: (a) plot in the plane negativity—concurrence; (b) plot of the difference $C-t$ versus the participation R.

the smaller the mean entanglement of formation E. For $R>3$ one has $E(R)=0$ [1].

C. Negativity and concurrence

In Ref. [1] we proposed a simple quantity t defined by Eq. (8), which characterized, quantitatively, to what extent the positivity of the partial transpose is violated. As shown in Fig. 4(b) the conditional average $t(R)$ does not depend on the measure applied and decreases monotonically with R. This dependence resembles the function $E(R)$, which suggests a possible link between both quantities.

To analyze such a relation between these measures of entanglement, following the strategy of Eisert and Plenio [35], we generated 10^5 random density matrices ρ, computing their concurrence C, entanglement $E=E(C)$, and negativity t. As expected, the points at the plot E versus t do not form a single curve. It means that both quantities, entanglement of formation and negativity, do *not* generate the same ordering in the space of 4×4 density matrices. However, large correlation coefficients (approximately 0.978 for the orthogonal measure and 0.967 for the unitary measure) reveal a statistical connection between these measures.

It is particularly useful to look at the plane concurrence versus negativity. The data presented in Fig. 5(a) are obtained with the measure μ_o. We observed, independently of the measure used, that all points are localized at or above the diagonal. This allows us to conjecture that for any density matrix ρ the following inequality holds:

$$t(\rho)\leqslant C(\rho). \qquad (17)$$

A similar observation was already reported in [35], where a modulus of the negative eigenvalue E_N of the partially transposed matrix ρ^{T_2} was used. Since for $N=4$ no more than one eigenvalue d_4' is negative [25], both quantities are equivalent and $t=2E_N$. Note that due to the conjecture (17) we can attribute a more specific meaning to negativity. By means of Eq. (15) and the fact that $h(x)$ decreases for $x>1/2$, negativity t allows us to obtain a lower bound for the entanglement of formation E.

Numerical investigations show that the difference $C-t$ is largest for mixed states with $R\approx2$, while it vanishes for $R\geqslant3$ and $R=1$ [see Fig. 5(b)]. In the former case all states are separable and $C=t=0$. The latter case corresponds to pure states for which $\alpha_2=\alpha_3=\alpha_4=0$ [14] and $C=\alpha_1=-2d_4'=t$. Thus the inequality (17) becomes sharp for separable states or pure states.

D. Mixed states with the same partition ratio R

As demonstrated in Fig. 2(b), the conditional probability $P_S(R)$ of encountering a separable state is similar for states with the same participation R, averaged over both product measures μ_o and μ_u. This does not mean, however, that the probability P_S is constant for each family of states $\rho=UdU^\dagger$ defined by a given vector d with fixed participation ratio R. To illustrate this issue we discuss the case $R=2$.

Consider a vector of eigenvalues $\vec{d}$ with r nonzero elements. This natural number ($r\in[1,4]$) is just the rank of the matrix ρ. Any state $\rho=UdU^\dagger$ can be expressed by the sum of r terms, $\rho_{ij}=\Sigma_{l=1}^{r}d_lU_{il}U_{jl}^*$. Moreover, the number of nonzero eigenvalues α_i entering the definition of concurrence (14) equals r [14].

Take any vector with $r=2$ nonzero elements. In this case the formula (14) reduces to $C=\alpha_1-\alpha_2$. Since, per definition, $\alpha_1\geqslant\alpha_2$, the concurrence is positive unless $\alpha_1=\alpha_2$. Such degenerate cases occur with probability zero (e.g., for diagonal rotation matrices U), so one arrives at a simple conclusion: For any set d of eigenvalues with $r\leqslant2$, the probability P_S that a random state $UdU^\dagger$ is separable is equal to zero.

For concreteness consider three vectors of eigenvalues characterized by $r=2$, 3, and 4. We put $\vec{d}_a=\{1/2,1/2,0,0\}$, $\vec{d}_b=\{2/3,1/6,1/6,0\}$, and $\vec{d}_c=\{x_1,x_2,x_2,x_2\}$, where $x_1=(1+\sqrt{3})/4$ and $x_2=(1-x_1)/3$. Each such vector generates an ensemble of density matrices $\rho=UdU^\dagger$, where U stands for a random unitary rotation matrix of the size $N=4$. Although all three ensembles are characterized by the same participation ratio $R=2$, the probabilities of generating a separable state are different. The case $\vec{d}_a$ is characterized by $r=2$, so $P_S=0$. Numerical results obtained of a sample of 10^5 random unitary matrices give $P_S\approx0.105$ and 0.200 for $\vec{d}_b$ and $\vec{d}_c$, respectively. Thus the probability P_S grows with the number r of pure states necessary to construct given mixed state ρ, or with the von Neuman entropy H_1.

On the other hand, the average quantities characterizing entanglement (negativity, concurrence, or entanglement of formation) decrease with r, provided the participation R is

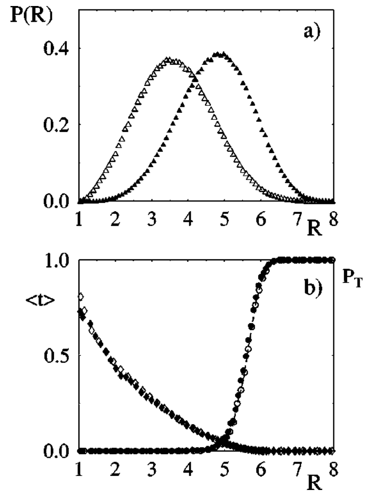

FIG. 6. Same in Fig. 2 for the 2×4 system ($N=8$). The circles in (b) represent the conditional probability of finding a state with positive partial transpose, $P_T(R)$. Diamonds represent the average negativity $t(R)$ obtained with the measures μ_o (open symbols) and μ_u (full symbols).

fixed. For example, the mean entanglement $\langle E\rangle$ equals 0.063, 0.057, and 0.042 for the ensembles $\vec{d}_a$, $\vec{d}_b$, and $\vec{d}_c$, respectively. Interestingly, in the latter case (or any other ensemble with $d_2=d_3=d_4$), one has $\alpha_3=\alpha_4$ and $C=t$.

IV. 2×4 CASE: POSITIVE PARTIAL TRANSPOSE DOES NOT ASSURE SEPARABILITY

A. Purity and positive partial transpose

For any system size the probability of finding the states with positive partial transpose depends on the measure used, as shown in Fig. 1 and Table I. On the other hand, for any N, the relations between purity and entanglement depend only weakly on the kind of product measure used. Figure 6(b) presents the conditional probability of $P_T(R)$ and the mean negativity t as a function of the degree of mixing R for the 2×4 system. For both quantities the results obtained with orthogonal and unitary product measures are difficult to distinguish. Thus the dependence of the total probability P_T on the measure used is strongly influenced by the likelihood of generating highly mixed states, described by the distribution $P(R)$.

These distributions for $N=8$ are shown in Fig. 6(a). The histogram for the unitary measure μ_u is shifted to larger values of R, with respect to the data obtained with the orthogonal measure. Quantitatively, the mean values read $\langle R\rangle_u\approx4.74>\langle R\rangle_o\approx3.66$. It is known that $P_T=1$ for $N>R-1$ [1]. The right histogram, corresponding to the unitary measure, has a larger overlap with this region, which causes $\langle P_T\rangle_u>\langle P_T\rangle_o$.

This observation is valid for an arbitrary matrix size, since for large N one has $\langle R(N)\rangle_u\approx N/2$, while $\langle R(N)\rangle_o\approx N/3$ [41]. For N large enough, the distributions $P(R)$ tend to Gaussians. They are centered at mean values, which depend on the measure, while the variance σ^2 is of the order of $N/5$ for both measures under consideration. Hence, the overlap with the interval $[N-1,N]$ is larger for the measure μ_u characterized by a larger mean value $\langle R\rangle_u$.

B. Entanglement of formation

Since for $N>4$ there exist no analytical methods to compute the entanglement of formation of an arbitrary mixed state ρ, we have relied on numerical computations. To perform the minimization present in the definition (12) we worked out an algorithm based on a random walk in the space of unitary matrices $U(M)$ with $M\geqslant N$. It is described in detail in Appendix B. Each run ends with an approximate *optimal decomposition* of the state ρ and provides an *upper* estimation of the entanglement E. To verify the accuracy of this technique we started with the case $N=4$, in which the explicit formula (15) is known. Computing numerically entanglement for 1000 randomly chosen $N=4$ mixed states we obtained a mean error of the order of 10^{-7}, while the maximal error was smaller than 10^{-4}.

At the beginning of each computation one has to choose the number M determining the number of pure states in the decomposition. Since for $N=4$ it is known that the cardinality of any state is not larger than 4 [14,25], it is sufficient to look for the optimal decomposition in the ($M=N=k=4$)-dimensional space. For larger systems the problem of finding the maximal possible cardinality is open. For each randomly generated mixed state ρ in the discussed 2×4 case, we started to look for the optimal decomposition with $M=N=8$, recorded the minimal entanglement $E_{M=8}$, and repeated computations with $M=9,10,\ldots,M_{max}$. It is known [42,7] that the maximal number of pure states does not exceed N^2, but in practice we analyzed $M\in[N,2N]$.

The number of degrees of freedom grows as M^2, so the process of searching for the optimal decomposition becomes less efficient with an increase in the number M. However, for certain states we found better estimations for entanglement; e.g., $E_{M=9}(\rho)<E_{M=8}(\rho)$. In these rare cases, improvements of the estimations of E were very small, and repeating several times our procedure with $M=8$ the same upper bounds for entanglement of formation were reproduced.

Thus our results do not contradict an appealing conjecture that the *cardinality* k of any 2×4 mixed system is not larger than $N=8$. Further work is still needed to verify whether this conjecture is true.

Note that the numerical algorithm for searching for the optimal decomposition and the entropy of formation may also be used to look for the generalized entropy of formation E_q, in the analogy to Eqs. (10) and (12), see [37]. We found it interesting to study the quantity E_2, which has an interpretation similar to the participation ratio R and equals unity for the separable states.

C. Volume of the bound entangled states

It is known [8] that for $N=8$ there exist bound entangled states, which cannot be brought into the singlet form. All entangled states satisfying the partial transposition criterion are bound entangled ones [7,8,10]. It was shown in [1] that they occupy a positive volume P_B. Therefore, $P_S=P_T-P_B$ is smaller than the volume P_T of the states with positive partial transpose. Strictly speaking, the volume P_B of entangled states with positive partial transpose should be considered as a lower bound of the volume of bound entangled states, since it is not proven yet that all states with negative partial transpose are free entangled.

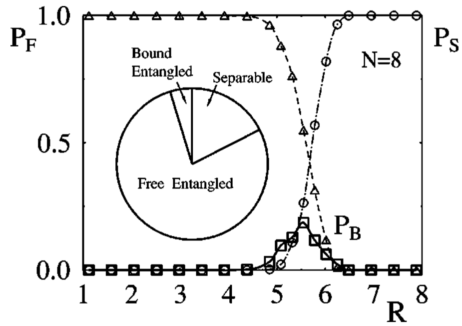

FIG. 7. Conditional probabilities of finding the separable states (○), free entangled states (△), and bound entangled states (□) as a function of the participation ratio *R*. Results are obtained with 10^5 random density matrices of the size $N=8$ distributed according to the measure μ_u. The lines are drawn to guide the eye. The inset shows the pie chart of the total probability of encountering separable states, bound entangled states (lower bound), and free entangled states (upper bound).

To estimate P_B, we generated 10^5 random density matrices of size $N=8$. We worked with the unitary product measure μ_u, since, as shown in Table I, the 2×4 states chosen according to the orthogonal measure μ_o very seldom satisfy the partial transposition criterion. To save computing time, we estimated the entanglement of formation E only in the 2223 cases with positive partial transpose. Setting an entanglement cutoff $E_c=0.0003$ (see Appendix B), we found that 473 states enjoyed the entanglement $E>E_c$. This gives a fraction of $P_B\approx 4.7\%$ of all states, or $P_B/P_T=21.3\%$ of the states with positive partial transpose. Although these numbers are influenced by systematic errors (bound entangled states with $E<E_c$ are regarded as separable, while separable states with numerically obtained upper estimations of the entanglement larger than E_c are considered as entangled), the dependence of the results obtained on the cutoff value E_c is weak. Moreover, these results do not depend on the exact values of the parameters characterizing the random walk (see Appendix B). Consequently, we obtained an estimate of the volume of separable states for this case, $P_S=P_T-P_B\approx 17.5\%$, as shown in the inset of Fig. 7.

D. Bound entanglement and purity

It is interesting to ask whether a certain degree of mixing favors the probability of finding the bound entangled states. Grouping all 10^5 analyzed states in 30 bins according to the participation ratio *R*, we computed the conditional probabilities of entanglement. These results are shown in Fig. 7. Probability P_S increases monotonically with *R*, while the probability of finding a free entangled state $P_F=1-P_T$ decays with the participation. On the other hand, the conditional probability $P_B(R)$ of finding a bound entangled state exhibits a clear maximum at $R\sim 5.5$. If the mean purity is concerned, the bound entangled states are thus sandwiched between free entangled states (generally of high purity) and the separable states are characterized by a high degree of mixing.

The above results suggest that for the bound entangled states there exists a minimal participation ratio *R* or a minimal rank *r*. Preparing a sketch analogous to Fig. 3 for $N=8$, one should put the bound entangled states close to the center of the figure, but outside the symbolic ‘‘needle of the compass,’’ which represents the separable states.

It is worth noting that the entanglement of formation for bound entangled states is rather small in comparison to the mean entanglement of formation for the free entangled states, which violates the partial transposition criterion. The average taken over all free entangled states is $\langle E\rangle_F\approx 0.05$; the average taken over all bound entangled states is $\langle E\rangle_B\approx 0.0033$ (which is much larger than the cutoff value E_c). The maximal entanglement found for a bound state was only $E_M=0.0746$.

V. CLOSING REMARKS

In this work we attempt to characterize the statistical properties of the set of separable mixed quantum states. A certain level of caution is always recommended for interpretation of any results of probabilistic calculations, especially if the space of the outcomes is infinite. Let us mention here the famous Bertrand paradox: What is the probability that a randomly chosen chord of a circle is longer than the side of the equilateral triangle inscribed within the circle? The answer depends on the construction of the randomly chosen chord, which determines the measure in infinite space of the possible outcomes.

Asking a question on the probability that a randomly chosen mixed state is separable, one should also expect that the answer will depend on the measure used. This is indeed the case, as demonstrated in this work for two products measures, and also shown by Slater [6] for a different measure related to the *monotone* metrics [43]. We reach, therefore, a simple conclusion, which is rather intuitive for an experimental physicist: the probability of finding an entangled state depends on the way the states are prepared, which determines the measure in space of mixed quantum states.

On the other hand, in this paper we provide arguments supporting the conjecture that some statistical properties of entangled states are universal and to a large extent do not depend (or depend rather weakly) on the measure used. Let us mention only the exponential decay of the volume of the set of separable states with size *N* of the problem or the important relation between the purity of mixed quantum states and the probability of finding a separable state.

Studying the simplest case $N=4$, we have shown that for an ensemble of pure states the distribution of entanglement of formation is rather flat in $[0,\ln 2]$. The more mixed states, the larger the peak at small values of entanglement and the larger the probability of finding a separable state. We have shown that the negativity *t*, a naive measure of entanglement, provides a lower bound for the entanglement of formation.

Analyzing a more sophisticated problem $N=8$, we developed an efficient numerical algorithm to estimate the entanglement of formation of any mixed state. In this way we could differentiate between separable states and the bound entangled states. About 79% of $N=8$ states satisfying the positive transposition criterion are separable. This result is obtained for random states generated according to the unitary product measure in the space of $N=8$ density matrices, but we expect to get comparable results for other, nonsingular measures. The mean entanglement of formation for the bound entangled states is much smaller than for the free entangled states. The relative probability of finding a bound entangled state for the 2×4 systems is largest for moderately mixed systems, characterized by the participation ratio close to $R=5.5$.

Even though this paper follows the previous work [1], the list of unresolved problems in this field is still very long. Let us collect here some of those related to this work, mentioning also those already discussed in the literature.

(a) $N=4$, (2×2 systems). (i) Check whether the dependence of the conditional probability on the participation ratio $P_S(R)$, obtained for two product measures [see Fig. 2(b)] holds also for the measures based on the monotonic metrics [6] or for the product Bures measure [44,45]. (ii) Prove the relation between the concurrence and the negativity: $C\geqslant t$. (iii) Find max$(C-t)$ as a function of the participation ratio R [see Fig. 4(b)]. (iv) Check whether the following conjecture is true: If $R(\vec{d}_1)=R(\vec{d}_2)$ and $H_1(\vec{d}_1)\geqslant H_1(\vec{d}_2)$, then $P_S(\rho_1)\geqslant P_S(\rho_2)$. The von Neuman entropy H_1 and the participation ratio R measure the degree of mixing of a given vector $\vec{d}$, while P_S denotes the probability that a random state $\rho_i=Ud_iU^\dagger$ is separable. (v) Find isoprobability surfaces in the simplex $\{d_1,d_2,d_3\}$, such that $P_S(\vec{d})=\text{const}$.

(b) $N=6$ (2×3 or 3×2 systems). (vi) Find a lower bound for the entanglement of formation E (in analogy to negativity t, which gives a lower bound for C and E in the case $N=4$). (vii) Find an explicit formula for E in this case.

(c) $N=8$ (2×4 or 4×2 systems). (viii) Find necessary and sufficient conditions for a bound entangled (or separable) state. (ix) Find the maximal entanglement of formation E of a bound entangled state. (x) Check whether the rank of bound entangled states is bounded from below. (xi) Check that the cardinality of any state is not larger than 8.

(d) *General questions.* (xii) Check whether all states violating the partial transpose criterion are free entangled. (xiii) Can we verify that the optimal decomposition of a given mixed state into a sum of pure states leading to the entanglement of formation, $E=E_1$, also gives the minimum of the generalized entanglement of formation E_q? (xiv) For what $N_A\times N_B$ composed systems is the cardinality k of any mixed state in the N-dimensional Hilbert space less than or equal to $N=N_AN_B$? (xv) Can we determine whether the entanglement of formation is additive?

Not all of the above problems are of the same importance. We regard the questions (i), (viii), and the last two general questions as the most relevant. The preliminary results of Slater [46] suggest that the relation $P_S(R)$ for monotonic metrics is similar to that obtained here for the product metric, at least for $N=4$. Concerning problem (viii): for separable states with $N=8$, some necessary conditions, stronger than the positive partial transpose, are known [47,48], but conditions sufficient for assuring separability are still most welcome. The problem of the additivity of the entanglement of formation is present in the literature (see, e.g., [14]). Performing numerical estimations of the entanglement of formation E for several states of $2\times N_B$ systems, we have not found any cases that violate questions (xiii) and (xv) [49]. Recent results of Lewenstein, Cirac, and Karnas [48] suggest that the answer to question (xiv) is negative for the systems $3\times N_B$ with $N_B>3$, but they do not contradict that statement for the $2\times N_B$ composed systems. Further effort is required to establish whether in this case the answer to question (xiv) is positive.

Note added in proof. After this work was completed Vidal proved that the negativity t of a mixed state does not grow under any local operations [52]. Therefore, negativity might be considered as a measure of entanglement.

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APPENDIX A: ROTATIONALLY INVARIANT PRODUCT MEASURES

In this appendix we show that a vector of an N-dimensional random orthogonal (unitary) matrix generates the Dirichlet measure (4) with $\lambda=1/2$ ($\lambda=1$) in the $(N-1)D$ simplex. Although these results seem not to be new, we have not found them in the literature in this form, and prove them here for the convenience of the reader, starting with the simplest case $N=2$.

Lemma 1. Let O be an $N\times N$ random orthogonal matrix distributed according to the Haar measure on $O(N)$. Then the vector $d_i=|O_{i1}|^2, i=1,\dots,N$ is distributed according to the statistical measure on the $(N-1)$-dimensional simplex (Dirichlet measure with $\lambda=1/2$).

Proof. Due to the rotational invariance of the Haar measure on $O(N)$ the vector O_{i1} is distributed uniformly on the $(N-1)$-dimensional sphere S^{N-1}. Thus $\Sigma_{i=1}^N d_i=1$.

For $N=2$ the vector $|O_{i1}|$ is distributed uniformly along the quarter of the circle of radius 1. Therefore, $x=\cos\phi$, where $\phi\in[0,\pi/2)$ and $P(\phi)=2/\pi$. Hence $P(x)=P(\phi)d\phi/dx=2/(\pi\sqrt{1-x^2})$. Another substitution $\xi=x^2$ gives the required result: $P(\xi)=P(x)dx/d\xi=1/[\pi\sqrt{\xi(1-\xi)}]$.

To discuss the general N-dimensional case, it is convenient to introduce the polar angles and to represent any point belonging to the $(N-1)D$ sphere as $x_N=\cos\theta_{N-2}$, $\rho=\sin\theta_{N-2}$, where $\rho^2=1-\Sigma_{i=1}^{N-1}x_i^2$. Uniform distribution of the points on the sphere is described by the volume element $d\Omega=\sin^{N-2}\theta_{N-2}d\theta_{N-2}\cdots\sin\theta_1 d\theta_1 d\phi$. Changing the polar variables into Cartesian, we obtain $P(\rho)\sim1/\cos\theta_{N-2}=1/\sqrt{1-\rho^2}$. The last change of variables $\xi_i:=x_i^2$ for $i=1,\dots,N$ allows us to receive $P(\xi_1,\dots,\xi_{N-1})\sim[\xi_1\xi_2\dots\xi_{N-1}(1-\xi_1-\xi_2-\cdots-\xi_{N-1})]^{-1/2}$, which gives the statistical measure $\Delta_{1/2}$ defined in Eq. (4). ■

Geometric interpretation of this result is particularly convincing for $N=3$. Then the vector O_{i1} covers uniformly the sphere S^2, while $|O_{i1}|$ is distributed uniformly in the first octant. The points $\{d_1,d_2,d_3\}=\{\xi_1,\xi_2,\xi_3\}$ lie at the plane $z=1-x-y$. Their projection into the x-y plane gives the statistical measure on the 2D simplex; i.e., the triangle $\{(0,0),(1,0),(0,1)\}$.

Lemma 2. Let U be an $N\times N$ random unitary matrix distributed according to the Haar measure on $U(N)$. Then the vector $d_i=|U_{i1}|^2, i=1,\ldots,N$ is distributed according to the uniform measure on the $(N-1)$-dimensional simplex (Dirichlet measure with $\lambda=1$).

Proof. We will use the Hurwitz parametrization of $U(N)$ [22], based on the angles $\varphi_{kl}\in[0,\pi/2]$ with $0\leqslant k<l\leqslant N-1$. Their distribution can be determined by the relation $\varphi_{kl}=\arcsin \xi_{k+1}^{1/(2k+2)}$, where ξ_k are the auxiliary independent random numbers distributed uniformly in $[0,1]$ (see Ref. [23]).

In the simplest case $N=2$, the vector $\vec{d}$ reads $|U_{i1}|^2=\{\cos^2\varphi_{01},\sin^2\varphi_{01}\}=\{\xi_1,1-\xi_1\}$ and the variable $d_1=\xi_1$ is distributed uniformly in the interval $[0,1]$ (one-dimensional simplex). For $N=3$ one obtains

$$\vec{d}=\{\cos^2\varphi_{12},\sin^2\varphi_{12}\cos^2\varphi_{01},\sin^2\varphi_{12}\sin^2\varphi_{01}\}=\{1-\xi_2^{1/2},\xi_2^{1/2}(1-\xi_1),\xi_2^{1/2}\xi_1\},$$

which is distributed uniformly in the simplex $\{(0,0),(1,0),(0,1)\}$.

In the general N-dimensional case we get

$$\begin{aligned}\vec{d}=\{&\cos^2\varphi_{N-2,N-1},\ \sin^2\varphi_{N-2,N-1}\cos^2\varphi_{N-3,N-1},\ \sin^2\varphi_{N-2,N-1}\sin^2\varphi_{N-3,N-1}\\ &\times\cos^2\varphi_{N-4,N-1},\ \ldots,\ \sin^2\varphi_{N-2,N-1}\cdots\sin^2\varphi_{1,N-1}\cos^2\varphi_{0,N-1},\ \sin^2\varphi_{N-2,N-1}\cdots\sin^2\varphi_{1,N-1}\sin^2\varphi_{0,N-1}\}.\end{aligned}$$

Using uniformly distributed random variables this vector may be written as

$$\{1-\xi_{N-1}^{1/(N-1)},\xi_{N-1}^{1/(N-1)}(1-\xi_{N-2}^{1/(N-2)}),\xi_{N-1}^{1/(N-1)}\xi_{N-2}^{1/(N-2)}(1-\xi_{N-3}^{1/(N-3)}),\ldots,\xi_{N-1}^{1/(N-1)}\cdots\xi_2^{1/2}(1-\xi_1),\xi_{N-1}^{1/(N-1)}\cdots\xi_2^{1/2}\xi_1\}.$$

This vector is uniformly distributed in the $(N-1)$-dimensional simplex, as explicitly shown in Appendix A of Ref. [1]. ■

The above lemmas allow one to generate random points distributed in the simplex according to the both measures, using vectors of random orthogonal (unitary) matrices. They may be constructed according to the algorithms presented in Ref. [23]. Alternatively, one may take a random matrix of a Gaussian orthogonal (unitary) ensemble, diagonalize it, and use one of its eigenvectors, as in Eq. (3). Random matrices pertaining to GOE (GUE) are obtained as symmetric (Hermitian) matrices with all elements given by independent random Gaussian variables. Several ensembles interpolating between GOE and GUE are known [21]. Statistics of eigenvectors during such a transition were studied, e.g., in [50], while the transitions between circular ensembles of unitary matrices were analyzed in [51].

APPENDIX B: ENTANGLEMENT OF FORMATION–A NUMERICAL ALGORITHM

1. Generating the random density matrix

In order to generate an $N\times N$ random density matrix we write $\rho=UdU^{\dagger}$ and use the product measure $\mu=\Delta_\lambda\times\nu_H$. The vector of eigenvalues d, taken according to the Dirichlet measure (4), can be obtained from unitary random matrices, as shown in Appendix A. The unitary random rotation matrix U distributed according to the Haar measure ν_H is generated by the algorithm presented in [22]. The random state ρ, generated according to a given product measure, may be decomposed into a mixture of N pure states determined by its eigenvectors,

$$\rho=\sum_{i=1}^{N}|\Psi_i\rangle\langle\Psi_i|. \tag{B1}$$

Note that the pure states $|\Psi_i\rangle$ are not normalized to unity, but their norms are given by the eigenvalues d_i. Expansion coefficients of each of these states are given by the elements of the random rotation matrix, $|\Psi_i\rangle=\sqrt{d_i}\{U_{1i},U_{2i},\ldots,U_{Ni}\}$.

There exist many other possible decompositions of the state ρ into a mixture of M pure states, with $M\geqslant N$. Let $\tilde{V}$ be a random unitary matrix of size M distributed according to the Haar measure on $U(M)$. Let V denote a rectangular matrix constructed from the N first columns of $\tilde{V}$. Any such $M\times N$ matrix allows one to write a legitimate decomposition ρ' of the same state ρ,

$$\rho'=\sum_{i=1}^{M}|\phi_i\rangle\langle\phi_i|, \tag{B2}$$

where

$$|\phi_i\rangle=\sum_{m=1}^{N}V_{im}|\Psi_m\rangle,\quad i=1,\ldots M. \tag{B3}$$

The unitarity of the rotation matrix $\tilde{V}$ assures the correct normalization $\mathrm{Tr}\,\rho'=\sum_{i=1}^{M}\langle\phi_i|\phi_i\rangle=1$.

Assume that the composite N-dimensional quantum system consists of two subsystems of size N_A and N_B, such that $N=N_AN_B$. It is then convenient to represent any vector $|\phi_i\rangle$ (of a nonzero norm $p_i=\langle\phi_i|\phi_i\rangle$) by a complex $N_A\times N_B$ matrix $A^{(i)}$, which contains all N elements of this vector. To describe the reduction of the state $|\phi_i\rangle$ into the second subsystem, we define an $N_B\times N_B$ Hermitian matrix,

$$B^{(i)} := [A^{(i)}]^{\dagger} A^{(i)}. \tag{B4}$$

Diagonalizing it numerically we find its eigenvalues $\tilde{b}_l^{(i)}, l = 1, N_B$. Rescaling them by the norm of the state p_i we get $b_l^{(i)} = \tilde{b}_l^{(i)}/p_i$, satisfying $\Sigma_{l=1}^{N_B} b_l^{(i)} = 1$. We compute the entropy of this partition,

$$E_B(|\phi_i\rangle) := -\sum_{l=1}^{N_B} b_l^{(i)} \ln b_l^{(i)}, \tag{B5}$$

giving the von Neuman entropy of the reduced state. The entanglement of the state ρ' with respect to the rotated decomposition (B2) is equal to the average entropy of the pure states involved,

$$E(\rho') = \sum_{i=1}^{M} p_i E_B(|\phi_i\rangle), \tag{B6}$$

where $\Sigma_{i=1}^{M} p_i = 1$.

The entanglement of formation E of the state ρ is then defined as a minimal value $E_B(\rho')$, where the minimum is taken over the set of decompositions ρ' given by Eq. (B2) [compare with the definition (12)]. The rotation matrix V_o for which the minimum is achieved is called the *optimal*. Our task is to find the optimal matrix in the space of M-dimensional unitary matrices where $M = N, N+1, \ldots, N^2$.

We have found it interesting to also consider the generalized entanglement

$$E_q(\rho') = \sum_{i=1}^{M} p_i E_q(|\phi_i\rangle), \tag{B7}$$

where

$$E_q(|\phi_i\rangle) := \frac{1}{1-q} \ln\left(\sum_{l=1}^{N_B} [b_l^{(i)}]^q \right). \tag{B8}$$

The standard quantity $E_B(\rho)$ is obtained in the limit $\lim_{q\to 1} E_q(\rho)$.

2. Search for the optimal rotation matrix

The search for the optimal rotation matrix V has to be performed in the M^2-dimensional space of unitary matrices. Starting with $M = N$ one has to consider the 16-dimensional space in the simplest case of $N = 4$. To obtain accurate minimization results in such a large space one should try to perform some more sophisticated minimization schemes; for example, the stimulated annealing. Fortunately, the optimal rotation matrix V_o is determined up to a diagonal unitary matrix containing M arbitrary phases. Therefore, one can hope to get reasonable results with a simple random walk, moving only then, if the entanglement decreases. Performing only the ‘‘down’’ movements in the M^2-dimensional space, one has a good chance of landing close to the M-dimensional manifold defined by optimal matrices equivalent to V_o. This corresponds to fixing the temperature to zero in the annealing scheme, and simplifies the search algorithm.

To perform small movements in the space of unitary matrices we will use $M \times M$ Hermitian random matrices H pertaining to the Gaussian unitary ensemble (GUE). They can be constructed by independent Gaussian variables with zero mean and the variance $(\sigma_{mn}^{\mathrm{Re}})^2 = (1+\delta_{mn})/M$ for the real part and $(\sigma_{mn}^{\mathrm{Im}})^2 = (1-\delta_{mn})/M$ for the imaginary part of each complex element $H_{mn} = H_{nm}^*$. We generate random matrix H and take $W = e^{i\chi H}$ as a unitary matrix, which might be arbitrarily close to the identity matrix. Our strategy consists in fixing the initial angle χ_0, performing random movements of this size, and then gradually decreasing the angle χ.

The detailed algorithm of estimating the entanglement of formation of a given $N \times N$ state ρ is listed below.

(1) Fix the number M of the components of the decomposition (B2). Start with $M = N$.

(2) Generate random unitary rotation matrix V of size M, which defines the decomposition ρ' in Eq. (B2). Compute the entanglement $E = E_B(\rho')$ according to Eqs. (B5),(B6).

(3) Set the initial angle $\chi = \chi_0$.

(4) Generate a random $M \times M$ GUE matrix H and compute $V' = V \exp(i\chi H)$. Calculate the entanglement E' for the decomposition ρ' generated by V'.

(5) If $E' < E$, accept the move (substitute $V := V'$ and $E := E'$) and continue with step (4). Otherwise, repeat steps (4) and (5) I_{change} times.

(6) Decrease the angle $\chi := \alpha\chi$, where $\alpha < 1$.

(7) Repeat steps (4)–(6) until $\chi < \chi_{end}$. Memorize the final value of the entanglement E.

(8) Repeat L_{mat} times steps (2)–(7) starting from a different initial random matrix V.

(9) Memorize the value E_M, defined as the smallest of L_{mat} repetitions of the above procedure.

(10) Set $M =: M+1$ and repeat the steps (2)–(9) until $M = M_{max}$.

(11) Find the smallest value of $E_M, M = N, \ldots, M_{max}$. This value $E_{min} = E_{M_*}$ gives the upper bound for the entanglement of formation of the mixed state ρ, while the size M_* of the optimal rotation V_* may be considered as the cardinality of ρ.

3. Remarks on estimating the entanglement of formation

The accuracy of the above algorithm may be easily tested for the case $N = 4$, for which the analytical formula (15) exists. Results mentioned in Sec. IV B, giving a mean error of the estimation of the entanglement smaller than 10^{-7}, were obtained with the following algorithm parameters: the initial angle $\chi_0 = 0.3$, the final angle $\chi_{end} = 0.0001$, the angle reduction coefficient $\alpha = 2/3$, the number of iterations with the angle fixed $I_{change} = 25$, and the number of realizations $L_{mat} = 3$. Using relatively slow routines interpreted by Matlab on a standard laptop computer we needed a couple of minutes to get the entanglement of any mixed state ρ. Although we performed test searches with $M = 4,5, \ldots, 8$, the optimal rotation was always found for $M = N = 4$.

The same algorithm was used for random states with $N = 2 \times 4 = 8$. In this case the simplest search with $M = N = 8$, performed in 64-dimensional space, requires much more computing time. It depends on all parameters characterizing the algorithm; one may therefore impose an additional bound on the total number I of generated random matrices V'. To estimate the volume of the bound entangled states we performed the above algorithm only for the states with positive partial transpose. Setting the final angle at $\chi_{end}=0.0002$, we obtained in a histogram $P(E)$ a flat local minimum at $E_m \sim 0.0003$. The minimum is located just to the right of the singular peak at even smaller values of E, corresponding to separable states. The cumulative distribution $P_c = \int_{E_m}^{\infty} P(E) dE$ was found not to be very sensitive to the position of the minimum E_m. We could, therefore, set the cutoff value E_c at the position of minimum E_m, and interpret the quantity P_c as the relative volume of the bound entangled states. In the computations described in Sec. IV C we took $\chi_0=0.3$, $\alpha=2/3$, $I_{change}=25$, and $L_{mat}=5$, and for $M=N=8$ obtained the mean number of iterations $\langle I \rangle$ of the order 5×10^4.

The other possibility of distinguishing the bound entangled states from the separable states consists in studying the dependence of the obtained upper bound of the entanglement E on the total number I of iterations performed. Numerical results obtained for the separable states show that E decreases with a computation time not slower than $E(I) = a/I$. Assuming a similar effectiveness of the algorithm for the nonseparable states (with a nonzero entanglement of formation E_{form}), we have $E(I)=E_{form}+b/I$. This allows us to design a simple auxiliary criterion: the state ρ is separable if (for all realizations of the random walk starting from the different matrices V) for sufficiently large number of iterations I one has $E(I)<E(I/2)/2$. If this condition is not fulfilled, the state ρ can be regarded as entangled. Using this method we obtained the estimation for the volume of bound entangled states similar to P_c.

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