Volume of the set of mixed entangled states II

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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, the recent developments of the theory of quantum information and quantum computing caused a rapid increase of the interest in studying 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 to fit some fast growing curves to these data nor to 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 \( \rho \). One may also ask a complementary question concerning the set of the separable states, which can be represented as a sum of product states.

Consider a quantum system described by the density matrix \( \rho \) which 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 \( \mu \), according to which the random density matrices \( \rho \) are drawn,

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

Representing any density matrix in the diagonal form \( \rho = U \rho U^\dagger \) we proposed \( \rho \) to use a product measure \( \mu = \Delta_1 \times \nu \), where \( \Delta_1 \) describes the uniform measure on the simplex \( \sum_{i=1}^{N} d_i = 1 \) and \( \nu \) stands for the Haar measure in the space of unitary matrices \( U(N) \). Based on the partial transposition criterion \( \frac{c}{c'} \) we found that under this measure the volume of the set of separable states is positive and decreases with the system size \( N \). Some more general analytical bounds were also provided by Vidal and Tarrach \( \frac{c}{c'} \). Recently Slater suggested estimating the same quantity using some other measures in the space of the density matrices \( \frac{c}{c'} \). 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. 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. Basing 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 \( \frac{c}{c'} \). For \( N > 6 \), however, there exist states, which are not separable and do satisfy this criterion \( \frac{c}{c'} \). These states cannot be distilled to the singlet form and are called bound entangled \( \frac{c}{c'} \). Since there are no explicit conditions allowing one to distinguish between separable and bound entangled states, in Ref. \( \frac{c}{c'} \) only the upper bound for the volume of separable states was considered for \( N > 6 \). In this paper we present an efficient numerical method of computing the entanglement of formation \( E \) \( \frac{c}{c'} \) for any density matrix. This method allows us to estimate the volume of bound entangled states, by taking a reasonably small cut-off entanglement \( E_c \) and counting these states satisfying the partial transposition criterion for which \( E > E_c \). Our numerical results are to large extent independent on the exact value of \( E_c \).
The paper is organized as follows. In section 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 next section is devoted to 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 \cite{4,3} and we study how this quantity changes with the purity of the mixed states. In section 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 Section V containing a list of open questions. In Appendix A we prove the first column) of an auxiliary random unitary matrix 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 $\nu_H$

$$d_i = |V_i|^2.$$ \hfill (3)

In the sequel we will thus refer to the measure defined by \cite{4} as the unitary product measure $\mu_u$.

As correctly pointed out by Slater \cite{3}, our choice of the measure is by far not the only one possible. He discussed several possible measures, and proposed to pick the measure on the $(N - 1)D$ simplex from a certain family of the Dirichlet distributions

$$\Delta(\nu_1, \ldots, \nu_{N-1}) = C_\lambda \nu_1^{\lambda-1} \nu_2^{\lambda-1} \cdots \nu_{N-1}^{\lambda-1} (1 - \nu_1 - \cdots - \nu_{N-1})^{\lambda-1}.$$ \hfill (4)

where $\lambda > 0$ is a free parameter and $C_\lambda$ 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 $\Delta_1$ corresponds to $\lambda = 1$. Slater distinguishes also the case $\lambda = 1/2$, which is related to the Fisher information metric \cite{4}, the Mahalonobis distance \cite{4} and Jeffreys’ prior \cite{4} and was used for many years in different contexts \cite{14,24}. 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

$$\mu_o := \Delta_{1/2} \times \nu_H$$ \hfill (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 \cite{22}, referred to as GUE and GOE. The measure $\mu_a$ is determined by squared components of an eigenvector of a GUE matrix, while the measure $\mu_o$ may defined by components of an eigenvector of GOE matrices \cite{23}. Some properties of the orthogonal measure $\mu_o$ have been recently studied in \cite{24}. Let us stress that the name of the product measure (orthogonal or unitary) is related to the distribution $\Delta$ on the simplex $d$, while the random rotations $U$ are always assumed to be distributed according to the Haar measure $\nu_H$ in $U(N)$.

It is interesting to consider the limiting cases of the distribution \cite{4}. For $\lambda \to 0$ one obtains a singular distribution concentrated on the pure states only \cite{4}, while in the opposite limit $\lambda \to \infty$, the distribution is peaked on the maximally mixed state $\rho_s$ described by the vector $d = \{1/N, \ldots, 1/N\}$. Changing the continuous parameter $\lambda$ 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 $\rho$ in the $N$ dimensional Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$. Dimension of the system $N$ is equal to the product $n_A n_B$ of the dimensions of the both subsystems. If the state $\rho \in \mathcal{H}$ can be expressed as $\rho = \rho_A \otimes \rho_B$, then $\rho = \sum_{i=1}^{n_A} \sum_{j=1}^{n_B} c_{ij} \rho_{ij}$, where $c_{ij}$ are complex numbers. If $c_{ij}$ are real numbers, then $\rho$ is a separable state. If $c_{ij}$ are complex numbers, then $\rho$ is a mixed state. If $c_{ij}$ are complex numbers, then $\rho$ is a pure state. If $\sum_{i=1}^{n_A} \sum_{j=1}^{n_B} |c_{ij}|^2 = 1$, then $\rho$ is a maximally mixed state. If $\sum_{i=1}^{n_A} \sum_{j=1}^{n_B} |c_{ij}|^2 < 1$, then $\rho$ is a mixed state. If $\sum_{i=1}^{n_A} \sum_{j=1}^{n_B} |c_{ij}|^2 > 1$, then $\rho$ is a pure state. If $\sum_{i=1}^{n_A} \sum_{j=1}^{n_B} |c_{ij}|^2 = 0$, then $\rho$ is a singular state.
with $\rho_A \in \mathcal{H}_A$ and $\rho_B \in \mathcal{H}_B$, it is called product state (or factorizable state). This occurs if and only if $\rho = \text{Tr}_B \rho \otimes \text{Tr}_A \rho$, where $\text{Tr}_A$ and $\text{Tr}_B$ denote the operations of partial tracing. In other words, for such states the description of the composite state is equivalent to the description in the both subsystems.

A given quantum state $\rho$ is called separable, if it can be represented by a sum of product states \[ \rho = \sum_{i=1}^{k} p_i \rho_{A_i} \otimes \rho_{B_i}, \tag{6} \]

where $\rho_{A_i}$ and $\rho_{B_i}$ are the states on $\mathcal{H}_B$ and $\mathcal{H}_B$ respectively. The smallest number $k$ of the product states used in the above decomposition is called the cardinality of the separable state $\rho$ \[. \]

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 \[. \]

Later Horodeccy demonstrated that for $N = 4$ and $N = 6$ this is also a sufficient condition \[. \]

To characterize quantitatively the violation of positivity we introduced \[. \] the negativity

\[ t := \sum_{i=1}^{N} |d_i^r| - 1, \tag{8} \]

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

### C. Relative volume in the space of the density matrices

In \[. \] 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 one, is obviously valid for any nonsingular measure.

To analyze the influence of the measure chosen for the volume of the separable states $P_s$, we picked several random density matrices (circa $10^6$) distributed according to the orthogonal and unitary product measures, and verified, whether their partial transpose \[. \] are 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 the 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 the section IV.

The symbols are labeled by the size of the first subsystem $n_A$. For both measures the symbols seem to lay on one curve, which would imply that $P_T(n_A, n_B) = P_T(n_A * n_B)$. However, this relation is only approximate, since $P_T(2 \times 6) = P_T(3 \times 4)$ as pointed out by Smolin \[. \] Numerical results for $P_T$ and $\langle t \rangle$ for $N \leq 12$ are collected in Table 1. 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 \[. \] 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 $N$.

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

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### Table 1. Probability $P_T$ of finding a mixed states of size $N$ with positive partial transpose and the mean negativity $\langle t \rangle$ for two product measures orthogonal $\mu_o$ and unitary $\mu_u$. For $N = 4$ and $N = 6$ one has $P_T = P_S$. 
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 (non-singular) probability measure used. 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 $\mu_u$, and $P_{To} \sim 3.0e^{-0.55N}$ for the orthogonal product measure $\mu_o$. Dependence of the probability $P_T$ on the measure chosen is due to the fact that each measure distinguishes states of a different purity. This issue is discussed in details 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 $H_1(q) = -\text{Tr}(q \ln q)$. Another quantity, called the participation ratio

$$R(q) = \frac{1}{\text{Tr}(q^2)},$$

is often more convenient for calculations. It varies from unity (for pure states) to $N$ (for the totally mixed state $q$ proportional to the identity matrix) and may be interpreted as an effective number of the states in the mixture. This quantity gives an lower bound for the rank $r$ of the matrix $q$, namely $r \geq R$. Moreover, it is related to the von Neumann-Renyi entropy of order two, $H_2(q) = \ln R(q)$. The latter, also called the purity of the state, together with other quantum Renyi entropies

$$H_q(q) = \frac{1}{1-q} \ln[\text{Tr}q^q]$$

is used, for $q \neq 1$, as a measure of how much a given state is mixed (see e.g. [28]).

Figure 2 presents the probability distributions $P(R)$ for $N=4$ density matrices generated according to the both product measures. As discussed before, the orthogonal measure $\mu_o$ is concentrated at less mixed states (lower values of $R$) than the unitary measure $\mu_u$. For example the mean values 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 non-smooth 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 3D simplex formed by $d_1,d_2$ and $d_3$.

![Figure 2](image_url)
the average mixture $\langle R \rangle_{\rho_A}$ grows monotonically with the parameter $\lambda$ (from 1 for $\lambda \to 0$ to 4 for $\lambda \to \infty$) also the probability $P_S$ 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 [29] for complementary, constructive results.

Above considerations allow us to sketch the set of entangled states in the case $N = 4$. In the 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 with a pinch of salt. In particular, the structure of the set of density matrices is not as simple and there exist several points inside the ball which do not correspond to density matrices. Furthermore, the 6-dimensional space of the pure states possesses the structure of the complex projective space $CP^3$, much more complicated than a hypersphere. In the sense of the Hilbert-Schmidt metric, $(\Delta_{HS}(\rho_1, \rho_2) = \sqrt{\text{Tr}[(\rho_1 - \rho_2)^2]})$, the set of the pure states forms a 6-dimensional subset of the 14-dimensional hypersphere of a radius $\sqrt{3}/2$ centered at $\rho_* = \frac{1}{4}$. Keeping this fact in mind, we represent this manifold by a circle in our oversimplified two-dimensional sketch.

![FIG. 3. Sketch of the set of mixed quantum states for $N = 4$: gray color represents the separable states](image)

The set of the separable states is visualized in Fig. 3 as a 'needle of a compass': it is convex, has a positive measure and includes the vicinity of the maximally mixed state $\rho_*$. 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 state, (localized closer to the center of the 'ball'), the larger probability of encountering a separable state. All states with $R \geq 3$ are separable; for simplicity this complicated set is symbolically represented by a smaller circle.

**B. Entanglement of formation**

After discussing the problem, how the probability of encountering a separable state changes with the degree of mixing $R$, we may discuss a related issue, how the average entanglement depends on $R$. For this purpose we need a quantitative measure of entanglement of a given mixed state. Several such quantities have recently been proposed and analyzed [12,30–40], 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 a minimal amount of entanglement necessary to create a given density matrix.

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

$$E(\psi) = -\text{Tr}\rho_A \ln \rho_A = -\text{Tr}\rho_B \ln \rho_B,$$

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

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

and the minimum is taken over all possible decompositions of the mixed state $\rho$ into pure states

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

The decomposition of $\rho$ 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 [24], since for any separable state $\rho_S$ one has $E(\rho_S) = 0$.

In Appendix B we present an algorithm allowing one to perform the minimization crucial for the definition [12]. It gives an upper estimation 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 qubits, discussed in this section, an analytical solution was found by Hill and Wooters [31], who introduced the concept of concurrence.

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

$$C(\rho) := \max\{0, \alpha_1 - \alpha_2 - \alpha_3 - \alpha_4\},$$
where $\alpha_i$s are the eigenvalues, in decreasing order, of the Hermitian matrix $\sqrt{\rho\sqrt{\rho}}$. Note that this matrix determines the Bures distance [14] between $\rho$ and $\tilde{\rho}$. In other words, $\alpha_i$s are the non-negative square roots of the moduli of the complex eigenvalues of the non Hermitian matrix $\rho\tilde{\rho}$.

Concurrence $C$ of a given state $\rho$ determines its entanglement of formation [13,15]

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

where

$$h(x) := -x \ln(x) - (1 - x) \ln(1 - x)$$

is the Shannon entropy of the 2-elements partition $\{x, 1-x\}$.

![FIG. 4. 2 × 2 system; a) The distributions $P(E)$ of the entanglement of formation obtained for the density matrices generated according to $\mu_o$ (white histogram, open symbols) and $\mu_u$ (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 $\mu$.](image)

Note that in the definition of entropy [11] the natural logarithm was used, (in contrast to the binary logarithm present in the paper [13]), so the entanglement $E \in [0, \ln 2]$. Two histograms in Figure 4 present the probability distribution $P(E)$ obtained for $N = 4$ random density matrices distributed according to both product measures $\mu_o$ and $\mu_u$. 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 gives favor to more pure, 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. 4a. 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 $\langle E \rangle_{\text{pure}} \approx 0.328$ 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 (11), we observe that the mean entanglement $\langle E \rangle$ decreases with increase of the parameter $\lambda$, as the distributions $\Delta_\lambda$ increasingly favor more mixed states.

Although the mean entanglement $\langle E \rangle$ strongly depends on the measure used, the conditional mean entanglement $\langle E \rangle(R)$, averaged over all states of the same degree of mixing $R$, is not sensitive to the choice of a measure, as demonstrated in figure 4b. 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 $R$, the smaller the mean entanglement of formation $E$. For $R > 3$ one has $\langle E \rangle(R) = 0$ [11].

**C. Negativity and concurrence**

In Ref. [11] we proposed a simple quantity $t$ defined by [8], which characterizes quantitatively, to what extent the positivity of partial transpose is violated. As shown in Fig. 4b the conditional average $\langle t \rangle(R)$ 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 the both quantities.

To analyze such a relation between these measures of entanglement, following the strategy of Eisert and Plenio [20], we generated $10^5$ random density matrices $\rho$ 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 the negativity, do not generate the same ordering in the space of $4 \times 4$ density matrices. However, large correlation coefficients (approximately 0.978 for the orthogonal measure and 0.967 for the unitary measure) reveals a statistical
connection between these measures.

A similar observation was already reported in [36], where a modulus of the negative eigenvalue $E_N$ of the partially transposed matrix $\rho^{T_2}$ was used. Since for $N = 4$ no more than one eigenvalue $d_i$ is negative [24], both quantities are equivalent and $t = 2E_N$. Note that due to the conjecture (17) we can attribute to negativity a more specific meaning. By means of equation (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 $E_r$.

Numerical investigations show that the difference $C - t$ is largest for mixed states with $R \approx 2$, while it vanishes for $R \geq 3$ and $R = 1$ (see Fig. 5b). In the former case all states are separable and $C = t = 0$. The latter case corresponds to pure states for which $\alpha_2 = \alpha_3 = \alpha_4 = 0$ [13] and $C = \alpha_1 - 2d_4^t = t$. 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.2b 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 $\mu_o$ and $\mu_u$. 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 $\rho$. Any state $\rho = UdU^\dagger$ can be expressed by the sum of $r$ terms, $\rho_{ij} = \sum_{l=1}^{r}d_lU_{il}U_{jl}^*$. Moreover, the number of nonzero eigenvalues $\alpha$ entering the definition of concurrence (14) equals to $r$ [13].

Take any vector with $r = 2$ nonzero elements. In this case the formula (14) reduces to $C = \alpha_1 - \alpha_2$. Since per definition $\alpha_1 \geq \alpha_2$, 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 with a simple conclusion:

For any set $\vec{d}$ of eigenvalues with $r \leq 2$ 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 an 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 $P_S \approx 0.105$ 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

FIG. 5. Ten thousands random density matrices of the 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 $R$.

It is particularly useful to look at the plane concurrence versus negativity. The data presented in Fig. 5a are obtained with the measure $\mu_u$. 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 $\rho$ the following inequality holds

$$t(\rho) \leq C(\rho).$$

A similar observation was already reported in [30], where...
given mixed state $\rho$, 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 fixed. For example, the mean entanglement, $\langle E \rangle$, equals 0.063, 0.057 and 0.042 for the ensembles $d'_a$, $d'_b$ and $d'_c$, 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 1. On the other hand, for any $N$ the relations between purity and entanglement depend only weakly on the kind of the product measure used.

![Purity and positive partial transpose](image)

**B. Entanglement of formation**

Since for $N > 4$ there exist no analytical methods to compute the entanglement of formation of an arbitrary mixed state $\rho$, we 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 $M \geq N$. It is described in detail in Appendix B. Each run ends with an approximate optimal decomposition of the state $\rho$ and provides an upper estimation of the entanglement $E$. To verify the accuracy of this technique we started with for 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 the 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, 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 $\rho$ in the discussed $2 \times 4$ case we started to look for the optimal entanglement decomposition with $M = N = 8$, recorded the minimal entanglement $E_{M=8}$, and repeated computations with $M = 9, 10, \ldots, M_{\text{max}}$. It is known 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 search for the optimal decomposition becomes less efficient with increase of 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, the 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 $2 \times 4$ 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 to search 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 [10] and [12], see [37]. We found it interesting to study the quantity $E_2$, which has a similar interpretation as the participation ratio $R$, and equals to unity for the separable states.

C. Volume of the bound entangled states

It is known 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. It was shown in [8] 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.

To estimate $P_B$ we generated $10^5$ random density matrices of size $N = 8$. We worked with the unitary product measure $\mu_u$, since, as shown in Table 1, the $2 \times 4$ states chosen according to the orthogonal measure $\mu_o$ very seldom satisfy the partial transposition criterion. To save the computing time we estimated the entanglement of formation $E$ only in the $2223$ cases with positive partial transpose. Setting an entanglement cut-off $E_c = 0.0003$, (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 cut-off 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 $R \approx 5.5$. 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 characterized by a high degree of mixing.

![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 $\mu_u$. 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).](image-url)
different measure related to the products measures, and also shown by Slater [6] for a that the answer will depend on the measure used. This chosen mixed state is separable, one should also expect possible outcomes.

determines the measure in the infinite space of the pos-
on the construction of the randomly chosen chord, which determines the measure in the 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 [3].

We reach, therefore, a simple conclusion, 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 the space of mixed quantum states.

On the other hand, this paper we provide arguments supporting the conjecture that some statistical properties of entangled states are universal and to a large extend 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 the separable states with the size N of the problem or the important relation between the purity of mixed quantum states and the probability to find a separable state.

Studying the simplest case N = 4 we have shown that the distribution of entanglement of formation is close to uniform in [0, ln2) for all pure states. The more mixed states, the larger peak at small values of entanglement, the larger 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 the 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, non-singular measures. Mean entanglement of formation for the bound entangled states is much smaller than for the free entangled states. 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 open problems in this field is still very long. Let us collect here some of them related to this work, mentioning also these, 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. 2b) holds also for the measures based on the monotone metrics [1] or for the product Bures measure [2,3].

(ii) Prove the relation between the concurrence and the negativity: C ≥ t.

(iii) Find max(C - t) as a function of the participation ratio R, (see Fig. 4b).

(iv) Check whether the following conjecture is true: If R(d_1) = R(d_2) and H_1(d_1) ≥ H_1(d_2) then P_S(ρ_1) ≥ P_S(ρ_2). The von Neuman entropy H_1 and the participation ratio R measure the degree of mixing of a given vector d, while P_S denotes the probability that a random state ρ_i = Ud_iU^† is separable.

(v) Find iso-probability surfaces in the simplex \{d_1, d_2, d_3\} such that P_S(d) =const.

B. N = 6, (2 × 3 or 3 × 2 systems)

(vi) Find a lower bound for the entanglement of formation E, (in the 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 whether all states violating the partial transpose criterion are free entangled.

(xii) Check whether the cardinality of any state is not larger than 8.

D. General questions

(xiii) Verify, whether 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 the cardinality $k$ of any mixed state in the $N$ dimensional Hilbert space is less or equal to $N = N_A N_B$?

(xv) Check whether the entanglement of formation is additive.

Not all of the above problems are of the same importance. As most relevant we regard the questions (i),(viii) and the last two general problems. Preliminary results of Slater suggest that the relation $P_S(R)$ for monotone metrics is similar to this obtained here for product metric, at least for $N = 4$. Concerning the question (viii): for separable states with $N = 8$, some necessary conditions, stronger than the positive partial transpose, are known, but the sufficient conditions assuring the separability are still most welcome. The problem of additivity of entanglement of formation is present in the literature (see e.g. [13]). Performing numerical estimations of the entanglement of formation $E$ for several states of $2 \times N_B$ systems we have not found any cases violating the statements (xiv) and (xv) [17]. Recent results of Lewenstein, Cirac and Karnas [18] suggest that the answer for the problem (xv) is negative for the systems $3 \times N_B$ with $N_B > 3$, but do not contradict this statement for the $2 \times N_B$ composed systems. Further effort is required to establish whether in this case the answer for the problem (xv) is positive.

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APPENDIX A: ROTATIONALLY INVARIANT PRODUCT MEASURES

In this appendix we show that a vector of a $N$-dimensional random orthogonal (unitary) matrix generates the Dirichlet measure 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 convenience of the reader, starting with the simplest case $N = 2$.

Lemma 1. Let $O$ be a $N \times N$ random orthogonal matrix distributed according to the Haar measure on $O(N)$. Then the vector $d_i = |O_{i1}|^2; \ i = 1, \ldots, N$ 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 $\sum_{i=1}^N d_i = 1$.

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: $P(\xi) = P(x) dx/d\xi = 1/(\pi \sqrt{(1-\xi)})$.

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 $\rho^2 = 1 - \sum_{i=1}^{N-1} x_i^2$. Uniform distribution of the points on the sphere is described by the volume element $d\Omega = \sin^{N-2} \theta_{N-2} \sin \theta_{N-1} d\theta_{N-2} \sin \theta_{N-1} d\theta_{N-1}$. Changing the polar coordinates into Cartesian we obtain $P(\rho) \sim 1/\cos \theta_{N-2} = 1/\sqrt{1-\rho^2}$. The last change of the variables $\xi_i := x_i^2$ for $i = 1, \ldots, N$ allows us to receive $P(\xi_1, \ldots, \xi_{N-1}) \sim [\xi_1 \xi_2 \cdots \xi_{N-1} (1 - \xi_1 - \xi_2 - \cdots - \xi_{N-1})]^{1/2}$, which gives the statistical measure $\Delta_{1/N}$ defined in Eq. (1).

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 $\{d_1, d_2, d_3\} = \{\xi_1, \xi_2, \xi_3\}$ lay 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 a $N \times N$ random unitary matrix distributed according to the Haar measure on $O(N)$. 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 $U(N)$ [23], based on the angles $\varphi_{kl} \in [0, \pi/2]$ with $0 \leq k < l \leq N - 1$. Their distribution can be determined by the relation $\varphi_{kl} = \arcsin \xi_{k+l}^{1/2(k+l+2)}$, where $\xi_k$ 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 $|U_{i1}|^2 = \{\cos^2 \varphi_{01} - \sin^2 \varphi_{01}\} = \{\xi_1 - \xi_1\}$ and the variable $d_i = \xi_1$ is distributed uniformly in the interval $[0, 1]$ (one dimensional simplex). For $N = 3$ one obtains $\vec{d} = \{\cos^2 \varphi_{12}, \sin^2 \varphi_{12} \cos^2 \varphi_{12}, \sin^2 \varphi_{12} \sin^2 \varphi_{12}\} = \{1 - \xi_2^2, \xi_2^2/(1 - \xi_1), \xi_2^2/(1 - \xi_1)\}$, which is distributed uniformly in the simplex $\{(0,0), (1,0), (0,1)\}$.

In the general $N$-dimensional case we get $\vec{d} = \{\cos^2 \varphi_{N-2,N-1}, \sin^2 \varphi_{N-2,N-1} \cos^2 \varphi_{N-3,N-1}, \sin^2 \varphi_{N-2,N-1} \sin^2 \varphi_{N-3,N-1} \cos^2 \varphi_{N-4,N-1}, \ldots, \sin^2 \varphi_{N-2,N-1} \sin^2 \varphi_{N-3,N-1} \sin^2 \varphi_{N-4,N-1}, \ldots, \sin^2 \varphi_{N-2,N-1} \sin^2 \varphi_{N-3,N-1} \sin^2 \varphi_{N-4,N-1} \sin^2 \varphi_{N-2,N-1} \cdots \sin^2 \varphi_{1,N-1} \sin^2 \varphi_{N-2,N-1}\}$. Using uniformly distributed random variables this vector may be written as $\{1 - \xi_{N-1}^{1/(N-1)} 1/(N-1), \xi_{N-1}^{1/(N-1)} 1/(N-1), \ldots, \xi_{N-1}^{1/(N-1)} 1/(N-1), \ldots, \xi_{N-1}^{1/(N-1)} 1/(N-1)\}$. For $N = 3$ we get $\{1 - \xi_2^{1/2}, \xi_2^{1/2}, (1 - \xi_1), (1 - \xi_1)\}$. For $N = 4$ we get $\{1 - \xi_3^{1/3}, \xi_3^{1/3}, (1 - \xi_2), (1 - \xi_2), (1 - \xi_2)\}$. For $N = 5$ we get $\{1 - \xi_4^{1/4}, \xi_4^{1/4}, (1 - \xi_3), (1 - \xi_3), (1 - \xi_3), (1 - \xi_3)\}$. For $N = 6$ we get $\{1 - \xi_5^{1/5}, \xi_5^{1/5}, (1 - \xi_4), (1 - \xi_4), (1 - \xi_4), (1 - \xi_4), (1 - \xi_4)\}$.
analyzed in \([54x-800]\). 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. \([4x-572]\). Alternatively, one may take a random matrix of Gaussian orthogonal (unitary) ensemble, diagonalize it, and use one of its eigenvectors as in \([\text{3}]\). 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 \([\text{32}]\). Statistics of eigenvectors during such a transition were studied e.g. in \([\text{34}]\), while the transitions between circular ensembles of unitary matrices were analyzed in \([\text{35}]\).

**APPENDIX B: ENTANGLEMENT OF FORMATION - A NUMERICAL ALGORITHM**

1. Generating random density matrix

In order to generate an \(N \times N\) random density matrix we write \(\rho = U dU^\dagger\) and use the product measure \(\mu = \Delta_A \times \nu_H\). The vector of eigenvalues \(d\), taken according to the Dirichlet measure \([\text{3}]\), can be obtained from unitary random matrices as shown in Appendix A. Unitary random rotation matrix \(U\) distributed according to the Haar measure \(\nu_H\) is generated with the algorithm presented in \([\text{33}]\). Random state \(\rho\), generated according to a given product measure, may be decomposed into a mixture of \(N\) pure states determined by its eigenvectors

\[
\rho = \sum_{i=1}^N |\Psi_i\rangle \langle \Psi_i|.
\]

(B1)

Note that the pure states \(|\Psi_i\rangle\) are not normalized to unity, but its 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 \(\rho\) into a mixture of \(M\) pure states, with \(M \geq N\). Let \(\hat{V}\) be a random unitary matrix of size \(M\) distributed according to the Haar measure on \(U(M)\). Let \(V\) denotes a rectangular matrix constructed of the \(N\) first columns of \(\hat{V}\). Any such \(M \times N\) matrix allows one to write a legitimate decomposition \(\rho'\) of the same state \(\rho\)

\[
\rho' = \sum_{i=1}^M |\phi_i\rangle \langle \phi_i|,
\]

(B2)

where \(|\phi_i\rangle = \sum_{m=1}^N V_{im} |\Psi_m\rangle; \ i=1, \ldots, M\).

Unitarity of the rotation matrix \(\hat{V}\) assures the correct normalization \(\text{Tr} \rho' = \sum_{i=1}^M \langle \phi_i | \phi_i \rangle = 1\).

Assume that the composite \(N\) dimensional quantum system consists of two subsystems of the size \(N_A\) and \(N_B\), such that \(N = N_A N_B\). It is then convenient to represent any vector \(|\phi_i\rangle\) (of a non zero 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 a \(N_B \times N_B\) Hermitian matrix

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

(B4)

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

\[
E_B(|\phi_i\rangle) := - \sum_{i=1}^{N_B} \hat{b}_l^{(i)} \ln \hat{b}_l^{(i)},
\]

(B5)

giving the von Neumman entropy of the reduced state. Entanglement of the state \(\rho'\) with respect to the rotated decomposition \([\text{32}]\) is equal to the average entropy of the pure states involved

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

(B6)

where \(\sum_{i=1}^M p_i = 1\).

The entanglement of formation \(E\) of the state \(\rho\) is then defined as a minimal value \(E_B(\rho')\), where the minimum is taken over the set of the decompositions \(\rho'\) given by \([\text{32}]\), (compare with the definition \([\text{12}]\)). 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 found it interesting to consider also the generalized entanglement

\[
E_q(\rho') = \sum_{i=1}^M p_i E_q(|\phi_i\rangle),
\]

(B7)

where

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

(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 $V_0$ 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 to land close to the $M$ dimensional manifold defined by optimal matrices equivalent to $V_0$. 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 $\langle \sigma_{m,n}^2 \rangle = (1 + \delta_{m,n})/M$ for the real part and $\langle \sigma_{m,n}^{\ast} \rangle = (1 - \delta_{m,n})/M$ for the imaginary part of each complex element $H_{m,n} = H_{n,m}^\ast$. 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 $\chi_0$, performing random movements of this size and then gradually decreasing the angle $\chi$.

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

1. Fix the number $M$ of the components of the decomposition $[2]$. Start with $M = N$.
2. Generate random unitary rotation matrix $V$ of size $M$, which defines the decomposition $\rho'$ in $[2]$. Compute the entanglement $E = E_B(\rho')$ according to $[13, 30]$.
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 $\rho'$ generated by $V'$.
5. If $E' < E$ accept the move (substitute $V := V'$ and $E := E'$) and continue with the step (4). In the other case repeat the steps (4-5) $I_{\text{change}}$ times.
6. Decrease the angle $\chi := \alpha \chi$, where $\alpha < 1$.
7. Repeat the steps (4-6) until $\chi < \chi_{\text{end}}$. Memorize the final value of the entanglement $E$.
8. Repeat $L_{\text{mat}}$ times the steps (2-7) starting from a different initial random matrix $V$.
9. Memorize the value $E_M$, defined as the smallest of $L_{\text{mat}}$ repetitions of the above procedure.
10. Set $M := M + 1$ and repeat the steps (2-9) until $M = M_{\text{max}}$.
11. Find the smallest value of $E_M$, $M = N, \ldots, M_{\text{max}}$. This value $E_{\text{min}} = E_M$, gives the upper bound for the entanglement of formation of the mixed state $\rho$, while the size $M_*$ of the optimal rotation $V_*$ may be considered as the cardinality of $\rho$.

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 $[13]$ exist. Results mentioned in the section IV B, giving the mean error of the estimation of the entanglement smaller than $10^{-3}$, were obtained with the following algorithm parameters: the initial angle $\chi_0 = 0.3$, the final angle $\chi_{\text{end}} = 0.0001$, the angle reduction coefficient $\alpha = 2/3$, the number of iterations with the angle fixed $I_{\text{change}} = 25$, the number of realizations $L_{\text{mat}} = 3$. 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 $\rho$. 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 impose therefore 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 $\chi_{\text{end}} = 0.0002$ we obtained in a histogram $P(E)$ a flat local minimum at $E_{\text{m}} \sim 0.0003$. The minimum is located just right to the singular peak at even smaller values of $E$, corresponding to separable states. The cumulative distribution $P_c = \int_{-\infty}^{E_{\text{m}}} P(E) dE$ was found not to be very sensitive on the position of the minimum $E_{\text{m}}$. We could, therefore, set the cut-off value $E_c$ to the position of minimum $E_{\text{m}}$, and interpret the quantity $P_c$ as the relative volume of the bound entangled states. In the computations described in section IV C we took $\chi_0 = 0.3$, $\alpha = 2/3$, $I_{\text{change}} = 25$ and $L_{\text{mat}} = 5$, and for $M = N = 8$ obtained the mean number of iterations $I$ of the order $5 \times 10^4$.

The other possibility to distinguish the bound entangled states from the separable states consists in studying the dependence of the obtained upper bound on the entanglement $E$ on the total number $I$ of iterations performed. Numerical results obtained for the separable states show that $E$ decreases with the computation time not slower than $E(I) = a/I$. Assuming a similar effectiveness of the algorithm for the nonseparable states (with a non zero entanglement of formation $E_{\text{form}}$), we have $E(I) = E_{\text{form}} + b/I$. This allows us to design a simple auxiliary criterion: the state $\rho$ 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 ful-
filled the state $\rho$ 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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