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Minimum distance of the boundary of the set of PPT states from the maximally mixed state using the geometry of the positive semidefinite cone

Shreya Banerjee[1] · Aryaman A. Patel[2] · Prasanta K. Panigrahi[1]

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Abstract
Using a geometric measure of entanglement quantification based on Euclidean distance of the Hermitian matrices (Patel and Panigrahi in Geometric measure of entanglement based on local measurement, 2016. arXiv:1608.06145), we obtain the minimum distance between the set of bipartite n-qudit density matrices with a positive partial transpose and the maximally mixed state. This minimum distance is obtained as $\frac{1}{\sqrt{d^n(d^n-1)}}$, which is also the minimum distance within which all quantum states are separable. An idea of the interior of the set of all positive semidefinite matrices has also been provided. A particular class of Werner states has been identified for which the PPT criterion is necessary and sufficient for separability in dimensions greater than six.

Keywords Entanglement · Separability · Partial transpose · Werner states · PPT criterion · Positive semidefinite cone

1 Introduction

Characterization of entanglement is of deep interest in the field of quantum information and quantum computation [1–3]. As is well known, there are two types of entangled states: distillable and non-distillable [4]. Distillable entangled states find application

✉ Shreya Banerjee
shreya93ban@gmail.com

Aryaman A. Patel
13me121.aaryaman@nitk.edu.in

Prasanta K. Panigrahi
panigrahi.iiser@gmail.com

1 Indian Institute of Science Education and Research Kolkata, Mohanpur, West Bengal 741246, India

2 National Institute of Technology Karnataka, Surathkal, Mangalore, Karnataka 575025, India

in quantum technology: quantum teleportation [5,6], quantum error correction [7,8], quantum cryptography [9–11], etc. The other class of entangled states that cannot be distilled is called bound entangled states, which has found application in steering and ruling out local hidden state models [12]. The Peres–Horodecki criterion provides a necessary and sufficient condition for separability in $2 \otimes 2$ and $2 \otimes 3$ dimensions. It fails to identify separable states in higher dimensions. Using this criterion, one can only identify the states that have positive partial transpose (PPT) in higher dimensions. By definition, such states, if entangled, are bound entangled states [13].

There have been various approaches to analyze the geometry of the quantum state space [14–16] and entanglement measures based on geometry [17–22]. Geometry has also been used in quantum computation to develop new algorithms [23,24]. Recently, quantification of entanglement has been carried out from a geometric perspective, for general n-qudit states [17]. Another related approach has used wedge product [25], which manifests naturally in a geometric setting of concurrence, a proven measure of entanglement and tangle in two-qubit pure states [26–28] as well as in atom entanglement [29], hybrid entanglement [30] and hyperentanglement [31]. This geometric approach makes essential use of the fact that measurement of a subsystem of an entangled state necessarily affects the remaining constituents in contrast to separable states. Using this approach and the geometry of $N = d^n$-dimensional positive semidefinite matrices, here we establish the radius for the absolutely PPT ball. This radius coincides with the largest separable ball [32]. As is well known, PPT criterion is not the sufficient condition for separability for states with dimension greater than 6. One can therefore conclude that the largest PPT ball coincides with the largest separable ball for arbitrary dimension revealing that the PPT criterion is useful to determine the largest separable ball. We further show that this criterion is necessary and sufficient to determine the separability of a particular class of n-qubit Werner states.

The paper is organized as follows: Sect. 2 describes classification of states based on their partial transpose and the general geometry of density matrices; in Sect. 3, the boundary of the PPT states has been calculated using the geometry of the positive semidefinite cone and its intersection with the state space of the density matrices; the distance of the general n-qudit states from the maximally mixed state of order N, where $N = d^n$ has been calculated in Sect. 4, starting with an example of the procedure of calculating the distance between a 2-qubit state and the normalized identity of order 4; in Sect. 5, the maximal distance from the normalized identity of a special class of Werner states to be separable and PPT have been discussed; we then conclude in Sect. 6 with directions for future work.

2 Classification and measurement-based geometry of n-dimensional density matrices

A general state ρ acting on $H_A \otimes H_B$ can be written as [33],

$$\rho = \sum_{ijkl} p_{kl}^{ij} \left|i\right\rangle \left\langle j\right| \otimes \left|k\right\rangle \left\langle l\right|, \tag{1}$$

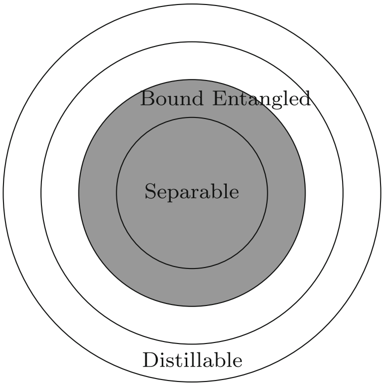

Fig. 1 Diagrammatic representation of the set of all mixed states, or a general arbitrary Hilbert space; the shaded region is the set of all PPT states and the white portion is the set of all NPT states

with its partial transpose defined as,

$$\rho^{\mathrm{T}_B} = \mathbb{I} \otimes T(\rho) = \sum_{ijkl} p_{kl}^{ij} \left|i\right\rangle \left\langle j\right| \otimes \left|l\right\rangle \left\langle k\right|. \tag{2}$$

Here, $\mathbb{I} \otimes T(\rho)$ is the map that acts on the composite system with identity map acting on system A and transposition map acting on B.

ρ is called PPT if its partial transpose ρ^{T_B} is a positive semidefinite operator. If ρ^{T_B} has a negative eigenvalue, it is called NPT. It is known from Peres–Horodecki criterion that for $2 \otimes 2$ and $2 \otimes 3$ dimensions, all PPT states are separable and all NPT states are entangled. For arbitrary $n \otimes m$ dimensions, some PPT states show entanglement, whereas all NPT states are necessarily entangled [33].

For a bipartite state ρ, $H = H_A \otimes H_B$ and for an integer $k \geq 1$, ρ is k-distillable if there exists a (non-normalized) state $\left|\psi\right\rangle \in H^{\otimes k}$ of Schmidt rank at most 2 such that,

$$\left\langle \psi\right| \sigma^{\otimes k} \left|\psi\right\rangle < 0, \sigma = \mathbb{I} \otimes T(\rho).$$

ρ is distillable if it is k-distillable for some integer $k \geq 1$ [13].

If a state ρ is PPT, it is non-distillable; hence, entangled PPT states have no distillable entanglement. Such states are called PPT bound entangled states. All distillable entangled states are NPT. The converse may not hold, i.e., whether all NPT states are distillable or not; although it is believed that the converse does not hold [13]. Figure 1 represents a schematic representation of the different classes of quantum states.

The Euclidean distance between any two Hermitian matrices ρ and σ is given by [17],

$$D(\rho, \sigma) = \sqrt{Tr(\rho - \sigma)^2}. \tag{3}$$

The set of all n-qudit density matrices, i.e., density matrices of order N where $N = d^n$, is considered as a convex compact set embedded in the closed $(N^2 - 1)$ ball $\mathbb{B}^{N^2-1}$ of radius $\sqrt{\frac{N-1}{N}}$, centered at normalized identity $\frac{\mathbb{I}}{N}$. This set always admits a regular

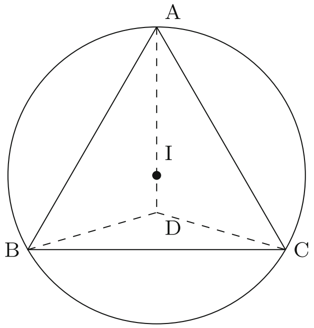

Fig. 2 Orthogonal basis represented by a 3-simplex, a regular tetrahedron, for bipartite 2-qubit systems. The sphere here represents the closed $\mathbb{B}^{15}$ ball centered at identity I. The set of all 2-qubit states admits a convex set embedded in this ball. The tetrahedron ABCD represents one of the orthogonal bases of this convex set. Its vertices A, B, C and D represent pure states as they lie on the surface of the ball

$N-1$ simplex with its vertices on the boundary of the ball as one of its orthogonal bases. The convex hull of a basis is represented by a regular m simplex centered at normalized identity $\frac{\mathbb{I}}{N}$ and circumscribed by $\mathbb{B}^{N^2-1}$, where $N-1 \leq m \leq N^2-1$. Each density matrix can thus be treated as a point in a simplex whose vertices are pure states.

We take the set of all 2-qubit density matrices (order 4) as an example. The geometry of this set implies a convex compact set embedded in closed $\mathbb{B}^{15}$ ball. One of its orthogonal bases can be represented by a tetrahedron, the usual 3-simplex, centered at $\frac{\mathbb{I}}{4}$ and circumscribed by the $\mathbb{B}^{15}$, i.e., the vertices of the tetrahedron will be pure states, as depicted in Fig. 2. The convex hull of this tetrahedron will admit to the set of all density matrices, which can be represented by another regular m' simplex, where $3 \leq m' \leq 15$, centered at $\frac{\mathbb{I}}{4}$ and circumscribed by $\mathbb{B}^{15}$.

Based on this geometry, a separability criterion is proposed in [17]. Due to the convex property of the simplices, if a density matrix lies in a simplex whose vertices are separable states, it is separable. Thus, in the following, an orthogonal basis of the set of all composite density matrices spanned by pure separable states can be constructed from the orthogonal bases of the constituents of the composite system.

As an example, we again consider the 2-qubit, i.e., $N=4$ case with bi-partitions A and B. We consider two orthogonal matrices π_A and σ_A as the antipodal points on the Bloch sphere of A. The diameter formed by these two points is a simplex of $N=2$ dimension, i.e., the dimension of A. Two similar points on the Bloch sphere of B are also chosen as π_B and σ_B. The matrices $\pi_A \otimes \pi_B$, $\pi_A \otimes \sigma_B$, $\sigma_A \otimes \pi_B$, $\sigma_A \otimes \sigma_B$ will represent the vertices of a regular tetrahedron in $N=4$, circumscribed in $\mathbb{B}^{15}$ ball, centered at $\frac{\mathbb{I}}{4}$. This tetrahedron is the said orthogonal basis of the set of all composite density matrices spanned by pure separable states. Henceforth, if one takes a measurement on any of the qubits of the composite system, both the post-measurement matrices will geometrically coincide with the constituent diameters of the Bloch spheres of the respective qubits, i.e., simplices of the constituent dimension, i.e., $N=2$.

To generalize, a bipartite n-qudit density matrix ρ with bi-partitions A–B is considered. To find out the separability criterion for ρ, a measurement on one of the bi-partitions is done [17]. Then, one checks whether both the post-measurement reduced density matrices ρ_A and ρ_B localize to the simplices of corresponding dimensions using Eq. (3). The distance between the reduced density matrices and the center of the closed ball homeomorphic to the corresponding simplex is calculated using Eq. (3), and if it lies within the bound given in Ref. [17], then it is certainly separable. A similar approach has been used in [25], where a bipartite $n-$qudit pure state is projected in a basis consisting of two orthonormal bases to check the separability of the state.

To check whether a state is PPT, we consider the geometry of the set of all positive semidefinite matrices, as all partially transposed PPT states are either positive semidefinite or positive definite.

A subset S of a vector space V is called a cone if $\forall x \in C$ and positive scalar α, $\alpha x \in C$. A cone C is called a convex cone if $\alpha x + \beta y \in C$.

The defining property of the set of all positive semidefinite matrices P of order N is that the scalar $x^T x$ is positive for each nonzero column vector x of N real numbers. Let P be the set of all positive semidefinite matrices, then $\forall X, Y \in P$ and $\alpha, \beta > 0$,

$$x^T(\alpha X + \beta Y)x = \alpha x^T Xx + \beta x^T Yx > 0,$$

i.e., P is a convex cone. The set of the positive semidefinite (PSD) matrices of order $N \times N$ hence forms a convex cone S_N in $\mathbb{R}^{N^2}$. The minimum distance to the boundary of this cone from the normalized identity is the radius of the ball within which every state is PPT.

A few interesting known properties of this cone are,

(a) it has non-empty interior containing positive definite matrices, which are full rank;
(b) the singular positive semidefinite matrices with at least one zero eigenvalue lie on the boundary of the cone.

To calculate the minimum distance of the boundary of this cone from the normalized identity of dimension N, i.e., the center of the closed ball $\mathbb{B}^{N^2-1}$, one needs to identify the geometry of the interior of the S_N cone. Each positive semidefinite matrix of order N is associated with a quadric. One can represent a diagonalized symmetric matrix of order 2 as a conic using the characteristic equation of the matrix. Let us consider the matrix

$$\begin{bmatrix} a & 0 \\ 0 & b \end{bmatrix}$$

with the eigenvector corresponding to eigenvalue a,

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

where the following equation represents the conic associated with it.

$$a{x_1}^2 + b{x_2}^2 = a \tag{4}$$

Analogously, each positive definite matrix of order 3 forms an ellipsoid and each positive semidefinite matrix will be a set of either intersecting planes or parallel planes. The matrix with all three eigenvalues zero would be represented by a point. This leads us to propose the following conjecture that:

The interior of the S_3 cone is comprised of ellipsoids, and its boundary is formed by intersecting and parallel planes with origin at (0,0,0).

Generalizing the conjecture for N dimensions,

Conjecture *The interior of the general S_N cone is comprised of conics associated with N-dimensional matrices. Its boundary is formed by conics of N' dimensions, i.e., $N' < N$ intersecting and parallel planes at the boundary and the origin at $(0, 0, 0.._{uptoN})$. The ball is embedded in a subspace of the cone as the origin of the general S_N cone is equidistant from each point on the surface of the $\mathbb{B}^{N^2-1}$ ball. [This is also supported by the fact that the origin of the cone is not a density matrix, since it does not satisfy the trace condition.]*

Taking a transposition of one of the subsystems of a bipartite system (the partial transpose) if one finds the resulting density matrix to lie within the cone formed by the positive semidefinite matrices, the density matrix of the bipartite system is assumed to be PPT.

The set of n-qudit density matrices (i.e., order of the matrix, $N = d^n$) is represented by convex sets homeomorphic to a closed ball of radius $R =$ centered at the maximally mixed state, the identity matrix of $d^n \times d^n$ dimension. Expectedly this contains entangled states with positive partial transpose and negative partial transpose. If the partial transpose of a density matrix is positive, then it will lie within the S_N cone. Now the minimum distance of the S_N cone from the maximally mixed state placed at the center of the $\mathbb{B}^{N^2-1}$ ball is the distance for which the density matrix would definitely be PPT.

3 Minimum distance within which a state would be definitely PPT

We consider a bipartite 2-qubit density matrix. In this case, there is no bound entanglement as the PPT criterion is necessary and sufficient for separability for $2 \otimes 2$ systems. If the density matrix is PPT, then the partial transpose of the matrix will lie within the cone S_4 of all positive semidefinite matrices of order 4. The set of all density matrices considered is homeomorphic to the closed ball $\mathbb{B}^{15}$.

Following the conjecture in Sect. 2, one can identify that the boundary of S_4 is formed by positive semidefinite matrices of order 4 which can be represented by ellipsoids, parallel planes and intersecting planes. The parallel planes intersect the set of density matrices at the pure states on the surface [1, 0, 0, 0], [0, 1, 0, 0], [0, 0, 1, 0] and [0, 0, 0, 1]. The ellipsoids on the boundary of the cone illustrate the curved surface

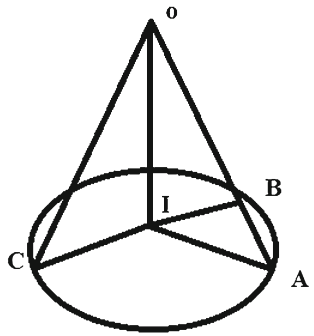

Fig. 3 Cross section of the $\mathbb{B}^{15}$ ball and S_4 cone, showing the center of the ball I and the origin of the cone O

of the cone, and the intersecting planes indicate the intersection boundary of the cone with the ball. In their 2−dimensional projections, they form a set of intersecting lines

$$\frac{x^2}{a^2} = \frac{y^2}{b^2}, \tag{5}$$

yielding,

$$\frac{y}{x} = \pm\frac{b}{a}. \tag{6}$$

where a and b are both nonzero eigenvalues of the system. Figure 3 depicts that.

From Fig. 3, $A\ and\ C$ are the points where the cone cuts the ball and IB is the perpendicular distance from I to the boundary of cone. The slope of the intersecting lines OC and OA is given by $\frac{b}{a}$. Slope of OA is also given by $\frac{OI}{IB}$.

Using Hilbert–Schmidt norm, the distance of the maximally mixed state from the origin of the S_4 cone is found to be $OI = \frac{1}{\sqrt{4}}$. The slope of the line OA is given by,

$$\frac{OI}{IB} = \frac{b}{a}, \tag{7}$$

The minimum value of IB is obtained as,

$$IB_{\min} = \frac{1}{\sqrt{4}}\left(\frac{a}{b}\right)_{\min}, \tag{8}$$

where the minimum value of $\frac{a}{b}$ is,

$$\left(\frac{a}{b}\right)_{\min} = \frac{\frac{1}{\sqrt{\lambda_{\max}}}}{\frac{1}{\sqrt{\lambda_{\min}}}} = \frac{\sqrt{\lambda_{\min}}}{\sqrt{\lambda_{\max}}}, \tag{9}$$

where λ is the eigenvalue of the matrix considered.

The intersecting part of the S_4 cone and the $\mathbb{B}^{15}$ ball is essentially convex, implying it is a subspace of any of the 15-simplices with vertices at [1,0,0,0], [0,1,0,0], [0,0,1,0] and [0,0,0,1]. Hence, we have, $\lambda_{\min} = \frac{1}{4}$ and $\lambda_{\max} = \frac{3}{4}$, which leads us to,

$$IB_{\min} = \frac{1}{\sqrt{12}} \tag{10}$$

The ratio of IB and a proper radius of $\mathbb{B}^{15}$ ball is given by,

$$\frac{IB_{\min}}{R^{15}} = \frac{1}{3}. \tag{11}$$

PPT criterion is necessary and sufficient for separability in bipartite $2 \otimes 2$ systems. Following that, a 4−dimensional state is absolutely separable if it lies within a distance of $\frac{1}{3}R$ of the maximally mixed state. This result matches with the separability criterion known for the 4-qubit Werner states [17].

For higher dimensions, the PPT criterion is not sufficient for separability. Instead, the criterion helps us to detect bound entangled states. For $N-$dimensional states, the cone of all PSD matrices intersects the $\mathbb{B}^{N^2-1}$ ball in $\mathbb{R}^{N^2-1}$. Considering the geometry of diagonalized PSD matrices of N^2-1 dimensions, one can infer that they are associated with either $M-$dimensional ellipsoids that form the curved surface of the cone where $M < (N^2-1)$ or intersecting lines that give the boundary of the cone or intersecting planes, which denote the points where the cone cuts the ball.

Considering the intersecting lines, we have the minimum distance IB of the boundary of the cone from the maximally mixed state as,

$$IB = \frac{1}{\sqrt{N}}\sqrt{\frac{\lambda_{\min}}{\lambda_{\max}}} \tag{12}$$

This minimum distance satisfies the following inequality:

$$\left(\lambda_1 - \frac{1}{N}\right)^2 + \left(\lambda_2 - \frac{1}{N}\right)^2 \geq 0, \tag{13}$$

λ_1 and λ_2 are two eigenvalues of the corresponding PSD matrix.

One can, then, obtain the minimum value of λ that corresponds to the minimum distance, $\lambda_{\min} = \frac{1}{N}$.

The intersection part of the $\mathbb{B}^{N^2-1}$ ball and S_N cone is essentially a subspace of the largest convex set embedded in the $\mathbb{B}^{N^2-1}$ ball, any of the N^2-1 simplices.

Considering the simplex of all density matrices, one can then obtain, $\lambda_{\max} = \frac{1}{N-1}$.

From Eq. (12), the maximum distance of ρ from $\mathbb{I}_N$ such that ρ is definitely PPT is,

$$IB_{\min} = \frac{1}{\sqrt{N(N-1)}}. \tag{14}$$

In [32], the boundary of largest separable ball was shown to lie at a distance $\frac{1}{\sqrt{N(N-1)}}$ from the maximally mixed state. The boundary of the absolutely PPT states therefore coincides with the boundary of largest separable ball (LSB). In [34], Bandyopadhyay and Roychowdhury found that NPT states exist just outside the boundary of the LSB, which is in agreement with the claim of this paper.

4 General distance of the partial transpose of a n-dimensional matrix from normalized identity

Any density matrix ρ of order $N \times N$ can be written as [35],

$$\rho = pP_{\psi} + (1-p)\rho'', \tag{15}$$

where $p \in [0, 1]$; P_{ψ} is a pure state and ρ'' any separable density matrix.

We consider a 2-qubit Werner state as,

$$\rho_{w_2} = pP_2^{\psi} + (1-p)\frac{\mathbb{I}}{4} \tag{16}$$

Where P_2^{ψ} is the Bell state, i.e., a pure state, and $\frac{\mathbb{I}}{4}$ is the normalized identity matrix of order 4, i.e., a separable state.

Partial transposition of ρ_{w_2} gives,

$$\rho_{w_2}^{\mathrm{T}_B} = p(P_2^{\psi})^{\mathrm{T}_B} + (1-p)\frac{\mathbb{I}}{4}. \tag{17}$$

The Euclidean distance between $\rho_{w_2}^{\mathrm{T}_B}$ and the normalized identity is given by,

$$D(\rho_{w_2}^{\mathrm{T}_B}, \mathbb{I}_4) = \sqrt{Tr\left(\rho_{w_2}^{\mathrm{T}_B} - \frac{\mathbb{I}}{4}\right)^2}, \tag{18}$$

where

$$Tr\left(\rho_{w_2}^{\mathrm{T}_B} - \frac{\mathbb{I}}{4}\right)^2 = Tr(\rho_{w_2}^{\mathrm{T}_B})^2 - \frac{Tr(\rho_{w_2}^{\mathrm{T}_B})}{2} + \frac{1}{4}, \tag{19}$$

and from Eq. (17),

$$Tr(\rho_{w_2})^{\mathrm{T}_B} = pTr(P_2^{\psi})^{\mathrm{T}_B} + (1-p)Tr\left(\frac{\mathbb{I}}{4}\right). \tag{20}$$

Using the eigenvalues of the partial transposition of a Bell state, i.e., $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, -\frac{1}{2})$ in a $2 \otimes 2$ bi-partition, the distance of the partially transposed 2-qubit Werner state from the maximally mixed state calculated from Eqs. (18), (19) and (20) is given as,

$$D(\rho_{w_2}^{\mathrm{T}_B}, \mathbb{I}_4)^2 = \frac{3p^2}{4}. \tag{21}$$

Equating this distance to the minimum distance to the boundary of the set of all PPT states found from Eq. (10) for $2 \otimes 2$ states, we can find the maximum value of p for ρ_{w_2} to be PPT, and, hence, separable, is $p = \frac{1}{3}$.

We can generalize this approach using Eq. (15).

Partial transpose of Eq. (15) yields,

$$\sigma^{\mathrm{T}_B} = p(\sigma^{\mathrm{T}_B})' + (1-p)(\sigma^{\mathrm{T}_B})'', \tag{22}$$

where σ^{T_B} is the partial transpose of ρ, $(\sigma^{\mathrm{T}_B})'$ is the partial transpose of P_ψ and $(\sigma^{\mathrm{T}_B})''$ is the partial transpose of ρ''.

We consider the Euclidean distance between σ^{T_B} and the normalized identity of order N:

$$D(\sigma^{\mathrm{T}_B}, \mathbb{I}_N) = \sqrt{Tr\left(\sigma^{\mathrm{T}_B} - \frac{\mathbb{I}}{N}\right)^2}, \tag{23}$$

yielding,

$$D(\sigma^{\mathrm{T}_B}, \mathbb{I}_N) = \sqrt{Tr(\sigma^{\mathrm{T}_B})^2 - \frac{2}{N}Tr(\sigma^{\mathrm{T}_B}) + \frac{1}{N}}, \tag{24}$$

where

$$Tr(\sigma^{\mathrm{T}_B}) = pTr(\sigma^{\mathrm{T}_B'}) + (1-p)Tr(\sigma^{\mathrm{T}_B''}), \tag{25}$$

and,

$$\begin{aligned} Tr(\sigma^{\mathrm{T}_B})^2 &= p^2 Tr(\sigma^{\mathrm{T}_B'})^2 + (1-p)^2 Tr(\sigma^{\mathrm{T}_B''})^2 \\ &\quad + 2p(1-p)Tr(\sigma^{\mathrm{T}_B'}\sigma^{\mathrm{T}_B''}). \end{aligned} \tag{26}$$

Using Eqs. (24), (25), and (26), we have the distance of the partially transpose of any density matrix characterized by the parameter p from the normalized identity as,

$$\begin{aligned} D(\sigma^{\mathrm{T}_B}, \mathbb{I}_N)^2 \leq & p^2 \sum_i \lambda_i{}^2 + (1-p)^2 \sum_j \lambda_j{}^2 + 2p(1-p) \sum_{i,j} \lambda_i \lambda_j \\ & - \frac{2}{N}\left(p \sum_i \lambda_i + (1-p) \sum_j \lambda_j\right) + \frac{1}{N}, \end{aligned} \tag{27}$$

as, $Tr(\sigma^{\mathrm{T}_B'}\sigma^{\mathrm{T}_B''}) \leq \sum_{i,j} \lambda_i \lambda_j$ [36]. Here, λ_i is the ith eigenvalue of the matrix $(\sigma^{\mathrm{T}_B})'$ and λ_j is the jth eigenvalue of the matrix $(\sigma^{\mathrm{T}_B})''$.

The spectrum of the partial transposition of a pure state $\rho = |\psi\rangle\langle\psi|$ is given in [37].

The Schmidt decomposition of $|\psi\rangle \in H = H^m \otimes H^n$ is given by,

$$|\psi\rangle = \sum_i \alpha_i |e_i\rangle \otimes |f_i\rangle \tag{28}$$

where $|e_i\rangle \otimes |f_i\rangle$ forms a bi-orthogonal basis, i.e., $\langle e_i|e_j\rangle = \langle f_i|f_j\rangle = \delta_{ij}$ and $0 \leq \alpha_i \leq 1$ along with $\sum_i \alpha_i^2 = 1$.
The partial transposition of ρ, ρ^{T_B}, has eigenvalues, α_i^2 for $i = 1, 2, \ldots r$, where r is the Schmidt rank; $\pm\alpha_i\alpha_j$ for $1 \leq i < j \leq r$ and 0 with multiplicity $min(m, n)|m - n| + \{min(n, m)\}^2 - r^2$. From the above condition, the trace of the partial transposition of a pure state is given by, $\sum_i \lambda_i = \sum_{i=1,2,..,r} \alpha_i^2 + \sum_{i,j}(\alpha_i\alpha_j - \alpha_i\alpha_j) = 1$.

The maximum value of the square of the eigenvalues of the partial transposition of a pure state is given by $\sum_i {\lambda_i}^2 \leq 1$ as $\forall i, \alpha_i \leq 1$, with the maximum condition holding when only one value of i survives and $\lambda_i = 1$. This condition ensures $Tr(\sigma^{\mathrm{T}_B}{}' \sigma^{\mathrm{T}_B}{}'') \leq \lambda_k$, where k corresponds to the index of the eigenvalue of the partially transposed separable state $(\sigma^{\mathrm{T}_B})''$ multiplied to the only surviving eigenvalue of the partial transposed matrix of the pure state.

From [38], all eigenvalues of partial transposition of any $m \otimes n$ state always lie within $[-1/2, 1]$. Since $(\sigma^{\mathrm{T}_B})''$ is the partial transposition of a separable state, $\lambda_j \in [0, 1] \forall j$, and $\sum_j \lambda_j$ as well as $\sum_j \lambda_j^2$ are necessarily positive.

Incorporating the above maximization conditions in Eq. (27), we have the maximum distance of the partial transpose of a density matrix characterized by p from the normalized identity as,

$$\begin{aligned} {D(\sigma^{\mathrm{T}_B}, \mathbb{I}_N)^2}_{\max} &= p^2 + (1-p)^2 \sum_j {\lambda_j}^2 + 2p(1-p)\lambda_k \\ &- \frac{2}{N}\left(p + (1-p)\sum_j \lambda_j\right) + \frac{1}{N} \end{aligned} \tag{29}$$

where λ_j is the jth eigenvalue of the matrix $(\sigma^{\mathrm{T}_B})''$ and k corresponds to the index of the eigenvalue of the partially transposed separable state $(\sigma^{\mathrm{T}_B})''$ multiplied to the only surviving eigenvalue of the partial transposed matrix of the pure state. Here, the inequality vanishes as we are considering the maximal distance and thus have taken $Tr(\sigma^{\mathrm{T}_B}{}' \sigma^{\mathrm{T}_B}{}'') = \lambda_k$.

If σ^{T_B} is positive semidefinite or positive definite, it lies either on the boundary of the convex cone S_N or inside it.

The maximum value of the distance for which the state ρ will be PPT corresponds to the distance to the boundary of the convex cone S_N from the normalized identity as found in Sect. 3. Using Eqs. (14) and (29), one can find the maximum value of the parameter $p = p_{\max}$ for which any density matrix of order $N \times N$ can be definitely PPT, i.e.,

$$D(\sigma^{\mathrm{T}_B}, \mathbb{I}_N)^2{}_{\max} = p_m^2 + (1-p_m)^2 \sum_j \lambda_j{}^2 + 2p_m(1-p_m)\lambda_k$$
$$- \frac{2}{N}\left(p_m + (1-p_m)\sum_j \lambda_j\right) + \frac{1}{N} = \frac{1}{N(N-1)}. \tag{30}$$

Solving Eq. (30) would give the desired maximum value of the parameter p.

5 PPT as a sufficient separability criterion for a class of Werner states in dimensions greater than 6

5.1 Separability criterion for pure states from measurement-based geometry

A composite pure state of a bipartite quantum system AB of $n \otimes m$ dimensions is said to be separable if it can be expressed as,

$$|\psi\rangle = \sum_{i,j} c_{i,j} |\psi_i\rangle \otimes |\psi_j\rangle . \tag{31}$$

where the set of all $|\psi_i\rangle$, $i = 1, n$ and $|\psi_j\rangle$, $j = 1, m$ are the bases of system A and B, respectively.

To find a geometrical interpretation of separability, one can consider a pure state of a 2-qubit system in computational basis as,

$$|\psi\rangle = a\,|0_A 0_B\rangle + b\,|0_A 1_B\rangle + c\,|1_A 0_B\rangle + d\,|1_A 1_B\rangle \tag{32}$$

which can be rewritten as,

$$\begin{aligned} |\psi\rangle &= |0_A\rangle\,(a\,|0_A\rangle + b\,|1_B\rangle) + |1_A\rangle\,(c\,|0_A\rangle + d\,|1_B\rangle) \\ &= \langle 0_A|\psi\rangle\,|0_A\rangle + \langle 1_A|\psi\rangle\,|1_A\rangle \end{aligned} \tag{33}$$

From Eq. (33) it is clear that the composite system will be separable iff the vectors $\langle 0_A|\psi\rangle$ and $\langle 1_A|\psi\rangle$ are parallel to each other. This condition along with Eq. (32) yields,

$$\frac{a}{c} = \frac{b}{d}. \tag{34}$$

This criterion for separability for pure states has been generalized for higher dimensions and multipartite cases in [25] using Wedge product and Lagrange's identity along with a measure of entanglement.

It can be seen that the vectors $\langle 0_A|\psi\rangle$ and $\langle 1_A|\psi\rangle$ are, respectively, the non-normalized reduced density matrices of system B after one takes a measurement of system A on bases $|0_A\rangle$ and $|1_A\rangle$, respectively. If they are parallel to each other, then after normalization the post-measurement reduced density matrix always gives

$p\,|0_A\rangle + q\,|1_B\rangle$ with $p^2 + q^2 = 1$, implying that, in case of separable pure states, measurement on one system does not affect the unmeasured system.

In light of geometric setting presented in Sect. 2, the state of a single-qubit quantum system is represented by a density matrix of order 2 and all such density matrices form a sphere in 3 dimension, namely the Bloch sphere ($\mathbb{B}$ ball). The pure states are on the surface of this sphere. In case of composite system AB of $2 \otimes 2$ qubits, the Bloch spheres of systems A and B form the bases of the system AB. For the pure separable states, as measurement on one system does not affect the state of other system, if the pre- and post-measurement normalized reduced density matrices of the unmeasured system lie on the same point on its constituent Bloch ball, the composite system is separable.

Generalizing in higher dimension, we consider a separable pure state of bi-partition AB of dimension $n \otimes m$ dimensions as,

$$|\psi\rangle = \sum_{i,j} c_{i,j}\,|\psi_i\rangle \otimes |\psi_j\rangle\,.$$

where the set of all $|\psi_i\rangle$, $i = 1, n$ and $|\psi_j\rangle$, $j = 1, m$ are the bases of systems A and B, respectively.

So, the normalized state of system B before any measurement can be written as,

$$|\psi_B\rangle = \sum_j d_j\,|\psi_j\rangle$$

Any measurement on system A will yield the state $\sum_j c_{i,j}\,|\psi_j\rangle$ for system B. Normalizing the post-measurement state of system B, one can get the same state as pre-measurement. Following the same approach as for the 2-qubit case, one can conclude that for pure separable states, measurement on any of the systems does not affect the state of the other party and hence the pre- and post-measurement density matrices of the state can be represented by the same point in their geometric setting. This approach has been further studied in [17].

5.2 Separability criterion from measurement-based geometry for bipartite *n*-qubit Werner states

A mixed state of a composite system AB ρ is said to be separable if it can be written as,

$$\rho = \sum_i q_i\,\rho_A^i \otimes \rho_B^i, \tag{35}$$

where $\sum_i q_i = 1$, ρ_A^i and ρ_B^i denotes the states of the composite systems A and B, respectively.

For separable mixed bipartite systems, the condition that after measuring one of the parties, pre- and post-measurement density matrices of the unmeasured system will coincide at the same point in Hilbert space is not in general true. We consider Werner states to check the measurement-based approach provided in the previous subsection.

A class of n-qubit Werner states can be written as,

$$\rho_w = p\,|\psi\rangle\,\langle\psi| + (1-p)\frac{\mathbb{I}}{N}, \tag{36}$$

where $N = 2^n$, $\frac{\mathbb{I}}{N}$ is normalized identity of order N and $|\psi\rangle\,\langle\psi|$ is n-qubit GHZ state.

To illustrate, we consider 2-qubit Werner state of this class with bi-partition A–B $(2 \otimes 2)$ as,

$$\rho_{w_2} = p\,|\psi\rangle\,\langle\psi| + (1-p)\frac{\mathbb{I}}{4}, \tag{37}$$

.

Here, $|\psi\rangle\,\langle\psi|$ is the maximally entangled Bell state.

A measurement on system A yields after normalization,

$$\rho^m_{w_2} = p\sigma_B + (1-p)\frac{\mathbb{I}}{2}, \tag{38}$$

where σ_B is either $|0\rangle\,\langle 0|$ or $|1\rangle\,\langle 1|$ depending on the choice of the measurement operator.

From Eq. (38), it can be seen that all post-measurement reduced density operators of the system can lie on any of the lines connecting the normalized identity matrix $\frac{\mathbb{I}}{2}$, which is effectively the center of the $\mathbb{B}^3$ ball, i.e., the Bloch Sphere and a pure density matrix σ_B. Hence, one can conclude geometrically they can lie on any radius of the Bloch sphere.

For ρ_{w_2} to be separable, from Eq. 35, we need the post-measurement reduced state itself to be a density matrix and hence following Sect. 2 of this paper, to lie inside all the 3-simplices (tetrahedrons) circumscribed by the Bloch sphere and centered at $\frac{\mathbb{I}}{2}$ (Fig. 4).

From Fig. 4, it is clear that for 2-qubit Werner states, the maximum value of p for which ρ_{w_2} would be separable is equal to the ratio at which the regular tetrahedron

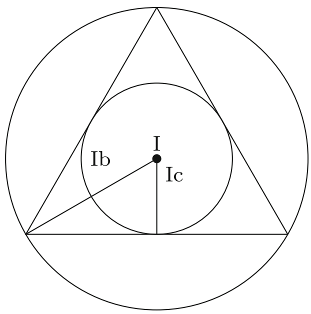

Fig. 4 Two-dimensional cross section of Bloch ball; here I at the center of the ball is the normalized identity, the triangle is the two-dimensional cross section of the 3-simplex, regular tetrahedron, and Ib and Ic are the inradius and circumradius of the tetrahedron

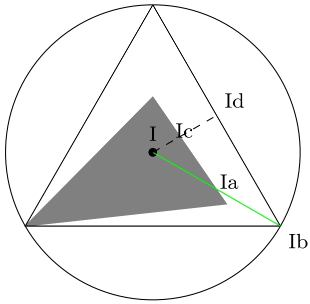

Fig. 5 Two-dimensional cross section of the m^2-1 ball; here I at the center of the ball is the normalized identity, the gray region is the two-dimensional cross section of the regular m^2-1-simplex, which intercepts the radius of the ball Ib at ratio $\frac{Ia}{Ib}$, and Ic is the inradius of the simplex

intercepts a radius of the Bloch sphere, i.e., the ratio of the inradius and circumradius of a regular tetrahedron, given by, $\frac{1}{3}$.

This result matches with the literature. Now to generalize the approach, we consider the $m \otimes m$ Werner state presented in Eq. (36) and take a measurement on bi-partition A.

The post-measurement reduced density matrix can be written as,

$$\rho_w^M = p\sigma_B + (1-p)\frac{\mathbb{I}}{m}. \tag{39}$$

It would lie on one of the proper radii (i.e., the radii which end with a density matrix) of the $\mathbb{B}^{m^2-1}$ ball centered at $\frac{\mathbb{I}}{m}$, and for ρ_w to be separable, the post-measurement reduced density matrix should lie inside all the m^2-1 simplices circumscribed by $\mathbb{B}^{m^2-1}$.

We consider Fig. 5. The maximum value of p for which the $N = m^2$-dimensional Werner state is separable is equal to the minimum ratio in which a m^2-1 simplex divides a proper radius of $\mathbb{B}^{m^2-1}$ ball. Here, the ratio is given by $\frac{Ia}{Ib}$, as every radius of the $\mathbb{B}^{m^2-1}$ ball is not a proper radius.

Following similar triangle approach, we have

$$\frac{Id}{Ib} = \frac{Ic}{Ia} = \frac{1}{m-1} \tag{40}$$

From the ratio of the inradius and circumradius of the regular simplices,

$$\frac{Ic}{Ib} = \frac{1}{m^2-1}. \tag{41}$$

Combining Eqs. (40) and (41), the maximum value of p, p_{maxsep} for which the state is separable, is found to be,

$$p_{\text{maxsep}} = \frac{Ia}{Ib} = \frac{1}{m+1} \tag{42}$$

A bi-partition of an n-qubit GHZ state consists of 2 parties A and B of k and l qubits, respectively, consists of nonzero and maximal entanglement if and only if k = 1 , l = n − 1 or, k = n − 1 and l = 1. Since the maximum value of p is given by the minimum ratio in which the simplex intercepts the proper radius of its circumsphere, substituting the $2^{(n-1)}$ as m in Eq. (43) we have,

$$p_{\text{maxsep}} = \frac{1}{2^{n-1}+1}. \tag{43}$$

5.3 PPT as a sufficient criterion of separability

Using the separability criterion established in the previous subsection following [17], one can show that for the class of Werner states explained in Eq. (36), PPT is a sufficient condition for separability even for dimensions greater than 6, i.e., for this class of states, if a system has a positive partial transpose for any bi-partition, it is also separable in that bi-partition. Previously, from Peres Horodecki criterion it was known that PPT is only a necessary condition for separability for systems in dimension greater than 6.

To establish the claim, the distance of this class of states from the normalized identity is calculated using Hilbert–Schmidt norm to be, $p\sqrt{\frac{N-1}{N}}$.

One can have the distance of the partially transposed Werner states from the maximally mixed states following Eq. (29) as,

$$D = p\sqrt{\frac{N-1}{N}}, \tag{44}$$

which equals the distance of these class of Werner states from the maximally mixed state.

We consider the 3-qubit Werner state with the $1 \otimes 2$ bi-partition given by,

$$\rho_{w_3} = pP_{\psi_3} + (1-p)\frac{\mathbb{I}}{3}, \tag{45}$$

.

Here, P_{ψ_3} is the GHZ state and $\frac{\mathbb{I}}{3}$ is the normalized identity matrix of order 3. Carrying out the partial transposition operation on ρ_{w_3} with $1 \otimes 2$ bi-partition, one can find the exact maximum value of p, for which the state will be PPT, to be $\frac{1}{5}$. The procedure is given in "Appendix A."

This procedure can be followed for states with higher numbers of qubits to find out the value of the maximum value of the parameter p for which the corresponding state will be PPT. Figure 6 depicts the values of the maximum value of p for varying n,

From Sect. 5.2, the maximum value of p for a state to be separable is given by,

$$p = \frac{1}{2^{n-1}+1}, \tag{46}$$

Figure 7 shows the maximum values of the parameter for which a Werner state is separable. These two plots, i.e., Figs. 6 and 7, coincide at each point.

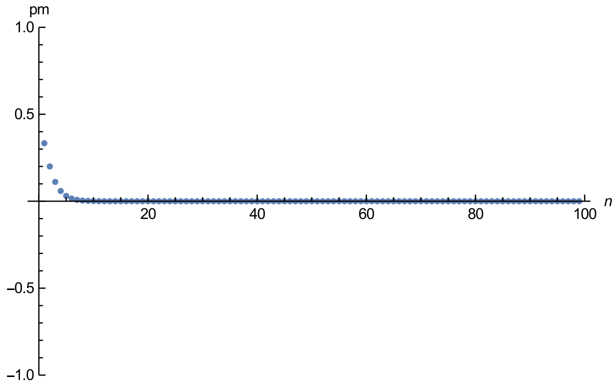

Fig. 6 Maximum value of the parameter p of n-qubit Werner states to be PPT with varying n

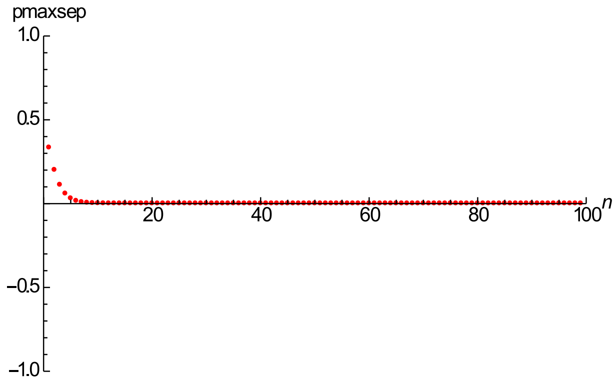

Fig. 7 Values of the parameter p of n-qubit Werner states for maximal distance taken with respect to the normalized identity with varying n for the state to be separable

Hence, within the distance $\frac{1}{2^{n-1}+1}\sqrt{\frac{2^n-1}{2^n}}$ from the normalized identity, any n-qubit Werner state is PPT as well as separable. Outside this limit, the states belong to this class do not have positive partial transpose and are entangled. From this, we can conclude that PPT criterion is necessary and sufficient for separability for these class of states. This is one of the main results of this paper.

6 Conclusion

In summary, using a geometric approach it has been shown that all the density matrices within the distance $\frac{1}{\sqrt{d^n(d^n-1)}}$ from the maximally mixed state have a positive partial transpose, which supports that NPT states lie just outside the boundary of the largest separable ball [34]. An idea of the interior geometry of the positive semidefinite cone and how it intersects the set of all density matrices has been provided. A class of Werner states has been found for which PPT criterion is necessary and sufficient for separability. The method provided here may be used to calculate limits for k-distillable states.

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7 Appendix A

Calculation for 3-qubit Werner state to be PPT

The 3-qubit Werner state with $1 \otimes 2$ bi-partition is given by

$$\rho_{w3} = pP_{\psi_3} + (1-p)\frac{\mathbb{I}}{8}, \tag{47}$$

where $N = 2^n$, $p \in [0, 1]$; P_ψ is 3-qubit GHZ state and $\frac{\mathbb{I}}{8}$ is the normalized identity matrix of order 8. Hence,

$$\rho_{w3} = \begin{pmatrix} \frac{1-p}{8}+\frac{p}{2} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{p}{2} \\ 0 & \frac{1-p}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1-p}{8} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-p}{8} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1-p}{8} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-p}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1-p}{8} & 0 \\ \frac{p}{2} & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1-p}{8}+\frac{p}{2} \end{pmatrix} \tag{48}$$

Carrying out the partial transposition operation, we have

$$\rho_{w3}^{\mathrm{T}_B} = \begin{pmatrix} \frac{1-p}{8}+\frac{p}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1-p}{8} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1-p}{8} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1-p}{8} & \frac{p}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{p}{2} & \frac{1-p}{8} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1-p}{8} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1-p}{8} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \frac{1-p}{8}+\frac{p}{2} \end{pmatrix} \tag{49}$$

Eigenvalues of $\rho_{w3}^{\mathrm{T}_B}$ are found to be,

$$\frac{1}{8}(1-5p), \frac{1-p}{8}, \frac{1-p}{8}, \frac{1-p}{8}, \frac{1-p}{8}, \frac{1}{8}(3p+1), \frac{1}{8}(3p+1), \frac{1}{8}(3p+1)$$

Hence, the maximum value of p such that the partially transposed Werner state is positive semidefinite is $\frac{1}{5}$.

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