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On the geometry of entangled states

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Abstract. The basic question that is addressed in this paper is finding the closest separable state for a given entangled state, measured with the Hilbert–Schmidt distance. While this problem is in general very difficult, we show that the following strongly related problem can be solved: find the Hilbert–Schmidt distance of an entangled state to the set of all partially transposed states. We prove that this latter distance can be expressed as a function of the negative eigenvalues of the partial transpose of the entangled state, and show how it is related to the distance of a state to the set of positive, partially transposed (PPT) states. We illustrate this by calculating the closest biseparable state to the W state and give a simple and very general proof for the fact that the set of W-type states is not of measure zero. Next we show that all surfaces with states whose partial transposes have constant minimal negative eigenvalue are similar to the boundary of PPT states. We illustrate this with some examples on bipartite qubit states, where contours of constant negativity are plotted on two-dimensional intersections of the complete state space.

In this paper we try to obain some insight into the geometrical structure of entangled states. The main goal will be to characterize the distance of an entangled state to the set of separable states. Related questions were addressed in the paper by Życzkowski and co-workers [1–3], Pittenger and Rubin [4] and Witte and Trucks [5] (see also the paper by Ozawa [6]), although here we attack the problem from a different perspective.

The concept of negativity will turn out to be very much related to the Hilbert–Schmidt distance of a state to the set of separable states. It originates from the observation due to Peres [7] that taking a partial transpose of a density matrix associated with a separable state is still a valid density matrix and thus positive (semi)definite. Subsequently Horodecki *et al.* [8] proved that this was a necessary and sufficient condition for a state to be separable if the dimension of the Hilbert space does not exceed 6. In higher-dimensional systems, no easy way of determining the separability of a state exists owing to the existence of bound entangled states. We shall therefore content ourselves to calculate the Hilbert–Schmidt distance of an entangled state to the set of positive, partially transposed (PPT) states (note that, in the case of two qubits, no bound entangled states exist).

This problem is highly related to calculating the distance of an entangled state to the set of partially transposed states, as the intersection of the set of all states

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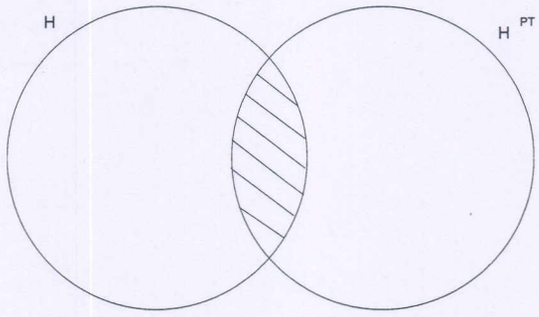


Figure 1. The set of all states is depicted by H and the set of all partial transposed states by H^{PT}. The intersection of both is the set of all PPT states.

with the set of all partially transposed states is equal to the set of all PPT states. This is visualized in figure 1, where the boundary of the convex set of states H consists of rank-deficient states. The set of partially transposed states is completely isomorphic with the set of states and can be seen as some kind of reflection of the set of states. The intersection of both sets is the convex set of PPT states.

From figure 1 it is immediately clear that the distance of an entangled state to the PPT state is equal to the distance of an entangled state to the set of partially transposed states if the closest partially transposed state is positive (semi)definite; this condition will turn out to be almost always true if the dimension of the Hilbert space is not too high.

Let us now calculate the closest partially transposed state to the entangled state. The key observation is the fact that the Hilbert–Schmidt norm is preserved under the partial transpose map. Therefore the proposed measure can be defined in the space of partial transposed density matrices as the minimal Hilbert–Schmidt distance of $\boldsymbol{\rho}^{\mathrm{PT}}$ to the surface of positive (semi)definite matrices with trace 1, this surface being the partial transpose of the boundary of PPT states. It is precisely due to this peculiar feature of the Hilbert–Schmidt distance that analytical results will be obtained. Note that the trace distance does not have this nice property.‡

We are therefore looking for the best positive semidefinite approximation of the indefinite matrix $\boldsymbol{\rho}^{\mathrm{PT}}$ in the Hilbert–Schmidt norm:

$$\min_{\boldsymbol{\sigma}\in H} \|\boldsymbol{\rho}^{\mathrm{PT}} - \boldsymbol{\sigma}\|_2 = \min_{\boldsymbol{\sigma}\in H}\{\mathrm{Tr}\,[(\boldsymbol{\rho}^{\mathrm{PT}} - \boldsymbol{\sigma})^2]\}^{1/2}. \tag{1}$$

Writing the eigenvalue decomposition $\boldsymbol{\rho}^{\mathrm{PT}} = \mathbf{U}\mathbf{D}\mathbf{U}^{\dagger}$, and absorbing $\mathbf{U}$ in $\boldsymbol{\sigma}$, this problem is equivalent to finding $\boldsymbol{\sigma}$ such that $\|\mathbf{D} - \boldsymbol{\sigma}\|$ is minimal. Using the eigenvalue decomposition $\boldsymbol{\sigma} = \mathbf{V}\mathbf{E}^2\mathbf{V}^{\dagger}$ with $\mathrm{Tr}\,(\mathbf{E}^2) = 1$, this can be written as a Lagrange constrained problem with cost function:

$$K = \|\mathbf{D} - \mathbf{V}\mathbf{E}^2\mathbf{V}^{\dagger}\|_2 - \lambda[\mathrm{Tr}\,(\mathbf{E}^2) - 1]. \tag{2}$$

‡ On the other hand it is well known that the minimal trace distance between a state and the set of PPT states is an entangled monotone owing to the contractive nature of completely positive maps. It is not known whether the same property holds in the case of the Hilbert–Schmidt distance; Ozawa [6] gave an example of a non-local completely positive map that can enlarge the Hilbert–Schmidt distance between two states, but this does not, of course, prove nor disprove the fact that the entanglement measure based on the Hilbert–Schmidt distance is not an entangled monotone.

It is immediately clear that the optimal unitary $\mathbf{V}$ is given by the identity: a positive definite matrix remains positive definite if off-diagonal elements are made zero. Differentiation leads to the result that the eigenvalues e_i^2 are either equal to 0 or equal to $d_i + \lambda$. Normalization fixes the value of λ. Straightforward calculations show that the e_j^2 corresponding to the negative eigenvalues d_j have to be chosen equal to zero and the others either equal to $d_i + \lambda$ or equal to 0, depending on the sign of $d_i + \lambda$. The algorithm for finding the closest partially transposed state therefore becomes the following.

(i) Calcuate the eigenvalue decomposition of $\boldsymbol{\rho}^{\mathrm{PT}} = \mathbf{UDU}^{\dagger}$.

(ii) Define $\mathbf{E}^2$ as the unique diagonal positive (semi)definite normalized matrix such that its elements are $e_i^2 = d_i + \lambda$ or $e_i^2 = 0$.

(iii) The closest partially transposed state $\boldsymbol{\rho}_{\mathrm{s}}$ is given by $\boldsymbol{\rho}_{\mathrm{s}} = (\mathbf{UE}^2\mathbf{U}^{\dagger})^{\mathrm{PT}}$. The Hilbert–Schmidt distance between both states is given by

$$\|\boldsymbol{\rho} - \boldsymbol{\rho}_{\mathrm{s}}\|_2 = \left(\frac{\left(\sum_{i \in I_{\mathrm{p}}} d_i + \sum_{i \in I_{\mathrm{n}}} d_i \right)^2}{n_{\mathrm{p}}} + \sum_{i \in I_{\mathrm{n}}} d_i^2 \right)^{1/2}, \tag{3}$$

where I_{n} is the set of all indices corresponding to the negative eigenvalues of $\boldsymbol{\rho}^{\mathrm{PT}}$, I_{p} is the set of indices corresponding to positive eigenvalues of $\boldsymbol{\rho}^{\mathrm{PT}}$ but for which $\mathbf{E}_i^2 = 0$, and n_{p} denotes the rank of $\mathbf{E}^2$.

If $\boldsymbol{\rho}_{\mathrm{s}}$ is a state, it is guaranteed to be the closest PPT state. Numerical investigations show that, for example, in the two-qubit case the positiveness of $\boldsymbol{\rho}_{\mathrm{s}}$ happens in most of the cases. If $\boldsymbol{\rho}_{\mathrm{s}}$ is not positive, then the distance to the set of partially transposed states calculated is a (fairly good) lower bound on the distance of the entangled state to the set of PPT states.

Let us illustrate the above procedure with an example. Suppose we want to find the closest biseparable 2×4 state to the three-qubit W state [9] $|W\rangle = (|001\rangle + |010\rangle + |100\rangle)/3^{1/2}$. The eigenvalue decomposition of $(|W\rangle\langle W|)^{\mathrm{PT}} = \mathbf{UDU}^{\dagger}$, with the partial transpose operation taken over the four-dimensional Hilbert space, is given by

$$\mathbf{D} = \mathrm{diag}\left(\frac{2}{3}, \frac{2^{1/2}}{3}, \frac{1}{3}, 0, 0, 0, 0, -\frac{2^{1/2}}{3} \right), \tag{4}$$

$$\mathbf{U} = \begin{pmatrix}
\cdot & \frac{1}{2^{1/2}} & \cdot & \cdot & \cdot & \cdot & \cdot & -\frac{1}{2^{1/2}} \\
\frac{1}{2^{1/2}} & \cdot & \cdot & \frac{1}{2^{1/2}} & \cdot & \cdot & \cdot & \cdot \\
\frac{1}{2^{1/2}} & \cdot & \cdot & -\frac{1}{2^{1/2}} & \cdot & \cdot & \cdot & \cdot \\
\cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot & \cdot \\
\cdot & \cdot & 1 & \cdot & \cdot & \cdot & \cdot & \cdot \\
\cdot & \frac{1}{2} & \cdot & \cdot & \cdot & \cdot & \frac{1}{2^{1/2}} & \frac{1}{2} \\
\cdot & \frac{1}{2} & \cdot & \cdot & \cdot & \cdot & -\frac{1}{2^{1/2}} & \frac{1}{2} \\
\cdot & \cdot & \cdot & \cdot & \cdot & 1 & \cdot & \cdot
\end{pmatrix}. \tag{5}$$

The eigenvalues $\mathbf{E}^2$ are readily obtained:

$$\mathbf{E}^2 = \mathrm{diag}\left(\frac{2}{3} - \frac{2^{1/2}}{9}, \frac{2^{3/2}}{9}, \frac{1}{3} - \frac{2^{1/2}}{9}, 0, 0, 0, 0, 0\right). \tag{6}$$

Taking the partial transpose leads to the state $\boldsymbol{\rho}_s$, where we use the notation $c = 2^{1/2}/18$:

$$\begin{pmatrix} 2c & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{3}-c & \frac{1}{3}-c & \cdot & \frac{1}{9} & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{3}-c & \frac{1}{3}-c & \cdot & \frac{1}{9} & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{9} & \frac{1}{9} & \cdot & \frac{1}{3}-2c & \cdot & \cdot & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & c & c & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & c & c & \cdot \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \end{pmatrix}. \tag{7}$$

The eigenvalue of $\boldsymbol{\rho}_s$ are non-negative and it is easy to show that $\boldsymbol{\rho}_s$ is biseparable. We have therefore found the closest biseparable 2×4 state to the $|W\rangle$ state, and the Hilbert–Schmidt distance to it is equal to $(\frac{2}{3})^{3/2}$.

Recently, the question arose whether the set of W-type states is of measure zero. Using the language of the Hilbert–Schmidt distance, this problem is readily solved. Indeed, the question is solved if we can prove that the state obtained by mixing the W state with a small random, completely separable mixed state remains outside the set of all convex combinations of biseparable states (with relation to whatever partition). As there is no biseparable pure state infinitesimally close to the W state, and a mixed state not infinitesimally close to a pure state is always at a finite distance from whatever pure state, it is proved that the set of W-type states is indeed not of measure zero. A different proof was given by Acin *et al.* [10]. Note that the above proof is very general and can be used in systems of arbitrary dimensions: whenever there exists a pure state ψ_1 that can probabilistically be converted into another state ψ_2 but not vice versa; the set of ψ_1-like states minus the set of the ψ_2-like states is of finite measure if there does not exist a ψ_2-like pure state infinitesimally close to ψ_1!

The concept of negativity is also connected to the concept of robustness of entanglement [11]. Indeed, let us calculate how much an entangled bipartite state of whatever dimension has to be mixed with the identity before it becomes PPT. In analogy with the previous derivation of the Hilbert–Schmidt distance, this amounts to the equivalent problem of how much one has to mix the partial transpose of $\boldsymbol{\rho}$ with the identity before it becomes positive semidefinite:

$$\min_t (1-t)\boldsymbol{\rho}^{\mathrm{PT}} + \frac{t}{4} I_4 \geqslant 0. \tag{8}$$

This problem is readily solved, and the solution is

$$t = \frac{|d_{\min}|}{|d_{\min}| + \frac{1}{4}}, \tag{9}$$

where $d_{\min}$ is the minimal negative eigenvalue of $\boldsymbol{\rho}^{\mathrm{PT}}$. The minimal t is therefore only a function of the negative eigenvalues. A geometrical implication of this fact is

that all surfaces of constant $d_{\min}$ are similar to the boundary of separable and entangled states; the set of all states with constant $d_{\min}$ can be generated by extrapolating all lines from the identity to the boundary of separable states such that the distance of the extrapolated state to the identity is a constant factor (greater than 1) of the distance of the separable state to the identity.

Let us now move to the case of two qubits. In this case, ρ^{PT} has at most one negative eigenvalue [12]. Numerical investigations indicate that in a vast majority of the states the optimal rank of $\mathbf{E}^2$ is equal to three and, if the rank is equal to two, this implies that ρ_{s} has a negative eigenvalue. For the states for $\mathbf{E}^2$ is rank 3, it follows that their distance to the set of partially transposed states is given by

$$\|\rho - \rho_{\mathrm{s}}\|_2 = \frac{2}{3^{1/2}}|d_{\min}|, \tag{10}$$

where $d_{\min}$ is the negative eigenvalue of ρ^{PT}. Surfaces of two-qubit states with constant negativity, defined as $N = 2|d_{\min}|$, have therefore two distinct properties: they are all similar to each other owing to the constant robustness and the Hilbert–Schmidt distance between them is almost everywhere constant.

Let us illustrate the above findings by explicitly calculating some two-dimensional intersections of the set of all bipartite qubit states including the maximally mixed state. In the following figures we use the metric based on the Hilbert–Schmidt distance $\|\rho_1 - \rho_2\|_2^2 = \mathrm{Tr}\,[(\rho_1 - \rho_2)^\dagger(\rho_1 - \rho_2)]$, and directions represented orthogonal to each other are orthogonal in the sense that $\mathrm{Tr}\,(A_1 A_2) = 0$. Rank-deficient density operators always lie on the boundary of the intersection.

Note that an explicit parametrization of the boundary between the entangled and separable states can easily be obtained; it is at most a quartic function of the mixing parameters of the states, as their analytic expression can be obtained by setting the determinant of the partial transpose equal to zero.

As a first example we consider the plane containing the maximally mixed state and the states

$$\begin{aligned} \rho_1 &= \tfrac{1}{2}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}(0 \quad 1 \quad 1 \quad 0), \\ \rho_2 &= \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}(1 \quad 0 \quad 0 \quad 0). \end{aligned} \tag{11}$$

The plane is plotted in figure 2 and the boundary of all (rank-deficient) states is given by the solid envelope. The starred line is the boundary between the convex set of separable states and the convex set of all states. The surfaces of constant negativity are indeed all similar to this boundary. The fact that the distance between these surfaces is not constant throughout the picture indicates that the closest separable states lie in other planes. Note that the Werner states lie along the

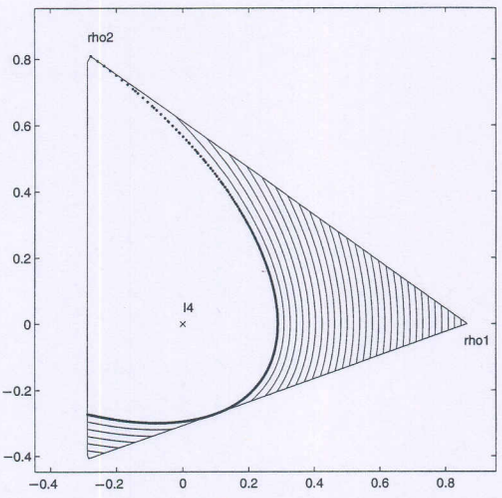


Figure 2. Intersection of the convex set of all states including states (11) and the maximally mixed state. The contours represent surfaces of constant negativity; the dotted curve is the boundary between separable and entangled states.

line between the maximally mixed state and the maximally entangled state ρ_1. The third extremal point in the undermost left corner is given by the rank 2 state

$$\rho = \begin{pmatrix} \cdot & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{4} & -\frac{1}{4} & \cdot \\ \cdot & -\frac{1}{4} & \frac{1}{4} & \cdot \\ \cdot & \cdot & \cdot & \frac{1}{2} \end{pmatrix}. \tag{12}$$

This state is called a quasidistillable state and has some remarkable properties; a single copy of it can be distilled infinitesimally close to the singlet state [13, 14], it is the state with minimal negativity for given entanglement of formation [12], and it has furthermore the strange property that no global unitary operation can increase its entanglement [15].

Let us now consider a different plane including the maximally mixed state and

$$\begin{aligned} \rho_1 &= \tfrac{1}{2} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} (0 \quad 1 \quad 1 \quad 0), \\ \rho_2 &= \tfrac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix} (1 \quad 1 \quad 0 \quad 0). \end{aligned} \tag{13}$$

This plane is obtained by rotating the previous plane around the axis $\rho_1 - I_4$. In this case, $\rho_1 - I_4$ is orthogonal to $\rho_2 - I_4$, and a completely different picture is obtained as shown in figure 3.

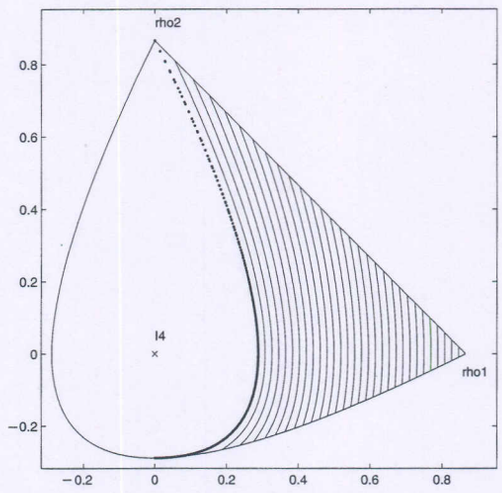


Figure 3. Intersection of the convex set of all states including states (13) and the maximally mixed state.

Further rotation of the plane leads to the following states.

$$\rho_1 = \tfrac{1}{2}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}(0 \quad 1 \quad 1 \quad 0),$$
$$\rho_2 = \tfrac{1}{2}\begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}(0 \quad 1 \quad 0 \quad 0). \tag{14}$$

The intersection of the state space by the plane is shown in figure 4.

The surfaces of constant negativity become straight lines, implying that the closest separable states lie in the same plane; the Hilbert–Schmidt distance between the surfaces of constant negativity has to be constant if they consist of parallel planes. Using the procedure previously outlined, it is indeed trivial to check that the separable state closest to the maximally entangled state ρ_1 lies in the defined plane and is given by

$$\rho_s = \begin{pmatrix} \frac{1}{6} & \cdot & \cdot & \cdot \\ \cdot & \frac{1}{3} & \frac{1}{6} & \cdot \\ \cdot & \frac{1}{6} & \frac{1}{3} & \cdot \\ \cdot & \cdot & \cdot & \frac{1}{6} \end{pmatrix}. \tag{15}$$

Let us rotate the plane further over the $\rho_1 - I_4$ axis:

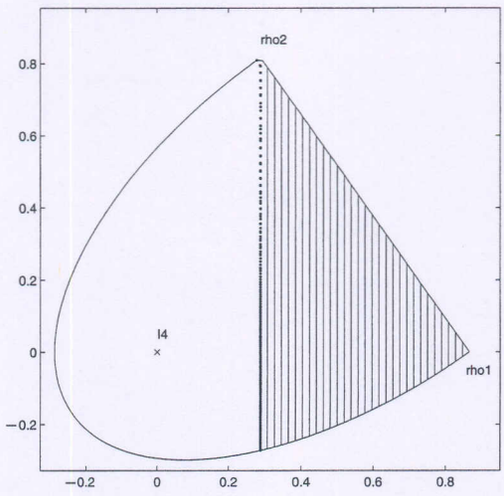


Figure 4. Intersection of the convex set of all states including states (14) and the maximally mixed state.

$$\rho_1 = \tfrac{1}{2}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}(0 \quad 1 \quad 1 \quad 0),$$
$$\rho_2 = \tfrac{1}{101}\begin{pmatrix} 10 \\ 0 \\ 0 \\ 1 \end{pmatrix}(10 \quad 0 \quad 0 \quad 1). \tag{16}$$

The resulting figure 5 combines the features of the previous figures. Three entangled disconnected regions arise, and once more we observe the strange shape of the boundary between entangled and separable states.

A plane with highly symmetric contour lines is obtained if ρ_1 and ρ_2 are both taken to be maximally entangled states:

$$\rho_1 = \tfrac{1}{2}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}(0 \quad 1 \quad 1 \quad 0),$$
$$\rho_2 = \tfrac{1}{2}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}(0 \quad 1 \quad -1 \quad 0). \tag{17}$$

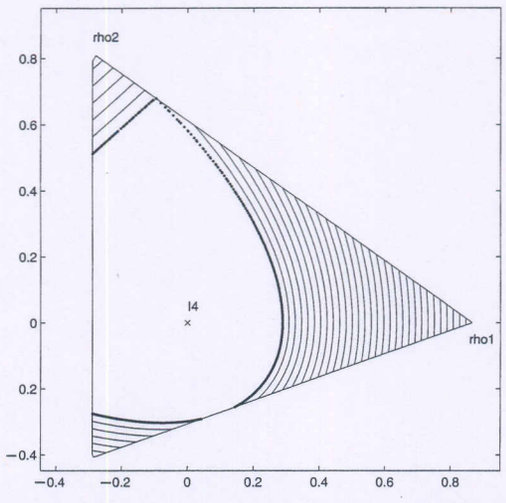


Figure 5. Intersection of the convex set of all states including states (16) and the maximally mixed state.

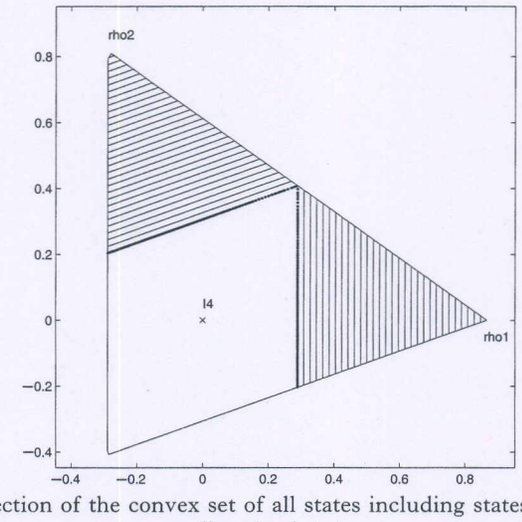


Figure 6. Intersection of the convex set of all states including states (17) and the maximally mixed state.

Indeed, only straight lines are obtained in figure 6. The third extremal state is in this case given by $\rho = \mathrm{diag}\,(\frac{1}{2}, 0, 0, \frac{1}{2})$.

Finally, we choose two random planes through the maximally mixed state and plot them in figure 7.

In conclusion, we have analysed the space of density operators from the perspective of the Hilbert–Schmidt metric. Because of the nice property that the Hilbert–Schmidt distance between two states is equal to the Hilbert–Schmidt distance between the partial transposes of the states, a very simple and elegant technique arose for calculating the closest PPT state to an entangled state. As an example the closest biseparable state to the three-qubit W state was calculated.

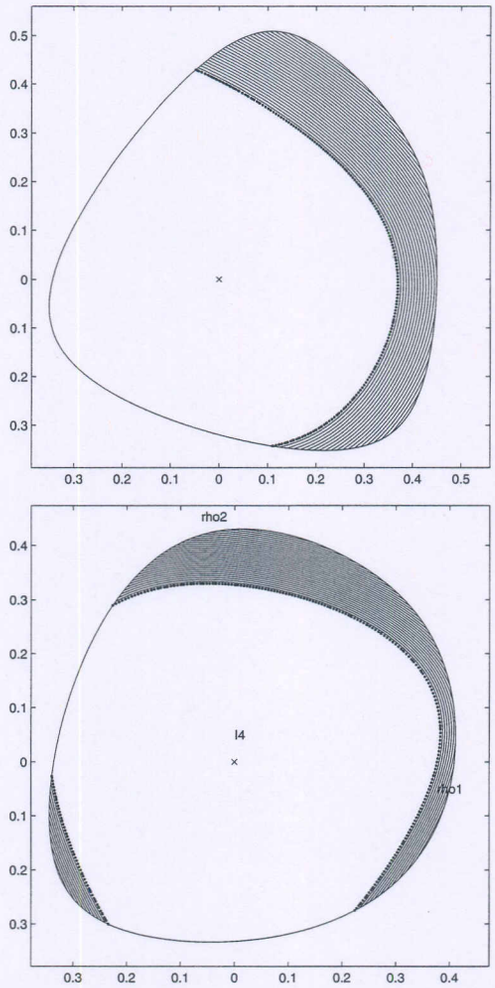


Figure 7. Contour plots of the negativity on random planes incuding the maximally mixed state.

Finally, the Hilbert–Schmidt distance was illustrated with some two-dimensional intersections of the space of density operators of mixed states of two qubits.

Acknowledgments

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