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Optimal Decompositions with Respect to Entropy and Symmetries

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Abstract. The entropy of a subalgebra, which has been used in quantum ergodic theory to construct a noncommutative dynamical entropy, coincides for N-level systems and Abelian subalgebras with the notion of maximal mutual information of quantum communication theory. The optimal decompositions of mixed quantum states singled out by the entropy of Abelian subalgebras correspond to optimal detection schemes at the receiving end of a quantum channel. It is then worthwhile studying in some detail the structure of the convex hull of quantum states brought about by the variational definition of the entropy of a subalgebra. In this Letter, we extend previous results on the optimal decompositions for 3-level systems.

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1. Introduction

The fact that a pure state on a large system need not be pure when regarded as a state over a smaller subsystem, is a well established quantum mechanical fact that is often referred to as *quantum entanglement*. In recent years, quantum entanglement has become more and more central to quantum computation, quantum cryptography and quantum information theory. Pure quantum states, e.g. one-dimensional Hilbert space projections, are not decomposable, whereas their restrictions to finite-dimensional subalgebras, are, in general, density matrices, that is mixed states. As such, they can be decomposed in infinitely many ways. In all instances, it is important to get hold of the degree of entanglement contained in a given quantum state, a notion that is better expressed in entropic terms [1]: interestingly enough, such a notion coincides [2] with the so-called *entropy of a subalgebra* which has been used to extend the Kolmogorov–Sinai dynamical entropy to quantum dynamical systems [3–5].

The fact that the same mathematical tool has emerged in two not obviously related quantum contexts, is certainly a sign that the notion of entropy of a subalgebra is fairly natural: beside providing quantitative statements on entanglement, it also evidences interesting new geometrical structures in the state space of the large system [6] that might be important to improve quantum detection.

Though the entropy of a subalgebra is easily defined, it is, unfortunately, quite difficult to compute analytically, mainly because of the intricacies of the variational principle it is based on. Only very limited results are available [6–11]. In [12, 13], the case of one spin $\frac{1}{2}$ particle as a subsystem of two spin $\frac{1}{2}$ particles was considered and solved. The problem goes back to [1] where some particular cases are already computed. In [6], Abelian subalgebras of 2×2 and 3×3 algebras were taken into account, the Abelian subalgebras representing possible measurement processes. Again, in order to achieve a reasonable understanding in as much an analytic way as possible, it was necessary to restrict to a highly symmetric state. However, already in such a relatively simple case, a hardly expected surprise appeared. The symmetric real quantum states are parametrized by a real parameter and, when that parameter becomes smaller than a certain *bifurcation value*, a kind of *phase transition* occurs: for larger values there is a unique optimal decomposition, whereas for smaller ones a whole convex hull of optimal decompositions appears.

In this Letter, we enlarge the class of three-dimensional states by allowing for complex symmetric density matrices and thus we lessen the symmetry. These states are now parametrized by two real parameters and it turns out that, if we can control their optimal decompositions with respect to a maximally Abelian subalgebra, then we are also able to control a larger part of the whole eight-dimensional state space, though not all of it. Surprisingly enough, the states in the neighborhood of the tracial state escape control, despite the tracial state being the least affected by quantum effects.

The study has been performed analytically as long as it proved possible, when not, we resorted to numerical calculations, whose support becomes less and less avoidable. However, the flatness of the maxima and minima involved in the mimimization routine asked for a thorough analytical study. The result is that phase-transitions are a typical feature even with a lower symmetry. Moreover, the location of bifurcation points in the parameter space corresponds to the subdivison of the state space into regions with different characteristic dimensionalities. While the details of the phase-transition depends on the convex functional used to measure the degree of entanglement, the presence of bifurcations and phase-transitions only depends on the relation between the larger and the smaller algebras involved (see [11] for the real, symmetric case).

The paper is organized as follows: in Section 2 we introduce the necessary definitions and results contained in [6]. In Section 3 we turn to the explicit three-dimensional examples and evaluate the entropy and the optimal decompositions of symmetric complex density matrices with respect to maximally Abelian subalgebras. Finally, using the results of the previous section, in Section 4, we discuss how far optimal decompositions of generic 3×3 density matrices can be controlled.

2. The Entropy of a Subalgebra

We consider finite-dimensional Hilbert spaces and finite-dimensional (matrix) algebras $\mathbf{M}$ of observables. Quantum states are either one-dimensional projections or density matrices, in which case there are infinitely many, physically different mixtures that are described by the same state $\hat{\rho}$. Each one of such mixtures is specified by (i) a set of weights $0 \leqslant \lambda_j \leqslant 1$, with $\sum_j \lambda_j = 1$, and (ii) a corresponding set of density matrices $\hat{\rho}_j$ such that $\hat{\rho} = \sum_j \lambda_j \hat{\rho}_j$.

The entropy of a subalgebra $\mathbf{N} \subseteq \mathbf{M}$ w.r.t. a state $\hat{\rho}$ singles out certain (optimal) decompositions among the many possible.

DEFINITION 1. Let $\mathbf{M}$ be a finite-dimensional full matrix algebra, $\mathbf{N} \subseteq \mathbf{M}$ a subalgebra, $\hat{\rho}$ a density matrix in (a state on) $\mathbf{M}$, $\hat{\rho} \upharpoonright \mathbf{N}$ its restriction to $\mathbf{N}$ and $S\left(\hat{\rho}\right) = -\mathrm{Tr}\, \hat{\rho} \log \hat{\rho}$ the von Neumann entropy of a state $\hat{\rho}$. Then, the entropy of $\mathbf{N}$ w.r.t. $\hat{\rho}$ is defined by

$$H_{\hat{\rho}}(\mathbf{N}) := \sup_{\hat{\rho}=\sum_j \lambda_j \hat{\rho}_j} \Big\{ S\left(\hat{\rho} \upharpoonright \mathbf{N}\right) - E_{\hat{\rho}}(\{\hat{\rho}_j \upharpoonright \mathbf{N}\} \Big\}, \tag{1}$$

where

$$E_{\hat{\rho}}(\{\hat{\rho}_j \upharpoonright \mathbf{N}\}) := \sum_j \lambda_j S\left(\hat{\rho}_j \upharpoonright \mathbf{N}\right) . \tag{2}$$

Remark 1. Because of finite-dimensionality, the sup in (1) is, in fact, a maximum corresponding to the minimum $E^*_{\hat{\rho}}(\mathbf{N})$ of $E_{\hat{\rho}}(\{\hat{\rho}_j \upharpoonright \mathbf{N}\})$ attained at one or more distinguished decompositions $\hat{\rho} = \sum_j \lambda^*_j \hat{\rho}^*_j$ which will be called 'optimal'.

Next, we report two general results from [6] and refer to [11] for further general considerations on optimal decompositions.

PROPOSITION 1. (a) *Let $\hat{\rho} = \sum_j \lambda^*_j \hat{\rho}^*_j$ be an optimal decomposition for a state $\hat{\rho}$ w.r.t. a subalgebra $\mathbf{N} \subseteq \mathbf{M}$. Let $\hat{\sigma} = \sum_\ell \mu_\ell \hat{\rho}^*_\ell$ be another state in the convex hull of the optimal states $\hat{\rho}^*_j$. Then, $\hat{\sigma} = \sum_\ell \mu_\ell \hat{\rho}^*_\ell$ is an optimal decomposition for $\hat{\sigma}$ w.r.t.* $\mathbf{N}$.

(b) *Let $\hat{\rho}$ and $\mathbf{N} \subseteq \mathbf{M}$ be such that there exist two different decompositions $\hat{\rho} = \sum_j \lambda^*_j \hat{\rho}^*_j$ and $\hat{\rho} = \sum_j \mu^*_j \hat{\sigma}^*_j$ which are optimal w.r.t.* $\mathbf{N}$.

Then, $\hat{\rho} = \alpha \sum_j \lambda^*_j \hat{\rho}^*_j + (1-\alpha) \sum_j \mu^*_j \hat{\sigma}^*_j$ is also an optimal decomposition of $\hat{\rho}$ w.r.t. $\mathbf{N}$.

As a consequence of the above proposition, the state space splits into regions that do not have common interior points. Furthermore, by convexity arguments [6], the search for optimal decompositions can be restricted to decompositions in terms of pure states (one-dimensional projections). Thence, it makes sense to introduce the following definition:

DEFINITION 2. Two one-dimensional projections will be called compatible w.r.t. $\mathbf{N} \subseteq \mathbf{M}$, if they belong to decompositions of some state $\hat{\rho}$ which are also optimal w.r.t. $\mathbf{N}$.

With $\mathbf{M}$ (isomorphic to) the full $N \times N$ matrix algebra, any maximally Abelian subalgebra $\mathbf{A} \subset \mathbf{M}$, generated by N orthogonal projections $\hat{a}_j$, identifies an orthonormal basis $\{|a_j\rangle\}$ of the underlying N-dimensional Hilbert space $\mathcal{H}_N$. In the following, we denote by $\phi(j)$, $j = 1, \ldots, N$, the components of vectors $|\phi\rangle \in \mathcal{H}_N$ w.r.t. the basis associated with $\mathbf{A}$.

LEMMA 1. *Two one-dimensional projections* $|\phi_1\rangle\langle\phi_1|$, $|\phi_2\rangle\langle\phi_2|$ *are compatible only if*

$$\sum_{j=1}^{N} \phi_1^*(j)\phi_2(j) \log \frac{|\phi_1(j)|^2}{|\phi_2(j)|^2} = 0. \tag{3}$$

Remarks 2. (1) The proof of the above Lemma can be found in [6]. Condition (3) is necessary for the stationarity of the functional (2), but not sufficient to guarantee that it attains a minimum. In order to exclude that $\hat{\rho} = \sum_j \lambda_j \hat{p}_j$, with one-dimensional projections $\hat{p}_j$ compatible w.r.t. $\mathbf{N}$, might correspond to a maximum of (2), one has to study second variations.

(2) Compatible states form compatible sets and the optimal decompositions of any state w.r.t. any subalgebra $\mathbf{N}$ are under control if we know all compatible sets (w.r.t. $\mathbf{N}$) of maximal size [6]

The presence of symmetries greatly helps to simplify the minimization procedure.

LEMMA 2. *Let* $\mathbf{M}$ *be a finite dimensional full matrix algebra,* $\hat{\rho}$ *a state,* $\hat{U} \in \mathbf{M}$ *a unitary operator and* $\mathbf{N} \subseteq \mathbf{M}$ *a subalgebra. Then,*

$$H_{\hat{\rho}}(\mathbf{N}_U) = H_{\hat{\rho}^U}(\mathbf{N}), \quad \textit{where } \mathbf{N}_U := \hat{U}\,\mathbf{N}\,\hat{U}^* \textit{ and } \hat{\rho}^U := \hat{U}^*\hat{\rho}\hat{U}. \tag{4}$$

Proof. Let $\hat{\rho} = \sum_j \lambda_j^U \sigma_j^U$ be an optimal decomposition w.r.t. $\mathbf{N}_U$. According to Definition 1, this means $E^*_{\hat{\rho}}(\mathbf{N}_U) = \sum_j \lambda_j^U S\left(\sigma_j^U \upharpoonright \mathbf{N}_U\right)$. Now,

$$\hat{\rho} \upharpoonright \mathbf{N}_U = \hat{\rho}^U \upharpoonright \mathbf{N} \quad \text{and} \quad \hat{\rho}^U = \sum_j \lambda_j^U \hat{U}^* \sigma_j^U \hat{U},$$

with the latter decomposition not necessarily optimal for $\hat{\rho}^U$ w.r.t. $\mathbf{N}$. Therefore,

$$E^*_{\hat{\rho}^U}(\mathbf{N}) \leqslant \sum_j \lambda_j^U S\left(\hat{U}^*\sigma_j^U \hat{U} \upharpoonright \mathbf{N}\right) = E^*_{\hat{\rho}}(\mathbf{N}_U).$$

Inverting the roles of $\hat{\rho}$, $\hat{\rho}^U$ and $\mathbf{N}$, $\mathbf{N}_U$, the Lemma is proved. □

COROLLARY 1. *Let $\hat{U} \in \mathbf{M}$ be a unitary operator.*

(a) *Let $\hat{\rho} = \sum_j \lambda_j \sigma_j$ be a decomposition of $\hat{\rho}$ which is optimal w.r.t. $\mathbf{N}_U$. Then, the map $\hat{\sigma}_i \mapsto \hat{U}^* \hat{\sigma}_i \hat{U}$ transforms it into a decomposition of $\hat{\rho}^U = \hat{U}^* \hat{\rho} \hat{U}$ which is optimal w.r.t. $\mathbf{N}$.*

(b) *Let $\mathbf{N}_U = \mathbf{N}$ and $\hat{\rho}^U = \hat{\rho}$ and $\hat{\rho} = \sum_j \lambda_j \sigma_j$ be a decomposition of $\hat{\rho}$ which is optimal w.r.t. $\mathbf{N}$. Then, the decomposition $\hat{\rho} = \sum_j \lambda_j \hat{U}^* \sigma_j \hat{U}$ must also be optimal w.r.t. $\mathbf{N}$.*

(c) *If a state $\hat{\rho}$ has a unique decomposition $\hat{\rho} = \sum_j \lambda_j \sigma_j$ which is optimal w.r.t. $\mathbf{N}$, then the effect of the map $\sigma_j \mapsto \hat{U}^* \sigma_j \hat{U}$ is to exchange the optimal states among themselves.*

Remark 3. As we shall see, more than one optimal decomposition may appear, in which case, according to Proposition 1, their whole convex span is optimal as well. The state space of an N-level system is the $N^2 - 1$-dimensional submanifold of $\mathbf{R}^{N^2}$ determined by the request that $\hat{\rho}$ be a positive normalized matrix. Given a suitable parametrization of $\hat{\rho}$, we shall say that bifurcation(s) or a phase-transition(s) occurs when there are subregions in the parameter manifold where optimal decompositions w.r.t. a given subalgebra are unique and others where they are not.

3. Totally Symmetric States

While in dimension 2 a fully analytic proof shows the existence of a unique optimal decomposition for any given state $\hat{\rho}$ and Abelian subalgebra $\mathbf{A}$ [7–9], already in three-dimensions this fails to be the case [6].

PROPOSITION 2. *Let $\mathbf{M}$ be the algebra of 3×3 complex matrices and $\mathbf{A} \subset \mathbf{M}$ a maximally Abelian subalgebra, its minimal projections identifying an orthonormal basis $|a_j\rangle$, $j = 1, 2, 3$. Let us then consider states $\hat{\rho}(x)$ given, with respect to the basis associated with $\mathbf{A}$ by totally symmetric and real density matrices*

$$\hat{\rho}(x) = \frac{1}{3} \begin{pmatrix} 1 & x & x \\ x & 1 & x \\ x & x & 1 \end{pmatrix}, \quad -1/2 \leqslant x \leqslant 1 . \tag{5}$$

It turns out that

(1) *$H_{\hat{\rho}(x)}(\mathbf{A})$ is attained at one or more optimal decompositions of the form*

$$\hat{\rho}(x) = \frac{1}{3} \sum_{j=0}^{2} \hat{U}^j |\psi_\theta\rangle\langle\psi_\theta| \hat{U}^{-j}, \tag{6}$$

where

$$|\psi_\theta\rangle = \frac{a+2b\cos(\theta)}{3}\,|a_1\rangle + \frac{a-2b\cos(\theta-\pi/3)}{3}\,|a_2\rangle + \\ + \frac{a-2b\cos(\theta+\pi/3)}{3}\,|a_3\rangle, \tag{7}$$

with

$$a=\sqrt{1+2x}, \qquad b=\sqrt{1-x}, \quad \text{and} \quad \hat{U}=\begin{pmatrix}0&0&1\\1&0&0\\0&1&0\end{pmatrix},$$

cyclically permuting the basis vectors $|a_j\rangle$, $j=1,2,3$.

Thus, to calculate $H_{\hat{\rho}(x)}(\mathbf{A})$*, one has to seek the angles* $\theta^*(x)$ *that minimize*

$$E(x;\theta) := -\sum_{j=1}^{3}|\psi_\theta^j|^2\log|\psi_\theta^j|^2\,, \tag{8}$$

where ψ_θ^j, $j=1,2,3$*, are the components of* $|\psi_\theta\rangle$ *with respect to* $|a_j\rangle$, $j=1,2,3$.

(2) *There exists a value* $x* = -0.415023$ *of the parameter* x *such that*

(a) *For* $x* \leqslant x \leqslant 1$*, there is a unique,* x*-independent, optimal angle* $\theta^*(x)=2\pi/3$ *and a unique optimal decomposition*

$$|\psi_{\theta^*(x)}\rangle = \frac{1}{3}\begin{pmatrix}a-b\\a-b\\a+2b\end{pmatrix}. \tag{9}$$

(b) *If* $-1/2 < x < x*$*, there are two* x*-dependent different optimal angles* $\theta^*_\pm(x)=2\pi/3\pm\alpha(x)$*, with* $\alpha(x)\neq 0$.

Correspondingly, two optimal vectors appear:

$$|\psi_{\theta^*_\pm(x)}\rangle = \frac{1}{3}\begin{pmatrix}a-2b\cos(\pi/3\mp\alpha(x))\\a-2b\cos(\pi/3\pm\alpha(x)\\a+2b\cos\alpha(x)\end{pmatrix}. \tag{10}$$

They cannot be mapped one into the other by a permutation: we shall refer to them as forming an 'optimal doublet'.

(c) *For* $x=-1/2$, $\alpha(x)=-\pi/6$ *the optimal vectors are*

$$|\psi_{\theta^*_+(-1/2)}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}-1\\0\\1\end{pmatrix}, \qquad |\psi_{\theta^*_-(-1/2)}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\-1\\1\end{pmatrix}. \tag{11}$$

One gets mapped into the other by a suitable cyclic permuatation, so they do not form an optimal doublet (see the second remark below).

Proof. See [6]. The results were partially analytical and partially numerically supported. □

Remarks 4. (1) Beside the cyclic permutations $\hat{U}^j$, $j = 0, 1, 2$, the state $\hat{\rho}(x)$ and the algebra **A** are also left invariant by the unitary operator

$$\hat{V}_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} . \tag{12}$$

Vectors forming optimal doublets (10) are exchanged one into the other by $\hat{V}_1$.

(2) Notice that, for $x = -\frac{1}{2}$, the optimal states do not form an optimal doublet, but they are of a quite different form with respect to (9).

(3) The point x^* at which a bifurcation occurs is also a point where we have a kind of ‘phase-transition’. Indeed, suppose $E(x;\theta)$ has a minimum at (x_0, θ^*), that is $\partial_\theta\, E(x_0;\theta^*) = 0$ and $\partial^2_\theta\, E(x_0;\theta^*) > 0$. Then, the continuity of $E(x;\theta)$ and the stationarity condition $\partial_\theta E(x;\theta) = 0$ implicitly define the optimal angles as continuous functions $x \mapsto \theta^*(x)$ in a neighborhood of (x_0, θ^*). Unless $\partial^2_\theta\, E(x^*;\theta) = 0$, this is always possible in a neighborhood of a point (x^*, θ) for which $\partial_\theta\, E(x^*;\theta) = 0$. For instance, one checks that

$$\partial^2_\theta E(x;\theta = 2\pi/3) = \frac{4b}{9}\left[(a+2b)\log\frac{(a+2b)^2}{(a-b)^2} \;-\; 6b\right] \tag{13}$$

vanishes at $x^* = -.415023$ [8], while $\theta = 2\pi/3$, which corresponds to a minimum of $E(x;\theta)$ for $x > x^*$, starts giving rise to a maximum of $E(x;\theta)$ with a bifurcation into two symmetric minima at $\theta_\pm(x) = 2\pi/3 \pm \alpha(x)$ as soon as $x < x^*$.

(4) Very much in the spirit of the above remark, the necessity of a bifurcation can be argued as follows (for more details, see [11]). Let us consider the vectors $|v\rangle := (0, -1, 1)/\sqrt{2}$ in (11) that are optimal at $x = -1/2$. When $x \to -1/2$, the vectors $|u\rangle := (a-b, a-b, a+2b)/3$ in (9), which are optimal for any $x \geqslant x^*$, transform into $|u^*\rangle := (-1, -1, 2)/\sqrt{6}$. There is no choice of phase and of cyclic permutation $\hat{U}^j$ such that $\hat{U}^j|u^*\rangle = \exp(i\phi)|v\rangle$, while the continuous transformation of $|u\rangle$ into $|v\rangle$ would certainly be possible if $\partial^2_\theta E(x;\theta^*(x))$ did not vanish at some x.

Proposition 2 tells us that, already for a state as in (6), optimal decompositions w.r.t. **A** are not unique. In order to study whether the occurrence of bifurcations and phase transitions of the type explained above is a more typical feature, we fix the three-dimensional context and the maximally Abelian subalgebra **A** of Proposition 2, but we allow the state some more freedom and consider density matrices of the form

$$\hat{\rho}(z) = \frac{1}{3}\begin{pmatrix} 1 & z & z^* \\ z^* & 1 & z \\ z & z^* & 1 \end{pmatrix}, \quad \text{where} \quad z = x + iy\,. \tag{14}$$

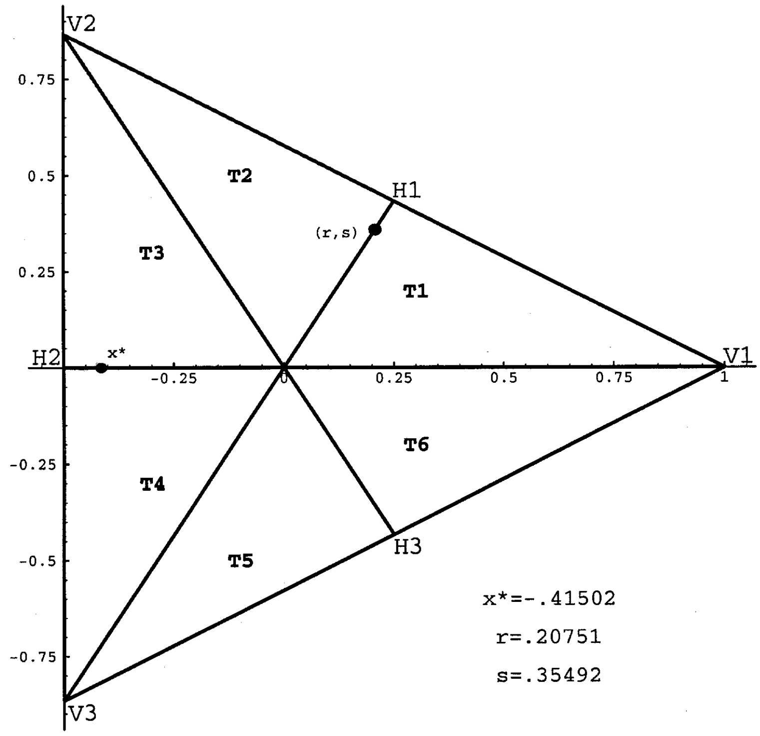

Figure 1. Triangle of possible states $\hat{\rho}(z)$, $z = x + iy$.

Positivity and normalization enforce the following bounds

$$-\tfrac{1}{2} \leqslant x \leqslant 1\,, \quad 0 \leqslant 1 - x + \sqrt{3}y \leqslant 1 \quad \text{and} \quad 0 \leqslant 1 - x - \sqrt{3}y \leqslant 1. \tag{15}$$

Therefore, the density matrices $\rho(z)$ as in (14) can be parametrized by the coordinates (x, y) of points belonging to the equilateral triangle **T** in Figure 1. The vertices $V1 = (1, 0)$, $V2 = (-1/2, \sqrt{3}/2)$ and $V3 = (-1/2, -\sqrt{3}/2)$ correspond to pure states, while the origin corresponds to the tracial state $\mathbb{1}/3$.

LEMMA 3. *It is possible to decompose $\hat{\rho}(z)$ as follows:*

$$\hat{\rho}(z) = \frac{1}{3}\sum_{j=0}^{2} \hat{U}^j |\psi_{\phi\theta}\rangle\langle\psi_{\phi\theta}|\hat{U}^{-j}\,, \tag{16}$$

where

$$\begin{aligned} |\psi_{\phi\theta}\rangle \;=\; & \frac{a + 2b\cos(\theta+\phi) - i2\sqrt{3}\eta\cos\theta}{3}\,|a_1\rangle + \\ & + \frac{a - 2b\cos(\theta+\phi-\pi/3) + i2\sqrt{3}\eta\cos(\theta-\pi/3)}{3}\,|a_2\rangle + \end{aligned}$$

$$+\frac{a - 2b\cos(\theta+\phi+\pi/3) + i2\sqrt{3}\eta\cos(\theta+\pi/3)}{3}\,|a_3\rangle\ , \tag{17}$$

with

$$a = \sqrt{1+2x}\ , \qquad b = \sqrt{1-x-3\eta^2}$$

and

$$\eta^2 = \frac{1}{6}\left[1 - x - \sqrt{(1-x)^2 - \frac{3y^2}{\sin^2\phi}}\right] \quad \textit{with} \quad \sin^2\phi \geqslant \frac{3y^2}{(1-x)^2}\ . \tag{18}$$

Thus, analogously to (8)*, the quantity* (2) *to be minimized reads*

$$E(x, y; \theta, \phi) := -\sum_{j=1}^{3} |\psi^j_{\theta\phi}|^2 \log |\psi^j_{\theta\phi}|^2\ , \tag{19}$$

where $\psi^j_{\theta\phi}$ *are the components of* $|\psi_{\theta\phi}\rangle$*, w.r.t.* $|a_j\rangle$*,* $j = 1, 2, 3$*.*

The decompositions of the form (16) play the same role for $\hat{\rho}(z)$ as those in (6) for $\hat{\rho}(x)$. Indeed,

PROPOSITION 3. $H_{\hat{\rho}(z)}(\mathbf{A})$ *is attained at one or more optimal decompositions of the form* (16)*. It is thus sufficient to look for 'optimal' angles* $\theta^*(x, y)$ *and* $\phi^*(x, y)$ *such that* (19) *achieve its minimum* $E(\theta^*(x, y), \phi^*(x, y))$*.*

Proof. In the case of $z = x$ real, the optimal decompositions were showed to be of the form (6), by the fact, which was proved numerically, that the minima $E(\theta^*(x))$ of (8) form a concave function of the parameter $x \in [-1/2, 1]$ [6]. The same strategy works for $z = x+iy$ complex, if the the minima $E(\theta^*(x, y), \phi^*(x, y))$ form a concave function of the real and imaginary parts of the complex parameter $z = x + iy$. This is indeed the case: Figure 2 shows the concavity of $E(\theta^*(x, y), \phi^*(x, y))$ over the upper half of the triangle **T** in Figure 1. □

In the numerical proof of the concavity of the surface spanned by the minima as functions of the parameters x, y, we can restrict to the upper half of the triangle **T** because of many useful symmetries enjoyed by the parametrization (17). In order to better discuss them, we introduce the following three unitary operators

$$\hat{V}_u = \hat{V}^*_u = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & u^* \\ 0 & u & 0 \end{pmatrix}\ , \quad \text{with } u = \begin{cases} 1, \\ \kappa \quad = \dfrac{-1\ + i\sqrt{3}}{2}, \\ \kappa^* \quad = \dfrac{-1\ - i\sqrt{3}}{2}. \end{cases} \tag{20}$$

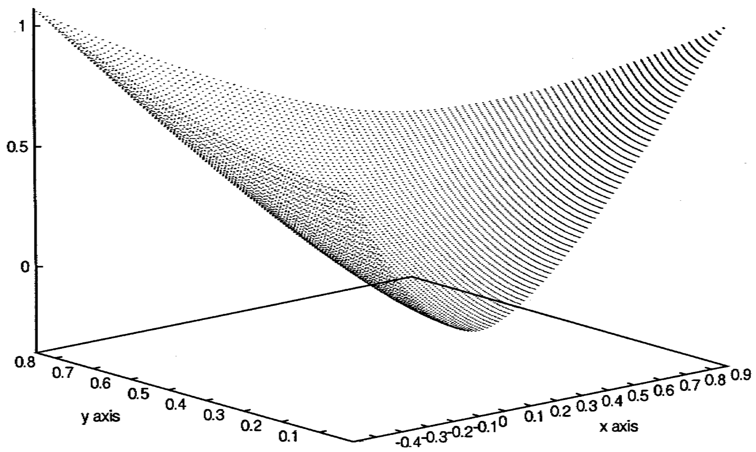

Figure 2. Concavity of the minima $E(x, y; \theta^*(x, y), \phi^*(x, y))$ on the upper half of the triangle **T**.

Remarks 5. (1) The operators of above transform symmetric states $\hat{\rho}(z)$ as follows

$$\hat{V}_u \hat{\rho}(z) \hat{V}_u = \hat{\rho}(uz^*), \quad \text{where } u = 1,\ \kappa,\ \kappa^*\ . \tag{21}$$

Therefore, unlike the case of real $z = x$, $\hat{V}_1$ does not represent a symmetry of the state $\hat{\rho}(z)$ for z complex. It is necessary to take the complex conjugate, too.

(2) Since $E(\theta, \phi)$ in (19) depends on y through η^2 in (18), it does not change when $y \to -y$. Thus, we can restrict to the upper half triangle in Figure 1. Notice that density matrices $\hat{\rho}(z)$ with $y < 0$ are reached from $\hat{\rho}(z)$ with $y > 0$ via a rotation by $\hat{V}_1$, which amounts to taking the complex conjugate of $\hat{\rho}(z)$.

(3) Because of (21), using $\hat{V}_u$, $u = 1$, κ and κ^*, the states $\hat{\rho}(z)$ labelled by z in **T1** can be mapped into states associated to the other triangles. If we identify the states $\hat{\rho}(z)$ with the points of the triangle z belongs to, then $\hat{V}_\kappa$ transforms **T1** onto **T2**, $\hat{V}_{\kappa^*}$ maps **T1** onto **T4**, while $\hat{V}_1$ reflects **T1** onto **T6**.

(4) Sending θ into $\theta + 2\pi/3$, we pass from $|\psi_{\theta\phi}\rangle$ to the cyclically permuted vector $\hat{U}_1|\psi_{\theta\phi}\rangle$. However, we know from Corollary 1 that, if the former is optimal, the latter is optimal, too. Therefore, we can restrict the search for 'optimal angles' to $0 \leqslant \theta \leqslant 2\pi/3$.

PROPOSITION 4. *In order to find all optimal decompositions of $\hat{\rho}(z)$ with respect to the maximally Abelian subalgebra* **A**, *one can minimize $E(x, y; \theta, \phi)$, with $z = x + iy$ in the triangle* **T1** *of Figure 1, and then act on the optimal vectors with the unitary operators $\hat{V}_u$ of* (20).

Proof. The unitary operators $\hat{V}_u$ in (20) leave the maximally Abelian subalgebra **A** invariant. Thus, the result follows from the previous remarks and the application of Lemma 3. □

As an application of the previous Proposition, we now concentrate on the borders of the triangle **T1** in Figure 1.

COROLLARY 2. *Each state* $\hat{\rho}(z)$ *with* z *on the lines* $(0,0) \to V1$ *and* $H1 \to V1$ *has a unique optimal decomposition w.r.t. the maximally Abelian subalgebra* **A**. *There is a bifurcation point on the line from* $(0,0)$ *to* $H1$.

Proof. The case of the line $(0,0) \to V1$ is known from [6], that of the line $H1 \to V1$ comes from numerical results some of them being collected in Table I.

Table I. Optimal values of $E(x, y; \theta, \phi)$ and optimal vector components $\psi_j^r + i\psi_j^i$ for states $\hat{\rho}(z)$ on the line from $H1$ to $V1$:

$$x = \tfrac{1}{4} + \frac{\sqrt{3}}{2}t\,, \qquad y = -\tfrac{t}{2} + \frac{\sqrt{3}}{4}, \quad t \in \left[0, \frac{\sqrt{3}}{2}\right].$$

t	$E(\theta^*(x,y), \phi^*(x,y))$	ψ_1^r	ψ_1^i	ψ_2^r	ψ_2^i	ψ_3^r	ψ_3^i
.001	.6931	.0004	0	.6124	.3533	.6124	−.3533
.01	.6933	.0046	0	.6135	.3514	.6135	−.3514
.1	.7074	.0472	0	.6231	.3325	.6231	−.3325
.2	.7383	.0949	0	.6319	.3100	.6319	−.3100
.4	.8275	.1940	0	.6433	.2593	.6433	−.2593
.6	.9380	.3048	0	.6443	.1958	.6443	−.1958
.8	1.058	.4519	0	.6233	.0962	.6233	−.0962

As to the appearance of a bifurcation, we use the third among the previous remarks and rotate with $\hat{V}_{\kappa^*}$, as in (21), the states parametrized by the line from $(0,0) \to H2$. The resulting states are parametrized by the line $(0,0) \to H1$. Therefore, by applying Lemma 3, the optimal decompositions corresponding to the line $(0,0) \to H1$ are obtained by rotating with $\hat{V}_{\kappa^*}$ those associated with the line $(0,0) \to H2$, which are known from [6] to suffer a phase transition at $(x^*, 0)$. At the point $z^* = r + is = -x^*/2 - ix^*\sqrt{3}/2$ a bifurcation occurs on the line $(0,0) \to H1$: optimal doublets for $x < x^*$ are rotated with $\hat{V}_{\kappa^*}$ into optimal doublets for $r < x < 1/4$ and $y = \sqrt{3}x$, $s < y < \sqrt{3}/4$. □

Table I shows numerically that, on the line $H1 \to V1$, no bifurcation occurs, that is the optimal decompositions are unique and the structure of the optimal vectors is such that each one of them is mapped into itself by transforming it with $\hat{V}_1$ and taking the complex conjugate. This reminds us of the case 2c) in Proposition 2 where doublets return to a singlet at $x = -1/2$. More details are given in

PROPOSITION 5. *In the interior of the triangle* **T1** *of Figure 1, a bifurcation occurs on any straight line from* $(1-x)/\sqrt{3}$ *to* 0 *with* $x \in [1/4, 1]$.

Proof. According to Proposition 3 and to the parametrization (17), ϕ must equal $\pi/2$ on the line from $H1$ to $V1$. Thus, the optimal vectors are of the form:

$$|\psi_\theta\rangle = \frac{1}{3}\begin{pmatrix} a - 2i\tilde{b}\,\mathrm{e}^{-i\theta} \\ a + 2i\tilde{b}\,\mathrm{e}^{-i(\theta-\pi/3)} \\ a + 2i\tilde{b}\,\mathrm{e}^{-i(\theta+\pi/3)} \end{pmatrix}, \qquad \tilde{b} = \sqrt{\frac{1-x}{2}}\,. \tag{22}$$

Tables I and II (see below) show that there are no bifurcations on the line from $H1$ to $V1$ and that only optimal singlets contribute to the minimum of (19), with $\theta = \pi/2$. Therefore, the vector (22) transforms into

$$|U_x\rangle := \frac{1}{3}\begin{pmatrix} a - 2\tilde{b} \\ a + \tilde{b}(1 + i\sqrt{3}) \\ a + \tilde{b}(1 - i\sqrt{3}) \end{pmatrix}\,, \tag{23}$$

which is left invariant by acting with $\hat{V}_1$ and taking the complex conjugate. By symmetry (see the discussion before Proposition 4), the same is true on the line from $H1$ to $V2$.

Concerning the interior of the triangle **T1** in Figure 1, some numerical results are summarized in Table III (see also Table II).

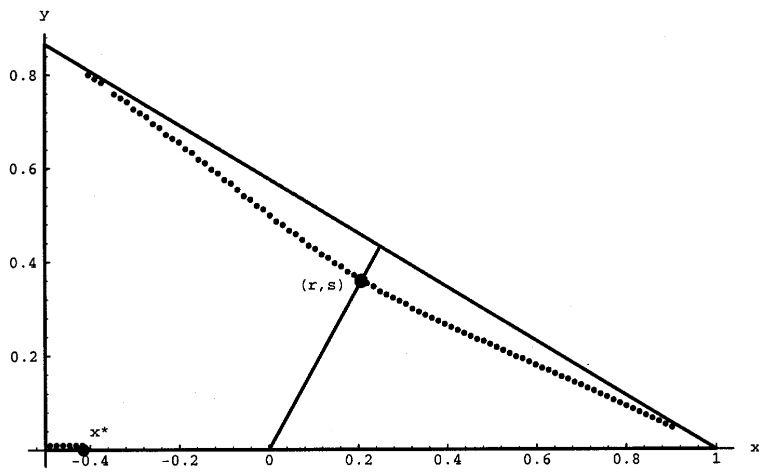

Figure 3. Curve of bifurcation points of $E(x, y; \theta, \phi)$.

The structure that emerges is depicted in Figure 3 and is as follows: (1) For points $z = x + iy$ below the bifurcation curve in the triangle **T1**, the 'optimal' angles are fixed to $\phi^* = \pi/2$ and $\theta^* = \pi/6$ and the optimal vectors are singlets. Indeed, they are of the form

$$|U_{x,y}\rangle := \frac{1}{3}\begin{pmatrix} a - \tilde{b}(\sqrt{1+c} + i\sqrt{3}\sqrt{1-c}) \\ a - \tilde{b}(\sqrt{1+c} - i\sqrt{3}\sqrt{1-c}) \\ a + 2\tilde{b}\sqrt{1+c} \end{pmatrix}\,, \tag{24}$$

Table II. Optimal values of θ, ϕ and $E(x, y; \theta, \phi)$ in **T1**.

x	y	$y_{\max}$	ϕ^*	θ^*	$E(x, y)$
.1	.1	.1732	$\pi/2$	$\pi/6$	.0665
.1	.1732	.1732	$\pi/2$	$\pi/6$	.1248
.3	.2	.4041	$\pi/2$	$\pi/6$	.3241
.3	.3	.4041	$\pi/2$	$\pi/6$	.4832
.3	.35	.4041	1.202	1.290	.5875
			1.939	1.851	.5875
.3	.4	.4041	1.692	1.602	.6886
			1.448	1.539	.6886
.3	.4041	.4041	$\pi/2$	$\pi/2$	.6977
.5	.1	.2886	$\pi/2$	$\pi/6$	.4632
.5	.2	.2886	$\pi/2$	$\pi/6$	.5833
.5	.25	.2886	1.281	1.257	.6815
			1.860	1.884	.6815
.5	.28	.2886	1.670	1.628	.7415
			1.471	1.513	.7415
.5	.2886	.2886	$\pi/2$	$\pi/2$	.7709
.8	.05	.1154	$\pi/2$	$\pi/6$	.8400
.8	.08	.1154	$\pi/2$	$\pi/6$	.8730
.8	.1	.1154	1.731	1.974	.9096
			1.410	1.166	.9096
.8	.105	.1154	1.688	1.775	.9196
			1.453	1.366	.9196
.8	.1154	.1154	$\pi/2$	$\pi/2$	.9553

where $c^2 = 1 - 3y^2/((1-x)^2$, thus invariant under $\hat{V}_1$ and complex conjugation. Since $c \to 1$ when $y \to 0$, the optimal vectors $|U_{x,y}\rangle$ continuously transform into the optimal vectors (9) with $y \to 0$. On the other hand, when $y \to (1-x)/\sqrt{3}$, $c \to 0$ and

$$|U_{x,y}\rangle \longrightarrow |U_x^*\rangle := \frac{1}{3}\begin{pmatrix} a - \tilde{b}(1 + i\sqrt{3}) \\ a - \tilde{b}(1 - i\sqrt{3}) \\ a + 2\tilde{b} \end{pmatrix} . \tag{25}$$

With a little more effort than in Remark 4.4, one can show that there is no choice of phase and of cyclic permutation $\hat{U}^j$ such that $\hat{U}^j|U_x^*\rangle = \exp(i\phi)|U_x\rangle$. This failure of continuity indicates the occurrence of one or more bifurcations when fixing $1/4 \leqslant x \leqslant 1$ and letting y vary from 0 to $(1-x)/\sqrt{3}$.

Table III. Optimal vector components $\psi_j^r + i\psi_j^i$ for states $\rho(z)$ in **T1**.

x	y	$y_{\max}$	ψ_1^r	ψ_1^i	ψ_2^r	ψ_2^i	ψ_3^r	ψ_3^i
.1	.1	.1732	.0504	−.0529	.0504	.0529	.9946	0
.1	.1732	.1732	.0534	−.0926	.0534	.0926	.9884	0
.3	.2	.4041	.1520	−.1236	.152	.1236	.9608	0
.3	.3	.4041	.1667	−.1961	.1667	.1961	.9313	0
.3	.35	.4041	.0537	−.0866	.3636	.3035	.8474	−.2168
			.0537	.0866	.8474	.2168	.3636	−.3035
.3	.4	.4041	.0175	.0120	.6779	.3222	.5694	−.3343
			.0175	−.0120	.5694	.3343	.6779	−.3222
.3	.4041	.4041	.0242	0	.6203	.339	.6203	−.339
.5	.1	.2886	.2393	−.0718	.2393	.0718	.9354	0
.5	.2	.2886	.2527	−.1524	.2527	.1524	.9087	0
.5	.25	.2886	.1432	−.0776	.4399	.2464	.831	−.1687
			.1432	.0776	.8310	.1687	.4399	−.2464
.5	.28	.2886	.1073	.0169	.7034	.2455	.6034	−.2624
			.1073	−.0169	.6034	.2624	.7034	−.2455
.5	.2886	.2886	.1342	0	.6399	.2853	.6399	−.2853
.8	.05	.1154	.3921	−.0573	.3921	.0573	.8281	0
.8	.08	.1154	.3991	−.0964	.3991	.0964	.8140	0
.8	.1	.1154	.3208	.0597	.7646	.0912	.5270	−.1509
			.3208	−.0597	.5270	.1509	.7646	−.0912
.8	.105	.1154	.3006	.0331	.7242	.1210	.5874	−.1547
			.3006	−.0331	.5874	.1547	.7242	−.1216
.8	.1154	.1154	.3230	0	.6447	.1793	.6447	−.1793

(2) The bifurcation points actually unfold along a curve which continuously connects the vertex $V1$ to the point (r, s) on the line $(0, 0) \to H1$ and, symmetrically, from (r, s) to $V2$, as showed in Figure 3. The program was asked to signal the first appearance of doublets of optimal vectors, whence the dots on the x-axis, between the real bifurcation point x^* and $-1/2$.

(3) For points above the bifurcation line the 'optimal' angles depend on z and the 'optimal' vectors appear in doublets which are mapped into themselves by 'rotating' with $\hat{V}_1$ and taking the complex conjugate.

(4) Taking into account the previous results, one could try, as in Remark 4.3, to detect the bifurcation points as those (x, y) in the triangle **T** where the determinant of the Hessian matrix $\partial^2_{uv} E(x, y; \pi/6, \pi/2)$, $(u, v) = (\theta, \phi)$, vanishes. The result is showed in Figure 4 for the upper half of **T**, confirming the result obtained in

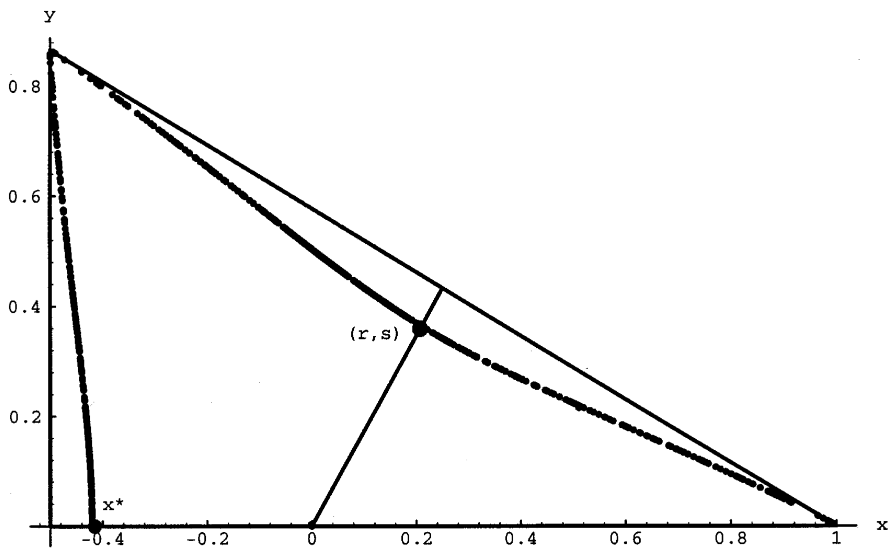

Figure 4. Zeroes of the determinant of the Hessian $\partial^2_{uv}E(x,y;\theta,\phi)$, $(u,v) = (\theta,\phi)$ at $\theta=\pi/6, \phi=\pi/2$.

Figure 3. For the lower half the result is specular, thus evidentiating the equilateral symmetry of the problem.

(5) Analogously to Remark 4.2, approaching the line $V1 \to H1$, the doublets become singlets again with 'optimal' angles $\phi^* = \theta^* = \pi/2$. □

4. Coverable State Space

According to Proposition 1 and Corollary 1, we do not only control the optimal decomposition of symmetric $\hat{\rho}(z)$, but also those of the density matrices that can be obtained from $\hat{\rho}(z)$ by generic unitary operators

$$\hat{V}_{\alpha\beta} = \hat{a}_1 + \mathrm{e}^{i\alpha}\hat{a}_2 + \mathrm{e}^{i\beta}\hat{a}_3 , \quad \text{where } \alpha,\ \beta \text{ real} \tag{26}$$

and $\hat{a}_j$, $j = 1,2,3$, are the minimal projections of the subalgebra **A**. In fact, they leave **A** invariant. Let then $\hat{p}_j(z)$ denote the projections onto the vectors that optimally decompose a given state $\hat{\rho}(z)$ in (14) w.r.t. **A**. Then, the first part of Proposition 1 ensures the density matrices $\hat{\rho}$

$$\hat{\rho} = \sum_j \lambda_j \hat{V}_{\alpha\beta}\hat{p}_j(z)\hat{V}^*_{\alpha\beta} , \tag{27}$$

are already optimally decomposed w.r.t. **A**.

LEMMA 4. *In the eight-dimensional real manifold of states of* 3*-level quantum systems, there is a subset of states, still parametrized by eight independent reals, for which the optimal decompositions are of the form* (27).

Proof. Let z belong to the region where the states $\hat{\rho}(z)$ have doublets of optimal decompositions. Then, for each such z, six different projections $\hat{p}_j(z)$ are available to be used in (27). However, the different doublets must satisfy $\hat{\rho}(z) = \sum_{j=1}^{3} \mu_j \hat{p}_j(z) = \sum_{j=4}^{6} \mu_j \hat{p}_j(z)$. Moreover, $\sum_{j=1}^{6} \lambda_j = 1$ provides a further constraint so that only 4 out of the 6 possible positive weights λ_j are independent. Together with α, β and $z = x + iy$, this makes for eight real independent parameters. □

Despite the right dimensionality, there are constraints on the subregion of allowed parameters that forbid complete control of the whole of state space.

PROPOSITION 6. *There exist density matrices with optimal decompositions w.r.t.* **A** *not of the form* (27).

Proof. Consider a vector (a, b, c) and assume it to belong to the optimal set of some $\hat{V}_{\alpha\beta}\hat{\rho}(z)\hat{V}^*_{\alpha\beta}$. Then, $(a, b, c) = (a, e^{i\alpha} b_0, e^{i\beta} c_0)$, for (a, b_0, c_0) in an optimal set of $\hat{\rho}(z)$. Therefore, using cyclic permutations and according to Corollary 1, (a, b, c) and $(b_0, e^{i\alpha} c_0, e^{i\beta} a) = (e^{-i\alpha} b, e^{i(\alpha-\beta)} c, e^{i\beta} a)$ must belong to the optimal set of $\hat{V}_{\alpha\beta}\hat{\rho}(z)\hat{V}^*_{\alpha\beta}$ and thus must be compatible in the sense of Lemma 1, that is

$$|a|\,|b| \log \frac{|b|^2}{|a|^2} \;+\; |b|\,|c|\, e^{i\gamma} \log \frac{|c|^2}{|b|^2} \;+\; |a|\,|c|\, e^{i\delta} \log \frac{|a|^2}{|c|^2} = 0 \,, \tag{28}$$

where γ and δ depend on α, β and on the phases of a, b and c. The above equality can always be arranged to have the form

$$A \;+\; e^{i\psi} B \;+\; e^{i\phi} C = 0 \,, \tag{29}$$

for unknown ψ, ϕ and $0 \leqslant A \leqslant B \leqslant C$. Solutions to (29) can be found only if the circle of radius C around the origin intersects the circle of radius B centered in A, that is if and only if $A + B \geqslant C$. It is no restriction to consider (not normalized) vectors $(1, b, c)$, so that, without any order relation between A, B and C, the three necessary inequalities $A + B \geqslant C$, $B + C \geqslant A$ and $C + A \geqslant B$ lead to

$$\frac{|c|}{|c| - 1} \log |c|^2 \geqslant \frac{|b|}{|b| - 1} \log |b|^2, \tag{30}$$

$$\frac{|c|}{|c| + 1} \log |c|^2 \geqslant \frac{|b|}{|b| + 1} \log |c|^2, \tag{31}$$

$$\frac{|b|}{|b| - 1} \log |b|^2 \geqslant \frac{|c|}{|c| + 1} \log |c|^2 \,. \tag{32}$$

The first two inequalities are always satisfied, whereas the third one is violated by $|b|$ close to $1 = |a|$ and sufficiently large $|c|$. □

Remark 6. Inequality (32) is violated by vectors like $(1, \varepsilon, \tilde{\varepsilon})$ that lie in a neighborhhod of the optimal set $(1, 0, 0)$, $(0, 1, 0)$ and $(0, 0, 1)$ of the tracial state.

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