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Squaring parametrization of constrained and unconstrained sets of quantum states

N Il'in¹, E Shpagina^{2,3}, F Uskov^{2,4} and O Lychkovskiy^{2,1,5} 

¹ Steklov Mathematical Institute of Russian Academy of Sciences, Gubkina str., 8, Moscow 119991, Russia

² Skolkovo Institute of Science and Technology, Skolkovo Innovation Center 3, Moscow 143026, Russia

³ Bauman Moscow State Technical University, 2nd Baumanskaya str., 5, Moscow 105005, Russia

⁴ Moscow State University, Faculty of Physics, GSP-1, 1-2 Leninskiye Gory, Moscow 119991, Russia

⁵ Russian Quantum Center, Novaya St. 100A, Skolkovo, Moscow Region, 143025, Russia

E-mail: ilyn@mi.ras.ru

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Abstract

A mixed quantum state is represented by a Hermitian positive semi-definite operator ρ with the unit trace. The positivity requirement is responsible for a highly nontrivial geometry of the set of quantum states. A known way to satisfy this requirement automatically is to use the map $\rho = \tau^2 / \text{tr } \tau^2$, where τ can be an arbitrary nonzero Hermitian operator. We elaborate the parametrization of the set of quantum states induced by the parametrization of the linear space of Hermitian operators by virtue of this map. In particular, we derive an equation for the boundary of the set. Further, we discuss how this parametrization can be applied to a set of quantum states constrained by some symmetry. We consider several examples of the squaring parametrisation of sets of qubits and qutrits constrained by various symmetries.

Keywords: parametrization of quantum states, generalized Bloch vector, mixed states, density matrix, Werner states, qubit, qutrit

(Some figures may appear in colour only in the online journal)

1. Introduction

A quantum state of a system with a Hilbert space $\mathcal{H} = \mathbb{C}^D$ with a finite dimension D is represented by a density operator $\rho \in \mathbb{C}^{D \times D}$, which should have unit trace and be Hermitian and positive semi-definite:

$$\text{tr } \rho = 1, \quad \rho^\dagger = \rho, \quad \rho \geq 0. \quad (1)$$

The latter non-linear condition is responsible for an extremely complicated structure of the set $\mathbb{M}$ of quantum states which shows up for $D > 2$ [1, 2]. To describe the shape of this set is an important problem with numerous applications in quantum information and condensed matter theory. In particular, it is often desirable to introduce a *parametrization* of $\mathbb{M}$, i.e. a map from some subset of $\mathbb{R}^{D^2-1}$ to $\mathbb{M}$. Should the system under consideration be a many-body system, and $\mathcal{H}$ be a tensor product of one-body Hilbert spaces, one would further wish to have a parametrization with this tensor product structure built in. Unfortunately, widely used parametrizations [3] either fail to explicitly incorporate the tensor product structure or impose the positivity condition in a rather opaque and computationally demanding form.

The purpose of the present paper is to fill this gap by elaborating a parametrization of the set $\mathbb{M}$ of quantum states which can account for the positivity in a straightforward manner, and is well-suited for many-body systems. The starting point for our reasoning is an observation made in [4] that any density operator ρ can be expressed as

$$\rho = \tau^2 / \text{tr } \tau^2, \quad (2)$$

where τ is some nonzero Hermitian operator. Obviously, the rhs of this equation satisfies all three conditions (1). Equation (2) establishes a map $\mathbb{H} \rightarrow \mathbb{M}$ between the real linear space $\mathbb{H}$ of Hermitian operators, and the set $\mathbb{M}$ of quantum states. This map has been used to introduce a measure in $\mathbb{M}$ induced by a measure in $\mathbb{H}$ [5]⁶. Here, we focus on the induced parametrization rather than the induced measure. Specifically, we employ the fact that $\mathbb{H}$ is easily parametrized in a manner preserving tensor structure [6]. This, in turn, induces a parametrization of $\mathbb{M}$ through the map (2). We will use the term ‘squaring parametrization’ for any parametrization obtained in this way.

We construct the squaring parametrization of $\mathbb{M}$, and discuss its properties and its relation to the widely used Bloch vector parametrization [7, 8] in section 2. In particular, within this parametrization we derive an equation for the boundary $\partial\mathbb{M}$ of $\mathbb{M}$.

In section 3, we study the squaring parametrization of the set of quantum states subject to linear constraints imposed by a symmetry. The usage and merits of the squaring parametrization are exemplified in the case of qubits and qutrits invariant under various symmetries. We conclude with the summary and outlook in section 4. Some technical results are relegated to the appendix.

2. An unconstrained set of quantum states

2.1. Preliminaries

2.1.1. Linear space of Hermitian operators. We start by recalling basic facts concerning $\mathbb{M}$ and $\mathbb{H}$ [1, 2, 6, 9]. The real linear space $\mathbb{H}$ is a space of Hermitian operators acting in the

⁶To be more exact, a slightly different map of the form $\rho = AA^\dagger / \text{tr } (AA^\dagger)$ with A being an arbitrary nonzero linear operator has been used in [5]. We choose the map (2) instead in order to minimize the number of parameters in the parametrization. This is further discussed in the footnote 7 in section 2.2.

Hilbert space $\mathcal{H} = \mathbb{C}^D$. These operators can be represented by $D \times D$ Hermitian matrices. The dimension of $\mathbb{H}$ equals D^2 .

One can introduce a scalar product in $\mathbb{H}$ according to

$$(\lambda, \lambda') \equiv D^{-1} \operatorname{tr}(\lambda \lambda'), \quad \lambda, \lambda' \in \mathbb{H}; \quad (3)$$

$\mathbb{H}$ is a real inner product space with respect to this scalar product.

One can always select in $\mathbb{H}$ an orthonormal basis consisting of a identity operator, $\mathbb{1}$, and $D^2 - 1$ generators λ_i of the $SU(D)$ group, satisfying

$$\lambda_i^\dagger = \lambda_i, \quad (4)$$

$$\operatorname{tr}(\lambda_i \lambda_j) = \delta_{ij} D, \quad (5)$$

$$\operatorname{tr} \lambda_i = 0, \quad (6)$$

$$[\lambda_i, \lambda_j] = 2if_{ijk} \lambda_k, \quad (7)$$

$$\{\lambda_i, \lambda_j\} = 2\delta_{ij} \mathbb{1} + 2d_{ijk} \lambda_k. \quad (8)$$

Here and in what follows, indices i, j, k run from 1 to $(D^2 - 1)$, a summation over repeated indices is implied, and f_{ijk} and d_{ijk} are totally antisymmetric and symmetric tensors, respectively. Relations (7) and (8) can be combined:

$$\lambda_i \lambda_j = \delta_{ij} \mathbb{1} + if_{ijk} \lambda_k + d_{ijk} \lambda_k. \quad (9)$$

In the simplest case of a single spin 1/2 there are three generators which can be chosen to be the Pauli matrices, σ^α . In the case of a many-body system, its Hilbert space $\mathcal{H}$ is a tensor product of Hilbert spaces of individual constituents, and one can choose the generators λ_i which inherit this tensor product structure. For example, a system consisting of N spins 1/2 has a Hilbert space $\mathcal{H} = (\mathbb{C}^2)^{\otimes N}$, $D = 2^N$, and one can choose

$$\lambda_i = \sigma_1^{\mu_{1i}} \otimes \sigma_2^{\mu_{2i}} \otimes \cdots \otimes \sigma_N^{\mu_{Ni}}, \quad (10)$$

where σ_n^μ acts in the space of the n th spin, and is equal to the μ th Pauli matrix in the case of $\mu = 1, 2, 3$ or an identity operator in the case of $\mu = 0$. Index i enumerates all possible combinations $\{\mu_{1i}, \mu_{2i}, \dots, \mu_{Ni}\}$ except one which consists of N zeros.

2.1.2. Set of quantum states. The set

$$\mathbb{M} \equiv \{\rho \mid \operatorname{tr} \rho = 1, \rho^\dagger = \rho, \rho \geq 0\} \subset \mathbb{H} \quad (11)$$

of all density operators ρ is a convex set of dimension $D^2 - 1$ embedded in $\mathbb{H}$. The positivity condition implies that inner points of $\mathbb{M}$ have D strictly positive eigenvalues, while points on its boundary, $\partial\mathbb{M}$, have at least one zero eigenvalue. In other words, the boundary is given by

$$\partial\mathbb{M} \equiv \{\rho \in \mathbb{M} \mid \operatorname{rank} \rho < D\}. \quad (12)$$

The extreme points of $\mathbb{M}$ are pure states, i.e rank-one projectors, $\rho^2 = \rho$.

2.2. Squaring parametrization

As is obvious from the above discussion, any quantum state ρ can be expanded as

$$\rho = \frac{1}{D}(\mathbb{1} + a_i \lambda_i), \quad (13)$$

where a_i , $i = 1, 2, \dots, D^2 - 1$ are real parameters. Such parametrization, known as the Bloch or the coherence vector parametrization [7, 8], does not ensure the positivity automatically. The positivity condition, $\rho \geq 0$, is fulfilled if and only if the Bloch vector $a = (a_1, a_2, \dots, a_{D^2-1})$ satisfies a set of $D - 1$ inequalities [7, 8]. The first inequality of this set reads

$$a^2 \leq D - 1, \text{ where } a^2 \equiv a_i a_i; \quad (14)$$

this ensures that $\text{tr} \rho^2 \leq 1$. Other inequalities are defined recursively—the j th inequality containing a polynomial in a_i of degree $j + 1$. The Bloch vector a corresponds to the state on the boundary of $\mathbb{M}$ if and only if at least one of these inequalities saturates (i.e. turns into an equality). The set of Bloch vectors subject to the aforementioned inequalities is isomorphic to the set $\mathbb{M}$ of quantum states; thus we will identify these sets.

An alternative way to describe $\mathbb{M}$ is to employ the squaring parametrization, which has the advantage of imposing positivity automatically. It is defined as follows. One introduces an auxiliary Hermitian operator τ parametrized by a real vector $b = (b_1, b_2, \dots, b_{D^2-1}) \in \mathbb{R}^{D^2-1}$,

$$\tau = \frac{1}{D}(\mathbb{1} + b_i \lambda_i). \quad (15)$$

The density operator ρ is then given by equation (2) [4, 5].

Obviously, for any $b \in \mathbb{R}^{D^2-1}$ the conditions (1) are satisfied. Conversely, for any density operator ρ one can choose $\tau = \sqrt{\rho}/\text{tr} \sqrt{\rho}$ (where $\sqrt{\dots}$ denotes a non-negative operator square root), and find a corresponding vector b . Thus we have established a surjective map $\mathbb{R}^{D^2-1} \rightarrow \mathbb{M}$, which constitutes the squaring parametrization. The explicit mapping between the auxiliary vector b and the Bloch vector a reads

$$a_i = \frac{2b_i + d_{ijk} b_j b_k}{1 + b^2}, \text{ where } b^2 \equiv b_i b_i. \quad (16)$$

Clearly, the established map, which we denote as $a(b)$, is not a one-to-one correspondence. As is discussed in appendix A, an inner point of $\mathbb{M}$ generically has 2^{D-1} preimage points in $\mathbb{R}^{D^2-1}$. The number of preimage points is smaller if the eigenvalues of ρ accidentally satisfy a certain sum rule; it is also smaller for boundary points of $\mathbb{M}$. In the case of a pure state, b is unique and equal to a , which follows from $\rho^2 = \rho$. The set of D^2 equations which determine the Bloch vector for pure states read [8]

$$a^2 = D - 1, \quad (17)$$

$$(D - 2)a_i = d_{ijk} a_j a_k. \quad (18)$$

We note that by defining τ according to equation (15) we have excluded those τ which are traceless, despite that they also produce a valid density operator ρ through the equation (2), unless $\tau = 0$. The advantage of the squaring parametrization defined by equations (15) and (2) is that the number of real parameters, $D^2 - 1$, coincides with the dimension of the space of quantum states $\mathbb{M}$. If we considered all nonzero τ , one redundant parameter would emerge⁷. We also note that provided we agree to consider only τ with a nonzero trace, the particular

⁷ If we employed the formula $\rho = AA^\dagger/\text{tr}(AA^\dagger)$ with A being an arbitrary $D \times D$ matrix, as in [5], the number of real parameters would be $2D^2$, which is more than twice larger than in the squaring parametrization considered in the present article.

value of $\text{tr } \tau$ is unimportant, and we can fix any overall normalization of τ . In particular, we will find it convenient to use a normalization different from that defined in equation (15) in section 3.

Describing a convex set of a complex structure like the set of quantum states $\mathbb{M}$ to a large extent reduces to describing its boundary, $\partial\mathbb{M}$. As an immediate corollary of the squaring parametrization, we obtain an equation satisfied by the boundary points. Indeed, a point of the boundary is a critical point of the map $a(b)$; hence, the Jacobian of this map should be zero on the boundary:

$$\det \left\| \frac{\partial a_i}{\partial b_j} \right\| = 0. \quad (19)$$

Of course, some of the solutions of this equation can be inner points of $\mathbb{M}$. This equation is one of the main results of the paper. Its usefulness will be exemplified below.

3. Constrained sets of quantum states

3.1. General remarks

Often, one is interested in a set $\mathbb{M}'$ of quantum states which are invariant under a certain symmetry,

$$\mathbb{M}' = \{ \rho \in \mathbb{M} \mid \forall \varphi \ U_\varphi \rho U_\varphi^\dagger = \rho, \}, \quad (20)$$

where unitary operators U_φ parameterised by a discrete or continuous parameter φ constitute a symmetry group. One can straightforwardly generalize the squaring parametrization to the present case. Specifically, for any $\rho \in \mathbb{M}'$ there exists at least one $\tau \in \mathbb{H}$ with a unit trace and symmetric with respect to the group U_φ ,

$$U_\varphi \tau U_\varphi^\dagger = \tau \quad \forall \varphi, \quad (21)$$

such that ρ can be obtained from τ according to equation (2). This follows from the fact that any ρ which is invariant under a symmetry group can be expanded as

$$\rho = \sum_l \frac{\omega_l}{\text{rank } \Pi_l} \Pi_l, \quad (22)$$

where Π_l are projectors invariant under the same symmetry group,

$$U_\varphi \Pi_l U_\varphi^\dagger = \Pi_l \quad \forall \varphi, l, \quad (23)$$

and $\omega_l \geq 0$ are the eigenvalues of the density matrix (probabilities) and satisfy $\sum_l \omega_l = 1$. As a consequence, τ chosen as a normalized positive square root of ρ (in full analogy with the reasoning below equation (15) for the unconstrained case) will satisfy equation (2) and, in addition, equation (21).

It appears practical to expand τ and ρ upon Hermitian operators which are explicitly invariant under the symmetry group. The maximal number of linearly independent symmetric Hermitian operators determines the dimension of $\mathbb{M}'$. We do not attempt to give a general prescription how to choose this basis of symmetric operators, and do not provide a general formula for $\dim \mathbb{M}'$. Neither do we provide a general analysis of the multiplicity of the squaring parametrization in the constrained case. Instead, we exemplify the technique by considering below a number of illustrative examples, addressing the above issues in each particular case.

It should be noted that while $\mathbb{M}'$ is a convex set, its extreme points (defined as points which cannot be represented as a convex combination of other points of $\mathbb{M}'$) are not necessarily pure states. In fact, they are, in general, normalized projectors of rank not necessarily equal to one, as is clear from equation (22).

3.2. Sets of Werner states of qubits

A Werner or rotationally invariant state of N spins $1/2$ (or qubits⁸) is a quantum state invariant under any unitary transformation of the form $U^{\otimes N}$, where U is a unitary rotation in the space of a single spin [10, 11]. The space of Werner states is rather well studied for a moderate number of spins [10–13] or under the additional permutation symmetry [14]. We employ Werner states as a convenient playground to visualize the squaring parametrization and demonstrate its merits.

We find it convenient to expand Werner states in a basis which makes explicit their symmetry but is not normalized. The basic building blocks of this basis are scalar and triple products of 2×2 sigma matrices of different spins:

$$\begin{aligned} (\sigma_n \sigma_m) &\equiv \delta_{\alpha\beta} \sigma_n^\alpha \otimes \sigma_m^\beta = \sigma_n^\alpha \otimes \sigma_m^\alpha, \\ (\sigma_n \sigma_m \sigma_l) &\equiv \varepsilon_{\alpha\beta\gamma} \sigma_n^\alpha \otimes \sigma_m^\beta \otimes \sigma_l^\gamma, \end{aligned} \quad (24)$$

where $\varepsilon_{\alpha\beta\gamma}$ is an absolutely antisymmetric Levi-Civita tensor with $\varepsilon_{123} = 1$. Here and in what follows, subscript indices of the σ -matrices label qubits. The superscript indices α, β and γ denote the x, y, z components of the σ -matrices; they are always repeated which implies summation. In the remainder of the paper, including the appendix, we will omit the tensor product notation, and substitute the identity operator $\mathbb{1}$ of any dimension by 1. In the case of two or three spins considered below in detail the basis in $\mathbb{H}'$ consists of operators of the form (24) and the identity operator. For larger number of spins, the basis operators involve products of operators of the form (24), such as $(\sigma_1 \sigma_2)(\sigma_3 \sigma_4 \sigma_5)$. Some remarks regarding the case of arbitrary number of spins, as well as some explicit expressions for the pairwise products of the basis operators analogue to equation (9), can be found in appendix B.

3.2.1. Two qubits. We start from a very simple example of a rotationally invariant state of two qubits. This state is given by

$$\rho = \frac{1}{4} (1 + a \sigma_1 \sigma_2). \quad (25)$$

The range of the only free parameter a must ensure the positivity of ρ . To find this range, we introduce the auxiliary operator τ ,

$$\tau = 1 + b \sigma_1 \sigma_2 \quad (26)$$

with $b \in \mathbb{R}$, and plug it into equation (2). Observe that here, and in the reminder of the paper, we use an overall normalization of τ different from the normalization of equation (15), which makes the formulae somewhat less bulky. The map $a(b)$ is found from equation (2) with the use of equation (B.1), and reads

$$a = \frac{2b(1-b)}{1+3b^2}. \quad (27)$$

⁸ We use terms ‘spin $1/2$ ’ and ‘qubit’ interchangeably throughout the paper. The same is true for the terms ‘spin 1’ and ‘qutrit’.

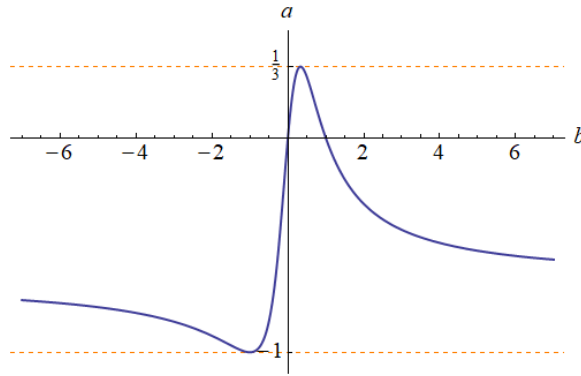


Figure 1. Squaring parametrization for the set of Werner states of two qubits, equation (25). Plotted is the map $a(b)$ given by equation (27). While the auxiliary parameter b runs from $-\infty$ to $+\infty$, the generalized Bloch parameter a automatically admits values only in the allowed range $[-1, \frac{1}{3}]$.

The latter rational function has a maximum of $\frac{1}{3}$ and a minimum of (-1) —see figure 1. Thus equation (25) defines a legitimate density matrix if and only if $a \in [-1, \frac{1}{3}]$.

Several observations related to the previous discussion are in order:

- The boundary $\partial\mathbb{M}' = \{-1, \frac{1}{3}\}$ of $\mathbb{M}' = [-1, \frac{1}{3}]$ satisfies equation (19), which in the present case reduces to $da/db = 0$.
- Each $a \in \mathbb{M}'$, except extreme points and the point $a = -2/3$, has two preimage points b .
- While one of the extreme points of $\mathbb{M}'$, $a = -1$, corresponds to the pure state, another one, $a = 1/3$, corresponds to the mixed state. This is in contrast to the unconstrained case, where all extreme points correspond to pure states. In fact, in the present case, two extreme points correspond to the states with a definite total spin (0 and 1, respectively).

The latter point deserves a special remark. One can see that for a constrained space of states, $\mathcal{M}'$, the condition $\rho^2 = \rho$, which have led, in particular, to equation (17) [8], does not necessarily determine all extreme points. Instead, some of the extreme points can be described by density matrices which are equal, up to a numerical factor, to a projector with the rank $r \geq 2$. This is equivalent to a condition

$$\rho^2 = r^{-1} \rho \quad (28)$$

with an unknown integer r , $1 \leq r < D$. This equation is sufficient to determine all extreme points in all specific cases considered in the present paper, as will be explicitly demonstrated. However, this is not the case for a general linear constraint. Furthermore, equation (28) can produce additional solutions which do not correspond to extreme points, as will be seen in the examples with three qubits, below. In the present case of two qubits, one obtains from equation (28) two extreme points,

$$\rho_0 = \frac{1}{4} (1 - \sigma_1 \sigma_2), \quad r = 1, \quad (29)$$

$$\rho_1 = \frac{1}{4} \left(1 + \frac{1}{3} \sigma_1 \sigma_2 \right), \quad r = 3, \quad (30)$$

in agreement with the analysis based on the squaring parametrization.

3.2.2. Translation-invariant Werner states of three qubits. A Werner (rotationally invariant) state of three qubits is given by

$$\rho = \frac{1}{8} (1 + a_{12} \sigma_1 \sigma_2 + a_{23} \sigma_2 \sigma_3 + a_{31} \sigma_3 \sigma_1 + a_{123} \sigma_1 \sigma_2 \sigma_3). \quad (31)$$

We would like to reduce the number of parameters from four to three or two for the purpose of visualization. To this end, we impose additional symmetries. In the present subsection, we require states to be translation invariant, which leads to a two-dimensionally constrained set of quantum states $\mathbb{M}'$. In the next subsection, we impose T -invariance and get a three-dimensional $\mathbb{M}'$.

A translational symmetry is a symmetry under cyclic permutations of qubits, $(1, 2, 3) \rightarrow (3, 1, 2) \rightarrow (2, 3, 1)$. Imposing this symmetry, we get a two-dimensional set of states of the form

$$\rho = \frac{1}{8} (1 + a_s (\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \sigma_3 \sigma_1) + a_t \sigma_1 \sigma_2 \sigma_3). \quad (32)$$

Introducing

$$\tau = 1 + b_s (\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \sigma_3 \sigma_1) + b_t \sigma_1 \sigma_2 \sigma_3, \quad (33)$$

we obtain from equation (2) with the use of equations (B.1)–(B.4), (B.7)

$$\begin{aligned} a_s &= 2 \frac{b_s - b_t^2}{1 + 9b_s^2 + 6b_t^2}, \\ a_t &= 2 \frac{b_t(1 - 3b_s)}{1 + 9b_s^2 + 6b_t^2}. \end{aligned} \quad (34)$$

These equations determine the shape of $\mathbb{M}'$, which is a triangle, as shown in figure 2. A direct way to see this is to find the boundary $\partial\mathbb{M}'$ from equation (19), which in the present case reads

$$\det \left\| \frac{\partial(a_s, a_t)}{\partial(b_s, b_t)} \right\| = 4 \frac{(1 + 3b_s)((1 - 3b_s)^2 - 12b_t^2)}{(1 + 9b_s^2 + 6b_t^2)^3} = 0. \quad (35)$$

The solutions of this equation determine three lines in the space of b variables:

$$\begin{aligned} b_s &= -\frac{1}{3}, \\ b_t &= \frac{1}{2\sqrt{3}}(1 - 3b_s), \\ b_t &= -\frac{1}{2\sqrt{3}}(1 - 3b_s). \end{aligned} \quad (36)$$

The map (34) converts these lines to three line segments,

$$\begin{aligned} a_s &= -\frac{1}{3}, & a_t &\in \left[-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right], \\ a_t &= \frac{1}{2\sqrt{3}}(1 - 3a_s), & a_s &\in \left[-\frac{1}{3}, \frac{1}{3}\right], \\ a_t &= -\frac{1}{2\sqrt{3}}(1 - 3a_s), & a_s &\in \left[-\frac{1}{3}, \frac{1}{3}\right], \end{aligned} \quad (37)$$

which form a triangle, as shown in figure 2.

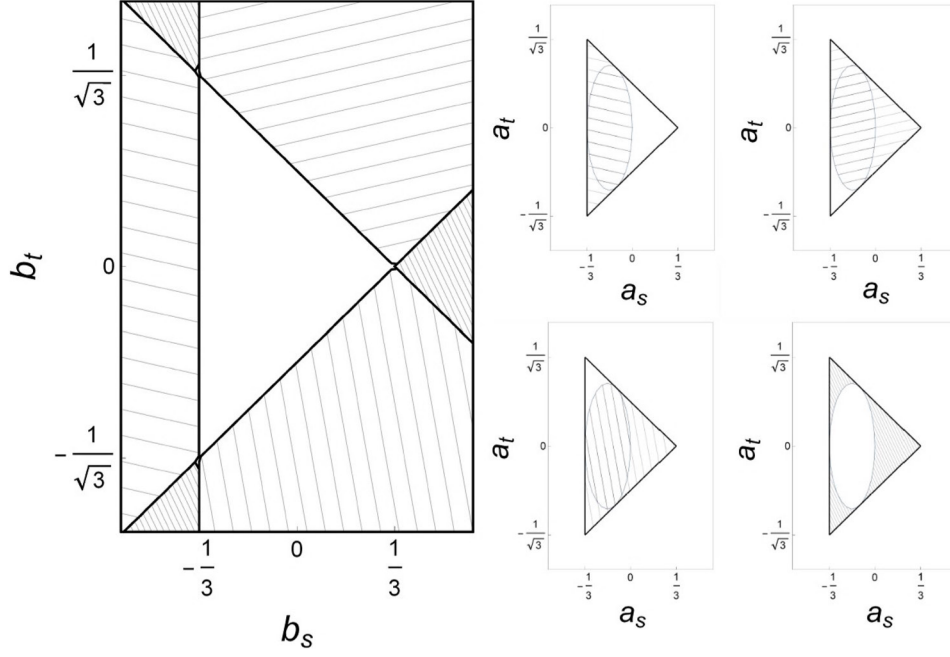


Figure 2. Squaring parametrization for the set $\mathbb{M}'$ of translation-invariant Werner states of three qubits, equation (32). The map $a(b)$ given by (34) is shown schematically: An area of a given hatching style in the (b_s, b_t) plane is mapped to the area of the same hatching style in the (a_s, a_t) plane. The set $\mathbb{M}'$ is represented by the triangle in the (a_s, a_t) plane. Points in this triangle have up to four preimage points in the (b_s, b_t) plane; thus, four sheets are required to visualize the map. The interior of the triangle is mapped onto itself. The ellipsoid inscribed in the triangle in the (a_s, a_t) plane is the limit of the image of a circle in the (b_s, b_t) plane with radius growing to infinity.

Figure 2 illustrates the map (34). A generic inner point of $\mathbb{M}'$ in the (a_s, a_t) plane has four preimage points in the (b_s, b_t) plane. The exception are the points of the ellipsoid inscribed in the triangle—each of these points has a single preimage point. The ellipsoid itself represents the limiting values of $a(b)$ for b growing to infinity (along fixed directions in the (b_s, b_t) plane). The extreme points of $\mathbb{M}'$ are the vertexes of the triangle. An alternative way to determine them is to use equation (28) as shown in appendix C. Remarkably, equations (37) replicate (36), up to the allowed range of variables.

3.2.3. *T*-invariant Werner states of three qubits. Now we turn to the case of Werner states of three qubits invariant under time reversal⁹. This transformation acts on products of sigma matrices as follow: $T(\sigma_i \sigma_k) = \sigma_i \sigma_k$ and $T(\sigma_1 \sigma_2 \sigma_3) = -\sigma_1 \sigma_2 \sigma_3$. Hence, the condition $T(\rho) = \rho$ with ρ given by equation (31) implies $a_{123} = 0$, and we obtain a three-dimensional set of states of the form

$$\rho = \frac{1}{8} (1 + a_{12} \sigma_1 \sigma_2 + a_{23} \sigma_2 \sigma_3 + a_{13} \sigma_1 \sigma_3). \quad (38)$$

⁹Time reversal is an antiunitary operation. A generalization of the definition (20) to the antiunitary case is straightforward.

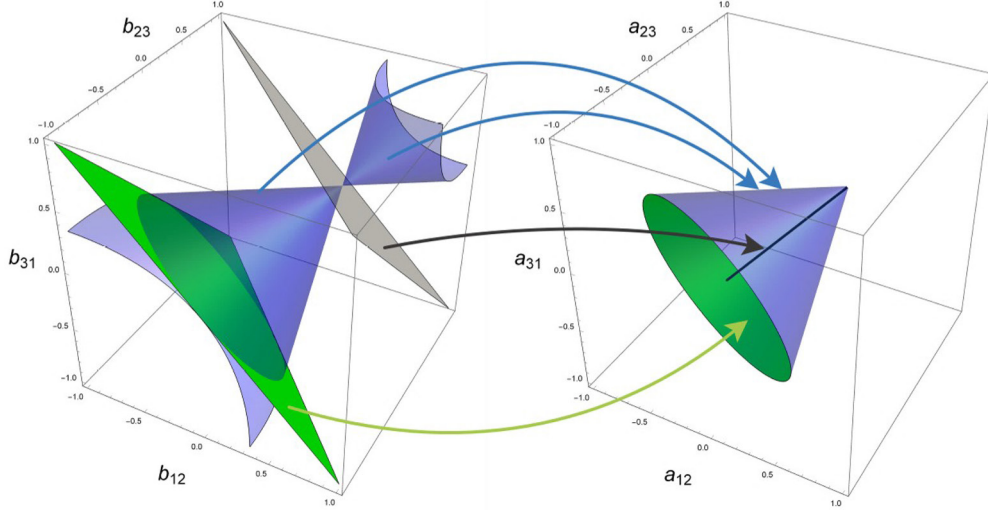


Figure 3. Squaring parametrization for the set of T -invariant Werner states of three qubits, equation (38). In the left panel, the solutions of the equation (19) for the boundary $\partial\mathbb{M}'$ are shown in the space of auxiliary parameters (b_{12}, b_{23}, b_{31}) . The same solutions in the space of generalized Bloch vectors (a_{12}, a_{23}, a_{31}) are shown in the right panel. The set $\mathbb{M}'$ is a truncated cone. Arrows illustrate the mapping (40) applied to solutions of equation (19).

Introducing

$$\tau = 1 + b_{12} \sigma_1 \sigma_2 + b_{23} \sigma_2 \sigma_3 + b_{13} \sigma_1 \sigma_3 \quad (39)$$

we get

$$a_{12} = 2 \frac{b_{12} - b_{12}^2 + b_{23}b_{13}}{1 + 3(b_{12}^2 + b_{23}^2 + b_{13}^2)}, \quad (40)$$

and analogous formulae for a_{23} and a_{13} .

The set $\mathbb{M}'$ determined by the map (40) is a truncated cone shown in figure 3. To see this let us determine the boundary $\partial\mathbb{M}'$ of the set. Equation (19) in the present case reads

$$\det \left\| \frac{\partial(a_{12}, a_{23}, a_{13})}{\partial(b_{12}, b_{23}, b_{13})} \right\| = 24 \frac{(A-1)(A+1)(B + \frac{2}{3}A - C - \frac{1}{3})}{(3B+1)^4} = 0, \quad (41)$$

where

$$A = b_{12} + b_{23} + b_{13}, \quad (42)$$

$$B = b_{12}^2 + b_{23}^2 + b_{13}^2, \quad (43)$$

$$C = 2(b_{12}b_{23} + b_{23}b_{13} + b_{13}b_{12}). \quad (44)$$

Solutions of equation (41) have the following form:

$$b_{12}^2 + b_{23}^2 + b_{13}^2 - 2(b_{12}b_{23} + b_{23}b_{13} + b_{13}b_{12}) + \frac{2}{3}(b_{12} + b_{23} + b_{13}) = \frac{1}{3}, \quad (45)$$

$$b_{12} + b_{13} + b_{23} = -1, \quad (46)$$

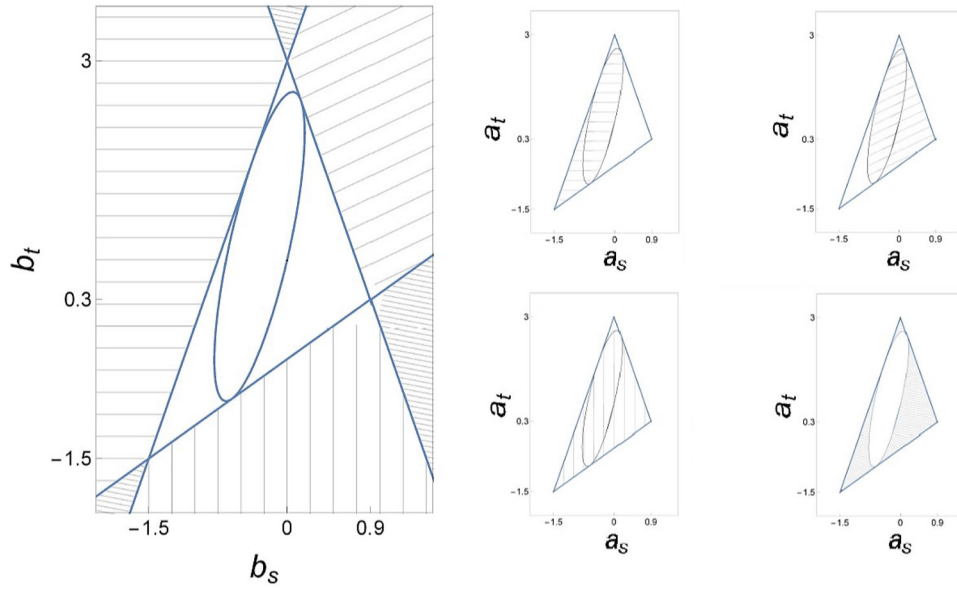


Figure 4. Squaring parametrization for the set $\mathbb{M}'$ of rotationally-invariant states of two qutrits, equation (50). The map $a(b)$ given by (51) is shown schematically by hatching in a way analogous to that in figure 2. The set $\mathbb{M}'$ is represented by the triangle in the (a_s, a_t) plane. Points in this triangle have up to four preimage points in the (b_s, b_t) plane; thus, four sheets are required to visualize the map. The interior of the triangle is mapped onto itself. The ellipsoid inscribed in the triangle in the (a_s, a_t) plane is the limit of the image of a circle in the (b_s, b_t) plane with radius growing to infinity.

$$b_{12} + b_{13} + b_{23} = 1. \quad (47)$$

Equation (45) describes a double cone with a vertex with co-ordinates $b_{12} = b_{13} = b_{23} = \frac{1}{3}$, while equations (46) and (47)—two parallel planes. The map (40) converts the double cone to a truncated cone, the first plane to the base of this truncated cone, and the second plane to the altitude of this cone, as shown in figure 3. In contrast to the previously considered cases, some of the solutions of equation (19) (specifically, those given by equation (47)) correspond to inner points of $\mathcal{M}'$.

$\mathbb{M}'$ has extreme points of two types, the tip of the cone and the directrix (the circle in the base of the cone). It is worth noting that in contrast to the previously considered cases, extreme points of the second type form a continuous set. Finding extreme points of $\mathcal{M}'$ with the help of equation (28) is described in appendix D.

3.3. Rotationally invariant states of two qutrits

In this section we consider a set of states of two spins one, or qutrits, which are invariant under global rotations of the basis. A unitary operator of rotations of a single spin one is given by

$$U_\varphi = e^{i\varphi S}, \quad (48)$$

where S is the operator of spin, and the direction and the magnitude of the vector φ correspond to the axis and angle of rotation, respectively. The rotational invariance of two qutrits is the invariance with respect to $U_\varphi \otimes U_\varphi$ for any φ . Note that, in contrast to the qubit case, the

rotational invariance is not equivalent to the Werner invariance, since U_φ does not exhaust all possible unitary transformations in the space of a qutrit.

A rotationally invariant density matrix of two qutrits is a linear combination of the identity operator and traceless operators $(\mathbf{S}_1\mathbf{S}_2)$ and $(\mathbf{S}_1\mathbf{S}_2)^2 - 4/3$. These three operators are linearly independent, and constitute a basis for $(\mathbf{S}_1\mathbf{S}_2)^3$ and higher powers of the scalar product $(\mathbf{S}_1\mathbf{S}_2)$. Thus, we expand

$$\tau = 1 + b_s(\mathbf{S}_1\mathbf{S}_2) + b_t \left((\mathbf{S}_1\mathbf{S}_2)^2 - \frac{4}{3} \right), \quad (49)$$

$$\rho = \frac{1}{9} \left(1 + a_s(\mathbf{S}_1\mathbf{S}_2) + a_t \left((\mathbf{S}_1\mathbf{S}_2)^2 - \frac{4}{3} \right) \right), \quad (50)$$

and the map (2) reads

$$a_s = 6 \frac{3b_s - b_s b_t}{12b_s^2 + 8b_t^2 - 12b_s b_t + 9}, \quad a_t = 3 \frac{3b_s^2 + 7b_t^2 - 12b_s b_t + 6b_t}{12b_s^2 + 8b_t^2 - 12b_s b_t + 9}. \quad (51)$$

The set $\mathbb{M}'$ determined by the map (51) is a triangle shown in figure 4. This can be revealed by an analysis completely analogous to that in the previous cases. Equation (16) leads to the equation for the boundary,

$$\left\| \frac{\partial(a_s, a_t)}{\partial(b_s, b_t)} \right\| = 108 \frac{(6b_s - 3 - 8b_t)(3b_s + 3 - b_t)(3b_s - 3 + b_t)}{(12b_s^2 - 12b_s b_t + 8b_t^2 + 9)^3} = 0, \quad (52)$$

with the solutions

$$b_t = \frac{3}{4}b_s - \frac{3}{8}, \quad (53)$$

$$b_t = 3 + 3b_s, \quad (54)$$

$$b_t = 3 - 3b_s, \quad (55)$$

$$a_t = \frac{3}{4}a_s - \frac{3}{8}, \quad a_s \in [-1.5, 0.9], \quad (56)$$

$$a_t = 3 + 3a_s, \quad a_s \in [-1.5, 0], \quad (57)$$

$$a_t = 3 - 3a_s, \quad a_s \in [0, 0.9]. \quad (58)$$

The latter three equations describe the sides of the triangle. The analysis of multiplicities of the map and its limiting values for b growing to infinity leads to results analogous to the case considered in section 3.2.2—see figure 4. Finding extreme points of $\mathcal{M}'$ with the help of equation (28) is described in appendix E.

4. Summary and outlook

To summarize, the squaring parametrization is a surjective nonlinear map from $\mathbb{R}^{D^2-1}$ to a set $\mathbb{M}$ of (in general, mixed) quantum states. This map is explicitly given by equation (16) which maps each point of $\mathbb{R}^{D^2-1}$ to a legitimate Bloch vector. The squaring parametrization has several attractive features. First, it automatically accounts for the positivity of a density operator and, at the same time, is able to explicitly preserve a tensor product structure of a many-body system. Second, it produces as a byproduct an equation for the boundary of $\mathbb{M}$

—see equation (19). Finally, the squaring parametrization can be adapted to describe sets of quantum states invariant under a symmetry group.

We believe that the squaring parametrization can be useful in a wide range of problems where a quantum density matrix of a sufficiently large dimension plays a role. In particular, we plan to incorporate it in a variational technique which is based on variation of a reduced density matrix (instead of a many-body wave function) and bounds the ground state energy from below (not from above) [15].

Acknowledgments

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Appendix A. Multiplicities of the squaring map in the unconstrained case

A density matrix ρ can be expanded as

$$\rho = \sum_{l=1}^D \omega_l \Pi_l. \quad (\text{A.1})$$

Here Π_l are projectors of rank 1 and $\omega_l \geq 0$ are the eigenvalues of ρ (i.e. probabilities),

$$\sum_{l=1}^D \omega_l = 1. \quad (\text{A.2})$$

If one considers the squaring map (2) as an equation with τ being unknown, all its solutions are given by

$$\tau = C \sum_{l=1}^D \eta_l \sqrt{\omega_l} \Pi_l, \quad (\text{A.3})$$

where C is a nonzero arbitrary constant and the set of $\eta_l \in \{-1, 1\}$ is such that

$$\sum_{l=1}^D \eta_l \sqrt{\omega_l} \neq 0. \quad (\text{A.4})$$

Clearly, the latter inequality is true for a generic point of $\mathbb{M}$. If we exclude from our consideration those rare points of $\mathbb{M}$ which do not satisfy equation (A.4) for some set of η_l , we can compute the multiplicity (i.e. the number of preimage points) of the squaring parametrization as defined by equations (2) and (15) in the following way. The number of nonzero ω_l is $\text{rank } \rho$. There are $2^{\text{rank } \rho}$ different combinations of $\eta_l \sqrt{\omega_l}$. These combinations can be partitioned in pairs, two members of each pair being different by an overall sign. This difference, as well as the freedom in choosing C , will disappear when τ is normalized according to equation (15). Thus the multiplicity of the map in a generic point is $2^{\text{rank } \rho - 1}$.

Appendix B. Rotationally invariant operators in the space of qubits

In order to use the squaring parametrization for Werner states of qubits one needs to be able to convolute products of scalar and triple products of sigma matrices. Here we give for reference a list of such convolutions involving at most five qubits:

$$(\sigma_1 \sigma_2)^2 = 3 - 2(\sigma_1 \sigma_2) \quad (\text{B.1})$$

$$(\sigma_1 \sigma_2)(\sigma_2 \sigma_3) = -i(\sigma_1 \sigma_2 \sigma_3) + (\sigma_1 \sigma_3) \quad (\text{B.2})$$

$$(\sigma_1 \sigma_2)(\sigma_1 \sigma_2 \sigma_3) = -(\sigma_1 \sigma_2 \sigma_3) - 2i(\sigma_1 \sigma_3) + 2i(\sigma_2 \sigma_3) \quad (\text{B.3})$$

$$(\sigma_1 \sigma_2 \sigma_3)(\sigma_1 \sigma_2) = -(\sigma_1 \sigma_2 \sigma_3) + 2i(\sigma_1 \sigma_3) - 2i(\sigma_2 \sigma_3) \quad (\text{B.4})$$

$$(\sigma_1 \sigma_2)(\sigma_2 \sigma_3 \sigma_4) = (\sigma_1 \sigma_3 \sigma_4) - i(\sigma_1 \sigma_3)(\sigma_2 \sigma_4) + i(\sigma_1 \sigma_4)(\sigma_2 \sigma_3) \quad (\text{B.5})$$

$$(\sigma_2 \sigma_3 \sigma_4)(\sigma_1 \sigma_2) = (\sigma_1 \sigma_3 \sigma_4) + i(\sigma_1 \sigma_3)(\sigma_2 \sigma_4) - i(\sigma_1 \sigma_4)(\sigma_2 \sigma_3) \quad (\text{B.6})$$

$$(\sigma_1 \sigma_2 \sigma_3)^2 = 6 - 2(\sigma_1 \sigma_2) - 2(\sigma_1 \sigma_3) - 2(\sigma_2 \sigma_3) \quad (\text{B.7})$$

$$\begin{aligned} (\sigma_1 \sigma_2 \sigma_3)(\sigma_1 \sigma_2 \sigma_4) = & +i(\sigma_1 \sigma_3 \sigma_4) + i(\sigma_2 \sigma_3 \sigma_4) \\ & - (\sigma_1 \sigma_3)(\sigma_2 \sigma_4) - (\sigma_1 \sigma_4)(\sigma_2 \sigma_3) + 2(\sigma_3 \sigma_4) \end{aligned} \quad (\text{B.8})$$

$$\begin{aligned} (\sigma_1 \sigma_2 \sigma_3)(\sigma_1 \sigma_4 \sigma_5) = & -i(\sigma_1 \sigma_2)(\sigma_3 \sigma_4 \sigma_5) + i(\sigma_1 \sigma_3)(\sigma_2 \sigma_4 \sigma_5) \\ & + (\sigma_2 \sigma_4)(\sigma_3 \sigma_5) - (\sigma_2 \sigma_5)(\sigma_3 \sigma_4) \end{aligned} \quad (\text{B.9})$$

$$\begin{aligned} (\sigma_1 \sigma_2)(\sigma_2 \sigma_3)(\sigma_3 \sigma_4) = & -i(\sigma_1 \sigma_2 \sigma_4) - i(\sigma_1 \sigma_3 \sigma_4) + (\sigma_1 \sigma_4) \\ & + (\sigma_1 \sigma_4)(\sigma_2 \sigma_3) - (\sigma_1 \sigma_3)(\sigma_2 \sigma_4) \end{aligned} \quad (\text{B.10})$$

$$\begin{aligned} (\sigma_1 \sigma_2)(\sigma_3 \sigma_4)(\sigma_1 \sigma_3)(\sigma_2 \sigma_4) = & 3 + i(\sigma_1 \sigma_2 \sigma_3) - i(\sigma_1 \sigma_2 \sigma_4) + i(\sigma_1 \sigma_3 \sigma_4) - i(\sigma_2 \sigma_3 \sigma_4) \\ & - 2(\sigma_1 \sigma_2) - 2(\sigma_1 \sigma_3) + 2(\sigma_1 \sigma_4) \\ & + 2(\sigma_2 \sigma_3) - 2(\sigma_2 \sigma_4) - 2(\sigma_3 \sigma_4) \\ & + (\sigma_1 \sigma_2)(\sigma_3 \sigma_4) + (\sigma_1 \sigma_3)(\sigma_2 \sigma_4). \end{aligned} \quad (\text{B.11})$$

It should be noted that the first nine of these equalities suffice to evaluate all other combinations of scalar and triple products—in particular, equations (B.10) and (B.11)—iteratively without exploiting the properties of σ -matrices. This can be used when implementing the manipulations with scalar and mixed products of a large number of qubits in computer algebra systems.

Also observe that equation (B.11) implies that operators $(\sigma_1 \sigma_2)(\sigma_3 \sigma_4)$ and $(\sigma_1 \sigma_3)(\sigma_2 \sigma_4)$ are not orthogonal with respect to the scalar product (3). This implies that in the case of the number of qubits being higher than three one has either to employ an additional orthogonalization procedure or cope with a nonorthogonal basis.

Appendix C. Translation invariant Werner states of three qubits

Here we solve equation (28) and this way find the extreme points of the set $\mathcal{M}'$ of the states of the form (32). We choose to work with projectors Π which are related to the solutions of equation (28) as $\Pi = r\rho$ and, obviously, satisfy the equation

$$\Pi^2 = \Pi. \quad (\text{C.1})$$

We further introduce $c \equiv r/D$. Substituting

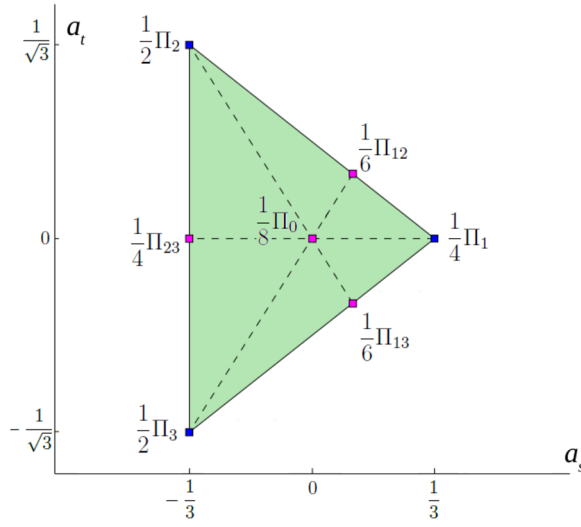


Figure C1. Set $\mathcal{M}'$ of the translation-invariant Werner states of three qubits, equation (32), with projectors determined from equation (28). A projector is turned into a density matrix by normalizing it by the numerical factor $1/r$, where r is the rank of the projector. Three of the solutions correspond to the extreme points of $\mathcal{M}'$ (vertices of the triangle), others can be obtained as equally weighted linear combinations of two or three ‘extreme’ solutions.

$$\Pi = c(1 + a_s(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1) + a_t\sigma_1\sigma_2\sigma_3), \quad (\text{C.2})$$

into equation (C.1) and using equations (B.1)–(B.3) one obtains

$$c = (1 + 9a_s^2 + 6a_t^2)^{-1}, \quad (\text{C.3})$$

$$a_s = 2c(a_s - a_t^2), \quad (\text{C.4})$$

$$a_t = 2ca_t(1 - 3a_s). \quad (\text{C.5})$$

The solutions of this system of equations correspond to seven projectors:

$$\Pi_0 = 1 \quad (\text{C.6})$$

$$\Pi_1 = \frac{1}{2} \left(1 + \frac{1}{3}(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1) \right), \quad (\text{C.7})$$

$$\Pi_2 = \frac{1}{4} \left(1 - \frac{1}{3}(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1) + \frac{1}{\sqrt{3}}\sigma_1\sigma_2\sigma_3 \right), \quad (\text{C.8})$$

$$\Pi_3 = \frac{1}{4} \left(1 - \frac{1}{3}(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1) - \frac{1}{\sqrt{3}}\sigma_1\sigma_2\sigma_3 \right), \quad (\text{C.9})$$

$$\Pi_{12} = \frac{3}{4} \left(1 + \frac{1}{9}(\sigma_1\sigma_2 + \sigma_2\sigma_3 + \sigma_3\sigma_1) + \frac{1}{3\sqrt{3}}\sigma_1\sigma_2\sigma_3 \right), \quad (\text{C.10})$$

$$\Pi_{23} = \frac{1}{2} \left(1 - \frac{1}{3} (\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \sigma_3 \sigma_1) \right), \quad (\text{C.11})$$

$$\Pi_{13} = \frac{3}{4} \left(1 + \frac{1}{9} (\sigma_1 \sigma_2 + \sigma_2 \sigma_3 + \sigma_3 \sigma_1) - \frac{1}{3\sqrt{3}} \sigma_1 \sigma_2 \sigma_3 \right). \quad (\text{C.12})$$

The extreme points of $\mathcal{M}'$ are given by $\Pi_1/4$, $\Pi_2/2$ and $\Pi_3/2$. All other projectors can be represented as equally weighted linear combinations of two or three of these ‘extreme’ projectors, e.g. $\Pi_{23} = \Pi_1 + \Pi_2$. Density matrices obtained from projectors (C.6)–(C.12) are shown in figure C1.

Appendix D. T -invariant Werner states of three qubits

Here we repeat the procedure described in appendix C for the states of the form (38). We consider a projector of the form

$$\Pi = c (1 + a_{12} \sigma_1 \sigma_2 + a_{23} \sigma_2 \sigma_3 + a_{31} \sigma_3 \sigma_1) \quad (\text{D.1})$$

and plug it to equation (C.1). Using equations (B.1) and (B.2) we obtain equations

$$c = \frac{1}{1 + 3(a_{12}^2 + a_{23}^2 + a_{31}^2)}, \quad (\text{D.2})$$

$$a_{12} = 2 \frac{a_{12} - a_{12}^2 + a_{23}a_{31}}{1 + 3(a_{12}^2 + a_{23}^2 + a_{31}^2)} \quad (\text{D.3})$$

and two more equations which can be obtained from equation (D.3) by cyclic permutation of indices in a_{ij} . The solutions of these equations correspond to the following projectors:

$$\Pi_0 = 1, \quad (\text{D.4})$$

$$\Pi_1 = \frac{1}{2} \left(1 + \frac{1}{3} \sigma_1 \sigma_2 + \frac{1}{3} \sigma_2 \sigma_3 + \frac{1}{3} \sigma_3 \sigma_1 \right), \quad (\text{D.5})$$

$$\Pi_2 = \frac{1}{2} \left(1 - \frac{1}{3} \sigma_1 \sigma_2 - \frac{1}{3} \sigma_2 \sigma_3 - \frac{1}{3} \sigma_3 \sigma_1 \right), \quad (\text{D.6})$$

$$\begin{aligned} \Pi_{3\pm} &= \frac{1}{4} \left(1 + a_{12} \sigma_1 \sigma_2 - \frac{a_{12} \mp k_{12} + 1}{2} \sigma_1 \sigma_3 - \frac{a_{12} \pm k_{12} + 1}{2} \sigma_2 \sigma_3 \right), \\ k_{12} &\equiv \sqrt{-3a_{12}^2 - 2a_{12} + 1}, \quad a_{12} \in [-1, \frac{1}{3}], \end{aligned} \quad (\text{D.7})$$

$$\begin{aligned} \Pi_{4\pm} &= \frac{3}{4} \left(1 + a_{12} \sigma_1 \sigma_2 + \frac{-3a_{12} \mp l_{12} + 1}{6} \sigma_1 \sigma_3 + \frac{-3a_{12} \pm l_{12} + 1}{6} \sigma_2 \sigma_3 \right), \\ l_{12} &\equiv \sqrt{-27a_{12}^2 + 6a_{12} + 1}, \quad a_{12} \in [-\frac{1}{9}, \frac{1}{3}]. \end{aligned} \quad (\text{D.8})$$

Note that $\Pi_{3\pm}$ and $\Pi_{4\pm}$ are one-parametric families of projectors parametrized by a_{12} .

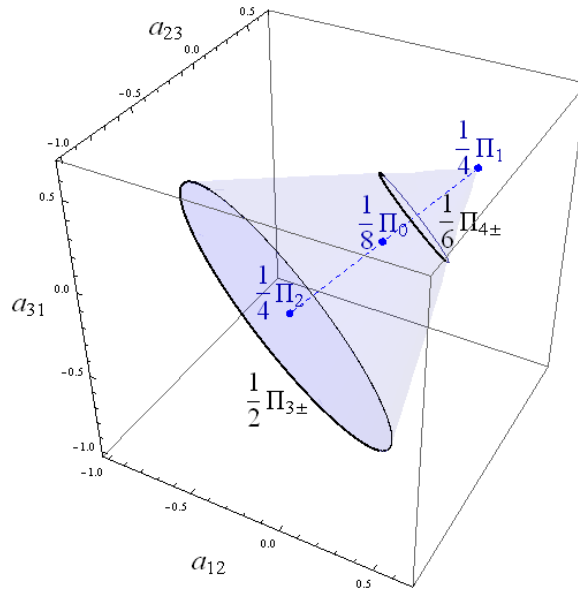


Figure D1. Solutions of equation (28) in the case of T -invariant Werner states of three qubits, equation (38). A projector is turned into a density matrix by normalizing it by the numerical factor $1/r$, where r is the rank of the projector. $\frac{1}{4}\Pi_1$ and $\frac{1}{2}\Pi_{3\pm}$ correspond to extreme points of $\mathcal{M}'$ (vortex and directrix, respectively).

Extreme points of $\mathcal{M}'$ are given by $\Pi_1/4$ (vertex) and $\Pi_{3\pm}/2$ (directrix). Density matrices obtained from projectors (D.4)–(D.8) are shown in figure D1.

Appendix E. States of two qutrits invariant under rotations

Here, we solve equation (28) and in this way find the extreme points of the set $\mathcal{M}'$ of the states of the form (50). This is done in complete analogy with appendix C. The results are illustrated in figure E1. The projectors read

$$\Pi_0 = 1 \quad (\text{E.1})$$

$$\Pi_1 = \frac{2}{3} \left(1 + \frac{3}{4}(\mathbf{S}_1 \mathbf{S}_2) + \frac{3}{4} \left((\mathbf{S}_1 \mathbf{S}_2)^2 - \frac{4}{3} \right) \right) \quad (\text{E.2})$$

$$\Pi_2 = \frac{8}{9} \left(1 - \frac{3}{8} \left((\mathbf{S}_1 \mathbf{S}_2)^2 - \frac{4}{3} \right) \right) \quad (\text{E.3})$$

$$\Pi_3 = \frac{4}{9} \left(1 - \frac{9}{8}(\mathbf{S}_1 \mathbf{S}_2) - \frac{3}{8} \left((\mathbf{S}_1 \mathbf{S}_2)^2 - \frac{4}{3} \right) \right) \quad (\text{E.4})$$

$$\Pi_4 = \frac{5}{9} \left(1 + \frac{9}{10}(\mathbf{S}_1 \mathbf{S}_2) + \frac{3}{10} \left((\mathbf{S}_1 \mathbf{S}_2)^2 - \frac{4}{3} \right) \right) \quad (\text{E.5})$$

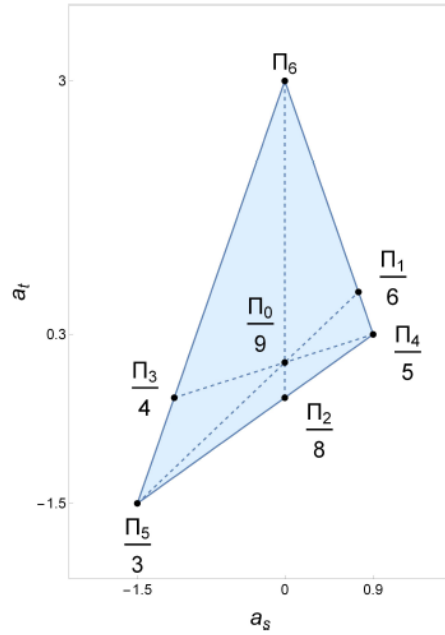


Figure E1. Set $\mathcal{M}'$ of the rotationally-invariant states of two qutrits, equation (50), with projectors determined from equation (28) (see caption to figure C1 for further details).

$$\Pi_5 = \frac{1}{3} \left(1 - \frac{3}{2}(\mathcal{S}_1 \mathcal{S}_2) - \frac{3}{2} \left((\mathcal{S}_1 \mathcal{S}_2)^2 - \frac{4}{3} \right) \right) \quad (\text{E.6})$$

$$\Pi_6 = \frac{1}{9} \left(1 + 3 \left((\mathcal{S}_1 \mathcal{S}_2)^2 - \frac{4}{3} \right) \right). \quad (\text{E.7})$$

The extreme points of $\mathcal{M}'$ are given by $\Pi_4/5$, $\Pi_5/3$ and Π_6 .

ORCID iDs

O Lychkovskiy  <https://orcid.org/0000-0003-1470-2399>

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