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The classification of three-parameter density matrices for a qutrit

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Abstract
The properties and structure of the eight-dimensional parameter space of three-state density matrices are examined using the $SU(3)$ generator expansion. Three-dimensional cross sections of the space of generalized Bloch vectors are determined by the Monte Carlo sampling method and an appropriate classification of 56 different three-parameter density matrices into ten types, according to the shape of the corresponding region of allowed values of three relevant parameters, is introduced. Positions of the representative points corresponding to the pure states are determined for all ten types.

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1. Introduction

With the quantum mechanical N-state system is associated an N-dimensional Hilbert space $\mathcal{H}_N$ [1]. Quantum observables are self-adjoint operators in Banach space $\mathcal{B}$ and can be represented by corresponding $N \times N$ Hermitian matrices. Density matrices, $\hat{\rho}$, for such a system are a subset of $\mathcal{B}$ possessing three fundamental properties: (i) Hermiticity, $\hat{\rho} = \hat{\rho}^\dagger$, (ii) normalization, $\mathrm{Tr}(\hat{\rho}) = 1$ and (iii) positivity, $\lambda_i \geqslant 0$ (here $\lambda_i, i = 1, 2, \ldots, N$, denote eigenvalues of the density matrix). Except for the case of a two-state system (a qubit), not much is known about the structure of the set $\mathcal{B}$. A deeper understanding of properties of this set is of interest in quantum mechanics and in quantum information science [2]. The set $\mathcal{B}$ is convex $\hat{\rho} = p\hat{\rho}' + (1-p)\hat{\rho}''$, for $0 \leqslant p \leqslant 1$, and density matrices satisfy inequalities $1/N^{k-1} \leqslant \mathrm{Tr}(\hat{\rho}^k) \leqslant 1$, for $\geqslant 2$.

The $SU(N)$ generators, $\hat{\mathbf{\Lambda}} \equiv (\hat{\Lambda}_1, \hat{\Lambda}_2, \ldots, \hat{\Lambda}_{N^2-1})$, can be used to expand an arbitrary $N \times N$ density matrix [3, 4]:

$$\hat{\rho} = \frac{1}{N}\left(\hat{1}_N + \sqrt{\frac{N(N-1)}{2}}\mathbf{b}\cdot\hat{\mathbf{\Lambda}}\right). \tag{1}$$

Here, $\hat{1}_N$ denotes the $N \times N$ unit matrix. The $SU(N)$ generators are Hermitian, $\hat{\Lambda}_k = \hat{\Lambda}_k^\dagger$, traceless , $\mathrm{Tr}(\hat{\Lambda}_k) = 0$ and orthogonal, $\mathrm{Tr}(\hat{\Lambda}_k \hat{\Lambda}_{k'}) = 2\delta_{kk'}$. The generators correspond to the Pauli and Gell-Mann matrices in the case of the two-state and three-state systems, respectively. Construction methods of $N \times N$ matrices $\hat{\Lambda}_k$ are known [5]. The expansion coefficients form the generalized Bloch vector consisting of $N^2 - 1$ real parameters, $\mathbf{b} \equiv (b_1, b_2, \ldots, b_{N^2-1})$, so that in (1)

$$\mathbf{b} \cdot \hat{\mathbf{\Lambda}} = \sum_{k=1}^{N^2-1} b_k \hat{\Lambda}_k.$$

There is a one-to-one correspondence between density matrices and *allowed* generalized Bloch vectors. The requirement $\mathrm{Tr}(\hat{\rho}^2) \leqslant 1$ leads to the conclusion that generalized Bloch vectors lie within a hyperball of unit radius

$$\mathbf{b} \cdot \mathbf{b} \leqslant 1. \tag{2}$$

Only in the case of the two-state system, $N = 2$, one finds a one-to-one correspondence between *all* two-dimensional density matrices, $\hat{\rho} = \frac{1}{2}(\hat{1}_2 + \mathbf{b} \cdot \hat{\mathbf{\Lambda}})$, and the set of three-dimensional real vectors (Bloch vectors), $\mathbf{b} = (b_1, b_2, b_3)$, that coincides with the *entire* Bloch ball, $\mathbf{b} \cdot \mathbf{b} \leqslant 1$. In this case $\hat{\mathbf{\Lambda}}$ denotes the vector of three 2×2 Pauli matrices. The boundary of the Bloch ball, the Bloch sphere $|\mathbf{b}| = 1$, corresponds to the pure states. On the other hand, the origin, $\mathbf{b} = 0$, corresponds to a completely random mixed state. Only in the case of qubit, the conditions $\mathrm{Tr}(\hat{\rho}^2) \leqslant 1$ and (iii) are equivalent. Since the states of all two-level systems can be mapped onto the states of a particle with spin $\frac{1}{2}$, physically the vector $\mathbf{b}$ is the spin polarization vector, related to the average spin via $\langle \hat{\mathbf{S}} \rangle = \mathrm{Tr}(\hat{\rho}\hat{\mathbf{S}}) = \frac{\hbar}{2}\mathbf{b}$.

Generally, *not* all vectors within the hyperball (2) correspond to the allowed density matrices [2]; certain vectors produce from (1) non-positive matrices. For $N \geqslant 3$, the positivity condition (iii) is not equivalent to the requirement $\mathrm{Tr}(\hat{\rho}^2) \leqslant 1$, since the former imposes certain additional restrictions on the Bloch vector [6]. Consequently, there is a one-to-one correspondence between the possible density matrices of the N-state system, with $N \geqslant 3$, and points that constitute a proper *subset* of the hyperball (2). Equation (1) shows that, with $\hat{\rho} \to \hat{\rho}(\mathbf{b})$, $\hat{\rho}' \to \hat{\rho}(\mathbf{b}')$ and $\hat{\rho}'' \to \hat{\rho}(\mathbf{b}'')$, the convex set of density matrices maps into a convex set of points $\mathbf{b} = p\mathbf{b}' + (1 - p)\mathbf{b}''$ in the parameter space, i.e. that all points on a line connecting two points in the set, $\mathbf{b}'$ and $\mathbf{b}''$, belong to the set.

In this paper, in section 2, we investigate in some detail the nontrivial geometry of the eight-dimensional parameter space of allowed density matrices in the case of a three-state system (a qutrit). Ability to describe, generate and control various qutrit states is of interest in the emerging field of quantum information technology (e.g. new quantum key distribution protocols [7–9], eavesdropping analysis [10, 11]) and, more significantly, in the field of quantum mechanics for fundamental tests [12]. Cloning [13] and experimental realization of entangled qutrits [14] are of importance for such applications. Here, in subsection 2.1, the qutrit 3×3 density matrix is parametrized using the $SU(3)$ generators. Also the case of pure states is described briefly. In subsections 2.2 and 2.3 we examine one-, two- and three-dimensional cross sections of the space of generalized Bloch vectors. These have, it turns out, intricate and complex structure. Appropriate classification of 28 different two-parameter density matrices into four types, according to the shape of the corresponding region of allowed parameter values, is summarized. Then, the more involved case of three-parameter density matrices is examined in some detail using the Monte Carlo sampling method and the analogous classification into ten types of 56 different combinations of three nonzero parameters is introduced. This classification is relevant for purposes of determining the suitability for various quantum information processing tasks. Summary and conclusions are offered in section 3.

2. Qutrit

2.1. The density matrix

The case of a three-state system is more involved than the $N = 2$ case. Using the $SU(3)$ generators to expand the corresponding 3×3 density matrix one obtains [4, 15]

$$\begin{aligned}\hat{\rho} &= \begin{pmatrix} \frac{1}{3} + a_3 + \frac{a_8}{\sqrt{3}} & a_1 - \mathrm{i}a_2 & a_4 - \mathrm{i}a_5 \\ a_1 + \mathrm{i}a_2 & \frac{1}{3} - a_3 + \frac{a_8}{\sqrt{3}} & a_6 - \mathrm{i}a_7 \\ a_4 + \mathrm{i}a_5 & a_6 + \mathrm{i}a_7 & \frac{1}{3} - \frac{2a_8}{\sqrt{3}} \end{pmatrix}. \\ &\equiv \frac{1}{3}(\hat{1}_3 + \sqrt{3}\mathbf{b} \cdot \hat{\mathbf{\Lambda}}). \end{aligned} \tag{3}$$

Clearly, this matrix is Hermitian and normalized. Here the generalized Bloch vector is related to the eight real parameters $\mathbf{a} \equiv (a_1, a_2, \ldots, a_8)$ via $\mathbf{b} \equiv \sqrt{3}\mathbf{a}$, and $\mathbf{\Lambda} \equiv (\Lambda_1, \Lambda_2, \ldots, \Lambda_8)$ denote the 3×3 Gell-Mann matrices [16]. Generally, for a mixed state, the eight parameters are independent. Their values are however constrained by following inequalities:

$$\begin{aligned} &0 \leqslant \frac{1}{3} \pm a_3 + \frac{a_8}{\sqrt{3}} \leqslant 1, \\ &0 \leqslant \frac{1}{3} - \frac{2a_8}{\sqrt{3}} \leqslant 1, \\ &\mathbf{a} \cdot \mathbf{a} \leqslant \frac{1}{3}, \\ &0 \leqslant \det(\hat{\rho}). \end{aligned} \tag{4}$$

The first two inequalities follow from the requirement that every diagonal element of $\hat{\rho}$, in any matrix representation, must be non-negative [17], and they are in fact special cases of the latter two inequalities [3, 4]. The third inequality is the same as (2), while the importance of the last inequality, for ensuring positivity of the density matrix (3), has been recently emphasized in [6].

The eight real quantities, $\mathbf{a}$, of the three-state density matrix (3) are directly observable parameters being related to the average values of physical quantities, for example, $\hat{S}_x, \hat{S}_y, \hat{S}_z, \hat{S}_x^2, \hat{S}_y^2, \{\hat{S}_x, \hat{S}_y\}, \{\hat{S}_y, \hat{S}_z\}$ and $\{\hat{S}_z, \hat{S}_x\}$, in the case of spin 1 particle. Here $\hat{\mathbf{S}} = (\hat{S}_x, \hat{S}_y, \hat{S}_z)$ indicates the corresponding spin operator, while $\{\hat{S}_i, \hat{S}_j\}$ denotes the anticommutator $\hat{S}_i\hat{S}_j + \hat{S}_j\hat{S}_i$, $(i, j = x, y, z)$. One has

$$\begin{aligned} a_1 &= \frac{\hbar\langle\hat{S}_x\rangle + \langle\{\hat{S}_z, \hat{S}_x\}\rangle}{2\sqrt{2}\hbar^2}, & a_2 &= \frac{\hbar\langle\hat{S}_y\rangle + \langle\{\hat{S}_y, \hat{S}_z\}\rangle}{2\sqrt{2}\hbar^2}, \\ a_3 &= 1 + \frac{\hbar\langle\hat{S}_z\rangle - 3\langle\hat{S}_x^2\rangle - 3\langle\hat{S}_y^2\rangle}{4\hbar^2}, & a_4 &= \frac{\langle\hat{S}_x^2\rangle - \langle\hat{S}_y^2\rangle}{2\hbar^2}, \\ a_5 &= \frac{\langle\{\hat{S}_x, \hat{S}_y\}\rangle}{2\hbar^2}, & a_6 &= \frac{\hbar\langle\hat{S}_x\rangle - \langle\{\hat{S}_z, \hat{S}_x\}\rangle}{2\sqrt{2}\hbar^2}, \\ a_7 &= \frac{\hbar\langle\hat{S}_y\rangle - \langle\{\hat{S}_y, \hat{S}_z\}\rangle}{2\sqrt{2}\hbar^2}, & \frac{a_8}{\sqrt{3}} &= \frac{\hbar\langle\hat{S}_z\rangle + \langle\hat{S}_x^2\rangle + \langle\hat{S}_y^2\rangle}{4\hbar^2} - \frac{1}{3}. \end{aligned} \tag{5}$$

A pure state of a three-level system is identified by three complex coefficients. The number of meaningful independent real parameters is reduced from $3 \times 2 = 6$ to $6 - 2 = 4$

by the normalization condition, and further because the overall phase of the state vector is arbitrary and physically meaningless. Thus

$$|\Psi\rangle \equiv \begin{pmatrix} A \\ B\,\mathrm{e}^{\mathrm{i}\beta} \\ C\,\mathrm{e}^{\mathrm{i}\gamma} \end{pmatrix}, \tag{6}$$

where $C = \sqrt{1 - A^2 - B^2}$ by the normalization condition, so that one has four independent real parameters A, B, β and γ. This gives the four-parameter density matrix, $|\Psi\rangle\langle\Psi|$. Comparison with (3) leads to the corresponding eight parameters

$$\begin{aligned} a_1 &= AB\cos\beta, & a_2 &= AB\sin\beta, \\ a_3 &= \tfrac{1}{2}(A^2 - B^2), & a_4 &= AC\cos\gamma, \\ a_5 &= AC\sin\gamma, & a_6 &= BC\cos(\gamma - \beta), \\ a_7 &= BC\sin(\gamma - \beta), & a_8 &= \tfrac{-2+3A^2+3B^2}{2\sqrt{3}}. \end{aligned} \tag{7}$$

These parameters satisfy $\mathbf{a} \cdot \mathbf{a} = \frac{1}{3}$, so that all points representing pure states lie on the Bloch hypersphere. There are no points within the Bloch sphere corresponding to pure states, i.e. the interior points, which are allowed by inequalities (4), represent mixed states. Conversely, there are no points lying on the hypersphere corresponding to the mixed states. Since in the case of pure states only four of the eight parameters (appearing in equation (7)) are independent, the regions of the seven-dimensional hypersphere containing pure states can at most be four dimensional. These regions extend continuously into the sphere to form the boundary separating allowed density matrices from the non-positive matrices. Boundary on the sphere consists of density matrices with *two* vanishing eigenvalues (representing pure states), while within the sphere it consists of density matrices with only *one* vanishing eigenvalue (and two non-zero eigenvalues) representing thus mixed states having nearby matrices with negative eigenvalues. The overall boundary forms a convex subset of points contained within the Bloch hypersphere. Extreme points are points that cannot be written as a convex combination of other points in the set. Hence, pure states are extreme points. Every mixed state is a convex sum of pure states. Therefore only the extreme points are pure states [18].

All this provides an operational criterion, in terms of the Bloch vector, whether the state in question is pure $\left(\mathbf{a} \cdot \mathbf{a} = \frac{1}{3}\right)$ or mixed $\left(\mathbf{a} \cdot \mathbf{a} < \frac{1}{3}\right)$. This discrimination can at times be a non-trivial task. In the case of a qutrit, the criterion is based on the experimental measurements of average values of eight independent observables and on equation (5).

2.2. One- and two-parameter density matrices

Inequalities (4) impose certain restrictions on the eight components of the vector $\mathbf{a}$ thereby inducing a complex structure on the set of allowed values of these parameters. General discussion, involving simultaneously all eight parameters, is complex [19] and one has to restrict attention to the simplest cases [3, 4, 6, 19].

Firstly, one assumes that only one of the eight parameters $a_1, a_2, \ldots, a_8$ is nonzero, while the remaining seven vanish. This yields, from (3), corresponding one-parameter 3×3 density matrices. Inequalities (4) imply that in such a case, the non-vanishing parameter a_k ($k = 1$ or $2, \ldots, 7$) must range in the interval $-\frac{1}{3} \leqslant a_k \leqslant \frac{1}{3}$, while the parameter a_8 represents a special case: $-\frac{1}{\sqrt{3}} \leqslant a_8 \leqslant \frac{1}{2\sqrt{3}}$. In all eight cases the corresponding one-parameter $\hat{\rho}$s are rank-3 matrices, implying that they describe mixed states. There is only one exception: $a_8 = -1/\sqrt{3}$, plus remaining seven $a_k \equiv 0$, produce a rank-1 density matrix describing therefore a pure state [20].

Secondly, one assumes that two of the eight parameters $a_1, a_2, \ldots, a_8$ are non-zero, while the remaining six vanish, yielding, from (3), corresponding two-parameter density matrices. This two-parameter case has been discussed in some detail for the three-state system in [3, 4, 6, 19] (and also for the four-state system in [21, 22]), and we here briefly summarize pertinent results. In the case of qutrit, there are $C_2^8 = \frac{8!}{2!6!} = 28$ combinations of different pairs (a_i, a_j) of nonzero parameters and one finds that these belong to one of the four distinct types of sets of allowed parameter values. This is in accord with the results reported in [19], and differs from results described in [6] since they obtained, using a different parametrization of the density matrix, *seven* distinct types. The parametrization of the qutrit density matrix (3), based on $SU(3)$ generators, leads to greater economy and appears to be, in this respect, advantageous.

One finds that the first type of two-parameter set of allowed values is most numerous, and corresponds to 17 pairs of parameters $(a_i, a_j) \equiv (x, y)$ with $ij = 12,\ 13,\ 14,\ 15,\ 16,\ 17,\ 23,\ 24,\ 25,\ 26,\ 27,\ 45,\ 46,\ 47,\ 56,\ 57$ or 67. For these pairs of parameters one has $x^2 + y^2 \leqslant \left(\frac{1}{3}\right)^2$, placing representative points on or inside the circle. All representative points correspond to mixed states.

The second type of two-parameter set of allowed values corresponds to three different pairs of parameters (a_i, a_j) with $ij = 18, 28$ or 38. The representative points are on or inside the triangle with vertices at $(x, y) = \left(0, -\frac{1}{\sqrt{3}}\right)$ and $\left(\pm\frac{1}{2}, \frac{1}{2\sqrt{3}}\right)$. Here also an infinite number of points represent mixed states; only vertices correspond to pure states.

The third type of two-parameter set of allowed values corresponds to four different pairs (a_i, a_j). For $ij = 34$ or 35, the representative points are on or inside the region delineated by the lines $y = \pm\frac{1}{3}\sqrt{1+3x}$ and confined within $-\frac{1}{3} \leqslant x \leqslant \frac{1}{3}$. Majority of points represent mixed states; only two points $\left(\frac{1}{3}, \pm\frac{\sqrt{2}}{3}\right)$ represent pure states. Appropriate description of $ij = 36$ or 37 cases is obtained by reversing the x-axis, $x \to -x$. The two points $\left(-\frac{1}{3}, \pm\frac{\sqrt{2}}{3}\right)$ represent pure states.

The last, fourth type of two-parameter set of allowed values corresponds to four different pairs of parameters (a_i, a_j) with $ij = 48, 58, 68$ or 78. The values of such pairs of parameters are confined within the elliptic region $x^2 + \frac{2}{3}\left(y + \frac{\sqrt{3}}{12}\right)^2 \leqslant \frac{1}{8}$. All representative points, except $\left(0, -\frac{1}{\sqrt{3}}\right)$, correspond to mixed states.

2.3. *Three-parameter density matrices*

Here one assumes that three of the eight parameters $a_1, a_2, \ldots, a_8$ are nonzero, while the remaining five vanish yielding, from (3), corresponding three-parameter density matrices. Such a case is much more involved than one- or two-parameter cases. There are $C_3^8 = \frac{8!}{3!5!} = 56$ combinations of different triplets (a_i, a_j, a_k) of nonzero parameters and one finds, by reducing analytically (as far as possible) the collection of inequalities (4), that these lead to ten distinct types of three-parameter sets of allowed values. The results are much more transparent, and succinctly presented, by employing the Monte Carlo (MC) sampling method [23]. One finds randomly instances of three nonzero parameters that represent isolated sample points belonging to the allowed set and displays resulting random distribution graphically. Each instance is in effect a constructive proof that inequalities (4), in a specific case, can in fact be satisfied. That all MC generated matrices were *density* matrices was confirmed in each instance by computing the corresponding eigenvalues and checking their non-negativity.

One finds that the first type of the set of allowed parameter values is most numerous and corresponds to 17 different triplets of parameters $(a_i, a_j, a_k) \equiv (x, y, z)$ with $ijk = 123$, $124, 125, 126, 127, 145, 147, 156, 167, 245, 246, 257, 267, 456, 457, 467$ or 567. For these

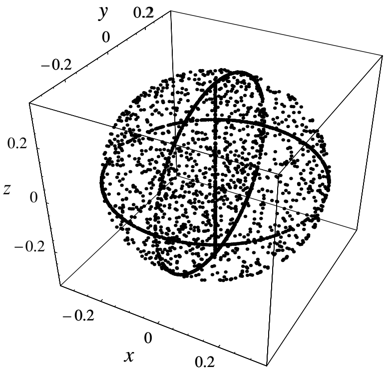

Figure 1. Allowed values of three nonzero parameters a_i, a_j and a_k, with $ijk = 123, 124, 125, 126, 127, 145, 147, 156, 167, 245, 246, 257, 267, 456, 457, 467$ or 567, belong to the outlined sphere. Here x stands for a_i, y for a_j and z for a_k.

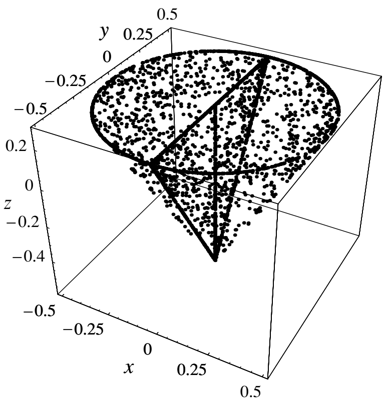

Figure 2. Allowed values of nonzero parameters a_i, a_j and a_k, with $ijk = 128, 138$ or 238 belong to the outlined region. The vertex as well as the points on the circle correspond to pure states.

triplets of parameters one has from (4), $x^2+y^2+z^2 \leqslant \left(\frac{1}{3}\right)^2$, placing representative points on or inside the sphere as depicted in figure 1. All representative points correspond to mixed states.

The second type of the set of allowed parameter values corresponds to three different triplets of parameters (a_i, a_j, a_k) with $ijk = 128, 138$ or 238. The representative points are on or inside the region depicted in figure 2. Asymmetry of the resulting three-dimensional region is apparent. The $x = 0$ cross section, and indeed a cross section obtained with any vertical plane passing through the origin, coincides with the second type of two-parameter density matrices. The infinite number of points in figure 2 represent mixed states; only the points on the circle $x^2 + y^2 = \left(\frac{1}{2}\right)^2$, lying in the plane $z = \frac{1}{2\sqrt{3}}$, as well as the one isolated point $\left(0, 0, -\frac{1}{\sqrt{3}}\right)$, correspond to pure states.

The third type of the set of allowed parameter values corresponds to eight different triplets of parameters (a_i, a_j, a_k) with two subtypes: one with $ijk = 134, 135, 234$ or 235, and second with $ijk = 136, 137, 236$ or 237. The representative points corresponding to the first subtype lie on or inside the region depicted in figure 3. The region corresponding to the second subtype is obtained by reversing axes y and z: $y \to -y$ and $z \to -z$. It is found that the $x = 0$ cross section coincides with the third type of the two-parameter density matrices. Similarly, the

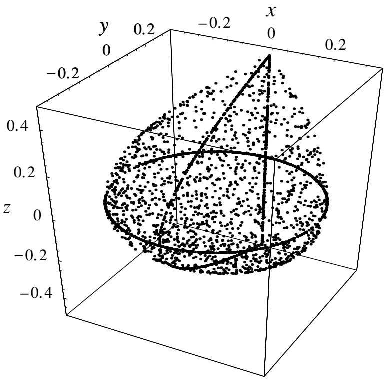

Figure 3. Allowed values of nonzero parameters a_i, a_j and a_k, with $ijk = 134, 135, 234$ or 235, belong to the outlined region.

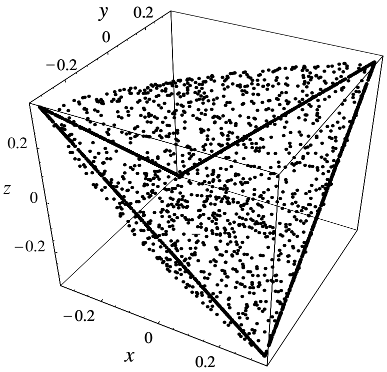

Figure 4. Allowed values of nonzero parameters a_i, a_j and a_k, with $ijk = 146, 157, 247$ or 256, belong to the outlined region. Four vertices represent pure states.

$z = 0$ cross section coincides with the first type of the two-parameter density matrices. Two points, $\left(0, \frac{1}{3}, \pm\frac{\sqrt{2}}{3}\right)$, represent pure states in the case of the first subtype, and $\left(0, -\frac{1}{3}, \pm\frac{\sqrt{2}}{3}\right)$ in the case of the second subtype.

The fourth type of the set of allowed parameter values corresponds to four different triplets of parameters (a_i, a_j, a_k) with $ijk = 146, 157, 247$ or 256. The representative points are on or inside the region depicted in figure 4. Here only four vertices $\left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)$, $\left(\frac{1}{3}, -\frac{1}{3}, -\frac{1}{3}\right)$, $\left(-\frac{1}{3}, \frac{1}{3}, -\frac{1}{3}\right)$ and $\left(-\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}\right)$, represent pure states.

The fifth type of the set of allowed parameter values corresponds to eight different triplets of parameters (a_i, a_j, a_k) with $ijk = 148, 158, 168, 178, 248, 258, 268$ or 278. The representative points are on or inside the region shown in figure 5. Here only three points, $\left(0, 0, -\frac{1}{\sqrt{3}}\right)$ and $\left(\pm\frac{1}{2}, 0, \frac{1}{2\sqrt{3}}\right)$, represent pure states.

The sixth type of the set of allowed parameter values corresponds to a couple of different triplets of parameters (a_i, a_j, a_k) with $ijk = 345$ or 367. The representative points are on or inside the region defined by the inequalities $|x| \leqslant \frac{1}{3}$, $|y| \leqslant \frac{1}{3}\sqrt{1 \pm 3x}$ and $|z| \leqslant \frac{1}{3}\sqrt{1 \pm 3x - 9y^2}$, where the upper (lower) sign corresponds to the 345 (367) case (see figure 6 corresponding to the 345 case; the 367 case is obtained by reversing axes $x \to -x$ and $z \to -z$). Pure states are located on the circle $y^2 + z^2 = \left(\frac{\sqrt{2}}{3}\right)^2$ lying in the plane $x = \pm\frac{1}{3}$, where again the upper (lower) sign corresponds to the 345 (367) case.

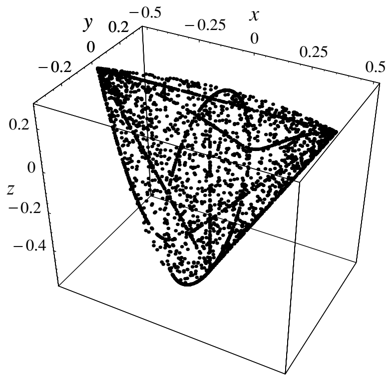

Figure 5. Allowed values of nonzero parameters a_i, a_j and a_k, with ijk = 148, 158, 168, 178, 248, 258, 268 or 278, belong to the outlined region.

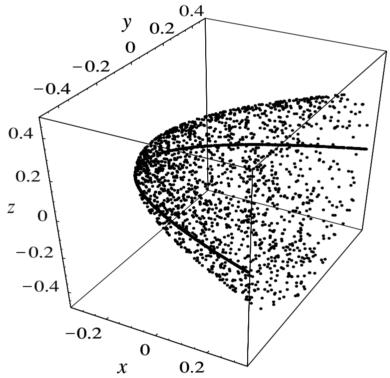

Figure 6. Allowed values of nonzero parameters a_3, a_4 and a_5 belong to the outlined region.

The seventh type of the set of allowed parameter values corresponds to four different triplets of parameters (a_i, a_j, a_k) with $ijk = 346, 347, 356$ or 357. The representative points are on or inside the region defined by the inequalities $|x| \leqslant \frac{1}{3}$, $|y| \leqslant \frac{1}{3}\sqrt{1+3x}$ and $|z| \leqslant \frac{1}{3}\sqrt{(1-9x^2-9y^2+27xy^2)/(1+3x)}$ (figure 7). Here only four points, $\left(\frac{1}{3}, \pm\frac{\sqrt{2}}{3}, 0\right)$ and $\left(-\frac{1}{3}, 0, \pm\frac{\sqrt{2}}{3}\right)$, represent pure states.

The eighth type of the set of allowed parameter values corresponds to a couple of triplets of parameters (a_i, a_j, a_k) with $ijk = 348$ or 358. The representative points are in the region depicted in figure 8. Pure states are located along the line defined via $-\frac{1}{\sqrt{3}} \leqslant z \leqslant \frac{1}{2\sqrt{3}}$, together with $x = \frac{1}{3}(1+\sqrt{3}z)$ and $|y| = \frac{\sqrt{2}}{3}\sqrt{1-\sqrt{3}z-6z^2}$. Additionally, there is a couple of pure states corresponding to the points $\left(\pm\frac{1}{2}, 0, \frac{1}{2\sqrt{3}}\right)$.

The ninth type of the set of allowed parameter values corresponds to a couple of different triplets of parameters (a_i, a_j, a_k) with $ijk = 368$ or 378. The representative points lie in the region depicted in figure 9. Pure states are located along the line $-\frac{1}{\sqrt{3}} \leqslant z \leqslant \frac{1}{2\sqrt{3}}$, together with $x = -\frac{1}{3}(1+\sqrt{3}z)$ and $|y| = \frac{\sqrt{2}}{3}\sqrt{1-\sqrt{3}z-6z^2}$. Additionally, there is a couple of pure states located at points $\left(\pm\frac{1}{2}, 0, \frac{1}{2\sqrt{3}}\right)$.

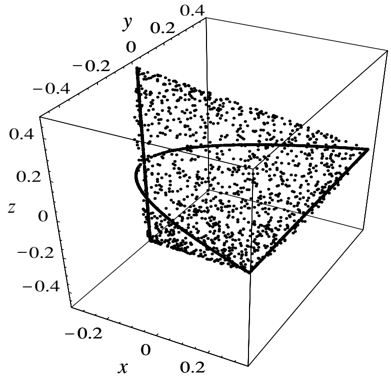

Figure 7. Allowed values of nonzero parameters a_i, a_j and a_k, with $ijk = 346, 347, 356$ or 357, belong to the outlined region. Four vertices represent pure states.

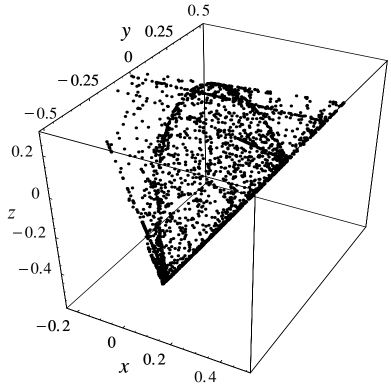

Figure 8. Allowed values of nonzero parameters a_i, a_j and a_k, with $ijk = 348$ or 358, belong to the outlined region.

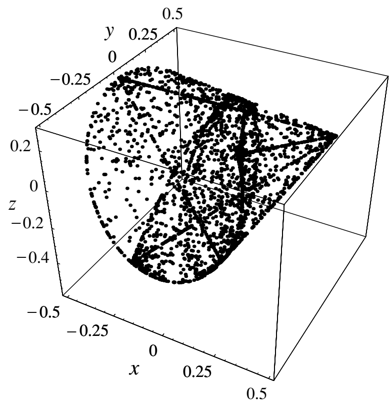

Figure 9. Allowed values of nonzero parameters a_i, a_j and a_k, with $ijk = 368$ or 378, belong to the outlined region.

The last, tenth type of three-parameter set of allowed values corresponds to six different triplets of parameters (a_i, a_j, a_k) with $ijk = 458, 468, 478, 568, 578$ or 678. The values

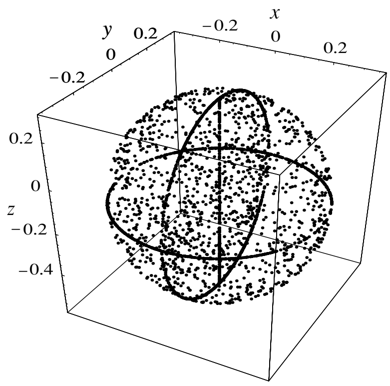

Figure 10. Allowed values of nonzero parameters a_i, a_j and a_k, with $ijk = 458, 468, 478, 568, 578$ or 678, belong to the outlined region.

of such triplets of parameters are confined within the region depicted in figure 10. All representative points, except $\left(0, 0, -\frac{1}{\sqrt{3}}\right)$, correspond to mixed states. This should be compared with the fourth type of two-parameter density matrices.

We repeat that in special cases when one of the three parameters a_i, a_j or a_k vanishes, one obtains the corresponding two-parameter section (one of the four types, discussed in subsection 2.2). Analogously, the regions shown in figures 1 to 10 represent sections of the four-parameter (a_i, a_j, a_k and a_l) regions of allowed parameter values (not shown for obvious reasons) in cases when one of these four parameters vanishes. In fact, analogous classification of all $C_4^8 = 70$ different combinations of four non-vanishing parameters can be performed analytically, but without the possibility of graphical presentation the results are complicated and not easily visualized, nor readily summarized. One finds, for example, that the quadruplets of non-vanishing parameters $a_i \equiv x, a_j \equiv y, a_k \equiv z$ and $a_l \equiv w$, with $ijkl = 4568, 4578, 4678$ and 5678, all belong to the same type. This means that the corresponding density matrices occupy the same region in the four-dimensional parameter space $xyzw$, and in particular, e.g. that the three-dimensional cross sections $a_i = 0$ are the same (these sections, $jkl = 568, 578$ and 678, are in fact depicted in figure 10). Similarly, the sections $a_j = 0$ (that is $ikl = 468, 478$ and 578), as well as $a_k = 0$ ($ijl = 458, 468$ and 568) are also of the form depicted in figure 10. Only the $a_l = 0$ sections ($ijk = 456, 457, 467$ and 567) belong to the type 1 of the three parameter classification and are therefore depicted in figure 1.

Finally we remark that, from equation (5), one obtains the expectation values of the eight relevant spin 1 observables, expressed via parameters $a_1, \ldots, a_8$:

$$\begin{aligned}
&\langle \hat{S}_x \rangle = \sqrt{2}\hbar(a_1 + a_6), \qquad \langle \hat{S}_y \rangle = \sqrt{2}\hbar(a_2 + a_7), \\
&\langle \hat{S}_z \rangle = \hbar(a_3 + \sqrt{3}a_8), \\
&\left\langle \hat{S}_x^2 \right\rangle = \frac{\hbar^2}{2}(4/3 - a_3 + 2a_4 + a_8/\sqrt{3}), \\
&\left\langle \hat{S}_y^2 \right\rangle = \frac{\hbar^2}{2}(4/3 - a_3 - 2a_4 + a_8/\sqrt{3}), \\
&\langle \{\hat{S}_x, \hat{S}_y\} \rangle = 2\hbar^2 a_5, \qquad \langle \{\hat{S}_y, \hat{S}_z\} \rangle = \sqrt{2}\hbar^2(a_2 - a_7), \\
&\langle \{\hat{S}_z, \hat{S}_x\} \rangle = \sqrt{2}\hbar^2(a_1 - a_6).
\end{aligned} \tag{8}$$

Then, from figures 1–10, one can directly predict possible ranges of experimental data for states described by various types of three-parameter density matrices. Additionally, global properties of these observables can be evaluated from equation (8) by generating, by the MC sampling method, nearly all density matrices pertaining to a given type. This amounts to determination, in the present case, of the corresponding average values of the three non-vanishing parameters $a_i \to x$, $a_j \to y$ and $a_k \to z$. Many of these vanish by symmetry apparent in figures 1–10. There is however some asymmetry (see [19] for a brief discussion of this point). The only nonzero average values found are: $\overline{z} \approx 0.158$ for type 2 of the three-parameter density matrices (see figure 2), $\overline{y} \approx \pm 0.023$ for type 3 (see figure 3), $\overline{z} \approx 0.017$ for type 5 (see figure 5), $\overline{x} \approx 0.054$ and $\overline{z} \approx -0.087$ for type 8 (see figure 8), $\overline{x} \approx -0.041$, and $\overline{z} \approx -0.068$ for type 9 (see figure 9), and $\overline{z} \approx -0.145$ for type 10 of the three-parameter density matrices (see figure 10). All results lie within ± 0.001 interval, with 95% confidence level. Thus, for example, in all three cases 128, 138 and 238 of type 2 three-parameter density matrices, the non-vanishing global averages are $\langle \hat{S}_z \rangle = \hbar\sqrt{3}\overline{z} \approx 0.273\hbar$ and $\langle \hat{S}_x^2 \rangle = \langle \hat{S}_y^2 \rangle = \frac{\hbar^2}{2}\overline{z}/\sqrt{3} \approx 0.0455\hbar^2$. Having in mind that every three-level system is formally equivalent to a fictitious spin 1, it is possible to extend directly these results to any three-level system.

3. Conclusion

In this paper we have investigated in some detail the properties and structure of the eight-dimensional parameter space of density matrices for a three-state quantum system, employing the $SU(3)$ generator expansion. In particular we studied three-dimensional cross sections of the space of generalized Bloch vectors which has, it turns out, rich and complex structure, thus providing some insight into the structure of the space of density matrices. A deeper understanding of properties of the Bloch vector space for a qutrit is of interest in quantum mechanics and in quantum information science. We have shown that one can classify 56 different three-parameter density matrices into ten different types, according to shape of the corresponding region of allowed values of three relevant parameters. All regions of the parametric space are convex, fit within the corresponding Bloch hypersphere and are bounded by density matrices with at least one vanishing eigenvalue, all being generic features of a larger class of N-state quantum systems. Finally, the cases of four, or five, ..., or eight nonzero parameter qutrit density matrices can in principle be investigated by the same Monte Carlo sampling method despite the fact that the resulting random distributions of sample points cannot be represented graphically. This method can be used to generate numerically nearly all density matrices via equation (3). This is often helpful if one wants to investigate some global properties by numerical experiments. In order to do that efficiently, one needs a parametrization of the density matrix with real values, and with simple ranges. We found that the Bloch vector provides one such natural parametrization and, moreover, it is based on actual experimental measurements of average values of the minimum set of eight independent observables, equation (5), needed to completely determine the density matrix.

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