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Positivity of the $N \times N$ density matrix expressed in terms of polarization operators

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Abstract
We use polarization operators known from the quantum theory of angular momentum to expand the $(N \times N)$-dimensional density operators. Thereby we construct generalized Bloch vectors representing density matrices. We study their properties and derive positivity conditions for any N. We also apply the procedure to study Bloch vector space for a qubit and a qutrit.

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1. Introduction

Recent advances in the fundamentals of quantum mechanics and in quantum information theory [1] resulted in the renewed interest in the properties and structure of the space of $(N \times N)$-dimensional density operators (matrices). Moreover, the composite (multipartite) systems exhibit the effect of entanglement which still makes things more interesting.

A quantum-mechanical N-level system is associated with the Hilbert space $\mathcal{H}_N$ ($\dim\mathcal{H}_N = N$). Density operators $\hat{\rho}$ for such systems are a subset $\mathcal{B}_\rho(\mathcal{H}_N)$ of $\mathcal{B}(\mathcal{H}_N)$—Banach space of self-adjoint operators represented by $N \times N$ Hermitian matrices. A density operator $\hat{\rho} \in \mathcal{B}_\rho(\mathcal{H}_N)$ possesses three fundamental properties

$$\text{(i)} \quad \hat{\rho} = \hat{\rho}^\dagger, \quad \text{Hermiticity;} \tag{1a}$$

$$\text{(ii)} \quad \mathrm{Tr}\{\hat{\rho}\} = 1, \quad \text{normalization;} \tag{1b}$$

$$\text{(iii)} \quad \lambda_j \geqslant 0, \quad \text{positivity;} \tag{1c}$$

where λ_j are the eigenvalues of the density operator $\hat{\rho}$. Strictly speaking we should say that density operators must be positive semidefinite. However, the phrase 'positive' is shorter, so we will use it, keeping in mind the strict sense. The set $\mathcal{B}_\rho(\mathcal{H}_N)$ is convex: that is, if

$\hat{\rho}_1, \hat{\rho}_2 \in \mathcal{B}_\rho(\mathcal{H}_N)$, then $\hat{\rho} = s\hat{\rho}_1 + (1-s)\hat{\rho}_2 \in \mathcal{B}_\rho(\mathcal{H}_N)$ for $s \in (0, 1)$. Density matrices must be normalized (as in (1*b*)), while for $k \geqslant 2$ satisfy the inequalities

$$\mathrm{Tr}\{\hat{\rho}^k\} \leqslant 1, \qquad \mathrm{Tr}\{\hat{\rho}^k\} \geqslant \frac{1}{N^{k-1}}. \tag{2}$$

For pure states $\hat{\rho} = |\Psi\rangle\langle\Psi|$, the first inequality becomes an equality (the second one is obviously satisfied). Pure states are also extremal—they cannot be given as a nontrivial convex combination of two other matrices. Maximally mixed states are represented by a diagonal matrix with all N elements equal to $1/N$. In this case, one has $\mathrm{Tr}\{\hat{\rho}^k\} = 1/N^{k-1}$. Finally it may be worth noting that for the two-level system condition, (1*c*) and $\mathrm{Tr}\{\hat{\rho}^2\} \leqslant 1$ are equivalent. But it is not the case for systems with higher dimensions, that is for $N \geqslant 3$. This is due to additional conditions which follow from requirement (1*c*).

Although the outlined fundamental properties of density matrices are simple and well known, not much is known about the structure of the set $\mathcal{B}_\rho(\mathcal{H}_N)$. Only the case of $N = 2$ (also called a qubit) seems to be an exception. When the usual Pauli matrices are taken as a basis then one can show that there exists a one-to-one correspondence between 2×2 density matrices and the set of three-dimensional real vectors (Bloch vectors). The set of such density matrices corresponds to the Bloch ball $\{\vec{\mathbf{b}} \in \mathbb{R}^3 : |\vec{\mathbf{b}}| \leqslant 1\}$. Equality occurs only for pure states which lie on the Bloch sphere $\{\vec{\mathbf{b}} \in \mathbb{R}^3 : |\vec{\mathbf{b}}| = 1\}$. For a maximally mixed state one has $|\vec{\mathbf{b}}| = 0$.

On the other hand, even for $N = 3$ the situation is not that simple. In two recent papers by Kimura [2] and by Byrd and Khaneja [3] the well-known Gell-Mann matrices $\hat{\Lambda}_j$ are used. $\hat{\Lambda}_j$'s are standard $SU(N)$ generators (see also [4, 5]) which are Hermitian, traceless and orthogonal in the sense that $\mathrm{Tr}\{\hat{\Lambda}_j\hat{\Lambda}_k\} = 2\delta_{jk}$. Expanding the $N \times N$ density matrix as (Byrd and Khaneja [3] adopt slightly different normalization of b_j coefficients)

$$\hat{\rho} = \frac{1}{N}\hat{\mathbf{1}}_N + \frac{1}{2}\sum_{j=1}^{N^2-1} b_j\hat{\Lambda}_j, \tag{3}$$

one establishes a one-to-one correspondence between density matrices and generalized Bloch vectors $\vec{\mathbf{b}} = (b_1, b_2, \ldots, b_{N^2-1}) \in \mathbb{R}^{N^2-1}$. Requirement that $\mathrm{Tr}\{\rho^2\} \leqslant 1$ generalizes the $N = 2$ case and implies that

$$|\vec{\mathbf{b}}| \equiv \sqrt{\sum_{j=1}^{N^2-1} b_j^2} \leqslant \sqrt{\frac{2(N-1)}{N}}. \tag{4}$$

Hence vectors $\vec{\mathbf{b}}$ lie within (N^2-1)-dimensional hypersphere.

The requirement of positivity imposes some additional restrictions on vector $\vec{\mathbf{b}}$. The hypersphere contains vectors corresponding to non-positive matrices [1]. So the generalized Bloch vectors constitute a subset inside the hypersphere. This set (and so the set of all $N \times N$ density matrices) has a complicated and asymmetric structure as briefly discussed in [2]. Investigations of the geometry of the space of density matrices are therefore difficult and complex. An example of such studies can, for instance, be found in [6].

The main aim of this work is to employ another parametrization of the set of $N \times N$ density matrices in order to construct the conditions for positivity. Hence, our work is somewhat similar in spirit to the papers [2, 3], though we will try to argue that the employed representation might be advantageous in future applications.

In the next section, we recall the concept of polarization operators and summarize their most important properties. We follow the terminology and notation used in the handbook [7]. Next we outline the idea of expansion of the density matrix in terms of polarization operators. These concepts are also discussed in the classic books by Biedenharn and Louck [8] and by

Blum [9] and also in other literature sources. Therefore, we state only the results essential for further developments. We also study the analogue of the generalized Bloch vector in the light of the conditions imposed upon a density operator. A more extensive presentation is given in [10].

The main part of our work is contained in section 3 where we present the general expressions which lead to the positivity conditions for any N.

The next sections give illustrations of the developed procedure for a qubit ($N = 2$) and for a qutrit ($N = 3$). For the latter we present all possible two-dimensional cross sections of the space of generalized Bloch vectors which possesses a complicated and asymmetric structure.

Finally, in the last section we give some concluding remarks and indicate some possible future applications and further developments.

2. Density matrix in terms of polarization operators

2.1. Polarization operators

The concept of polarization operators (in the terminology of section 2.4 of [7]) appears in the context of quantum-mechanical theory of angular momentum. This theory is extremely well documented, e.g., [7–9]. Therefore, we reduce the information given here as much as possible referring the reader mainly to chapter 2.4 of [7].

Let $\mathcal{E}_j$ denote, for a given but fixed value of $j\left(j = \frac{1}{2}, 1, \frac{3}{2}, 2, \dots\right)$, the space spanned by eigenvectors $|jm\rangle$ of angular momentum operator. Obviously, dim $\mathcal{E}_j = (2j + 1)$, so it may be identified with $\mathcal{H}_{N=2j+1}$, a Hilbert space for any $N = 2j + 1$-level system.

Polarization operators are defined as

$$\mathbf{T}_{LM}(j) = \sqrt{\frac{2L+1}{2j+1}} \sum_{m,m'} C^{jm}_{jm',LM} |jm\rangle\langle jm'|, \tag{5}$$

with $C^{jm}_{jm',LM}$ being Clebsch–Gordan coefficients (CGC). Properties of CGC imply that $L = 0, 1, 2, \dots, 2j$ with corresponding M's. There are $(2j + 1)^2$ polarization operators and they constitute a basis in the operator space $\mathcal{B}(\mathcal{H}_{N=2j+1})$.

In general, polarization operators are non-Hermitian, but due to the symmetry properties of CGC they satisfy the relation

$$\mathbf{T}^{\dagger}_{LM}(j) = (-1)^M \mathbf{T}_{L-M}(j). \tag{6}$$

For any j an operator $\mathbf{T}_{00}(j) = (2j + 1)^{-1/2}\hat{\mathbf{1}}_{N=2j+1}$ so its trace equals $(2j + 1)^{1/2}$. All other operators $\mathbf{T}_{LM}(j)$ (i.e., for $L \geqslant 1$) are traceless.

Polarization operators have the property

$$\mathrm{Tr}\left\{\mathbf{T}_{L_1M_1}(j)\mathbf{T}_{L_2M_2}(j)\right\} = (-1)^{M_1}\delta_{L_1L_2}\delta_{M_1,-M_2}, \tag{7}$$

which together with (6) ensures that they form an orthogonal basis in $\mathcal{B}(\mathcal{H}_{N=2j+1})$ (this is in the sense of Hilbert–Schmidt scalar product $\langle \hat{A}, \hat{B}\rangle = \mathrm{Tr}\{\hat{A}^{\dagger}\hat{B}\}$).

Polarization operators are well known and the given references (especially section 2.4 of [7]) list their other properties such as commutators, anticommutators, products and traces of n-fold products, etc.

Commutation relations for polarization operators follow from the properties of CGC and show that $\mathbf{T}_{LM}(j)$'s are just another realization of the representation of the $SU(N = 2j + 1)$ group, only with specific structural constants. This explains why we have called the representation used in papers [2, 3] the 'standard one'. We note that Biedenharn and Louck [8] give some interesting comments on the structure of the $SU(N)$ representation generated by operators $\mathbf{T}_{LM}(j)$. Discussion of these issues, although quite interesting, goes beyond the scope of this work, but perhaps deserves some further study.

2.2. Decomposition of density matrix

Polarization operators $\mathbf{T}_{LM}(j)$ constitute an orthonormal basis in $\mathcal{B}(\mathcal{H}_{N=2j+1})$. Henceforth, we will remember that $N = 2j + 1$ and drop the argument j. The density matrix for a N-level system (see [7], equation 2.4.13) can be expanded as

$$\hat{\rho} = V_{00}\mathbf{T}_{00} + \sum_{L=1}^{2j}\sum_{M=-L}^{M=L} V_{LM}\mathbf{T}_{LM} = \frac{1}{N}\hat{\mathbf{1}}_N + \vec{\mathbf{V}}\cdot\vec{\mathbf{T}}, \tag{8}$$

with coefficients V_{LM} being in general complex (since $\mathbf{T}_{LM}$ are non-Hermitian). They may also be called a generalized Bloch vector. We have separated the (00) term since $\mathbf{T}_{00}$ is the only polarization operator with nonzero trace. Its properties imply that $V_{00} = (2j+1)^{-1/2} = N^{-1/2}$ which explains the second equality in (8). We note that the second equality also defines the product $\vec{\mathbf{V}}\cdot\vec{\mathbf{T}}$. Due to relations (6) and (7) it follows that $V_{LM} = \mathrm{Tr}\{\mathbf{T}^{\dagger}_{LM}\hat{\rho}\}$. Moreover equation (6) implies that $V^{*}_{LM} = (-1)^{M}V_{L-M}$. This means that V_{L0} (there are $n-1$ of them) are real, while $N(N-1)$ components $V_{LM}(L \geqslant 1, M \neq 0)$ are specified by $N(N-1)$ real numbers. Therefore, the expansion (8) ensures normalization and Hermiticity of the density matrix, just like the corresponding generalized Bloch vector in the standard $SU(N)$ representation. We also note that linear combinations of the $\mathbf{T}_{LM}$ operators can be constructed to specify the observables necessary to determine the numbers V_{LM} experimentally. Thus, the fact that $\mathbf{T}_{LM}$ are non-Hermitian does not present any difficulties.

Density matrices must satisfy inequalities (2). Due to tracelessness of $\mathbf{T}_{LM}$ $(L \neq 0)$ operators and to relation (7) we obtain

$$\mathrm{Tr}\{\hat{\rho}^2\} = \frac{1}{N} + \mathrm{Tr}\{(\vec{\mathbf{V}}\cdot\vec{\mathbf{T}})^2\} = \frac{1}{N} + \sum_{L=1}^{2j}\sum_{M=-L}^{L} V_{LM}V^{*}_{LM} = \frac{1}{N} + |\vec{\mathbf{V}}|^2 \leqslant 1. \tag{9}$$

It implies that the generalized Bloch vectors $\vec{\mathbf{V}}$ form a subset within a hypersphere of radius $R = \sqrt{(N-1)/N}$. This result is analogous to relation (4) for the standard $SU(N)$ representation. The structure of this subset (for $N \geqslant 3$) is pretty complicated because requirement of positivity imposes additional restrictions. Pure states (for which $\mathrm{Tr}\{\hat{\rho}^2\} = 1$) lie on the surface of the hypersphere, while a maximally mixed state (for which $\mathrm{Tr}\{\hat{\rho}^2\} = 1/N$) corresponds to $|\vec{\mathbf{V}}| = 0$. The shorter the vector $\vec{\mathbf{V}}$, the density operator represented by it corresponds to a 'more mixed' state. The length of $\vec{\mathbf{V}}$ can be considered as a kind of measure of 'mixedness' [11].

3. Positivity of the density operator

The density operator, being normalized and Hermitian, must also be positive. This requirement may be formulated in many ways. For example, operator $\hat{\rho}$ is positive if for all $|\psi\rangle \in \mathcal{H}_N$ one has $\langle\psi|\hat{\rho}|\psi\rangle \geqslant 0$. Another formulation is given via the eigenvalues, as in (1*c*). We concentrate on the latter approach since it was also used by the authors of papers [2, 3].

Investigation of the eigenvalues of the $N \times N$ density matrix is done by means of the characteristic polynomial of a variable $\lambda \in \mathbb{R}$: $W(\lambda) = \det(\lambda\hat{\mathbf{1}}_N - \hat{\rho})$ (see [12]). It can be shown that $W(\lambda)$ may be written as

$$W(\lambda) = \sum_{k=0}^{N}(-1)^k S_k^{(N)}\lambda^{N-k}, \tag{10}$$

with $S_0^{(N)} \equiv 1$, and $S_N^{(N)} = \det \hat{\rho}$. Coefficients $S_k^{(N)}$, $(k = 1, 2, \ldots, N)$, are constructed recursively by Newton's formula

$$kS_k^{(N)} = \sum_{m=1}^{k} (-1)^{m-1} S_{k-m}^{(N)} \operatorname{Tr}\{\hat{\rho}^m\}. \tag{11}$$

Obviously $S_1^{(N)} \equiv \operatorname{Tr}\{\hat{\rho}\} = 1$ due to normalization of the density operator. Computation of subsequent $S_k^{(N)}$'s is straightforward.

The question of positivity is answered by the following theorem:

$$\left\{S_k^{(N)} \geqslant 0, \text{ for all } k = 1, 2, \ldots, N\right\} \quad \Longleftrightarrow \quad \left\{\forall_j \lambda_j \geqslant 0, \text{ that is } \hat{\rho} \text{ positive}\right\}. \tag{12}$$

To check positivity of operator $\hat{\rho}$ one needs to check positivity of the corresponding coefficients $S_k^{(N)}$. Clearly, the requirement that $S_k^{(N)} \geqslant 0, (k = 2, \ldots, N)$ imposes restrictions on the components of vector $\vec{\mathbf{V}}$, thereby inducing a complex structure on the set of all allowed $\vec{\mathbf{V}}$'s.

Using equation (11) one obtains $S_2^{(N)} = (1 - \operatorname{Tr}\{\hat{\rho}^2\})/2$. Its positivity reproduces the requirement $0 \leqslant |\vec{\mathbf{V}}|^2 \leqslant (N-1)/N$, as already discussed after equation (9). So, for a qubit $(N = 2)$ the requirement that $\operatorname{Tr}\{\hat{\rho}^2\} \leqslant 1$ is equivalent to the requirement of positivity. For higher dimensions $S_k^{(N)}(k = 2, \ldots, N)$ must be checked for positivity. Going further, we use Newton's binomial to expand powers of $\hat{\rho}$ expressed as in (8) Then, we have

$$\operatorname{Tr}\{\hat{\rho}^k\} = \sum_{m=0}^{k} \binom{k}{m} \frac{T_m}{N^{k-m}} = \frac{1}{N^{k-1}} + \frac{k(k-1)}{2N^{k-2}} |\vec{\mathbf{V}}|^2 + \sum_{m=3}^{k} \binom{k}{m} \frac{T_m}{N^{k-m}}, \tag{13}$$

where we have denoted $T_m = \operatorname{Tr}\{(\vec{\mathbf{V}} \cdot \vec{\mathbf{T}})^m\} \in \mathbb{R}$, due to Hermiticity of $\hat{\rho}$. In (13) we understand that $(\vec{\mathbf{V}} \cdot \vec{\mathbf{T}})^0 = \hat{\mathbf{1}}_N$ so that $T_0 = N$. Tracelessness of polarization operators implies that $T_1 = 0$, while (9) gives $T_2 = |\vec{\mathbf{V}}|^2$. So the problem is now reduced to computation of the quantities T_m for $m \geqslant 3$. Directly from the definition, one has

$$T_k = \sum_{L_1=1}^{2j} \sum_{M_1=-L_1}^{L_1} \cdots \sum_{L_k=1}^{2j} \sum_{M_k=-L_k}^{L_k} V_{L_1M_1} \cdots V_{L_kM_k} \operatorname{Tr}\left\{\mathbf{T}_{L_1M_1} \cdots \mathbf{T}_{L_kM_k}\right\}. \tag{14}$$

Multiple trace is known (see [7], equation (2.4.24)) so we can find any T_k and therefore the traces $\operatorname{Tr}\{\hat{\rho}^k\}$. The resulting expressions are complicated but the multiple trace is not zero only when $\sum_{i=1}^{k} M_i = 0$ which greatly reduces the number of terms.

For further purposes we write down the trace for $k = 3$. It reads

$$\operatorname{Tr}\{\rho^3\} = \frac{1}{N^2} + \frac{3}{N} |\vec{\mathbf{V}}|^2 + T_3. \tag{15}$$

Then, coefficients $S_k^{(N)}$ follow by combining the recurrence relation (11) with (13). Since $S_0^{(N)} = S_1^{(N)} = 1$ and $T_0 = N, T_1 = 0$, we obtain for $n \geqslant 2$

$$nS_n^{(N)} = S_{n-1}^{(N)} + \sum_{k=2}^{n} (-1)^{k-1} S_{n-k}^{(N)} \left[\frac{1}{N^{k-1}} + \sum_{m=2}^{k} \binom{k}{m} \frac{T_m}{N^{k-m}}\right], \tag{16}$$

which is the sought recurrence relation for coefficients $S_n^{(N)}$. The first nontrivial coefficients are (with $T_2 = |\vec{\mathbf{V}}|^2$))

$$S_2^{(N)} = \frac{N-1}{2N} - \frac{1}{2} T_2, \tag{17a}$$

$$S_3^{(N)} = \frac{(N-1)(N-2)}{6N^2} - \frac{N-2}{2N} T_2 + \frac{1}{3} T_3. \tag{17b}$$

Theorem (12) states that positivity of $\hat{\rho}$ is equivalent to the conditions that $S_k^{(N)} \geqslant 0$ for all $k = 1, 2, \ldots, N$. Relation (16) together with (14) allows one to compute these quantities for any finite N. The computations might be lengthy because multiple traces are fairly complex. Nevertheless, the proposed approach can be applied in a closed form for any N. On the other hand, Kimura [2] gives specific expressions only for $N \leqslant 4$, Byrd and Khaneja [3] up to $N \leqslant 9$. Our presentation is free from such restrictions. We give quite specific expressions valid for any N.

4. Example: qubit

The formalism introduced above can now be applied in some specific cases. The simplest one is a qubit ($j = 1/2$, $N = 2$), which within the 'standard' $SU(N)$ framework was represented by Pauli matrices and Bloch vector. Following [7] one easily constructs matrices $\mathbf{T}_{LM}$ with $L = 0, 1$. Then, using the property (6) we can write

$$\hat{\rho} = \frac{1}{N}\hat{\mathbf{1}}_2 + \sum_{M=-1}^{1} V_{1M}\mathbf{T}_{1M} = \begin{pmatrix} \dfrac{1}{2} - \dfrac{x}{\sqrt{2}} & -\alpha - \mathrm{i}\beta \\ -\alpha + \mathrm{i}\beta & \dfrac{1}{2} + \dfrac{x}{\sqrt{2}} \end{pmatrix}, \tag{18}$$

where V_{1M}'s are parametrized by real numbers x, α and β: $V_{10} = x$, $V_{11} = \alpha + \mathrm{i}\beta$. This matrix is clearly Hermitian and normalized. The requirement of positivity $S_2^{(2)} \geqslant 0$ (equivalent to the condition $\mathrm{Tr}\{\hat{\rho}^2\} \leqslant 1$) gives

$$|\vec{\mathbf{V}}|^2 = V_{10}^2 + 2|V_{11}|^2 = x^2 + 2(\alpha^2 + \beta^2) \leqslant \tfrac{1}{2}, \tag{19}$$

which is an analogue of relation $|\vec{\mathbf{b}}| \leqslant 1$ for Bloch sphere. The surface $x^2 + 2(\alpha^2 + \beta^2) = 1/2$ is a prolate spheroid and corresponds to the 'standard' Bloch sphere. All allowed vectors $\vec{\mathbf{V}}$ representing a two-dimensional density matrix lie within this spheroid, while pure states occupy its surface. Hence, the presented description of the density matrix yields results fully equivalent to the 'standard' one.

5. Example: qutrit

5.1. Construction

Now we discuss the next example. It is a 3-level system, sometimes called a qutrit. So we have $N = 3$ and $j = 1$. The operator basis is spanned by nine polarization operators $\mathbf{T}_{LM}(1)$ with $L = 0, 1, 2$ and $M = -L, \ldots, L$. We do not write them down, because they are easily found from definition (5) and are explicitly given in [7] (equations (2.6.18) and (19)). Expanding $\hat{\rho}$ as in the prescription (8) we need eight components V_{LM}. Due to relation (6) these components can be expressed by eight real variables. This is done as follows:

$$\begin{aligned} &V_{10} = x, && V_{11} = -V_{1-1}^* = a + \mathrm{i}b, && \\ &V_{20} = y, && V_{21} = -V_{2-1}^* = \alpha_1 + \mathrm{i}\beta_1, && V_{22} = V_{2-2}^* = \alpha_2 + \mathrm{i}\beta_2. \end{aligned} \tag{20}$$

With the aid of this notation the density matrix for a qutrit is of the form

$$\hat{\rho} = \begin{pmatrix} \dfrac{1}{3} + \dfrac{x}{\sqrt{2}} + \dfrac{y}{\sqrt{6}} & -\dfrac{a + \mathrm{i}b}{\sqrt{2}} - \dfrac{\alpha_1 + \mathrm{i}\beta_1}{\sqrt{2}} & \alpha_2 + \mathrm{i}\beta_2 \\ -\dfrac{a - \mathrm{i}b}{\sqrt{2}} - \dfrac{\alpha_1 - \mathrm{i}\beta_1}{\sqrt{2}} & \dfrac{1}{3} - \dfrac{2}{\sqrt{6}}y & -\dfrac{a + \mathrm{i}b}{\sqrt{2}} + \dfrac{\alpha_1 + \mathrm{i}\beta_1}{\sqrt{2}} \\ \alpha_2 - \mathrm{i}\beta_2 & -\dfrac{a - \mathrm{i}b}{\sqrt{2}} + \dfrac{\alpha_1 - \mathrm{i}\beta_1}{\sqrt{2}} & \dfrac{1}{3} - \dfrac{x}{\sqrt{2}} + \dfrac{y}{\sqrt{6}} \end{pmatrix}. \tag{21}$$

It is clearly Hermitian and normalized, as it should be.

To identify matrix (21) as a true density matrix one must be sure that it is positive. The positivity conditions correspond to the inequalities $S_2^{(3)} \geqslant 0$ and $S_3^{(3)} \geqslant 0$. The first one, as already discussed, is equivalent to $0 \leqslant |\vec{\mathbf{V}}|^2 \leqslant 2/3$, which with parametrization (20) reads

$$0 \leqslant |\vec{\mathbf{V}}|^2 = x^2 + y^2 + 2\big(a^2 + b^2 + \alpha_1^2 + \beta_1^2 + \alpha_2^2 + \beta_2^2\big) \leqslant \tfrac{2}{3}, \tag{22}$$

with the left inequality being trivial. $S_3^{(3)}$ follows immediately from (17*b*) and it reads

$$S_3^{(3)} = \tfrac{1}{3}\big[\tfrac{1}{9} - \tfrac{1}{2}|\vec{\mathbf{V}}|^2 + T_3\big] \geqslant 0. \tag{23}$$

Next we need to find T_3 according to (14). Computing the triple trace as given in [7] (equation (2.4.24)) and using identifications (20) we obtain

$$\begin{aligned} T_3 = \frac{3x^2y - y^3}{\sqrt{6}} + 3\sqrt{2}x(a\alpha_1 + b\beta_1) + \sqrt{\frac{3}{2}}y\big(2\alpha_2^2 + 2\beta_2^2 - a^2 - b^2 - \alpha_1^2 - \beta_1^2\big) \\ + 3\big[\alpha_2\big(a^2 - b^2 - \alpha_1^2 + \beta_1^2\big) + 2\beta_2\big(ab - \alpha_1\beta_1\big)\big]. \end{aligned} \tag{24}$$

Both quantities $|\vec{\mathbf{V}}|^2$ and T_3 are real, as they should be. Using the above relations one expresses $S_3^{(3)}$ via the introduced eight real variables. Moreover, one easily checks that $S_3^{(3)} = \det\hat{\rho}$, as is should be.

5.2. *Parametrization with two nonzero variables*

A general analytical discussion of positivity conditions (22) and (23) together with (24) seems to be extremely difficult if not virtually impossible, because there are eight real parameters. Therefore, we will restrict our attention to a simpler case. Namely, we will assume that only two of the real parameters $(x, y, a, b, \alpha_1, \beta_1, \alpha_2, \beta_2)$ are nonzero while the other six are taken to be zero. Similar procedure was employed by Kimura [2] and Byrd with Khaneja [3]. Then, there are 28 different pairs of nonzero parameters. We shall show that these 28 pairs split into 7 distinct types.

We shall denote the pair of nonzero parameters by (s, t) and next we will indicate to which pairs taken from the set $(x, y, a, b, \alpha_1, \beta_1, \alpha_2, \beta_2)$ it corresponds. Then we will give the conditions (22) and (23) written in terms of parameters s, t. The formal expressions for these conditions are common to all representatives of the given type. To discuss (23) we introduce the quantity

$$F = \tfrac{1}{9} - \tfrac{1}{2}\big|\vec{\mathbf{V}}\big|^2 + T_3 \geqslant 0, \tag{25}$$

which will be a function of two variables s and t and the inequality obviously follows from (23). After presenting the basic properties of each of the seven types we will briefly state the properties which are common to all of them.

5.2.1. Type I. Type I corresponds to only one pair of parameters, that is to $(s, t) = (x, y)$. Then, requirements (22) and (25) translate into the following ones:

$$\big|\vec{\mathbf{V}}\big|^2 = x^2 + y^2 \leqslant \frac{2}{3}, \qquad F(x, y) = \frac{1}{9} - \frac{x^2 + y^2}{2} + \frac{3x^2y - y^3}{\sqrt{6}} \geqslant 0. \tag{26}$$

The first requirement restricts x, y to within the dashed circle in figure 1 (left). Then, the second one implies that the allowed points must lie on or within the solid triangle. There are three pure states.

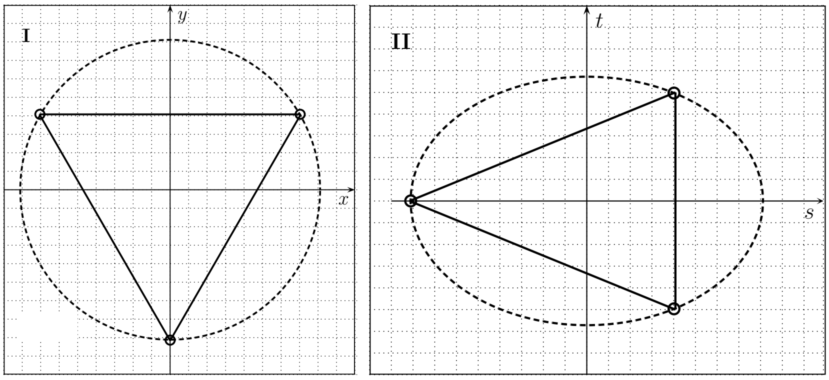

Figure 1. Type I (left) and type II (right). Allowed states lie on the solid lines and inside the triangles. The grid unit in all figures corresponds to actual value equal to 0.1. Small circles—pure states. Type I: circle radius $R = \sqrt{2/3}$; pure states $(\pm 1/\sqrt{2}, 1/\sqrt{6})$ and $(0, -\sqrt{2/3})$. Type II: semi-axes of the ellipse $a = \sqrt{2/3}$, $b = 1/\sqrt{3}$; pure states $(1/\sqrt{6}, \pm 1/2)$ and $(-\sqrt{2/3}, 0)$.

5.2.2. Type II. Type II has two representatives $(s, t) = (y, \alpha_2), (y, \beta_2)$. Then relations (22) and (25) give

$$|\vec{\mathbf{V}}|^2 = s^2 + 2t^2 \leqslant \frac{2}{3}, \qquad F(s, t) = \frac{1}{9} - \frac{s^2}{2} - t^2 + \frac{6t^2 s - s^3}{\sqrt{6}} \geqslant 0. \tag{27}$$

The first inequality places the allowed values of parameters on and inside the dashed ellipse in figure 1 (right). The second one restricts s and t to the solid triangle. There are also three pure states.

5.2.3. Type III. It has two cases $(s, t) = (a, \alpha_2), (\beta_1, \alpha_2)$. From (22) and (25) we get

$$|\vec{\mathbf{V}}|^2 = 2(s^2 + t^2) \leqslant \tfrac{2}{3}, \qquad F(s, t) = \tfrac{1}{9} - s^2 - t^2 + 3s^2 t \geqslant 0. \tag{28}$$

The first condition gives allowed values of parameters s and t within a dashed circle (figure 2 (left)). Second one restricts the values of s, t to a figure drawn by solid lines. Moreover we have two pure states.

5.2.4. Type IV. In this case, we also have two possibilities $(s, t) = (b, \alpha_2), (\alpha_1, \alpha_2)$. The conditions following from (22) and (25) are the same as for type III only with t replaced by $-t$. So type IV is just a mirror image of type III.

5.2.5. Type V. Type V has four representatives, namely $(s, t) = (y, a), (y, b), (y, \alpha_1), (y, \beta_1)$. From (22) with (25) we have

$$|\vec{\mathbf{V}}|^2 = s^2 + 2t^2 \leqslant \frac{2}{3}, \qquad F(s, t) = \frac{1}{9} - \frac{s^2}{2} - t^2 - \frac{3t^2 s + s^3}{\sqrt{6}} \geqslant 0. \tag{29}$$

The first requirement puts the allowed points on and within a dashed ellipse (figure 3). Second condition implies that the values of s and t are to the right of the straight line $s = -\sqrt{2/3}$ and within a solid ellipse. In this case, there is only one pure state.

5.2.6. Type VI. This type is most numerous, it is specified by 11 cases. They are $(s, t) = (a, b), (a, \alpha_1), (a, \beta_1), (a, \beta_2), (b, \alpha_1), (b, \beta_1), (b, \beta_2), (\alpha_1, \beta_1), (\alpha_1, \beta_2), (\beta_1, \beta_2), (\alpha_2, \beta_2)$. Then, requirements (22) and (25) yield

$$|\vec{\mathbf{V}}|^2 = 2(s^2 + t^2) \leqslant \tfrac{2}{3}, \qquad F(s, t) = \tfrac{1}{9} - s^2 - t^2 \geqslant 0, \tag{30}$$

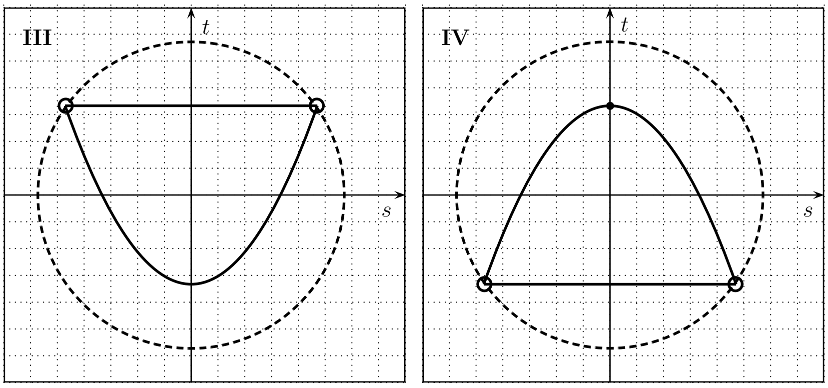

Figure 2. Type III (left) and type IV (right). The dashed circles radii are $R = 1/\sqrt{3}$. Allowed states lie on the solid lines and inside the figure drawn by them. For type III the straight line is $t = 1/3$, while the parabola is given by $t = 3s^2 - 1/3$; pure states (small circles) are at $(\pm\sqrt{2}/3, 1/3)$. Type IV is just a mirror image: $t \to -t$.

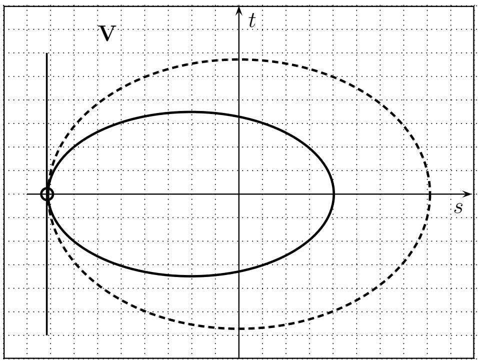

Figure 3. Type V. Allowed states lie on and inside the solid ellipse. Its centre is at $(-1/2\sqrt{6}, 0)$ and its semi-axes are equal to $\sqrt{3/8}$ and $1/\sqrt{8}$. The dashed ellipse has semi-axes $\sqrt{3/8}$ and $1/\sqrt{3}$. A single pure state occurs at $(-\sqrt{2/3}, 0)$.

because in this case we find $T_3 = 0$. Both conditions specify circles. The first one gives a dashed circle in figure 4, while the next yields the more restrictive smaller (solid) circle. No pure states are allowed here.

5.2.7. Type VII. The last type is given by six pairs, that is by $(s, t) = (x, a)$, (x, b), (x, α_1), (x, β_1), (x, α_2), (x, β_2). Then relations (22) and (25) give the requirements

$$|\vec{\mathbf{V}}|^2 = s^2 + 2t^2 \leqslant \frac{2}{3}, \qquad F(s, t) = \frac{1}{9} - \frac{s^2}{2} - t^2 \geqslant 0, \tag{31}$$

since in this case we also have $T_3 = 0$. The first condition restricts the allowed values of s and t to a larger (dashed in figure 4) ellipse. The second one places the allowed points to within and on a smaller (solid) ellipse. As in the previous type there are no pure states.

5.2.8. Features common to all seven types. All types are characterized by the two-parameter behaviour of $|\vec{\mathbf{V}}|^2$ and $F(s, t)$, the latter proportional to $\det \hat{\rho}$. The requirement $F(s, t) \geqslant 0$

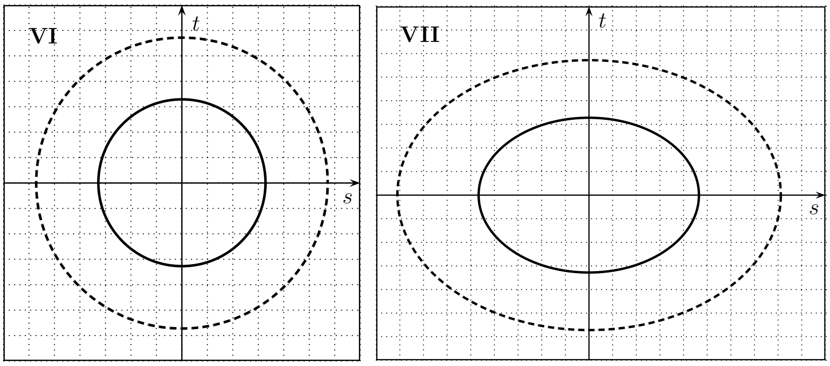

Figure 4. Type VI (left) and type VII (right). The allowed states lie on and within the solid curves. For type VI the radii of the circles are $1/\sqrt{3}$ and $1/3$. The dashed ellipse for type VII has semi-axes equal to $\sqrt{2/3}$ and $1/\sqrt{3}$, while for the solid one we have semi-axes $\sqrt{2}/3$ and $1/3$. There are no pure states.

is always more restrictive than that imposed upon the length of the Bloch vector $\vec{\mathbf{V}}$. That shows that the set of all density matrices is a proper subset of the hyperball determined by $|\vec{\mathbf{V}}|^2 \leqslant 2/3$.

The allowed values of parameters lie on and inside the solid contours which correspond to $F(s,t) = 0$. Since for pure states we have $|\vec{\mathbf{V}}|^2 = 2/3$ and $\det \hat{\rho} = 0$, it is not surprising that pure states are situated at the extremal points of solid contours.

Inside these contours $F(s,t)$ is obviously positive and for all cases attains its maximal value equal to $1/9$ at the point $(0,0)$ which corresponds to $\vec{\mathbf{V}} = 0$, that is to a maximally mixed state.

6. Final remarks

We have presented and discussed the representation of the $N \times N$ density matrix in terms of polarization operators $\mathbf{T}_{LM}(j)$. This idea is not new (see, for example [7–9]), but it seems that it was not previously used to discuss the important issue of positivity. The usefulness of this approach, as it seems to us, stems from the fact that polarization operators are expressed in terms of quantities known from the quantum theory of angular momentum which facilitates all considerations and allows derivation of expressions valid for any $N = 2j + 1$. For example, it is straightforward to find commutators, products, traces over products, etc. This can be done analytically, but also with the aid of computer programs allowing symbolic mathematics. These possibilities seem to indicate that the discussed approach is indeed useful in practice.

Polarization operators $\mathbf{T}_{LM}(j)$ constitute a basis in the space of $N \times N$ matrices (operators). Expansion of the density matrix (as in (8)) establishes a relationship between these and $\vec{\mathbf{V}}$'s—generalized Bloch vectors. Normalization is then automatically ensured. Hermiticity follows from the requirement $V^*_{LM} = (-1)^M V_{L-M}$ for the components of $\vec{\mathbf{V}}$. This also reduces the number of independent real parameters to $N^2 - 1$ and fixes the dimension of the space of generalized Bloch vectors.

The density operator must be also positive. We have investigated this question with the formalism allowing one to check whether the positivity conditions are met by given Hermitian and normalized matrix. Successive positivity requirements (that is inequalities $S_k^{(N)} \geqslant 0$ for $k \geqslant 2$) are derived for any N. These requirements specify and restrict the space of vectors $\vec{\mathbf{V}}$.

Expression (14) allows computation of the quantities T_m which, in turn, are used to compute coefficients $S_k^{(N)}$ as in (16). In particular, the requirement $S_2^{(N)} \geqslant 0$ entails $\mathrm{Tr}\{\hat{\rho}^2\} \leqslant 1$ which, in terms of Bloch vector yields $|\vec{\mathbf{V}}|^2 \leqslant (N-1)/N$. So, all vectors $\vec{\mathbf{V}}$ lie within an (N^2-1)-dimensional hyperball of radius equal to $\sqrt{(N-1)/N}$. However, further conditions $S_k^{(N)} \geqslant 0$ (for $k \geqslant 3$) severely restrict the set of allowed Bloch vectors. This set is a proper subset of the mentioned hyperball and it possesses quite a complicated structure. In the two previous sections, we employed the presented procedure to a qubit ($N = 2$) and to qutrit ($N = 3$). The former is quite simple, while the analysis of a qutrit gives support to all given remarks.

Finally, we would like to indicate some possibilities which probably deserve further attention. Polarization operators are spherical irreducible tensors [7]. Therefore, their tensor products preserve their character. This fact seems to be promising in the investigations of entangled states. We hope that this can provide new insights into the structure and geometry of entangled states. As indicated by Biedenharn and Louck [8], polarization operators constitute just another (non-standard) set of $SU(N)$ generators. This set is endowed with an interesting structure as it follows from inspection of the structure constants appearing in the commutators of polarization operators (see [7], equations (2.4.19) and (20)). Investigations based upon this fact go beyond the scope of this work, but seem to be an interesting subject for future studies of the space of allowed generalized Bloch vectors and therefore of the geometry of the space of density operators.

We end this paper with the hope that the revitalized expansion of the density operator in terms of polarization operators will prove useful in other investigations. The presented discussion of the correspondence between density operators and generalized Bloch vectors (especially in the light of requirement of positivity) is applicable to any dimension. The quantities appearing here are strongly connected with angular momentum theory and thereby well known. This, to our minds, indicates that the representation discussed here may be more practical than the 'standard' one.

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