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Parameterizing qudit states

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Quantum systems with a finite number of states at all times have been a primary element of many physical models in nuclear and elementary particle physics, as well as in condensed matter physics. Today, however, due to a practical demand in the area of developing quantum technologies, a whole set of novel tasks for improving our understanding of the structure of finite-dimensional quantum systems has appeared.

In the present article we will concentrate on one aspect of such studies related to the problem of explicit parameterization of state space of an N-level quantum system. More precisely, we will discuss the problem of a practical description of the unitary $SU(N)$-invariant counterpart of the N-level state space $\mathfrak{P}_N$, i.e., the unitary orbit space $\mathfrak{P}_N/SU(N)$. It will be demonstrated that the combination of well-known methods of the polynomial invariant theory and convex geometry provides useful parameterization for the elements of $\mathfrak{P}_N/SU(N)$. To illustrate the general situation, a detailed description of $\mathfrak{P}_N/SU(N)$ for low-level systems: qubit ($N = 2$), qutrit ($N = 3$), quatrit ($N = 4$) — will be given.

Key words and phrases: density matrix parameterization, quantum system, qubit, qutrit, quatrit, qudit, polynomial invariant theory, convex geometry

1. Introduction

Quantum mechanics is a unitary invariant probabilistic theory of finite-dimensional systems. Both basic features, the invariance and the randomness, strongly impose on the mathematical structure associated with the state

space $\mathfrak{P}$ of a quantum system. In particular, the geometrical concept of the convexity of the state space originates from the physical assumption of an ignorance about the quantum states. Furthermore, the convex structure of the state space, according to the Wigner [1] and Kadison [2] theorems about quantum symmetry realization, leads to unitary or anti-unitary invariance of the probability measures (short exposition of the interplay between these two theorems see e.g. in [3]). In turn of the action of unitary/anti-unitary transformations $\varrho \longrightarrow \varrho' = U\varrho U^{\dagger}$ sets the equivalence relation $\varrho \simeq \varrho'$ between the states $\varrho, \varrho' \in \mathfrak{P}$ and defines the factor space $\mathfrak{P}/U$. This space is a fundamental object containing all physically relevant information about a quantum system. An efficacious way to describe $\mathcal{O}[\mathfrak{P}_N] \coloneqq \mathfrak{P}_N/SU(N)$ for an N-level quantum system is a primary motivation of the present article. The properties of $\mathcal{O}[\mathfrak{P}_N]$, as a semi-algebraic variety, are reflected in the structure of the center of the enveloping algebra $\mathfrak{U}(\mathfrak{su}(N))$. Hence, it is pertinently to describe $\mathcal{O}[\mathfrak{P}_N]$ using the algebra of real $SU(N)$-invariant polynomials defined over the state space $\mathfrak{P}_N$. Following this observation in a series of our previous publications [4]–[8], we develop description of $\mathcal{O}[\mathfrak{P}_N]$ using the classical invariant theory [9].

It is worth noting that within this description of the state space the entanglement properties of binary composite systems can be analyzed as well. In [5], [6] qubit-qubit and qubit-qutrit pairs were studied from this standpoint. In particular, the optimal integrity basis for the polynomial $SU(2) \times SU(2)$ invariant ring of a two-qubit system was proposed and the separability criterion was formulated via polynomial inequalities in three $SU(4)$ Casimir invariants and two determinants of the so-called correlation and the Schlienz–Mahler entanglement matrices, which are the $SU(2) \times SU(2)$ polynomial scalars.

On the other hand, $\mathfrak{P}_N/SU(N)$ is related to the co-adjoint orbits space $\mathfrak{su}^*(N)/SU(N)$ and hence it is natural to describe $\mathfrak{P}_N/SU(N)$ directly in terms of non-polynomial variables — the spectrum of density matrices. Below we will describe a scheme which combines these points of view and provides description of the orbit space $\mathfrak{P}_N/SU(N)$ in terms of one second order polynomial invariant, the Bloch radius of a state and additional non-polynomial invariants, the angles corresponding to the projections of a unit $(N-2)$-dimensional vector on the weight vectors of the fundamental representation of $SU(N)$.

The article is organised as follows. The next section is devoted to brief statements of general results about the state space $\mathfrak{P}_N$ of N-dimensional quantum systems, including discussion of its convexity (Section 2.1) and semi-algebraic structure (Section 2.2). Particularly, the set of polynomial inequalities in an (N^2-1)-dimensional Bloch vector and the equivalent set of inequalities in $N-1$ polynomial $SU(N)$-invariants will be presented for arbitrary N-level quantum systems. Section 3 contains information on the orbit space $\mathcal{O}[\mathfrak{P}_N]$ — the factor space of the state space under equivalence relation against the unitary group adjoint action. In Section 3.3.1 we introduce a new type of parameterization of a qubit, a qutrit and a quatrit based on the representation of the orbit space of a qudit as a spherical polyhedron on $\mathbb{S}_{N-2}$. This parameterization allows us to give a simple formulation of the conception of the hierarchy of subsystems inside one another. In Section 3.3.2 we present

formal elements of the suggested scheme for an arbitrary final-dimensional system. Section 4 contains a few remarks on possible applications of the introduced version of the qudit parameterization.

2. The state space

The state space of a quantum system $\mathfrak{P}_N$ comes in many faces. One can discuss its mathematical structure from several points of view: as a topological set, as a measurable space, as a convex body, as a Riemannian manifold.[1] Below we concentrate mainly on a brief description of $\mathfrak{P}_N$ as a convex body realized as a semi-algebraic variety in $\mathbb{R}^{N^2-1}$ following in general the publications [4]–[8].

2.1. The state space as a convex body

According to the Hilbert space formulation of the quantum theory, a possible state of a quantum system is associated to a self-adjoint, positive semi-definite *"density operator"* acting on a Hilbert space. Considering a non-relativistic N-dimensional system whose Hilbert space $\mathcal{H}$ is $\mathbb{C}^N$, the density operator can be identified with the Hermitian, unit trace, positive semi-definite $N \times N$ *density matrix* [14], [15].

The set of all possible density matrices forms the *state space* $\mathfrak{P}_N$ of an N-dimensional quantum system. It is a subset of the space of complex $N \times N$ matrices:

$$\mathfrak{P}_N = \{\varrho \in M_N(\mathbb{C}) \,|\, \varrho = \varrho^\dagger,\ \varrho \geqslant 0,\ \mathrm{Tr}\,\varrho = 1\}.$$

A generic non-minimal rank matrix ϱ describes the *mixed state*, while the singular matrices with $\mathrm{rank}\,(\varrho) = 1$ are associated to *pure states*. Since the set of N-th order Hermitian matrices has a real dimension N^2, and due to the finite trace condition $\mathrm{Tr}\,(\varrho) = 1$, the dimension of the state space is $\dim(\mathfrak{P}_N) = N^2 - 1$. The semi-positivity condition $\varrho \geqslant 0$ restricts it further to a certain (N^2-1)-dimensional *convex body*. The convexity of $\mathfrak{P}_N$ is the fundamental property of the state space. The next propositions summarize results on a general pattern of the state space $\mathfrak{P}_N$ as a convex set with an interior $\mathrm{Int}\,(\mathfrak{P}_N)$ and a boundary $\partial\mathfrak{P}_N$ [10].

Proposition 1. Given two states $\varrho_1, \varrho_2 \in \mathrm{Int}(\mathfrak{P}_N)$ and a "probability" $p \in [0,1]$, consider the convex combination

$$\varrho_p := (1-p)\varrho_1 + p\varrho_2,$$

then $\varrho_p \in \mathrm{Int}(\mathfrak{P}_N)$.

Proposition 2. The boundary $\partial\mathfrak{P}_N$ consists of non-invertible matrices of all possible non-maximal ranks:

$$\partial\mathfrak{P}_N = \{\varrho \in \mathfrak{P}_N \,|\, \det(\varrho) = 0\}\,.$$

[1] Here is a short and extremely subjective list of publications on these issues [10]–[13].

The subset of pure states $\mathfrak{F}_N \subset \partial\mathfrak{P}_N$, $\mathfrak{F}_N = \{\varrho \in \partial\mathfrak{P}_N \,|\, \mathrm{rank}(\varrho) = 1\}$, contains N extreme boundary points $\mathscr{P}_i(\varrho)$ which generate the whole $\mathfrak{P}_N$ by taking the convex combination:

$$\varrho = \sum_{i=0}^{N} r_i \mathscr{P}_i(\varrho), \quad \sum_{i=0}^{N} r_i = 1, \quad r_i \geqslant 0. \tag{1}$$

In (1) every extreme component $\mathscr{P}_i(\varrho)$ can be related to the standard rank-one projector by a common unitary transformation $U \in SU(N)$ and transposition $P_{i(1)}$ interchanging the first and i-th position:

$$\mathscr{P}_i(\varrho) = U P_{i(1)}\, \mathbf{diag}(1, 0, \ldots, 0)\, P_{i(1)}\, U^{\dagger}.$$

For any dimension of the quantum system the subset of extreme states provides important information about the properties of all possible states, even the pure states comprise a manifold of a real dimension $\dim(\mathfrak{F}_N) = 2N - 2$, smaller than that dimension of the whole state space boundary $\dim(\partial\mathfrak{P}_N) = N^2 - 2$.

2.2. The state space as a semi-algebraic variety

According to the decomposition (1), the neighbourhood of a generic point of $\mathfrak{P}_N(\mathbb{R}^{N^2-1})$ is locally homeomorphic to $(U(N)/U(1)^N) \times D^{N-1}$, where the component D^{N-1} is an $(N-1)$-dimensional disc (cf. [10], [13]). Following this result, below we will describe how the state space $\mathfrak{P}_N$ can be realized as a convex body in $\mathbb{R}^{N^2-1}$ defined via a finite set of polynomial inequalities involving the Bloch vector of a state. In order to formalize the description of the state space, we consider the universal enveloping algebra $\mathfrak{U}(\mathfrak{su}(\mathrm{N}))$ of the Lie algebra $\mathfrak{su}(\mathrm{N})$. Choosing the orthonormal basis $\lambda_1, \lambda_2, \ldots, \lambda_{N^2-1}$ for $\mathfrak{su}(\mathrm{N})$,

$$\mathfrak{su}(\mathrm{N}) = \sum_{i=1}^{\mathrm{N}^2-1} \xi_i \lambda_i, \tag{2}$$

the density matrix will be identified with the element from $\mathfrak{U}(\mathfrak{su}(\mathrm{N}))$ of the form:

$$\varrho(N) = \frac{1}{N}\mathbb{I}_N + \sqrt{\frac{N-1}{2N}} \sum_{i=1}^{\mathrm{N}^2-1} \xi_i \lambda_i. \tag{3}$$

The analysis (see e.g. consideration in [4], [6]) shows the possibility of description of the state space via polynomial constraints on the Bloch vector of an N-level quantum system.

Proposition 3. If a real (N^2-1)-dimensional vector $\vec{\xi} = (\xi_1, \xi_2, \ldots, \xi_{N^2-1})$ in (3) satisfies the following set of polynomial inequalities:

$$S_k(\vec{\xi}) \geqslant 0, \quad k = 1, 2, \ldots N, \tag{4}$$

where $S_k(\vec{\xi})$ are coefficients of the characteristic equation of the density matrix ϱ:

$$\det \|x - \varrho\| = x^N - S_1 x^{N-1} + S_2 x^{N-2} - \cdots + (-1)^N S_N = 0, \tag{5}$$

then the equation (3) defines the states $\varrho \in \mathfrak{P}_N$.

The inequalities (4), which guarantee the semi-positivity of the density matrix, remain unaffected by unitary changes of the basis of the Lie algebra and thus the semi-algebraic set (4) can be equivalently rewritten in terms of the elements of the $SU(N)$-invariant polynomial ring $\mathbb{R}[\mathfrak{P}_N]^{\mathrm{SU(N)}}$. This ring can be equivalently represented by the integrity basis in the form of homogeneous polynomials $\mathcal{P} = (t_1, t_2, \dots, t_N)$,

$$\mathbb{R}\left[\xi_1, \xi_2, \dots, \xi_{N^2-1}\right]^{\mathrm{SU(N)}} = \mathbb{R}\left[t_1, t_2, \dots, t_N\right].$$

The useful, from a computational point of view, polynomial basis $\mathcal{P}$ is given by the *trace invariants* of the density matrix:

$$t_k := \mathrm{Tr}(\varrho^k). \tag{6}$$

The coefficients S_k, being $SU(N)$-invariant polynomial functions of the density matrix elements, are expressible in terms of the trace invariants via the well-known determinant formulae:

$$S_k = \frac{1}{k!} \det \begin{pmatrix} t_1 & 1 & 0 & \cdots & 0 \\ t_2 & t_1 & 2 & \cdots & 1 \\ t_3 & t_2 & t_1 & \cdots & \\ \vdots & \vdots & \vdots & \vdots\vdots\vdots & k-1 \\ t_k & t_{k-1} & t_{k-2} & \cdots & t_1 \end{pmatrix}.$$

Aiming at more economic description of $\mathfrak{P}_N$, we pass from $N^2 - 1$ Bloch variables to $N-1$ independent trace variables t_k. Pay for such a simplification is necessity to take into account additional constraints on t_k which reflect the Hermicity of the density matrix. Below we give the explicit form of these constraints in terms of $\mathcal{P} = (t_1, t_2, \dots, t_N)$.

In accordance with the classical results, the *Bézoutian*, the matrix $\mathrm{B} = \Delta^T \Delta$, constructed from the Vandermonde matrix Δ, accommodates information on the number of distinct roots (via its rank), numbers of real roots (via its signature), as well as the Hermicity condition. A real characteristic polynomial has all its roots *real and distinct* if and only if the Bézoutian is positive definite. For generic invertible density matrices — matrices with all eigenvalues different, the positivity of the Bézoutian reduces to the requirement

$$\det \|\mathrm{B}\| > 0. \tag{7}$$

Noting that the entries of the Bézoutian are simply the trace invariants:

$$\mathrm{B}_{ij} = t_{i+j-2}, \tag{8}$$

one can get convinced that the determinant of the Bézoutian is nothing else than the *discriminant* of the characteristic equation of the density matrix, $\mathrm{Disc} = \prod_{i>j} \left(r_i - r_j\right)^2$, rewritten in terms of the trace polynomials[2]

$$\mathrm{Disc}(t_1, t_2, \dots, t_N) := \det \|\mathrm{B}\|. \tag{9}$$

Hence, we arrive at the following result.

Proposition 4. The following set of inequalities in terms of the trace $SU(N)$-invariants,

$$\mathrm{Disc}\,(t_1, t_2, \dots, t_N) \geqslant 0, \quad S_k\,(t_1, t_2, \dots, t_N) \geqslant 0, \quad t_1 = 1, \tag{10}$$

define the same semi-algebraic variety as the inequalities (4) in $N^2 - 1$ Bloch coordinates do.

3. Orbit space $\mathfrak{P}_N/SU(N)$

3.1. Parameterizing $\mathfrak{P}_N/SU(N)$ via polynomial invariants

Proposition 4 is a useful starting point for establishing a stratification of the $\mathfrak{P}_N$ under the adjoint action of the $SU(N)$ group. It turns out that, due to the unitary invariant character of the inequalities (10), they accommodate all nontrivial information on possible strata of unitary orbits on the state space $\mathfrak{P}_N$. Indeed, it is easy to find the link between the description of $\mathfrak{P}_N$ given in the previous section and the well-known method developed by Abud–Sartori–Procesi–Schwarz (ASPS) for construction of the orbit space of compact Lie group [16]–[18]. The basic ingredients of this approach can be very shortly formulated as follows.

Consider a compact Lie group G acting linearly on a real d-dimensional vector space V. Let $\mathbb{R}[V]^{\mathrm{G}}$ be the corresponding ring of the G-invariant polynomials on V. Assume $\mathcal{P} = \left(t_1, t_2, \dots, t_q\right)$ is a set of homogeneous polynomials that form the integrity basis, $\mathbb{R}[\xi_1, \xi_2, \dots, \xi_d]^{\mathrm{G}} = \mathbb{R}[t_1, t_2, \dots, t_q]$. Elements of the integrity basis define the polynomial mapping:

$$t:\ V \to \mathbb{R}^q; \quad (\xi_1, \xi_2, \dots, \xi_d) \to \left(t_1, t_2, \dots, t_q\right). \tag{11}$$

Since the map t is constant on the orbits of G, it induces a homeomorphism of the orbit space V/G and the image X of t-mapping; $V/G \simeq X$ [19]. In order to describe X in terms of $\mathcal{P}$ uniquely, it is necessary to take into account the *syzygy ideal* of $\mathcal{P}$, i.e.,

$$I_{\mathcal{P}} = \left\{h \in \mathbb{R}\left[y_1, y_2, \dots, y_q\right] : h\left(p_1, p_2, \dots, p_q\right) = 0,\ \text{in } \mathbb{R}[V]\right\}.$$

Let $Z \subseteq \mathbb{R}^q$ denote the locus of common zeros of all elements of $I_{\mathcal{P}}$, then Z is an algebraic subset of $\mathbb{R}^q$ such that $X \subseteq Z$. Denoting by $\mathbb{R}[Z]$ the restriction

[2] The dependence of the discriminant on trace invariants only up to order N pointed in the left side of (9) assumes that all higher trace invariants t_k with $k > N$ in (9) are expressed via polynomials in $t_1, t_2, \dots, t_N$ (the Cayley–Hamilton Theorem).

of $\mathbb{R}[y_1, y_2, \dots, y_q]$ to Z, one can easily verify that $\mathbb{R}[Z]$ is isomorphic to the quotient $\mathbb{R}[y_1, y_2, \dots, y_q]/I_{\mathcal{P}}$ and thus $\mathbb{R}[Z] \simeq \mathbb{R}[V]^{\mathrm{G}}$. Therefore, the subset Z essentially is determined by $\mathbb{R}[V]^{\mathrm{G}}$, but to describe X the further steps are required. According to [17], [18], the necessary information on X is encoded in the structure of the $q \times q$ matrix with elements given by the inner products of gradients, $\mathrm{grad}(t_i)$:

$$\|\mathrm{Grad}\|_{ij} = \left(\mathrm{grad}\,(t_i)\,, \mathrm{grad}\,\left(t_j\right)\right). \tag{12}$$

Hence, applying the ASPS method to the construction of the orbit space $\mathfrak{P}_N/SU(N)$, one can prove the following proposition.

Proposition 5. The orbit space $\mathfrak{P}_N/SU(N)$ can be identified with the semi-algebraic variety, defined as points satisfying two conditions:

a) The integrity basis for $SU(N)$-invariant ring contains only N independent polynomials, i.e., the syzygy ideal is trivial and the integrity basis elements of $\mathbb{R}[\mathfrak{P}_N]^{\mathrm{SU}(N)}$ are subject to only semi-positivity inequalities

$$S_k\,(t_1, t_2, \dots, t_N) \geqslant 0;$$

b) ASPS inequality $\mathrm{Grad}(z) \geqslant 0$ is equivalent to the semi-positivity of the Bézoutian, provided by existence of the d-tuple where $\chi = (1, 2, \dots, d)$:

$$\mathrm{Grad}\,(t_1, t_2, \dots, t_d) = \chi \mathrm{B}\,(t_1, t_2, \dots, t_d)\,\chi^T. \tag{13}$$

3.2. $\mathfrak{P}_N/SU(N)$ — as a Δ_{N-1}-simplex of eigenvalues

The decomposition of the density matrix (1) over the extreme states explicitly displays the equivalence relation between states,

$$\varrho \overset{SU(N)}{\simeq} \varrho' \text{ if } \varrho' = U\varrho U^{\dagger}, \quad U \in SU(N).$$

Matrices with the same spectrum are unitary equivalent. Furthermore, since the eigenvalues of the density matrix $\mathbf{r} = (r_1, r_2, \dots, r_N)$ in (1) can be always disposed in a decreasing order, the orbit space $\mathfrak{P}_N/SU(N)$ can be identified with the following ordered $(N-1)$-simplex:

$$\Delta_{N-1} = \left\{ \mathbf{r} \in \mathbb{R}^N \,\middle|\, \sum_{i=1}^{N} r_i = 1,\ 1 \geqslant r_1 \geqslant r_2 \geqslant \cdots \geqslant r_N \geqslant 0 \right\}. \tag{14}$$

3.3. $\mathfrak{P}_N/SU(N)$ — as a spherical polyhedron on $\mathbb{S}_{N-2}$

We are now ready to combine the above stated methods of the description of the state space $\mathfrak{P}_N$, the polynomial invariant theory and convex geometry for writing down certain parameterization of density matrices. Based on the extreme decomposition of states (1), the parameterization of the elements of $\mathfrak{P}_N$ reduces to fixing the coordinates on the flag manifolds of $SU(N)$ and the simplex Δ_N of eigenvalues of density matrices. In the remaining

part of the article, we will describe $\mathfrak{P}_N/SU(N)$ in terms of the second order polynomial invariant, which is determined uniquely by the Euclidean length r of the Bloch vector, and $N-2$ angles on the sphere $\mathbb{S}_{N-2}$, whose radius in its turn is given as $\sqrt{\frac{N-1}{N}}\,r$.

3.3.1. Qubit, qutrit and quatrit

In order to demonstrate the main idea of the parameterization, we start with its exemplification by considering three the lowest-level systems, qubit, qutrit and quatrit and afterwards the general case of an N-level system will be briefly outlined.

Qubit. A two-level system, the qubit, is described by a three-dimensional Bloch vector $\vec{\xi} = \{\xi_1, \xi_2, \xi_3\}$:

$$\varrho(2) = \frac{1}{2}\,(\mathbb{I}_2 + \xi_i\sigma_i)\,. \tag{15}$$

The qubit state with the spectrum $\mathbf{r} = \{r_1, r_2\} \in \Delta_1$ is characterized by the only one independent second order $SU(2)$-invariant polynomial $t_2 = r_1^2 + r_2^2$. Introducing the length of the qubit Bloch vector, $r = \sqrt{\xi_1^2 + \xi_2^2 + \xi_3^2}$, we see that[3]

$$t_2 = \frac{1}{2} + \frac{1}{2}\,r^2.$$

Hence, the eigenvalues of the qubit density matrix (15) can be parameterized as

$$r_i = \frac{1}{2} + r\mu_i. \tag{16}$$

It will be explained later that the coincidence of the constants $\mu_1 = 1/2$ and $\mu_2 = -1/2$ in (16) with the standard weights of the fundamental $SU(2)$ representation, when the diagonal Pauli matrix σ_3 is used for the Cartan element of $\mathfrak{su}(2)$ algebra, is not accidental. Below we will give a generalization of (16) for the qudit, an arbitrary N-level system. With this aim it is sapiential to start with considering the $N = 3$ and $N = 4$ cases.

Qutrit. We assume that a generic qutrit state ($N = 3$) has the spectrum $\mathbf{r} = \{r_1, r_2, r_3\}$ from the simplex Δ_2 and thus is an eight-dimensional object. According to the normalization chosen in (3), it is characterized by the 8-dimensional Bloch vector $\vec{\xi} = (\xi_1, \xi_2, \dots, \xi_8)$,

$$\varrho(3) = \frac{1}{3}\,\mathbb{I}_3 + \frac{1}{\sqrt{3}}\,\sum_{i=1}^{8}\,\xi_i\lambda_i. \tag{17}$$

[3]The semi-positivity of state (15) dictates the constraint, $S_2 = 1/2(1 - t_2) \geqslant 0$, which restricts the value of the Bloch vector length: $0 \leqslant r \leqslant 1$.

A qutrit has two independent $SU(3)$ trace invariant polynomials, the first one, $t_2 = r_1^2 + r_2^2 + r_3^2$, is expressible via the Euclidean length of the Bloch vector, $r^2 = \sum_{i=1}^{8} \xi_i^2$,

$$t_2 = \frac{1}{3} + \frac{2}{3}\, r^2, \tag{18}$$

and the third order polynomial invariant, $t_3 = r_1^3 + r_2^3 + r_3^3$, which rewritten in terms of eight components of the Bloch vectors reads:

$$\begin{aligned} t_3 = \frac{1}{9} + \frac{2}{3} r^2 + \frac{2}{\sqrt{3}} \xi_1 \, (\xi_4\xi_6 + \xi_5\xi_7) + \\ + \frac{2}{\sqrt{3}}\, \xi_2\, (\xi_5\xi_6 - \xi_4\xi_7) + \frac{1}{\sqrt{3}}\, \xi_3\, (\xi_4^2 + \xi_5^2 - \xi_6^2 - \xi_7^2) + \\ + \frac{1}{9} \xi_8\, (6\,(\xi_1^2 + \xi_2^2 + \xi_3^2) - 3\,(\xi_4^2 + \xi_5^2 + \xi_6^2 + \xi_7^2) - 2\xi_8^2)\,. \end{aligned} \tag{19}$$

Now we want to rewrite (19) in terms of the Bloch vector of a length r and an additional $SU(3)$ invariant. Having this in mind, it is convenient to pass to new coordinates linked to the structure of the Cartan subalgebra of $\mathfrak{su}(3)$. Choosing the latter as the span of the diagonal SU(3) Gell-Mann matrices and noting that the state (17) is $SU(3)$-equivalent to the diagonal state:

$$\varrho(3) \overset{SU(3)}{\simeq} \frac{1}{3}\, \mathbb{I}_3 + \frac{1}{\sqrt{3}}\, (\mathcal{J}_3 \lambda_3 + \mathcal{J}_8 \lambda_8), \tag{20}$$

one can consider two coordinates $(\mathcal{J}_3, \mathcal{J}_8)$ in the Cartan subalgebra of $\mathfrak{su}(3)$ as independent coordinates in $\mathfrak{P}_3/SU(3)$. Taking into account that for the given values of the second trace invariant (18) the coefficients obey relation $\mathcal{J}_3^2 + \mathcal{J}_8^2 = r^2$, we pass to the polar coordinates on the $(\mathcal{J}_3, \mathcal{J}_8)$-plane,

$$\mathcal{J}_3 = r\, \cos\left(\frac{\varphi}{3}\right), \quad \mathcal{J}_8 = r\, \sin\left(\frac{\varphi}{3}\right). \tag{21}$$

In terms of new variables (r, φ) the expression (19) for the $SU(3)$-polynomial invariant t_3 simplifies,

$$t_3 = \frac{1}{9} + \frac{2}{3}\, r^2 + \frac{2}{9} r^3 \sin\varphi, \tag{22}$$

and the image of the ordered simplex Δ_2 in $(\mathcal{J}_3, \mathcal{J}_8)$-plane under the mapping (21) is given by the triangle $\triangle ABC$:

$$\Delta_2 \mapsto \left\{ 0 \leqslant \mathcal{J}_3 \leqslant \frac{\sqrt{3}}{2}, \quad \frac{1}{\sqrt{3}}\, \mathcal{J}_3 \leqslant \mathcal{J}_8 \leqslant \frac{1}{2} \right\},$$

depicted in the figure 1.

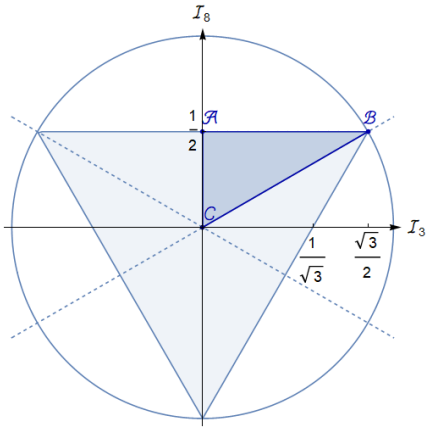

Figure 1. The image of the ordered simplex Δ_2 in $(\mathcal{I}_3, \mathcal{I}_8)$-plane under the mapping (21)

In the figure 1 the Δ_2-simplex of the qutrit eigenvalues is mapped to the triangle $\triangle ABC$ inscribed in a unit-radius circle $\mathcal{I}_3^2 + \mathcal{I}_8^2 = 1$. Its inner part $\triangle ABC$ comprises the points of the maximal rank-3 states $\mathfrak{P}_{3,3}$ with $1 > r_1 > r_2 > r_3 > 0$. All these points generate the *regular* $SU(3)$ orbits $\mathcal{O}_{123}$ of dimension $\dim(\mathcal{O}_{123}) = 6$. The points on the line AB also generate regular orbits $\mathcal{O}_{123}$, however the corresponding states have $\mathrm{rank}(\varrho) = 2$. In contrast to the above case, the line $AC/\{A\}$ and line $BC/\{B\}$ correspond to the subspace of $\mathfrak{P}_{3,3}$, but now the eigenvalues of the states are degenerate, either $r_1 = r_2 > r_3$, or $r_1 > r_2 = r_3$, hence representing the *degenerate orbits* $\mathcal{O}_{1|23}$ and $\mathcal{O}_{12|3}$, respectively. The dimensions of both types of orbits are the same, $\dim(\mathcal{O}_{1|23}) = \dim(\mathcal{O}_{12|3}) = 4$. Finally, the single point $C(0,0)$ represents a maximally mixed state which belongs also to the set of rank-3 states.

The polar form of the invariants (21) prompts us to introduce a unit 2-vector $\vec{n} = (\cos(\varphi/3), \sin(\varphi/3))$ and represent the qutrit eigenvalues as

$$r_i = \frac{1}{3} + \frac{2}{\sqrt{3}}\, r\, \vec{\mu}_i \cdot \vec{n}, \tag{23}$$

with the aid of the weights of the fundamental $SU(3)$ representation:

$$\vec{\mu}_1 = \left(\frac{1}{2}, \frac{1}{2\sqrt{3}}\right), \quad \vec{\mu}_2 = \left(-\frac{1}{2}, \frac{1}{2\sqrt{3}}\right), \quad \vec{\mu}_3 = \left(0, -\frac{1}{\sqrt{3}}\right). \tag{24}$$

Gathering all together, we convinced that the representation (23) is nothing else than the well-known trigonometric form of the roots of the 3-rd order characteristic equation of the qutrit density matrix:

$$r_1 = \frac{1}{3} - \frac{2}{3}\, r\, \sin\left(\frac{\varphi + 4\pi}{3}\right), \quad r_2 = \frac{1}{3} - \frac{2}{3}\, r\, \sin\left(\frac{\varphi + 2\pi}{3}\right), \\ r_3 = \frac{1}{3} - \frac{2}{3}\, r\, \sin\left(\frac{\varphi}{3}\right). \tag{25}$$

It is in order to present a 3-dimensional geometric picture associated to the parameterization (23). The three drawings in the figure 2 with different values of r show that (23) are parametric form of the arc of the red circle which is the intersection $\Delta_2 \cap \mathbb{S}_1(\sqrt{2/3}\, r)$.

The picture in the figure 2 illustrates a geometrical meaning of the parameterization of qutrit eigenvalues (25) in terms of the Bloch radius r and the angle $\varphi \in [0, \pi]$. Consider an intersection of a qutrit simplex Δ_2 with 2-sphere $r_1^2 + r_2^2 + r_3^2 = 1/3 + (2/3)r^2$. The intersection depends on a value of a qutrit Bloch vector. For $r = 0$ the sphere and the simplex Δ_2 intersect at point $C = (1/3, 1/3, 1/3)$, while for $0 < r < 1$ the intersection is an arc $\mathcal{C}_r$ of a circle on the plane $r_1 + r_2 + r_3 = 1$ of the radius $\sqrt{2/3}\, r$ centered at the point $C(1/3, 1/3, 1/3)$. The intersection for $r = 1$ takes place at $B(1, 0, 0)$. The ordering of eigenvalues $1 \geqslant r_1 \geqslant r_2 \geqslant r_3 \geqslant 0$ determines the length of the arc $\mathcal{C}_r$. For any r, the arc $\mathcal{C}_r$ is described by (25), the depicted curve in the figure corresponds to the fixed value $r = 1/4$. Furthermore, varying r within the interval $r \in [0, 1]$, provides the slices covering the whole simplex $\Delta_2 = [0, \pi] \times \mathcal{C}_r$.

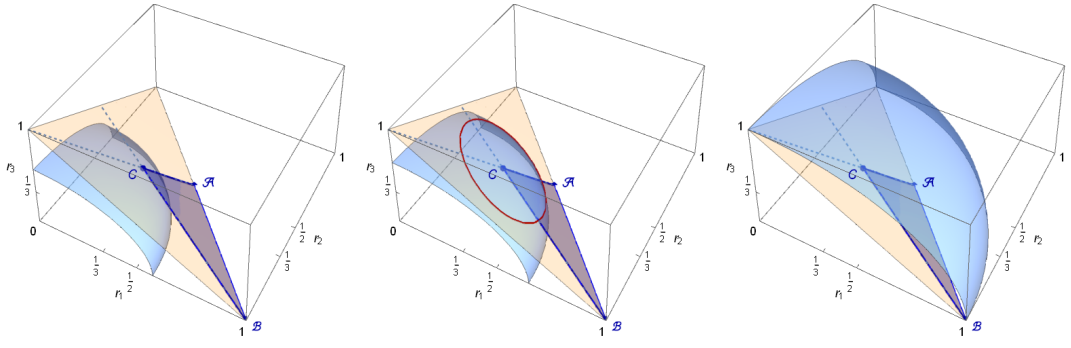

Figure 2. The geometrical meaning of the parameterization of qutrit eigenvalues (25) in terms of the Bloch radius r and the angle $\varphi \in [0, \pi]$

Qutrit Boundary. The introduced parameterization is very useful for analyzing the structure of a qutrit boundary states. The qutrit space $\mathfrak{P}_3$ admits decomposition

$$\mathfrak{P}_3 = \mathfrak{P}_{3,3} \cup \mathfrak{P}_{3,2} \cup \mathfrak{P}_{3,1} \tag{26}$$

into 8d-component of maximal rank-3, 7d-component of rank-2 and extreme pure states. Every component of (26) can be associated with the corresponding domains in the orbit space $\partial\mathcal{O}[\mathfrak{P}_3]$. Particularly, the boundary $\partial\mathcal{O}[\mathfrak{P}_3]$ consists of two components and is described as follows:

— **Qubit inside Qutrit.** For a chosen decreasing order of the qutrit eigenvalues, $r_1 \geqslant r_2 \geqslant r_3$, the rank-2 states belong to the edge Δ_3, given by equation $r_3 = 0$, which in the parameterization (25) reads:

$$\text{rank-2 states}: \quad \left\{ r = \frac{1}{2\,\sin(\varphi/3)} \text{ for } \varphi \in [0, \pi) \right\}. \tag{27}$$

Considering (27) as a polar equation for a plane curve, we find that the rank-2 states $\mathfrak{P}_{3,2}$ can be associated to the part of a 3-order plane curve. Indeed, rewriting (27) in Cartesian coordinates $x = r\cos\varphi$, $y = r\sin\varphi$,

$$(x^2 + y^2)(y - 3a) + 4a^3 = 0,$$

we identify this curve with the famous Maclaurin trisectrix with a special choice of $a = 1/2$.

For the boundary states (27), the equations (25) reduce to

$$r_1 = \frac{1}{2}(1 + r^*_{2\subset 3}), \quad r_2 = \frac{1}{2}(1 - r^*_{2\subset 3}), \tag{28}$$

where

$$r^*_{2\subset 3} = \frac{2}{\sqrt{3}}\sqrt{r^2 - \frac{1}{4}}. \tag{29}$$

These expressions for non-vanishing eigenvalues of a qutrit indicate the existence of a "qubit inside qutrit" whose effective radius is $r^*_{2\subset 3}$. Since the radius of the Bloch vector of rank-2 states associated to a qubit in qutrit lies in the interval $1/2 \leqslant r < 1$, the length of its Bloch vector, $r^*_{2\subset 3}$, takes the same values as a single isolated qubit, $0 \leqslant r^*_{2\subset 3} < 1$.

— **Orbit space of pure states of qutrit.** The boundary $\partial\mathcal{O}[\mathfrak{P}_{3,1}]$ corresponding to all pure states $\mathfrak{P}_{3,1}$ is attainable by $SU(3)$ transformation from the point, $r = 1$ for $\varphi = \pi$.

Quatrit. Now, following the qutrit case, consider a 4-level system, the quatrit, whose mixed state is described by the Bloch vector $\vec{\xi} = \{\xi_1, \xi_2, \dots, \xi_{15}\}$,

$$\varrho(4) = \frac{1}{4}\,\mathbb{I}_4 + \frac{3}{2\sqrt{6}}\sum_{i=1}^{15}\xi_i\lambda_i.$$

The integrity basis for a quatrit ring of $SU(4)$-invariant polynomials $\mathbb{R}[\xi_1, \dots, \xi_{15}]^{\mathrm{SU}(4)}$ consists of three polynomials $\mathbb{R}[t_2, t_3, t_4]$. Using the compact notations (see details in Appendix 5.1), they can be represented in terms of the Casimir invariants of $\mathfrak{su}(4)$ algebra in the following form:

$$\begin{gathered} t_2 = \frac{1}{4} + \frac{3}{4}\,r^2, \quad t_3 = \frac{1}{16} + \frac{9}{16}\,r^2 + \frac{3}{16}\,\vec{\xi}\cdot\vec{\xi}\vee\vec{\xi}, \\ t_4 = \frac{1}{64} + \frac{9}{32}\,r^2 + \frac{3}{16}\,\vec{\xi}\cdot\vec{\xi}\vee\vec{\xi} + \frac{9}{64}r^4 + \frac{1}{64}\,\vec{\xi}\vee\vec{\xi}\cdot\vec{\xi}\vee\vec{\xi}. \end{gathered} \tag{30}$$

From the expressions (30) one can see that apart from the length r of the Bloch vector, there are two independent parameters required to unambiguously

characterize the quatrit eigenvalues. To find them, let us proceed as in the qutrit case. Consider the diagonal form corresponding to a quatrit state:

$$\varrho(4) \overset{SU(4)}{\simeq} \frac{1}{4}\mathbb{I}_4 + \frac{3}{2\sqrt{6}}\left(\mathcal{I}_3\lambda_3 + \mathcal{I}_8\lambda_8 + \mathcal{I}_{15}\lambda_{15}\right). \tag{31}$$

The coefficients $\mathcal{I}_3, \mathcal{I}_8$ and $\mathcal{I}_{15}$ in (31) are invariants under the adjoint $SU(4)$ transformations of ϱ. By equivalence relation (31), the quatrit state space is projected to the following convex body:

$$0 \leqslant \mathcal{I}_3 \leqslant \sqrt{\frac{2}{3}}, \quad \frac{\mathcal{I}_3}{\sqrt{3}} \leqslant \mathcal{I}_8 \leqslant \frac{\sqrt{2}}{3}, \quad \frac{\mathcal{I}_8}{\sqrt{2}} \leqslant \mathcal{I}_{15} \leqslant \frac{1}{3}. \tag{32}$$

The 2-dimensional slice $\mathcal{I}_{15} = 1/3$ of this body corresponds to rank-3 states, see the figure 3. In terms of new invariants, all states with a given length of Bloch vector r belong to a 2-sphere: $\mathcal{I}_3^2 + \mathcal{I}_8^2 + \mathcal{I}_{15}^2 = r^2$. Hence, the corresponding spherical angles φ and θ of these invariants,

$$\mathcal{I}_3 = r\sin\theta\cos\frac{\varphi}{3}, \quad \mathcal{I}_8 = r\sin\theta\sin\frac{\varphi}{3}, \quad \mathcal{I}_{15} = r\cos\theta, \tag{33}$$

can be used as two additional parameters needed for the parameterization of a quatrit eigenvalues.

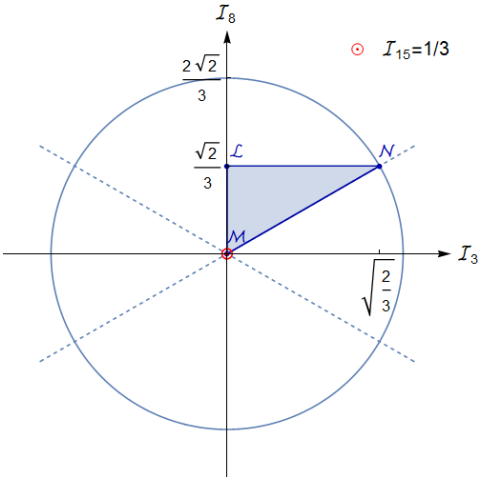

Figure 3. Slice of the convex body (32) as a result of cutting by the plane $\mathcal{I}_{15} = 1/3$

Let us now, in accordance with (33), introduce the unit 3-vector $\vec{n} = (\sin\theta\cos(\varphi/3), \sin\theta\sin(\varphi/3), \cos\theta)$ and parameterize 4-tuple of the eigenvalues of the density matrix $\mathbf{r} = (r_1, r_2, r_3, r_4)$ via the following projections:

$$r_i = \frac{1}{4} + \sqrt{\frac{3}{2}}\, r\, \vec{n}\cdot\vec{\mu}_i, \tag{34}$$

where 3-vectors $\vec{\mu}_1, \vec{\mu}_2, \vec{\mu}_3$ and $\vec{\mu}_4$ denote the weights of the fundamental $SU(4)$. Explicitly the weights read:

$$\begin{gathered} \vec{\mu}_1 = \left(\frac{1}{2}, \frac{1}{2\sqrt{3}}, \frac{1}{2\sqrt{6}}\right), \quad \vec{\mu}_2 = \left(-\frac{1}{2}, \frac{1}{2\sqrt{3}}, \frac{1}{2\sqrt{6}}\right), \\ \vec{\mu}_3 = \left(0, -\frac{1}{\sqrt{3}}, \frac{1}{2\sqrt{6}}\right), \quad \vec{\mu}_4 = \left(0, 0, -\frac{3}{2\sqrt{6}}\right). \end{gathered} \tag{35}$$

Note that the weights $\vec{\mu}_i$ are normalised in a way leading to a unit norm of the simple roots of algebra $\mathfrak{su}(4)$ and obey relations:

$$\sum_{i=1}^{4} \vec{\mu}_i = 0, \quad \text{and} \quad \sum_{i=1}^{4} \mu_i^\alpha \, \mu_i^\beta = \frac{1}{2}\, \delta^{\alpha\beta}. \tag{36}$$

Using these expressions, we arrive at the following parameterization of a quatrit eigenvalues:

$$\begin{gathered} r_1 = \frac{1}{4} - \frac{1}{\sqrt{2}}\, r \left(\sin\theta \sin\frac{\varphi + 4\pi}{3} - \frac{1}{2\sqrt{2}} \cos\theta\right), \\ r_2 = \frac{1}{4} - \frac{1}{\sqrt{2}}\, r \left(\sin\theta \sin\frac{\varphi + 2\pi}{3} - \frac{1}{2\sqrt{2}} \cos\theta\right), \\ r_3 = \frac{1}{4} - \frac{1}{\sqrt{2}}\, r \left(\sin\theta \sin\frac{\varphi}{3} - \frac{1}{2\sqrt{2}} \cos\theta\right), \\ r_4 = \frac{1}{4} - \frac{3}{4}\, r \cos\theta. \end{gathered} \tag{37}$$

To ensure the chosen ordering of the eigenvalues $r_i \in \Delta_3$, the Bloch radius should vary in the interval $r \in [0, 1]$ and angles φ, θ be defined over the domains:

$$\frac{\pi}{6} < \frac{\varphi}{3} < \frac{\pi}{2}, \quad \cot\theta \geqslant \frac{1}{\sqrt{2}} \sin\left(\frac{\varphi}{3}\right). \tag{38}$$

A geometric interpretation of (37), in full analogy with the qutrit case, is described in figure 4.

In the figure 4 the 3-sphere $\sum_i^4 r_i^2 = 1/4 + (3/4)r^2$ intersects the hyperplane $\sum_i^4 r_i = 1$ in the positive quadrant. The intersection occurs iff $1/4 \leqslant 1/4 + (3/4)r^2 \leqslant 1$, and represents the 2-sphere $\mathbb{S}_2(\frac{\sqrt{3}}{2}\, r)$ centered at the point $D = (1/4, 1/4, 1/4, 1/4)$. The intersection with the ordered simplex Δ_3 is given by a spherical polyhedron with 3 or 4 vertices, depending on the Bloch radius r.

The boundary of a quatrit orbit space $\partial\mathcal{O}[\mathfrak{P}_4]$ can be decomposed into 2d-component of rank-3, 1d-component of rank-2 and extreme zero-dimensional component of rank-1, corresponding to pure states:

$$\partial\mathcal{O}[\mathfrak{P}_4] = \partial\mathcal{O}[\mathfrak{P}_{4,3}] \cup \partial\mathcal{O}[\mathfrak{P}_{4,2}] \cup \partial\mathcal{O}[\mathfrak{P}_{4,1}].$$

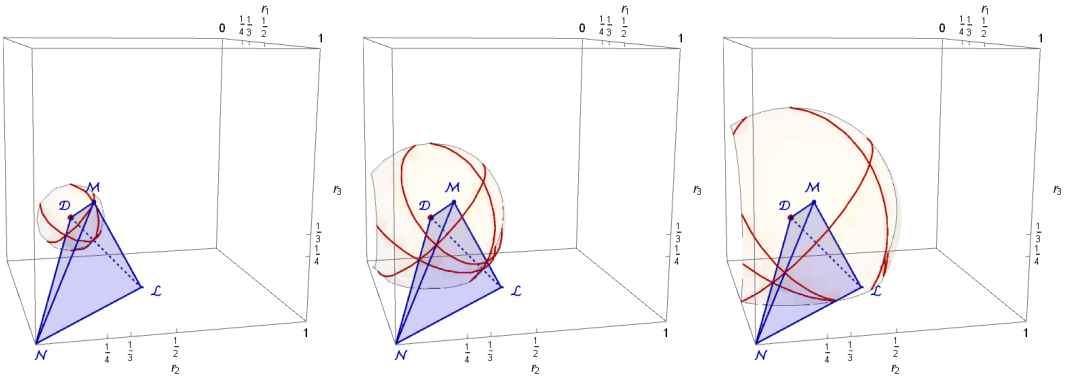

Figure 4. A geometric illustration of (37)

Qutrit inside Quatrit. The boundary component $\mathcal{O}[\mathfrak{P}_{4,3}]$ of rank-3 states is determined by the intersection of 3D simplex Δ_3 with the hyperplane:

$$r_4 = 0. \tag{39}$$

Parameterizing quatrit eigenvalues in terms of angles, the solution to the equation (39) is

$$\cos\theta = \frac{1}{3\,r}, \quad \text{if} \quad r \in \left[\frac{1}{3}, 1\right]. \tag{40}$$

Hence, the parametric form of the 2-dimensional surface $\mathcal{O}[\mathfrak{P}_{4,3}]$ is given in terms of the remaining three non-vanishing eigenvalues:

$$\begin{gathered} r_1 = \frac{1}{3} - \frac{1}{\sqrt{2}}\, f(r)\, \sin\left(\frac{\varphi + 4\pi}{3}\right), \quad r_2 = \frac{1}{3} - \frac{1}{\sqrt{2}}\, f(r)\, \sin\left(\frac{\varphi + 2\pi}{3}\right), \\ r_3 = \frac{1}{3} - \frac{1}{\sqrt{2}}\, f(r) \sin\left(\frac{\varphi}{3}\right), \end{gathered} \tag{41}$$

where $f(r) = \sqrt{r^2 - \frac{1}{9}}$.

Consequences of the above derived formulae deserve few comments.

1. According to the formula (41) for the eigenvalues of boundary rank-3 states, their expressions are similar to the qutrit eigenvalues given in (25). This observation prompts us to introduce the conception of the *"effective qutrit inside quatrit"*, whose Bloch radius value is determined by the Bloch radius of a quatrit:

$$r^*_{3\subset 4} = \frac{3}{2\sqrt{2}} \sqrt{r^2 - \frac{1}{9}}.$$

Note that since the admissible range of the Bloch radius of rank-3 quatrit states is $r \in [1/3, 1]$, then the effective radius $r^*_{3\subset 4}$ takes values in the interval $0 \leqslant r^*_{3\subset 4} < 1$.

2. The idea to identify qutrit inside quatrit is based on the establishing correspondence on the level of orbit spaces $\mathfrak{P}_{4,3}$ and $\mathfrak{P}_{3,3}$. The generic qutrit state in (26) is 8-dimensional, while $\dim(\mathfrak{P}_{4,3}) = 14$. Thus, one can speak about the correspondence between quatrit rank-3 states and qutrit states only modulo unitary transformations.
3. In favour of the idea considering "effective qutrit inside quatrit" is a relation between the polynomial invariants for states on bulk and boundary. Particularly, using expressions for trace polynomials given in Appendix 5.2, we get:
$$t_2^{(4,3)}(r) = t_2^{(3,3)}\left(r^*_{3\subset 4}\right).$$

Qubit inside Qutrit inside Quatrit. In Δ_3 the rank-2 boundary component $\mathcal{O}[\mathfrak{P}_{4,2}]$ is comprised from points on a line given by its intersection with two hypersurfaces:
$$r_4 = 0, \quad r_3 = 0.$$

Following in complete analogy with the rank-3 states, we arrive at "matryoshka" structure with "effective qubit inside qutrit which in turn is inside quatrit". The Bloch radius of this effective qubit is given by the Bloch radius of a quatrit:
$$r^*_{2\subset 3\subset 4} = \frac{3}{\sqrt{6}}\sqrt{r^2 - \frac{1}{3}}.$$

Note that for rank-2 states $r \in [1/\sqrt{3}, 1]$ and hence $0 < r^*_{2\subset 3\subset 4} < 1$.

Finally, the rank-1 boundary component $\mathcal{O}[\mathfrak{P}_{4,1}]$ is generated by one point $\mathbf{r} = (1,0,0,0)$ which represents all pure states in Δ_3.

3.3.2. Generalization to N-level system

Now after examining main features of the introduced parameterization for a qutrit and quatrit, we are ready to give a straightforward generalization to the case of an arbitrary N-level system. With this aim, we will use the Cartan subalgebra of $SU(N)$ as span of the following diagonal $N \times N$ Gell-Mann matrices:
$$H_1 = \operatorname{diag}(1,-1,0,\dots,0),$$
$$H_2 = \frac{1}{\sqrt{3}}\operatorname{diag}(1,1,-2,\dots,0),$$
$$H_k = \frac{2}{\sqrt{2k(k-1)}}\operatorname{diag}\left(\overbrace{1,1,\dots,1}^{k\ times},-k,0,\dots,0\right),$$
$$H_{N-1} = \frac{2}{\sqrt{2N(N-1)}}\operatorname{diag}\left(\overbrace{1,1,\dots,1}^{(N-1)\ times},-(N-1)\right).$$

The corresponding weights of the fundamental $SU(N)$ representation are

$$\vec{\mu}_1 = \left(\frac{1}{2}, \frac{1}{2\sqrt{3}}, \dots, \frac{1}{\sqrt{2k(k+1)}}, \dots, \frac{1}{\sqrt{2N(N-1)}}\right),$$

$$\vec{\mu}_2 = \left(-\frac{1}{2}, \frac{1}{2\sqrt{3}}, \dots, \frac{1}{\sqrt{2k(k+1)}}, \dots, \frac{1}{\sqrt{2N(N-1)}}\right),$$

$$\vec{\mu}_3 = \left(0, -\frac{2}{2\sqrt{3}}, \dots, \frac{1}{\sqrt{2k(k+1)}}, \dots, \frac{1}{\sqrt{2N(N-1)}}\right),$$

$$\vec{\mu}_k = \left(\overbrace{0, 0, \dots, 0}^{(k-2)\ times}, -\sqrt{\frac{k-1}{2k}}, \dots, \frac{1}{\sqrt{2k(k+1)}}, \dots, \frac{1}{\sqrt{2N(N-1)}}\right),$$

$$\vec{\mu}_N = \left(\overbrace{0, 0, \dots, 0}^{(N-2)\ times}, \dots, -\sqrt{\frac{N-1}{2N}}\right).$$

It is easy to verify that the following relations are true:

$$\sum_{i=1}^{N} \vec{\mu}_i = 0, \quad \text{and} \quad \sum_{i=1}^{N} \mu_i^\alpha \, \mu_i^\beta = \frac{1}{2}\, \delta^{\alpha\beta}.$$

Taking into account these observations, one can write down the following parameterization for the roots $\mathbf{r}$ of the Hermitian $N \times N$ matrix:

$$r_i = \frac{1}{N} + \sqrt{\frac{2(N-1)}{N}}\, r\, \vec{\mu}_i \cdot \vec{n}, \tag{42}$$

where $\vec{n} \in \mathbb{S}_{N-2}(1)$ and parameter r provides the fulfillment of the correspondence with a value of the second order invariant,

$$t_2 = \frac{1}{N} + \frac{N-1}{N}\, r^2.$$

Writing the traceless part of the density matrix as the expansion over the Cartan subalgebra H of $\mathfrak{su}(N)$,

$$\varrho(N) - \frac{1}{N}\, \mathbb{I}_N \overset{SU(N)}{\simeq} \sqrt{\frac{(N-1)}{2N}} \sum_{\lambda \in H} \mathcal{J}_s \lambda_s,$$

we see that $N-2$ angles of the unit norm vector $\vec{n}$ (42) are related to the invariants $\mathcal{J}_3^2, \mathcal{J}_8^2, \dots, \mathcal{J}_{N^2-1}^2$, whose values are constrained by the Bloch radius r:

$$\sum_{s=2}^{N} \mathcal{J}_{s^2-1}^2 = r^2. \tag{43}$$

Finally, it is worth to give the geometric arguments which are emphasizing the introduced parameterization (42) of qudit eigenvalues. With this goal consider the intersection $\mathbb{S}_{N-1}(R) \cap \Sigma_{N-1}$ of $(N-1)$-sphere of radius R and hyperplane $\Sigma_{N-1} : \sum_i^N r_i = 1$ in $\mathbb{R}^N$. Let us describe the hyperplane in parametric form, with parameters $s_1, s_2, \dots, s_{N-1}$:

$$\mathbf{r} = \mathbf{d} + \mathbf{e}^{(1)} s_1 + \mathbf{e}^{(2)} s_2 + \cdots + \mathbf{e}^{(N-1)} s_{N-1}, \tag{44}$$

where N-vector $\mathbf{d}$ fixes the point $P \in \Sigma_{N-1}$ and the basis vectors (Darboux frame) obey conditions:

$$\mathbf{d} \cdot \mathbf{e}^{(\alpha)} = 0, \quad \mathbf{e}^{(\alpha)} \cdot \mathbf{e}^{(\beta)} = \delta^{\alpha\beta}, \quad \alpha, \beta = 1, 2, \dots, N-1.$$

Using this parameterization, the equation for $(N-1)$-sphere reduces to the constraint

$$\mathbf{d}^2 + s_1^2 + s_2^2 + \cdots + s_{N-1}^2 = R^2$$

for all points of intersection $\mathbb{S}_{N-1}(R) \cap \Sigma_{N-1}$. Hence, the intersection is nothing else as the $(N-2)$-sphere of radius $R_{N-2} = \sqrt{R^2 - \mathbf{d}^2}$ centered at a point associated to the vector $\mathbf{d} \in \Sigma_{N-1}$. Now if we fix the point P such that $\mathbf{d} = (1/N, \dots, 1/N)$, express the parameters in (44) in terms of the Bloch radius and the components of the unit vector by relation $s_\alpha = \sqrt{2(N-1)/N}\, r\, n_\alpha$ and define the frame vectors $\mathbf{e}^{(\alpha)}$, so that[4]

$$e_i^{(\alpha)} = \sqrt{2}\, \mu_\alpha^{(i)}, \quad i = 1, 2, \dots, N, \quad \text{while} \quad \alpha = 1, 2, \dots, N-1,$$

we arrive at the representation (42) with the radius of intersection sphere $R_{N-2} = \sqrt{(N-1)/N}\, r$.

Passing from hyperplane Σ_{N-1} to its subset, the simplex Δ_{N-1}, we note that $\mathbb{S}_{N-1}(R) \cap \Delta_{N-1}$ will be determined uniquely for every chosen order of the eigenvalues and the value of r. For an arbitrary N, a special analysis is required to write down explicitly $\mathbb{S}_{N-1}(R) \cap \Delta_{N-1}$. Here we only note that the intersection is given by one out of all possible tillings of $\mathbb{S}_{N-2}$ by the spherical polyhedra. For $N = 3$ such polyhedron degenerates to an arc of a circle, whereas for $N = 4$ the intersection will be given by two types of polyhedra, either a spherical triangle, or a spherical quadrilateral, depending on the value of the Bloch radius r.

4. Concluding remarks

Since the introduction of the concept of mixed quantum states, the problem of an efficient parameterization of density matrices in terms of independent variables became one of the important tasks of numerous studies. Starting with the famous Bloch vector parameterization [20], several alternative types of "coordinates" for points of quantum states have been suggested [21]–[30]. According to the generalization of Bloch vector parameterization, initially introduced for a 2-level system, the Bloch vector for an N-level system is a real

[4]Here α component of i-th weights $\vec{\mu}^{(i)}$ determines i-th component of basis vector $\mathbf{e}^{(\alpha)}$.

(N^2-1)-dimensional vector. However, owing to the unitary symmetry of an isolated quantum system, those N^2-1 parameters can be divided into two special subsets. The first subset is given by $N-1$ unitary invariant parameters, and the second one is compiled from the coordinates on a certain flag manifold constructed from the $SU(N)$ group. Introduction of the coordinates on both subsets has a long history. A description of the former set of $SU(N)$-invariant parameters is related to the classical problem of determination of roots of a polynomial equation, while the latter corresponds to a description of the homogeneous spaces of $SU(N)$ group [5].

In the present article we have discussed the first part of the problem of parameterization of $N \times N$ density matrices and proposed a general form of parameterization of N-tuple of its eigenvalues in terms of a length r of the Bloch vector and $N-2$ angles on sphere $\mathbb{S}_{N-2}(\sqrt{(N-1)/N}r)$. We expect that this parameterization will be useful from a computational point of view in many physical applications including the models of elementary particles. Particularly, in forthcoming publications it will be used for the evaluation of very recently introduced indicators of quantumness/classicality of quantum states which are based on the potential of the Wigner quasidistributions to attain negative values [35]–[37].

5. Appendix

5.1. Constructing Casimir invariants for $\mathfrak{su}(N)$ algebra

In this Appendix we collect few notions and formulae explaining the construction of the polynomial Casimir invariants on the Lie algebra $\mathfrak{g} = \mathfrak{su}(N)$ of the group $G = SU(N)$.

Consider algebra $\mathfrak{g} = \sum_i^{N^2-1} \xi_i \lambda_i$, spanned by the orthonormal basis $\{\lambda_i\}$ with the multiplication rule

$$\lambda_i \lambda_j = \frac{2}{N}\delta_{ij} + (d_{ijk} + \imath f_{ijk})\,\lambda_k, \tag{45}$$

defined via the symmetric d_{ijk} and anti-symmetric f_{ijk} structure constants. Let $\{\omega^i\}$ be the dual basis in $\mathfrak{g}^*$, i.e., $\omega^i(\lambda_j) = \delta^i_j$, and introduce the G-invariant symmetric tensor S of order r:

$$S = S_{i_1 i_2 \ldots i_r}\, \omega^{i_1} \otimes \omega^{i_2} \cdots \otimes \omega^{i_r}. \tag{46}$$

The G-invariance of tensor S means that

$$\sum_{s=1}^{r} f^m_{i i_s} S_{i_1 i_2 \ldots i_{s-1} m i_{s+1} \ldots i_r} = 0. \tag{47}$$

[5] Among the important contributions to the problem of parameterizing $SU(N)$, we would like to mention the following publications that influenced the present work: [31]–[34].

Using the tensor S, one can construct the elements of the enveloping algebra $\mathcal{U}(\mathfrak{g})$:

$$C_r = S_{i_1 i_2 \ldots i_r} \lambda_{i_1} \lambda_{i_2} \ldots \lambda_{i_r}, \tag{48}$$

which turns to belong to the center of $\mathcal{U}(\mathfrak{g})$, i.e., $[C_r, \lambda_i] = 0$, for all generators λ_i. Having in mind the solution to the invariance equations (47), one can build the polynomials in $N^2 - 1$ real variables $\vec{\xi} = (\xi_1, \xi_2, \ldots \xi_{N^2-1})$:

$$\mathfrak{C}_r(\vec{\xi}) = \sum_i S_{i_1 i_2 \ldots i_r} \xi_{i_1} \xi_{i_2} \ldots \xi_{i_r},$$

which are invariant under the adjoint $SU(N)$-transformations:

$$p(\overrightarrow{\mathrm{Ad}_g(\xi)}) = p(\vec{\xi}).$$

It can be proved that the symmetric tensors $k^{(r)}$ defined in the given basis of algebra as $k^{(r)}_{i_1 i_2 \ldots i_r} = \mathrm{Tr}\left(\lambda_{\{i_1} \lambda_{i_2} \ldots \lambda_{i_r\}}\right)$, satisfy invariance equation (47) and form the basis for the polynomial ring of G-invariants. The tensors $k^{(r)}$ admit decomposition with the aid of the lowest symmetric invariants tensors, δ_{ij} and d_{ijk}. Particularly, the following combinations are valid candidates for the basis:

$$\begin{aligned} k^{(4)}_{i_1 i_2 i_3 i_4} &= d_{\{i_1 i_2\} s} d_{\{i_3 i_4\} s}, \\ k^{(5)}_{i_1 i_2 i_3 i_4 i_5} &= d_{\{i_1 i_2\} s} d_{s i_3 t} d_{\{i_4 i_5\} t}, \\ k^{(6)}_{i_1 i_2 i_3 i_4 i_5 i_6} &= d_{\{i_1 i_2\} s} d_{s i_3 t} d_{t, i_4, u} d_{\{i_5 i_6\} u}. \end{aligned}$$

As an example, for N-level system the G-invariant polynomials up to order six read:

$$\begin{aligned} \mathfrak{C}_2 &= (N-1)\, \vec{\xi}^{\,2}, \\ \mathfrak{C}_3 &= (N-1)\, \vec{\xi} \cdot \vec{\xi} \vee \vec{\xi}, \\ \mathfrak{C}_4 &= (N-1)\, \vec{\xi} \vee \vec{\xi} \cdot \vec{\xi} \vee \vec{\xi}, \\ \mathfrak{C}_5 &= (N-1)\, \vec{\xi} \vee \vec{\xi} \vee \vec{\xi} \vee \vec{\xi} \cdot \vec{\xi}, \\ \mathfrak{C}_6 &= (N-1)\, (\vec{\xi} \vee \vec{\xi} \vee \vec{\xi})^2. \end{aligned} \tag{49}$$

In the equation (49) the Casimir invariants are represented in a dense vectorial notation using the auxiliary (N^2-1)-dimensional vector defined via the symmetrical structure constants d_{ijk} of the algebra $\mathfrak{su}(N)$:

$$(\vec{\xi} \vee \vec{\xi})_k := \sqrt{\frac{N(N-1)}{2}}\, d_{ijk}\, \xi_i \xi_j.$$

5.2. Polynomial $SU(N)$-invariants on $\mathfrak{P}_N$

In this section the explicit formulae for polynomial invariants for quatrit will be given in terms of the suggested parameterization of density matrices. Since the traceless part of the density matrices, $\varrho - \frac{1}{N} I_N = \sqrt{\frac{(N-1)}{2N}}\ \mathfrak{g}$, belongs

to the algebra $\mathfrak{su}(N)$, all trace polynomials t_k can be expanded over the $\mathfrak{su}(N)$ Casimir invariants. The corresponding decomposition of independent polynomials for the quatrit ($N = 4$) read:

$$t_2 = \frac{1}{4}(1 + 3\mathfrak{C}_2),$$

$$t_3 = \frac{1}{4^2}(1 + 3\mathfrak{C}_2 + \mathfrak{C}_3),$$

$$t_4 = \frac{1}{4^3}\left(1 + 6\mathfrak{C}_2 + 4\mathfrak{C}_3 + \mathfrak{C}_2^2 + \mathfrak{C}_4\right).$$

In order to derive the explicit form of polynomials $\mathfrak{C}_2$ and $\mathfrak{C}_3$, the knowledge of components of the symmetric structure tensor d is needed. It is convenient at first to express the invariants for diagonal states, characterized by $\mathcal{I}_3$, $\mathcal{I}_8$ and $\mathcal{I}_{15}$, and afterwards rewrite them for generic states using parameterization (33). With this aim, we collect (up to permutations) in the table 1 all non-zero coefficients d_{ijk} for the Cartan subalgebra of $\mathfrak{su}(3)$ and $\mathfrak{su}(4)$.

Table 1
Symmetric structure constants for the Cartan subalgebra of $\mathfrak{su}(3)$ and $\mathfrak{su}(4)$

i.j.k	3.3.8	3.3.15	8.8.8	8.8.15	15.15.15
$d_{ijk}^{\mathrm{SU(4)}}$	$\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$-\frac{1}{\sqrt{3}}$	$\frac{1}{\sqrt{6}}$	$-\sqrt{\frac{2}{3}}$
$d_{ijk}^{\mathrm{SU(3)}}$	$\frac{1}{\sqrt{3}}$		$-\frac{1}{\sqrt{3}}$		

Taking into account the values for structure constant d from the table 1, the Casimir invariants of the third and fourth order of a quatrit read:

$$\mathfrak{C}_3 = 9\,\mathcal{I}_{15}\left(\mathcal{I}_3^2 + \mathcal{I}_8^2\right) + 9\sqrt{2}\,\mathcal{I}_8\left(\mathcal{I}_3^2 - \frac{1}{3}\,\mathcal{I}_8^2\right) - 6\,\mathcal{I}_{15}^3, \tag{50}$$

$$\mathfrak{C}_4 = 9\,\left(\mathcal{I}_3^2 + \mathcal{I}_8^2\right)^2 + 36\sqrt{2}\,\mathcal{I}_8\,\mathcal{I}_{15}\left(\mathcal{I}_3^2 - \frac{1}{3}\,\mathcal{I}_8^2\right) + 12\,\mathcal{I}_{15}^4. \tag{51}$$

Finally, plugging expressions (33) into (50) and (51), we arrive at the representation of the $\mathfrak{su}(4)$ Casimir invariants in terms of quatrit Bloch radius r and two angles (θ, φ):

$$\mathfrak{C}_3 = \frac{3}{4}\,r^3\left[4\sqrt{2}\sin^3(\theta)\sin(\varphi) - 3\cos(\theta) - 5\cos(3\theta)\right],$$

$$\mathfrak{C}_4 = \frac{3}{8}r^4\left[32\sqrt{2}\sin^3(\theta)\cos(\theta)\sin(\varphi) + 4\cos(2\theta) + 7\cos(4\theta) + 21\right],$$

as well as directly for the trace polynomial invariants,

$$t_2 = \frac{1}{4} + \frac{3}{4}r^2,$$

$$t_3 = \frac{1}{16} + \frac{9}{16}r^2 + \frac{3}{64}r^3\left(4\sqrt{2}\sin^3\theta\sin\varphi - 3\cos\theta - 5\cos(3\theta)\right),$$

$$t_4 = \frac{1}{64} + \frac{9}{32}r^2 + \frac{3}{64}r^3\left(4\sqrt{2}\,\sin^3\theta\sin\varphi - 3\cos\theta - 5\cos(3\theta)\right) + \\ + \frac{3}{512}r^4\left(32\sqrt{2}\sin^3\theta\cos\theta\sin\varphi + 4\cos(2\theta) + 7\cos(4\theta) + 45\right).$$

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Параметризация состояний кудита

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Квантовые системы с конечным числом состояний всегда были основным элементом многих физических моделей в ядерной физике, физике элементарных частиц, а также в физике конденсированного состояния. Однако сегодня, в связи с практической потребностью в области развития квантовых технологий, возник целый ряд новых задач, решение которых будет способствовать улучшению нашего понимания структуры конечномерных квантовых систем.

В статье мы сфокусируемся на одном из аспектов исследований, связанных с проблемой явной параметризации пространства состояний N-уровневой квантовой системы. Говоря точнее, мы обсудим вопрос практического описания унитарного пространства орбит — $SU(N)$-инвариантного аналога N-уровневого пространства состояний $\mathfrak{P}_N$. В работе будет показано, что сочетание хорошо известных методов теории полиномиальных инвариантов и выпуклой геометрии позволяет получить удобную параметризацию для элементов $\mathfrak{P}_N/SU(N)$. Общая схема параметризации $\mathfrak{P}_N/SU(N)$ будет детально проиллюстрирована на примере низкоуровневых систем: кубита ($N = 2$), кутрита ($N = 3$), куатрита ($N = 4$).

Ключевые слова: параметризация матрицы плотности, квантовая система, кубит, кутрит, куатрит, кудит, теория полиномиальных инвариантов, выпуклая геометрия