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Hilbert–Schmidt volume of the set of mixed quantum states

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Abstract

We compute the volume of the convex (N^2-1)-dimensional set $\mathcal{M}_N$ of density matrices of size N with respect to the Hilbert–Schmidt measure. The hyper-area of the boundary of this set is also found and its ratio to the volume provides information about the structure of $\mathcal{M}_N$. Similar investigations are also performed for the smaller set of all real density matrices. As an intermediate step, we analyse volumes of the unitary and orthogonal groups and of the flag manifolds.

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1. Introduction

Although the notion of a density matrix is one of the fundamental concepts discussed in the elementary courses of quantum mechanics, the structure of the set $\mathcal{M}_N$ of all density matrices of size N is not easy to characterize [1–3]. The only exception is the case $N = 2$, for which $\mathcal{M}_2$ embedded in $\mathbb{R}^3$ has the appealing form of the *Bloch ball*. Its boundary, $\partial\mathcal{M}_2$, consists of pure states and forms the *Bloch sphere*. For larger numbers of states the dimensionality of $\mathcal{M}_N$ grows quadratically with N, which makes its analysis involved. In particular, for $N > 2$ the set of pure states forms a $(2N-2)$-dimensional manifold, of measure zero in the (N^2-2)-dimensional boundary $\partial\mathcal{M}_N$.

In this work, we compute the volume of $\mathcal{M}_N$ with respect to the Hilbert–Schmidt (HS) measure. The HS measure is defined by the HS metric which is distinguished by the fact that it induces the flat, Euclidean geometry into the set of mixed states. The (hyper)area of the boundary of the space of the density matrices, $\partial\mathcal{M}_N$, is also computed, as well as the area of (hyper)edges of this set—the HS volume of the subspace of density matrices of an arbitrary rank $k < N$. In the special case of $k = 1$, we obtain a well-known formula for the volume of the space of pure states, equivalent to the complex projective manifold $\mathbb{C}P^{N-1}$.

A similar analysis is also performed for the set of real density matrices. To calculate the volume of the set of complex (real) mixed states, we use the volume of the unitary (orthogonal) groups and the volume of the complex (real) flag manifolds—these results are described in the appendix.

The motivation for such a study is twofold. On one hand, the complex structure of the set of mixed quantum states is interesting in itself. It is well known that for $N > 2$ the $D = N^2 - 1$ dimensional set $\mathcal{M}_N$ is neither a D-ball nor a polytope, but what does it look like? More like a ball or more like a polytope? Instead of using techniques of differential geometry and computing the average curvature on the boundary of the set $\mathcal{M}_N$, we compute the volume of its boundary and compare it with the volume of the $D-1$ sphere, which surrounds the ball of the same volume as $\mathcal{M}_N$. Such a comparison shows us to what extent the shape of the body of mixed quantum states differs from the ball, in that sense that more (hyper)area of the surface is needed to cover the same volume.

Complementary information characterizing the structure of a given set is obtained by calculating the ratio between the area of its boundary and its volume. Among all D-dimensional bodies of a fixed volume, such a ratio is the smallest for the D-ball. Hence computing such a ratio for the D-dimensional body of mixed quantum states we may compare it with similar ratios obtained for D-balls, D-cubes and D-simplices.

On the other hand, our investigations might be useful in characterizing the absolute volume of the subset of mixed states distinguished by a certain attribute. For instance, if ϱ describes a composite system, one may ask, what is the volume of the set of separable (entangled) mixed states [4, 5]. Furthermore, assume we are given a concrete mixed quantum state ϱ, it is natural to ask whether ϱ is in some sense typical, e.g., whether its von Neumann entropy is close to the average taken over the entire set $\mathcal{M}_N$ with respect to the HS measure. To compute such averages (see, e.g., [6]) it is useful to know the volume of $\mathcal{M}_N$ and to make use of integrals developed for such a calculation.

2. Geometry of $\mathcal{M}_N$ with respect to the Hilbert–Schmidt metric

The set of mixed quantum states $\mathcal{M}_N$ consists of Hermitian, positive matrices of size N, normalized by the trace condition

$$\mathcal{M}_N := \{\varrho : \varrho = \varrho^\dagger; \varrho \geqslant 0; \operatorname{Tr}\varrho = 1; \dim(\rho) = N\}. \tag{2.1}$$

It is a compact convex set of dimensionality $D = N^2 - 1$. Any density matrix may be diagonalized by a unitary rotation,

$$\varrho = U\Lambda U^{-1} \tag{2.2}$$

where Λ is a diagonal matrix of eigenvalues Λ_i. Due to the trace condition they satisfy $\sum_{i=1}^N \Lambda_i = 1$, so the space of spectra is isomorphic with a $(N-1)$-dimensional simplex Δ_{N-1}.

Let B be a diagonal unitary matrix. Since $\varrho = UB\Lambda B^\dagger U^\dagger$, in the generic case of a non-degenerate spectrum the unitary matrix U is determined up to N arbitrary phases entering B. To specify uniquely the unitary matrix of eigenvectors U, it is thus sufficient to select a point on the coset space $Fl_{\mathbb{C}}^{(N)} := U(N)/[U(1)]^N$, called the complex *flag manifold*. The generic density matrix is thus determined by $(N-1)$ parameters determining eigenvalues and $N^2 - N$ parameters related to eigenvectors, which sum up to the dimensionality D of $\mathcal{M}_N$. Although for degenerate spectra the dimension of the flag manifold decreases (see, e.g., [3, 7]), these cases of measure zero do not influence the estimation of the volume of the entire set of density matrices. Several different distances may be introduced into the set $\mathcal{M}_N$ (see for instance [7, 8]). In this work we shall use the Hilbert–Schmidt metric, which induces the flat geometry.

The Hilbert–Schmidt distance between any two density operators is defined as the Hilbert–Schmidt (Frobenius) norm of their difference,

$$D_{\mathrm{HS}}(\varrho_1, \varrho_2) = \|\varrho_1 - \varrho_2\|_{\mathrm{HS}} = \sqrt{\mathrm{Tr}[(\varrho_1 - \varrho_2)^2]}. \tag{2.3}$$

The set of all mixed states of size two acquires under this metric the geometry of the Bloch ball $\mathbf{B}^3$ embedded in $\mathbb{R}^3$. Its boundary, $\partial\mathbf{B}^3 = \mathbf{S}^2$ contains all pure states and is called the *Bloch sphere*. To show this let us use the Bloch representation of a $N = 2$ density matrix

$$\varrho = \frac{\mathbb{I}}{N} + \vec{\tau} \cdot \vec{\lambda} \tag{2.4}$$

where $\vec{\lambda}$ denotes the vector of three rescaled traceless Pauli matrices $\{\sigma_x, \sigma_y, \sigma_z\}/\sqrt{2}$. They are normalized according to $\mathrm{Tr}\,\lambda_i^2 = 1$. The three-dimensional Bloch vector $\vec{\tau}$ is real due to Hermiticity of ϱ. Positivity requires $\mathrm{Tr}\,\varrho^2 \leqslant 1$ and this implies $|\vec{\tau}| \leqslant 1/\sqrt{2} =: R_2$. Demanding equality one distinguishes the set of all pure states, $\varrho^2 = \varrho$, which form the Bloch sphere of radius R_2. Consider two arbitrary density matrices and express their difference $\varrho_1 - \varrho_2$ in the representation (2.4). The entries of this difference consist of the differences between components of both Bloch vectors $\vec{\tau}_1$ and $\vec{\tau}_2$. Therefore

$$D_{\mathrm{HS}}\big(\varrho_{\vec{\tau}_1}, \varrho_{\vec{\tau}_2}\big) = D_{\mathrm{E}}(\vec{\tau}_1, \vec{\tau}_2) \tag{2.5}$$

where D_{E} is the Euclidean distance between both Bloch vectors in $\mathbb{R}^3$. This proves that with respect to the HS metric the set $\mathcal{M}_2$ possesses the geometry of a ball $\mathbf{B}^3$. The unitary rotations of a density matrix $\varrho \to U\varrho U^\dagger$ correspond to the rotations of $\vec{\tau}$ in $\mathbb{R}^3$. This is due to the fact that the adjoint representation of $SU(2)$ is isomorphic with $SO(3)$.

The Hilbert–Schmidt metric induces a flat geometry inside $\mathcal{M}_N$ for arbitrary N. Any state ϱ may be represented by (2.4), but now the $\vec{\lambda}$ represents an operator-valued vector which consists of $D = N^2 - 1$ traceless Hermitian generators of $SU(N)$, which fulfil $\mathrm{Tr}\,\lambda_i\lambda_j = \delta_{ij}$. This generalized Bloch representation of density matrices for arbitrary N was introduced by Hioe and Eberly [9], and recently used in [10]. The case $N = 3$, related to the Gell-Mann matrices, is discussed in detail in a paper by Arvind *et al* [11]. The generalized Bloch vector $\vec{\tau}$ (also called *coherence vector*) is D dimensional. In the general case of an arbitrary N the right-hand side of (2.5) denotes the Euclidean distance between two Bloch vectors in $\mathbb{R}^{N^2-1}$. Positivity of ρ implies the bound for its length

$$|\vec{\tau}| \leqslant D_{\mathrm{HS}}(\mathbb{I}/N, |\psi\rangle\langle\psi|) = \sqrt{\frac{N-1}{N}} =: R_N. \tag{2.6}$$

In contrast to the Bloch sphere, the complex projective space $\mathbb{C}\mathbf{P}^{N-1}$, which contains all pure states, forms for $N > 2$ only a measure zero, simply connected $2(N-1)$-dimensional subset of the $(N^2 - 2)$-dimensional sphere of radius R_N embedded in $\mathbb{R}^{N^2-1}$. Thus not every vector $\vec{\tau}$ of the maximal length R_N represents a quantum state. This is related to the fact that for $N \geqslant 3$ the adjoint representation of $SU(N)$ forms only a subset of $SO(N^2 - 1)$, (see, e.g., [12]). Sufficient and necessary conditions for a Bloch vector to represent a pure state were given in [11] for $N = 3$, and in [13] for an arbitrary N. Furthermore, by far not all vectors of length shorter then R_N represent a quantum state, as not all the points inside a hyper-sphere belong to the simplex inscribed inside it. Necessary conditions for a Bloch vector to represent a quantum-mixed state were recently provided by Kimura [14]. On the other hand, there exists a smaller sphere inscribed inside the set $\mathcal{M}_N$. Its radius reads [2]

$$r_N = D_{\mathrm{HS}}(\mathbb{I}/N, \varrho_{N-1}) \frac{1}{\sqrt{N(N-1)}} = \frac{R_N}{N-1} \tag{2.7}$$

where ϱ_{N-1} denotes any state with the spectrum $\left(\frac{1}{N-1}, \ldots, \frac{1}{N-1}, 0\right)$.

3. Hilbert–Schmidt measure

Any metric in the space of mixed quantum states generates a measure, inasmuch as one can assume that drawing random density matrices from each ball of a fixed radius is equally likely. The balls are understood with respect to a given metric. In this work we investigate the measure induced by the Hilbert–Schmidt distance (2.3). The infinitesimal distance takes a particularly simple form

$$(\mathrm{d}s_{\mathrm{HS}})^2 = \mathrm{Tr}[(\mathrm{d}\varrho)^2] \tag{3.1}$$

valid for any dimension N. Making use of the diagonal form $\rho = U\Lambda U^{-1}$ we may write

$$\mathrm{d}\varrho = U[\mathrm{d}\Lambda + U^{-1}\,\mathrm{d}U\,\Lambda - \Lambda U^{-1}\,\mathrm{d}U]U^{-1}. \tag{3.2}$$

Thus (3.1) can be rewritten as

$$(\mathrm{d}s_{\mathrm{HS}})^2 = \sum_{i=1}^{N} (\mathrm{d}\Lambda_i)^2 + 2\sum_{i<j}^{N} (\Lambda_i - \Lambda_j)^2 |(U^{-1}\,\mathrm{d}U)_{ij}|^2. \tag{3.3}$$

Since the density matrices are normalized, $\sum_{i=1}^{N} \Lambda_i = 1$, thus $\sum_{i=1}^{N} \mathrm{d}\Lambda_i = 0$. Hence one may consider the variation of the Nth eigenvalue as a dependent one, $\mathrm{d}\Lambda_N = -\sum_{i=1}^{N-1} \mathrm{d}\Lambda_i$, which implies

$$\sum_{i=1}^{N} (\mathrm{d}\Lambda_i)^2 = \sum_{i=1}^{N-1} (\mathrm{d}\Lambda_i)^2 + \left(\sum_{i=1}^{N-1} \mathrm{d}\Lambda_i\right)^2 = \sum_{i,j=1}^{N-1} \mathrm{d}\Lambda_i\, g_{ij}\, \mathrm{d}\Lambda_j. \tag{3.4}$$

The corresponding volume element gains a factor $\sqrt{\det g}$, where g is the metric in the $(N-1)$-dimensional simplex Δ_{N-1} of eigenvalues. From (3.4) one may read out the explicit form of the metric g_{ij}

$$g = \begin{bmatrix} 1 & & 0 \\ & \ddots & \\ 0 & & 1 \end{bmatrix} + \begin{bmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{bmatrix}. \tag{3.5}$$

It is easy to check that the spectrum of the $(N-1)$-dimensional matrix g consists of one eigenvalue equal to N and the remaining $N-2$ eigenvalues equal to unity, so that $\det g = N$. Thus the Hilbert–Schmidt volume element is given by

$$\mathrm{d}V_{\mathrm{HS}} = \sqrt{N} \prod_{j=1}^{N-1} \mathrm{d}\Lambda_j \prod_{j<k}^{1\cdots N} (\Lambda_j - \Lambda_k)^2 \left| \prod_{j<k}^{1\cdots N} 2\,\mathrm{Re}(U^{-1}\,\mathrm{d}U)_{jk}\, \mathrm{Im}(U^{-1}\,\mathrm{d}U)_{jk} \right| \tag{3.6}$$

and has the following product form

$$\mathrm{d}V = \mathrm{d}\mu(\Lambda_1, \Lambda_2, \ldots, \Lambda_N) \times \mathrm{d}\nu_{\mathrm{Haar}}. \tag{3.7}$$

The first factor depends only on the eigenvalues Λ_i, while the latter one depends on the eigenvectors of ϱ which compose the unitary matrix U.

Any unitary matrix may be considered as an element of the Hilbert–Schmidt space of operators with the scalar product $\langle A|B\rangle = \operatorname{Tr} A^\dagger B$. This suggests the following definition of an invariant metric of the unitary group $U(N)$,

$$(\mathrm{d}s)^2 := -\operatorname{Tr}(U^{-1}\,\mathrm{d}U)^2 = \sum_{jk=1}^{N} |(U^{-1}\,\mathrm{d}U)_{jk}|^2 = \sum_{j=1}^{N} |(U^{-1}\,\mathrm{d}U)_{jj}|^2 + 2\sum_{j<k=1}^{N} |(U^{-1}\,\mathrm{d}U)_{jk}|^2. \tag{3.8}$$

This metric induces the unique Haar measure ν_{Haar} on $U(N)$, invariant with respect to unitary transformations, $\nu_{\mathrm{Haar}}(W) = \nu_{\mathrm{Haar}}(UW)$, where W denotes an arbitrary measurable subset of $U(N)$. Integrating the volume element corresponding to (3.8) over the unitary group we obtain the volume

$$\operatorname{Vol}[U(N)] = \frac{(2\pi)^{N(N+1)/2}}{1!2!\cdots(N-1)!}. \tag{3.9}$$

Integrating the volume element with the diagonal terms in (3.8) omitted (in that case the diagonal elements of U are fixed by $U_{ii} \geqslant 0$) we obtain the volume of the complex flag manifold, $Fl_{\mathbb{C}}^{(N)} := U(N)/[U(1)^N]$,

$$\operatorname{Vol}\big[Fl_{\mathbb{C}}^{(N)}\big] = \frac{\operatorname{Vol}[U(N)]}{(2\pi)^N} = \frac{(2\pi)^{N(N-1)/2}}{1!2!\cdots(N-1)!}. \tag{3.10}$$

Both results are known in the literature for almost fifty years [15]. However, since many different conventions in defining the volume of the unitary group are in use [16–22] we sketch a derivation of the above expressions in the appendix and provide a list of related results.

Comparing formulae (3.6) and (3.8) we recognize that the measure ν, responsible for the choice of eigenvectors of ϱ, is the natural measure on the complex flag manifold $Fl_{\mathbb{C}}^{(N)} = U(N)/[U(1)^N]$ induced by the Haar measure on $U(N)$. Since the trace is unitarily invariant, it follows directly from the definition (3.1) that the volume element with respect to the HS measure is invariant with respect to the group of unitary rotations, $\mathrm{d}V_{\mathrm{HS}}(\varrho) = \mathrm{d}V_{\mathrm{HS}}(U\varrho U^\dagger)$. Such a property is characteristic of any *product measure* of the form (3.7). Several product measures with different choices of μ were examined in [5, 6, 22, 23].

Integrating the volume element (3.6) with respect to the eigenvectors of ϱ distributed according to the Haar measure one obtains the probability distribution in the simplex of eigenvalues

$$P_{\mathrm{HS}}^{(2)}(\Lambda_1,\ldots,\Lambda_N) = C_N^{\mathrm{HS}}\,\delta\left(1-\sum_{j=1}^{N}\Lambda_j\right)\prod_{j<k}^{N}(\Lambda_j-\Lambda_k)^2 \tag{3.11}$$

where for future convenience we have decorated the symbol P with the superscript $^{(2)}$ consistent with the exponent in the last factor. As discussed in the following section the normalization constant C_N^{HS} may be expressed [6] in terms of the Euler gamma function $\Gamma(x)$ [24]

$$C_N^{\mathrm{HS}} = \frac{\Gamma(N^2)}{\prod_{j=0}^{N-1}\Gamma(N-j)\Gamma(N-j+1)}. \tag{3.12}$$

The above joint probability distribution, derived by Hall [26], defines the measure μ_{HS} in the space of diagonal matrices and the *Hilbert–Schmidt* measure (3.6) in the space of density matrices $\mathcal{M}_N$.

Interestingly, the very same measure may be generated by drawing random pure states $|\phi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ of a composite $N \times N$ system according to the Fubini–Study measure on $\mathbb{C}\mathbf{P}^{N^2-1}$. Then the density matrices of size N obtained by partial trace, $\varrho = \operatorname{Tr}_2(|\phi\rangle\langle\phi|)$, are distributed according to the HS measure [6, 26, 27]. Alternatively, one may generate a random matrix A of the Ginibre ensemble (non-Hermitian complex matrix with all entries independent Gaussian variables with zero mean and a fixed variance) and obtain a HS distributed random density matrix by a projection $\varrho = A^\dagger A/\mathrm{Tr}\, A^\dagger A$ [6]. A similar approach was recently advocated by Tucci [25], who used the name 'uniform ensemble' for just such an ensemble of density matrices generated according to the HS measure.

4. Volume of the set of mixed states

For convenience let us introduce generalized normalization constants

$$\frac{1}{C_N^{(\alpha,\beta)}} := \int_0^\infty \mathrm{d}\Lambda_1 \cdots \mathrm{d}\Lambda_N \delta\left(\sum_{i=1}^N \Lambda_i - 1\right) \prod_{i=1}^N \Lambda_i^{\alpha-1} \prod_{i<j} |\Lambda_i - \Lambda_j|^\beta \tag{4.1}$$

with $\alpha, \beta > 0$. These constants may be calculated using the formula for the Laguerre ensemble, discussed in the book of Mehta [29],

$$\int_0^\infty \mathrm{d}\Lambda_1 \cdots \mathrm{d}\Lambda_N \exp\left(-\sum_{i=1}^N \Lambda_i\right) \prod_{i=1}^N \Lambda_i^{\alpha-1} \prod_{i<j} |\Lambda_i - \Lambda_j|^\beta$$
$$= \prod_{j=1}^N \left[\frac{\Gamma[1 + j\beta/2]\Gamma[\alpha + (j-1)\beta/2]}{\Gamma[1 + \beta/2]}\right]. \tag{4.2}$$

Substituting $x_i^2 = \Lambda_i$ we may bring the latter integral to the Gaussian form. Expressing it in spherical coordinates we get the integral (4.1) and eventually obtain

$$\frac{1}{C_N^{(\alpha,\beta)}} := \frac{1}{\Gamma[\alpha N + \beta N(N-1)/2]} \prod_{j=1}^N \left[\frac{\Gamma[1 + j\beta/2]\Gamma[\alpha + (j-1)\beta/2]}{\Gamma[1 + \beta/2]}\right]. \tag{4.3}$$

By definition $C_N^{\mathrm{HS}} = C_N^{(1,2)}$ and the special case of the above expression reduces to (3.12).

To obtain the Hilbert–Schmidt volume of the set of mixed states $\mathcal{M}_N$ one has to integrate the volume element (3.6) over eigenvalues and eigenvectors. By definition the first integral gives $1\big/C_N^{\mathrm{HS}}$, while the second is equal to the volume of the flag manifold. To make the diagonalization transformation (2.2) unique, one has to restrict to a certain order of eigenvalues, say, $\Lambda_1 < \Lambda_2 < \cdots < \Lambda_N$ (a generic density matrix is not degenerate), which corresponds to a choice of a certain Weyl chamber of the eigenvalue simplex Δ_{N-1}. In other words, different permutations of the vector of N generically different eigenvalues Λ_i belong to the same unitary orbit. The number of different permutations (Weyl chambers) equals to $N!$, so the volume reads

$$V_N^{(2)} := \mathrm{Vol}_{\mathrm{HS}}(\mathcal{M}_N) = \frac{\sqrt{N}}{N!} \frac{\mathrm{Vol}\big(Fl_{\mathbb{C}}^{(N)}\big)}{C_N^{\mathrm{HS}}}. \tag{4.4}$$

The square root stems from the volume element (3.6), and the index $^{(2)}$ refers to the general case of complex density matrices. Making use of (3.12) and (3.10) we arrive at the final result[4]

$$V_N^{(2)} = \sqrt{N}(2\pi)^{N(N-1)/2} \frac{\Gamma(1)\cdots\Gamma(N)}{\Gamma(N^2)}. \tag{4.5}$$

Substituting $N = 2$ we are pleased to receive $V_2^{(2)} = \pi\sqrt{2}/3$—exactly the volume of the Bloch ball $\mathbf{B}^3$ of radius $R_2 = 1/\sqrt{2}$. This result may be also found in the notes of Caves [22], who also derived an explicit integral for the volume of the set of mixed states for arbitrary N.

[4] Apart from the first factor $\sqrt{N}$, the same formula has already appeared in the work of Tucci [25].

The next result $V_3^{(2)} = \pi^3/(840\sqrt{3})$ allows us to characterize the difference between the set $\mathcal{M}_3 \subset \mathbb{R}^8$ and the ball $\mathbf{B}^8$. The set of mixed states is inscribed into the sphere of radius $R_3 = \sqrt{2/3} \approx 0.816$, while the maximal ball contained inside has the radius $r_3 = R_3/2 \approx 0.408$. Using equation (6.1) we find the radius of the 8-ball of volume V_3 is $\rho_3 \approx 0.519$. The distance from the centre of $\mathcal{M}_3$ to its boundary varies with the direction in $\mathbb{R}^8$ from r_3 to R_3, in contrast to the $N = 2$ case of the Bloch ball, for which $R_2 = r_2 = \rho_2 = 1/\sqrt{2}$. The average HS-distance from the centre of $\mathcal{M}_3$ to its boundary is equal to ρ_3. Similar calculations performed for $N = 4$ give the maximal radius $R_4 = \sqrt{3/4} \approx 0.866$, the minimal radius $r_4 = R_4/3 \approx 0.289$ and the 'mean' radius $\rho_4 \approx 0.428$ which generates the ball $\mathbf{B}^{15}$ of the same volume as V_4. In general, let ρ_N denote the radius of a ball $\mathbf{B}^{N^2-1}$ of the same volume as the set $\mathcal{M}_N$.

The volume V_N tends to zero if $N \to \infty$, but there is no reason to worry about it. The same is true for the volume of the N-ball, see (6.1). This is just a consequence of the choice of the units. We are comparing the volume of an object in $\mathbb{R}^N$ with the volume of a hypercube C^N of side one, and it is easy to understand that, the larger the dimension, the smaller the volume of the ball inscribed into it.

5. Area of the boundary of the set of mixed states

The boundary of the set of mixed states is far from being trivial. Formally it may be written as a solution of the equation $\det \varrho = 0$ which contains all matrices of a lower rank. The boundary $\partial\mathcal{M}_N$ contains orbits of different dimensionality generated by spectra of different rank and degeneracy (see, e.g., [3, 7]). Fortunately all of them are of measure zero besides the generic orbits created by unitary rotations of diagonal matrices with all eigenvalues different and one of them equal to zero; $\Lambda = \{0, \Lambda_2 < \Lambda_3 < \cdots < \Lambda_N\}$. Such spectra form the $(N-2)$-dimensional simplex Δ_{N-2}, which contains $(N-1)!$ the Weyl chambers—this is the number of possible permutations of elements of Λ which all belong to the same unitary orbit.

Hence the hyper-area of the boundary may be computed in a way analogous to (4.4),

$$S_N^{(2)} := \mathrm{Vol}_{\mathrm{HS}}(\mathcal{M}_N) = \frac{\sqrt{N-1}}{(N-1)!}\frac{\mathrm{Vol}\big(Fl_{\mathbb{C}}^{(N)}\big)}{C_{N-1}^{(3,2)}}. \tag{5.1}$$

The change of the parameter α in (4.1) from 1 to 3 is due to the fact that by setting one component of an N-dimensional vector to zero the corresponding Vandermonde determinant of size N leads to the determinant of size $N-1$ for $\beta = 1$ and to the square of the determinant for $\beta = 2$. Applying (3.12) and (3.10) we obtain an explicit result

$$S_N^{(2)} = \sqrt{N-1}(2\pi)^{N(N-1)/2}\frac{\Gamma(1)\cdots\Gamma(N+1)}{\Gamma(N)\Gamma(N^2-1)}. \tag{5.2}$$

For $N = 2$ we get $S_2^{(2)} = 2\pi$—just the area of the Bloch sphere $\mathbf{S}^2$ of radius $R_2 = 1/\sqrt{2}$. The area of the 7-dim boundary of $\mathcal{M}_3$ reads $S_3^{(2)} = \sqrt{2}\pi^3/105$.

In an analogous way we may find the volume of edges, formed by the unitary orbits of the vector of eigenvalues with two zeros. More generally, states of rank $N-n$ are unitarily similar to diagonal matrices with n eigenvalues vanishing, $\Lambda = \{0, \ldots, 0, \Lambda_{n+1} < \Lambda_{n+2} < \cdots < \Lambda_N\}$. These edges of order n are $N^2 - n^2 - 1$ dimensional, since the dimension of the set of such spectra is $N - n - 1$, while the orbits have the structure of $U(N)/[U(n) \times (U(1))^{N-n}]$ and dimensionality $N^2 - n^2 - (N-n)$. Repeating the reasoning used to derive (5.1) we obtain the volume of the hyperedges

$$S_{N,n}^{(2)} = \frac{\sqrt{N-n}}{(N-n)!}\frac{1}{C_{N-n}^{(1+2n,2)}}\frac{\mathrm{Vol}\big(Fl_{\mathbb{C}}^{(N)}\big)}{\mathrm{Vol}\big(Fl_{\mathbb{C}}^{(n)}\big)}. \tag{5.3}$$

Note that for $n = 0$ this expression gives the volume $V_N^{(2)}$ of the set $\mathcal{M}_N$, for $n = 1$ the hyperarea $S_N^{(2)}$ of its boundary $\partial\mathcal{M}_N$ and for $n \geqslant 2$ the area of the edges of rank $N - n$. In the extreme case of $n = N - 1$, the above formula gives correctly the volume of the set of pure states (the states of rank one), $\mathrm{Vol}(\mathbb{C}\mathbf{P}^{N-1}) = (2\pi)^{N-1}/\Gamma(N)$, see appendix.

6. The ratio: area/volume

Certain information about the structure of a convex body may be extracted from the ratio γ of the (hyper)area of its boundary to its volume. The smaller the coefficient γ (with the diameter of the body kept fixed), the better the body investigated may be approximated by a ball, for which such a ratio is minimal. And conversely, the larger γ, the less the body resembles a ball, since more (hyper)area is needed to bound a given volume.

To analyse simple examples let us recall the volume of the N-dimensional unit ball $\mathbf{B}^N \subset \mathbb{R}^N$ and the volume S_N of the unit N-sphere $\mathbf{S}^N \subset \mathbb{R}^{N+1}$

$$B_N := \mathrm{Vol}(\mathbf{B}^N) = \frac{\mathrm{Vol}(\mathbf{S}^{N-1})}{N} = \frac{\pi^{\frac{N}{2}}}{\Gamma\left(\frac{N}{2}+1\right)} \sim \frac{1}{\sqrt{2\pi}}\left(\frac{2\pi e}{N}\right)^{\frac{N}{2}}, \tag{6.1}$$

where the Stirling expansion [24] was used for large N. For small N we obtain the well-known expressions, $S_1 = 2\pi$, $S_2 = 4\pi$, $S_3 = 2\pi^2$, $S_4 = 8\pi^2/3$ and $B_2 = \pi$, $B_3 = 4\pi/3$, $B_4 = \pi^2/2$. If the spheres and balls have radius L then the scale factor L^N has to be supplied. In odd dimensions the volume of the sphere simplifies, $\mathrm{Vol}(\mathbf{S}^{2k-1}) = 2\pi^k/(k-1)!$.

Since the boundary of a N-ball is formed by a $N-1$ sphere, $\partial\mathbf{B}^N = \mathbf{S}^{N-1}$, the ratio γ for a ball of radius L reads

$$\gamma(\mathbf{B}^N) := \frac{\mathrm{Vol}(\partial\mathbf{B}^N)}{\mathrm{Vol}(\mathbf{B}^N)} = \frac{N}{L}. \tag{6.2}$$

Intuitively this ratio will be the smallest possible among all N-dimensional sets of the same volume. Hence let us compare it with an analogous result for a hypercube $\Box_N$ of side L and volume L^N. The cube has 2^N corners and $2N$ faces, of area L^{N-1} each. We find the ratio

$$\gamma(\Box_N) := \frac{\mathrm{Vol}(\partial\Box_N)}{\mathrm{Vol}(\Box_N)} = 2\frac{N}{L} \tag{6.3}$$

which grows twice as fast as for N-balls. Another comparison can be made with simplices $\triangle_N$, generated by $(N+1)$ equally distant points in $\mathbb{R}^N$. The simplex $\triangle_2$ is a equilateral triangle, while $\triangle_3$ is a regular tetrahedron. The volume of a simplex of side L reads $\mathrm{Vol}(\triangle_N) = [L^N\sqrt{(N+1)/2^N}]/N!$. Since the boundary of $\triangle_N$ consists of $N+1$ simplices $\triangle_{N-1}$ we obtain

$$\gamma(\triangle_N) := \frac{\mathrm{Vol}(\partial\triangle_N)}{\mathrm{Vol}(\triangle_N)} = \sqrt{\frac{2N}{N+1}}\frac{N(N+1)}{L}. \tag{6.4}$$

In this case the ratio γ grows quadratically with N, which reflects the fact that simplices do have much 'sharper' corners, in contrast to the cubes, so more (hyper)area of the boundary is required to cover a given volume. Furthermore, if one defines a hyper-diamond as two simplices glued along one face, its volume is twice the volume of $\triangle_N$ while its boundary consists of $2N$ simplices $\triangle_{N-1}$, so the coefficient γ grows exactly as N^2.

Interestingly, the ratio γ of the N-cube is the same as for the N-ball inscribed in, which has much smaller volume. The same property is characteristic for the N-simplex. Hence another possibility to characterize the shape of any convex body F is to compute the ratio $\chi_1 := \mathrm{Vol}[\mathbf{B}_1(F)]/\mathrm{Vol}(F)$, and $\chi_2 := \mathrm{Vol}(F)/\mathrm{Vol}[\mathbf{B}_2(F)]$, where $\mathbf{B}_1(F)$ is the largest ball inscribed in F while $\mathbf{B}_2(F)$ is the smallest ball in which F may be inscribed. As stated above for cubes and simplices one has $\gamma(F) = \gamma[\mathbf{B}_1(F)]$.

Such quotients may be computed for the rather complicated convex body of mixed quantum states analysed with respect to the Hilbert–Schmidt measure. Using expressions (4.4) and (5.1) we find

$$\gamma_N := \frac{\mathrm{Vol}(\partial\mathcal{M}_N)}{\mathrm{Vol}(\mathcal{M}_N)} = \frac{N!\sqrt{N-1}}{\sqrt{N}(N-1)!}\frac{C_N^{(1,2)}}{C_{N-1}^{(3,2)}} = \sqrt{N(N-1)}(N^2-1). \tag{6.5}$$

The first coefficients read $\gamma_2 = 3\sqrt{2}$, $\gamma_3 = 8\sqrt{6}$ and $\gamma_4 = 15\sqrt{12}$, so they grow with N faster than N^2. A direct comparison with the results received for balls or cubes would be unfair, since here N does not denote the dimension of the set $\mathcal{M}_N \subset \mathbb{R}^D$. Substituting the right dimension, $D = N^2 - 1$, we see that the area/volume ratio for the mixed states increases with the dimensionality as $\gamma \sim D^{3/2}$. The linear scaling factor L, equal to the radius R_N, tends asymptotically to unity and does not influence this behaviour.

Note that the set of mixed states is convex and is inscribed into the sphere of radius R_N, so for each finite N the ratio γ_N remains finite. On the other hand, the fact that this coefficient increases with the dimension D much faster than for balls or cubes, sheds some light on the intricate structure of the set $\mathcal{M}_N$. It touches the hypersphere $\mathbf{S}^{N^2-2}$ of radius R_N along the $(2N-2)$-dimensional manifold of pure states. However, to be characterized by such a value of the coefficient γ it is a rather 'thin' set, and a lot of hyper-area of the boundary is used to encompass its volume. In fact, for any mixed state $\varrho \in \mathcal{M}_N$ its distance to the boundary $\partial\mathcal{M}_N$ does not exceed the radius $r_N \sim 1/N$. Another comparison can be made with the D-ball of radius $L = r_N = [N(N-1)]^{-1/2}$, inscribed into $\mathcal{M}_N$. Although its volume is much smaller than this of the larger set of mixed states, its area to volume ratio, $\gamma = D/L$, is exactly equal to (6.5) characterizing $\mathcal{M}_N$. In other words, for any dimensionality N the set of mixed quantum states belongs to the class of bodies for which $\gamma(F) = \gamma(\mathbf{B}_1(F))$ holds.

Using the notion of the effective radius ρ_N, introduced in section 4, we may express the coefficients χ_i for the set $\mathcal{M}_N$ as a ratio between radii raised to the power equal to the dimensionality, $D = N^2 - 1$. The exact values of $\chi_1 = (r_N/\rho_N)^D$ and $\chi_2 = (\rho_N/R_N)^D$, as well as their product $\chi = \chi_1\chi_2$, may be readily obtained from (4.5). Let us only note the large N behaviour, $\chi(\mathcal{M}_N) = (N-1)^{-N^2+1}$, so it grows with the dimensionality D as $D^{-D/2}$ while $\chi(\mathbf{B}^N) = 1$, $\chi(\square_N) = N^{-N/2}$ and $\chi(\triangle_N) \approx N^{-N}$.

7. Rebits: real density matrices

Even though from the physical point of view one should in general consider the entire set $\mathcal{M}_N$ of complex density matrices, we propose now to discuss its proper subset: the set of real density matrices. This set, denoted by $\mathcal{M}_N^{\mathbb{R}}$, is of smaller dimension $D_1 = N(N+1)/2 - 1 < D = N^2 - 1$, and any reduction of dimensionality simplifies the investigations. While complex density matrices of size two are known as qubits, the real density matrices are sometimes called *rebits* [28]. In the sense of the HS metric the space of rebits forms the full circle $\mathbf{B}^2$, which may be obtained as a slice of the Bloch ball $\mathbf{B}^3$ along a plane containing $\mathbb{I}/2$.

To find the volume of the set $\mathcal{M}_N^{\mathbb{R}}$ we will repeat the steps (3.2)–(4.5) for real symmetric density matrices which may be diagonalized by an orthogonal rotation, $\varrho = O\Lambda O^T$. The expressions

$$\mathrm{d}\varrho = O[\mathrm{d}\Lambda + O^{-1}\,\mathrm{dO}\Lambda - \Lambda O^{-1}\,\mathrm{dO}]O^{-1} \tag{7.1}$$

and

$$(\mathrm{d}s_{\mathrm{HS}})^2 = \sum_{i=1}^{N} (\mathrm{d}\Lambda_i)^2 + 2\sum_{i<j}^{N} (\Lambda_i - \Lambda_j)^2 |(O^{-1}\,\mathrm{d}O)_{ij}|^2 \tag{7.2}$$

allow us to obtain the HS volume element, analogous to (3.6),

$$\mathrm{d}V_{\mathrm{HS}}^{(1)} = \sqrt{N} \prod_{j=1}^{N-1} \mathrm{d}\Lambda_j \prod_{j<k}^{1\cdots N} |\Lambda_j - \Lambda_k| \cdot \left| \prod_{j<k}^{1\cdots N} \sqrt{2}(O^{-1}\,\mathrm{d}O)_{jk} \right|. \tag{7.3}$$

As in the complex case the measure has the product form, and the last factor is the volume element of the orthogonal group (see appendix). Orthogonal orbits of a non-degenerate diagonal matrix form real flag manifolds $Fl_{\mathbb{R}}^{(N)} = O(N)/[O(1)]^N$ of the volume

$$\mathrm{Vol}\big[Fl_{\mathbb{R}}^{(N)}\big] = \frac{\mathrm{Vol}[O(N)]}{2^N} = \frac{(2\pi)^{N(N-1)/4}\pi^{N/2}}{\Gamma[1/2]\cdots\Gamma[N/2]}. \tag{7.4}$$

Here $O(1)$ is the reflection group $\mathbb{Z}_2$ with volume 2.

The volume element (7.3) leads to the following probability measure in the simplex of eigenvalues

$$P_{\mathrm{HS}}^{(1)}(\Lambda_1,\ldots,\Lambda_N) = C_N^{(1,1)}\delta\left(1 - \sum_{j=1}^{N}\Lambda_j\right)\prod_{j<k}^{N}|\Lambda_j - \Lambda_k| \tag{7.5}$$

with the normalization constant given in (4.3). Note the linear dependence on the differences of eigenvalues, in contrast to the quadratic form present in (3.11). Taking into account the number $N!$ of different permutations of the elements of the spectrum Λ we obtain the expression for the volume of the set of $\mathcal{M}_N^{\mathbb{R}}$,

$$V_N^{(1)} := \mathrm{Vol}_{\mathrm{HS}}\big(\mathcal{M}_N^{\mathbb{R}}\big) = \frac{\sqrt{N}}{N!}\frac{\mathrm{Vol}\big(Fl_{\mathbb{R}}^{(N)}\big)}{C_N^{(1,1)}} \tag{7.6}$$

which gives

$$V_N^{(1)} = \frac{\sqrt{N}}{N!}\frac{2^N(2\pi)^{N(N-1)/4}\Gamma\big[\frac{N+1}{2}\big]}{\Gamma\big[\frac{N(N+1)}{2}\big]\Gamma\big[\frac{1}{2}\big]}\prod_{k=1}^{N}\Gamma\left[1+\frac{k}{2}\right]. \tag{7.7}$$

As in the complex case we find the volume of the boundary of $\mathcal{M}_N^{\mathbb{R}}$, and in general, the volume of edges of order n with $0 \leqslant n \leqslant N-1$. In the case of real density matrices these edges are $N(N+1)/2 - 1 - n(n+1)/2$ dimensional, since the dimension of the set of such spectra is $N-n-1$, and the orbits have the structure of $O(N)/[O(n)\times(O(1))^{N-n}]$ and dimensionality $N(N-1)/2 - n(n-1)/2$. In analogy to (5.3) we obtain

$$S_{N,n}^{(1)} = \frac{\sqrt{N-n}}{(N-n)!}\frac{1}{C_{N-n}^{(1+n,1)}}\frac{\mathrm{Vol}\big(Fl_{\mathbb{R}}^{(N)}\big)}{\mathrm{Vol}\big(Fl_{\mathbb{R}}^{(n)}\big)} \tag{7.8}$$

which for $n = 1$ gives the volume S of the boundary $\partial\mathcal{M}_N^{\mathbb{R}}$, and allows us to compute the ratio area to volume,

$$\gamma\big(\mathcal{M}_N^{\mathbb{R}}\big) := \frac{\mathrm{Vol}\big(\partial\mathcal{M}_N^{\mathbb{R}}\big)}{\mathrm{Vol}\big(\mathcal{M}_N^{\mathbb{R}}\big)} = \frac{N!\sqrt{N-1}}{\sqrt{N}(N-1)!}\frac{C_N^{(1,1)}}{C_{N-1}^{(2,1)}} = \sqrt{N(N-1)}(N-1)(1+N/2). \tag{7.9}$$

The product of the last two factors is equal to the dimensionality of the set of real density matrices, $D_1 = N(N+1)/2 - 1$. Therefore, just as in the complex case, the ratio area to volume for $\mathcal{M}_N^{\mathbb{R}}$ coincides with such a ratio $\gamma = D_1/L$ for the maximal ball of radius $L = r_N = [N(N-1)]^{-1/2}$ contained in this set. In the simplest case of $N = 2$ we receive $V_2^{(1)} = \pi/2$—the volume of the circle $\mathbf{B}^2$ of radius $R_2 = 1/\sqrt{2}$. The volume of the boundary, $S = \pi\sqrt{2}$, is equal to the circumference of the circle of radius $R_2 = 1/\sqrt{2}$, and gives $\gamma = 2\sqrt{2}$ in agreement with (7.9).

8. Concluding remarks

We have found the volume V and the surface area S of the $D = N^2 - 1$ dimensional set of mixed states $\mathcal{M}_N$ acting in the N-dimensional Hilbert space, and its subset $\mathcal{M}_N^{\mathbb{R}}$ containing real symmetric matrices. Although the volume of the unitary (orthogonal) group depends on the definition used, as discussed in the appendix, the volume of the set of mixed states has a well-specified, unambiguous meaning. For instance, for $N = 2$ the volume V_2 may be interpreted as the ratio of the volume of the Bloch ball (of radius R_2 fixed by the Hilbert–Schmidt metric), to the volume of the cube spanned by three orthonormal vectors of the HS space: the rescaled Pauli matrices, $\{\sigma_x, \sigma_y, \sigma_z\}/\sqrt{2}$.

On one hand, these explicit results may be applied for estimation of the volume of the set of entangled states [4, 5, 30–32], or yet another subset of $\mathcal{M}_N$. It is also likely that some integrals obtained in this work will be useful in such investigations.

On the other hand, outcomes of this paper advance our understanding of the properties of the set of mixed quantum states. The ratio of the hyperarea of the boundary of D-balls to their volume grows linearly with the dimension D. The same ratio for D-simplices behaves as D^2, while for the sets of complex and real density matrices it grows with the dimensionality D as $D^{3/2}$. Hence these geometrical properties of the convex body of mixed states are somewhere in between the properties of D-balls and D-simplices.

Furthermore, we have shown that for any N the sets of complex (real) density matrices belong to the family of sets for which the ratio area to volume is equal to such a ratio computed for the maximal ball inscribed into this set.

It is necessary to emphasize that a similar problem of estimating the volume of the set of mixed states could also be considered with respect to other probability measures. In particular, analogous results presented by us in [33] for the measure [26, 34] related to the Bures distance [35, 36] allow us to investigate similarities and differences between the geometry of mixed states induced by different metrics.

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Appendix. Volumes of the unitary groups and flag manifolds

Although the volume of the unitary (orthogonal) group and the complex (real) flag manifold that we use in our calculations were computed by Hua many years ago [15], one may find in more recent literature related results, which in some cases seem to be contradictory. However, different authors used different definitions of the volume of the unitary group [16–20, 22], so we review in this appendix the three most common definitions and compare the results.

A.1. Unitary group $U(N)$

We shall recall (3.8) the metric of the unitary group $U(N)$ induced by the Hilbert–Schmidt scalar product and used by Hua [15]

$$(\mathrm{d}s)^2 := -\mathrm{Tr}(U^{-1}\,\mathrm{d}U)^2 = \sum_{j=1}^{N} |(U^{-1}\,\mathrm{d}U)_{jj}|^2 + 2\sum_{j<k=1}^{N} |(U^{-1}\,\mathrm{d}U)_{jk}|^2 \qquad \text{(A1)}$$

which is left- and right-invariant under unitary transformations. The volume element is then given by the product of independent differentials times the square root of the determinant of the metric tensor. One has still the freedom of an overall scale factor for (A1) which appears then correspondingly in the volume element. To keep invariance the ratio of the prefactors c_{diag} and c_{off} of the diagonal and off-diagonal terms has to be fixed. Nevertheless one may introduce different scalings of the volume elements which we call $\mathrm{d}\nu_A$, $\mathrm{d}\nu_B$, $\mathrm{d}\nu_C$:

$$\mathrm{d}\nu_A := \left|\prod_{i=1}^{N}(U^{-1}\,\mathrm{d}U)_{ii}\prod_{j<k}^{1\cdots N} 2\,\mathrm{Re}(U^{-1}\mathrm{d}U)_{jk}\,\mathrm{Im}(U^{-1}\,\mathrm{d}U)_{jk}\right| \qquad c_{\mathrm{diag}} = 1 \quad c_{\mathrm{off}} = 2 \qquad \text{(A2)}$$

$$\mathrm{d}\nu_B := 2^{-N(N-1)/2}\,\mathrm{d}\nu_A \qquad c_{\mathrm{diag}} = 1 \quad c_{\mathrm{off}} = 1 \qquad \text{(A3)}$$

$$\mathrm{d}\nu_C := 2^{-N/2}\,\mathrm{d}\nu_B \qquad c_{\mathrm{diag}} = 1/2 \quad c_{\mathrm{off}} = 1. \qquad \text{(A4)}$$

The product in (A2), consistent with (A1), has to be understood in the sense of alternating external multiplication of differential forms. Only the first convention (A2) labelled by the index $_A$ was used in the main part of this work. Note that the normalization (A4) corresponds to the rescaled line element $(\mathrm{d}s)^2 = -\frac{1}{2}\,\mathrm{Tr}(U^{-1}\,\mathrm{d}U)^2$. In general we may scale

$$\mathrm{d}\nu_X := (c_{\mathrm{diag}})^{N/2}(c_{\mathrm{off}})^{N(N-1)/2}\,\mathrm{d}\nu_B \qquad \text{(A5)}$$

where the label $_X$ denotes a certain choice of the prefactors c_{diag} and c_{off} for diagonal or off-diagonal elements in (A1). All these volumes correspond to the Haar measure which is unique up to an overall constant scale factor. Thus we deduce that

$$\mathrm{Vol}_A[U(N)] = 2^{N(N-1)/2}\,\mathrm{Vol}_B[U(N)] \qquad \text{and} \qquad \mathrm{Vol}_C[U(N)] = 2^{-N/2}\,\mathrm{Vol}_B[U(N)]. \qquad \text{(A6)}$$

In order to determine the volume of the unitary group let us recall the fibre bundle structure $U(N-1) \to U(N) \to \mathbf{S}^{2N-1}$, see, e.g., [37]. This topological fact implies a relation between the volume of the unit sphere $\mathbf{S}^{2N-1}$ and the volume of the unitary group defined by the measure $\mathrm{d}\nu_B$ (A3), for which all components of the vector $(U^{-1}\,\mathrm{d}U)_{jk}$ have unit prefactors,

$$\mathrm{Vol}_B[U(N)] = \mathrm{Vol}_B[U(N-1)] \times \mathrm{Vol}[\mathbf{S}^{2N-1}]. \qquad \text{(A7)}$$

To prove this equality by a direct calculation, it is convenient to parametrize a unitary matrix of size N as

$$U_N = \begin{bmatrix} \mathrm{e}^{\mathrm{i}\phi} & 0 \\ 0 & U_{N-1} \end{bmatrix} \begin{bmatrix} \sqrt{1-|h|^2} & -h^\dagger \\ h & \sqrt{\mathbb{I} - h\otimes h^\dagger} \end{bmatrix} \qquad \text{(A8)}$$

where $\phi \in [0, 2\pi)$ is an arbitrary phase and h is a complex vector with $N-1$ components such that $|h| \leqslant 1$. This representation shows (we may also arrange the two matrices in (A8) in the opposite order) the relation

$$U(N)/[U(1) \times U(N-1)] = \mathbb{C}\mathbf{P}^{N-1} \qquad \text{(A9)}$$

since the second factor represents the complex projective space $\mathbb{C}\mathbf{P}^{N-1}$. In fact, if one calculates the metric (A1) we find

$$(\mathrm{d}s_N)^2 \cong (\mathrm{d}s_1)^2 + (\mathrm{d}s_{N-1})^2 + 2(\mathrm{d}s_h)^2 \tag{A10}$$

where $(\mathrm{d}s_N)^2$ means the metric for $U(N)$ (the sign $\cong$ shall indicate that we have omitted some shifts in $(\mathrm{d}s_1)^2$ and $(\mathrm{d}s_{N-1})^2$ that are not relevant for the volume) and $(\mathrm{d}s_h)^2$ means the metric of the complex projective space $\mathbb{C}\mathbf{P}^{N-1}$ with radius 1

$$(\mathrm{d}s_h)^2 = \mathrm{d}h^\dagger\,\mathrm{d}h + \frac{(h^\dagger\,\mathrm{d}h + \mathrm{d}h^\dagger h)^2}{4(1-|h|^2)} + \frac{(h^\dagger\,\mathrm{d}h - \mathrm{d}h^\dagger h)^2}{4}. \tag{A11}$$

It is easy to see by diagonalizing this metric (eigenvalues $1-|h|^2$, $1/(1-|h|^2)$, and otherwise 1) that the corresponding volume is that of the real ball $\mathbf{B}^{2N-2}$ with radius 1 and dimension $2N-2$. Thus one obtains

$$\mathrm{Vol}_X[U(N)] = \mathrm{Vol}_X[U(N-1)] \times \mathrm{Vol}_X[U(1)] \times c_{\mathrm{off}}^{N-1}\,\mathrm{Vol}[\mathbf{B}^{2N-2}] \tag{A12}$$

which for the measure (A3) with $c_{\mathrm{diag}} = c_{\mathrm{off}} = 1$ reduces to (A7). Applying this relation $N-1$ times we obtain

$$\mathrm{Vol}_B[U(N)] = \mathrm{Vol}[\mathbf{S}^{2N-1}] \times \cdots \times \mathrm{Vol}[\mathbf{S}^3] \times \mathrm{Vol}[\mathbf{S}^1]. \tag{A13}$$

Taking into account that Vol $[\mathbf{S}^{2N-1}] = 2\pi^N/(N-1)!$ and making use of the relation (A6), we may write an explicit result for the volumes calculated with respect to different definitions (A2)–(A4)

$$\mathrm{Vol}_X[U(N)] = a_X^U \frac{2^N \pi^{N(N+1)/2}}{0!1!\cdots(N-1)!} \tag{A14}$$

where the proportionality constants read $a_A^U = 2^{N(N-1)/2}$, $a_B^U = 1$ and $a_C^U = 2^{-N/2}$. The result for $\mathrm{Vol}_A[U(N)]$ was rigorously derived in [15], $\mathrm{Vol}_B[U(N)]$ was given in [18], while $\mathrm{Vol}_A[U(N)]$ and $\mathrm{Vol}_C[U(N)]$ were compared in [22]. In particular, $\mathrm{Vol}_A[U(1)] = \mathrm{Vol}_B[U(1)] = 2\pi$, while $\mathrm{Vol}_C[U(1)] = \sqrt{2}\pi$ and $\mathrm{Vol}_A[U(2)] = 8\pi^3, \mathrm{Vol}_B[U(2)] = 4\pi^3, \mathrm{Vol}_C[U(2)] = 2\pi^3$.

In general, the volume of a coset space may be expressed as a ratio of the volumes. Consider for instance the manifold of all pure states of dimensionality *N*. It forms the complex projective space $\mathbb{C}\mathbf{P}^{N-1} = U(N)/[U(N-1) \times U(1)]$. Therefore

$$\mathrm{Vol}_X[\mathbb{C}\mathbf{P}^{N-1}] = \frac{\mathrm{Vol}_X[U(N)]}{\mathrm{Vol}_X[U(1)]\,\mathrm{Vol}_X[U(N-1)]} \tag{A15}$$

which gives the general result

$$\mathrm{Vol}_X[\mathbb{C}\mathbf{P}^k] = a_X^{\mathrm{CP}} \frac{\pi^k}{k!} = a_X^{\mathrm{CP}}\,\mathrm{Vol}[\mathbf{B}^{2k}]. \tag{A16}$$

The scale factors read $a_A^{\mathrm{CP}} = 2^k$ and $a_B^{\mathrm{CP}} = a_C^{\mathrm{CP}} = 1$. For instance $\mathrm{Vol}_A[\mathbb{C}\mathbf{P}^1] = 2\pi$ which corresponds to the circle of radius $\sqrt{2}$, while $\mathrm{Vol}_B[\mathbb{C}\mathbf{P}^1] = \mathrm{Vol}_C[\mathbb{C}\mathbf{P}^1] = \pi$, equal to the area of the circle of radius 1. The latter convention is natural if one uses the Fubini–Study metric in the space of pure states, $D_{\mathrm{FS}}(|\varphi\rangle, |\psi\rangle) = \arccos(\sqrt{\kappa})$, where the transition probability is given by $\kappa = |\langle\varphi|\psi\rangle|^2$. Then the largest possible distance $D_{\mathrm{FS}} = \pi/2$, obtained for any orthogonal states, sets the geodesic length of the complex projective space to π which corresponds to the geodesic distance of two opposite points on the unit circle, being identified. It is worth adding that $\mathrm{Vol}_C[\mathbb{C}\mathbf{P}^k] = \mathrm{Vol}[\mathbf{S}^{2k+1}]/\mathrm{Vol}[\mathbf{S}^1]$ and this relation was used in [20] to *define* the volume Vol_C of complex projective spaces. We see therefore that different conventions adopted in (A2)–(A4) lead to different sizes (geodesic lengths) of the manifolds analysed.

Unitary orbits of a generic mixed state with a non-degenerate spectrum have the structure of a (N^2-N)-dimensional complex flag manifold $Fl_{\mathbb{C}}^{(N)} = U(N)/[U(1)]^N$. Hence its volume reads

$$\mathrm{Vol}_X\big[Fl_{\mathbb{C}}^{(N)}\big] = \frac{\mathrm{Vol}_X[U(N)]}{(\mathrm{Vol}_X[U(1)])^N} = a_X^{\mathrm{Fl}} \frac{\pi^{N(N-1)/2}}{1!2!\cdots(N-1)!} \tag{A17}$$

with convention-dependent scale constants $a_A^{\mathrm{Fl}} = 2^{N(N-1)/2}$ [15] and $a_B^{\mathrm{Fl}} = a_C^{\mathrm{Fl}} = 1$ [20]. It is easy to check that the relation

$$\mathrm{Vol}_X\big[Fl_{\mathbb{C}}^{(N)}\big] = \mathrm{Vol}_X[\mathbb{C}\mathbf{P}^1] \times \mathrm{Vol}_X[\mathbb{C}\mathbf{P}^2] \times \cdots \times \mathrm{Vol}_X[\mathbb{C}\mathbf{P}^{N-1}] \tag{A18}$$

holds for any definition (A2)–(A4), since the scale constants do cancel.

For completeness we also discuss the group $SU(N)$, the volume of which is *not* equal to $\mathrm{Vol}[U(N)]/\mathrm{Vol}[U(1)]$ [16, 19, 20]. To show this let us parametrize a matrix $Y_N \in SU(N)$ v

$$Y_N = \begin{bmatrix} \mathrm{e}^{\mathrm{i}\phi} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}[\phi/(N-1)]} Y_{N-1} \end{bmatrix} \begin{bmatrix} \sqrt{1-|h|^2} & -h^\dagger \\ h & \sqrt{\mathbb{I} - h \otimes h^\dagger} \end{bmatrix} = VW \tag{A19}$$

where $\phi \in [0, 2\pi)$ is an arbitrary phase and h is a complex vector with $N-1$ components such that $|h| \leqslant 1$. Condition $\det Y_N = 1$ implies $\mathrm{Tr}\, Y_N^{-1}\,\mathrm{d}Y_N = 0$. For instance, the metric (A1) gives, if the volume is concerned

$$(\mathrm{d}s)^2 \cong -\mathrm{Tr}(V^{-1}\,\mathrm{d}V)^2 - \mathrm{Tr}(W^{-1}\,\mathrm{d}W)^2. \tag{A20}$$

Since the first factor V is block diagonal the first term is equal to $(\mathrm{d}\phi)^2 N/(N-1) - \mathrm{Tr}\big(Y_{N-1}^{-1}\mathrm{d}Y_{N-1}\big)^2$, while the second one gives the metric on $\mathbb{C}\mathbf{P}^{N-1}$. Integrating an analogous expression in the general case of an arbitrary metric and using (A15), we obtain the following result

$$\mathrm{Vol}_X[SU(N)] = \frac{\mathrm{Vol}_X[U(N)]}{\mathrm{Vol}_X[U(N-1)]} \sqrt{\frac{N}{N-1}}\, \mathrm{Vol}_X[SU(N-1)] \tag{A21}$$

which iterated $N-1$ times gives the correct relation

$$\mathrm{Vol}_X[SU(N)] = \sqrt{N}\, \frac{\mathrm{Vol}_X[U(N)]}{\mathrm{Vol}_X[U(1)]} \tag{A22}$$

with the stretching factor $\sqrt{N}$. For instance, working with the measure (A4) and making use of (A14) we obtain $\mathrm{Vol}_C[SU(N)] = \sqrt{N} 2^{(N-1)/2} \pi^{(N+2)(N-1)/2}/[1!\cdots(N-1)!]$, so in particular, $\mathrm{Vol}_C[SU(2)] = 2\pi^2$, $\mathrm{Vol}_C[SU(3)] = \sqrt{3}\pi^5$ and $\mathrm{Vol}_C[SU(4)] = \sqrt{2}\pi^9/3$, consistently with the results obtained in [16, 20, 22, 38].

A.2. Orthogonal group $O(N)$

The analysis of the orthogonal group is simpler, since $(O^{-1}\,\mathrm{d}O)^T = -(O^{-1}\,\mathrm{d}O)^T$, so the diagonal elements of $\mathrm{Tr}(O^{-1}\mathrm{d}O)^2$ vanish. Thus we shall consider only two metrics (analogous to the measures (A2)–(A4)) with different scalings,

$$(\mathrm{d}s_A)^2 := -\mathrm{Tr}(O^{-1}\,\mathrm{d}O)^2 = 2 \sum_{j<k=1}^{N} |(O^{-1}\,\mathrm{d}O)_{jk}|^2 \tag{A23}$$

used in section 7 of this work, and

$$(\mathrm{d}s_B)^2 = (\mathrm{d}s_C)^2 := -\frac{1}{2}\,\mathrm{Tr}(O^{-1}\,\mathrm{d}O)^2 = \sum_{j<k=1}^{N} |(O^{-1}\,\mathrm{d}O)_{jk}|^2 \tag{A24}$$

which both lead to the Haar measure on the orthogonal group.

To obtain the volume of $O(N)$ we proceed as in the unitary case and parametrize an orthogonal matrix of size N as

$$O_N = \begin{bmatrix} O_1 & 0 \\ 0 & O_{N-1} \end{bmatrix} \begin{bmatrix} \sqrt{1-|h|^2} & -h^T \\ h & \sqrt{\mathbb{I} - h \otimes h^T} \end{bmatrix} \tag{A25}$$

where $O_1 \in O(1) = \pm$, while h is here a real vector with $N-1$ components such that $|h| \leqslant 1$. Representing the metric $(\mathrm{d}s_B)^2$ by these two matrices we see that the term containing only the vector h gives the metric of a real projective space. Integrating the resulting volume element (with scale factor 1) we obtain the volume of $\mathbb{R}\mathbf{P}^{N-1}$, equal to $\frac{1}{2}\,\mathrm{Vol}[\mathbf{S}^{N-1}]$. Taking into account a factor of two resulting from $O(1)$ we arrive at $\mathrm{Vol}_B[O(N)] = \mathrm{Vol}_B[O(N-1)]\,\mathrm{Vol}[\mathbf{S}^{N-1}]$, which applied recursively leads to

$$\mathrm{Vol}_B[O(N)] = \mathrm{Vol}[\mathbf{S}^{N-1}] \times \cdots \times \mathrm{Vol}[\mathbf{S}^1] \times \mathrm{Vol}[\mathbf{S}^0] = \prod_{k=1}^{N} \frac{2\pi^{k/2}}{\Gamma(k/2)} \tag{A26}$$

where $\mathrm{Vol}[\mathbf{S}^0] = \mathrm{Vol}[O(1)] = 2$. To get an equivalent result for the metric (A23) we have to take into account the factor $\sqrt{2}$ which occurs for each of $N(N-1)/2$ off-diagonal elements. Doing so we obtain

$$\mathrm{Vol}_A[O(N)] = 2^{N(N-1)/4}\,\mathrm{Vol}_B[O(N)] = 2^{N(N+3)/4} \prod_{k=1}^{N} \frac{\pi^{k/2}}{\Gamma(k/2)} \tag{A27}$$

in agreement with Hua [15]. In particular, $\mathrm{Vol}_A[O(1)] = \mathrm{Vol}_B[O(1)] = 2$, while $\mathrm{Vol}_A[O(2)] = 4\sqrt{2}\pi$, $\mathrm{Vol}_B[O(2)] = 4\pi$ and $\mathrm{Vol}_A[O(3)] = 32\sqrt{2}\pi^2$, $\mathrm{Vol}_B[O(3)] = 16\pi^2$.

In full analogy with the unitary case we obtain the volume of the real projective manifold

$$\mathrm{Vol}_X[\mathbb{R}\mathbf{P}^{N-1}] = \frac{\mathrm{Vol}_X[O(N)]}{\mathrm{Vol}_X[O(1)]\,\mathrm{Vol}_X[O(N-1)]}. \tag{A28}$$

For the metric (A24) this expression reduces to $\mathrm{Vol}_B[\mathbb{R}\mathbf{P}^k] = \frac{1}{2}\,\mathrm{Vol}[\mathbf{S}^k]$. Hence, this metric may be called the 'unit sphere' metric, while the convention (A23) may be called the 'unit trace' metric.

In the similar way we find the volume of the real flag manifolds, used in analysis of real density matrices,

$$\mathrm{Vol}_X\big[Fl_{\mathbb{R}}^{(N)}\big] = \frac{\mathrm{Vol}_X[O(N)]}{(\mathrm{Vol}_X[O(1)])^N} = \frac{1}{2^N}\,\mathrm{Vol}_X[O(N)]. \tag{A29}$$

Exactly as in the complex case we observe that the relation

$$\mathrm{Vol}_X\big[Fl_{\mathbb{R}}^{(N)}\big] = \mathrm{Vol}_X[\mathbb{R}\mathbf{P}^1] \times \mathrm{Vol}_X[\mathbb{R}\mathbf{P}^2] \times \cdots \times \mathrm{Vol}_X[\mathbb{R}\mathbf{P}^{N-1}] \tag{A30}$$

is satisfied for any definition of the metric.

Computation of the volume of the special orthogonal group $SO(N)$ is much easier than in the complex case, since there are no diagonal elements in the metric and hence, no stretching factors. For any normalization one gets

$$\mathrm{Vol}_X[SO(N)] = \frac{\mathrm{Vol}_X[O(N)]}{\mathrm{Vol}_X[O(1)]} = \frac{1}{2}\,\mathrm{Vol}_X[O(N)]. \tag{A31}$$

In particular, we get $\mathrm{Vol}_B[SO(2)] = 2\pi$ and $\mathrm{Vol}_B[SO(3)] = \mathrm{Vol}_C[SO(3)] = 8\pi^2$. The latter results seem to be inconsistent with $\mathrm{Vol}_C[SU(2)] = 2\pi^2$, since there exists a one to two relation between both groups. This paradox is resolved by analysing the scale effects [20]: the volume of $SU(2)$ is twice as large as the volume of the real projective manifold conjugated to $SO(3)$ of the appropriate geodesic length, $\mathrm{Vol}_C[\mathbb{R}\mathbf{P}^3] = \pi^2$.

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