

Bures volume of the set of mixed quantum states

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Abstract

We compute the volume of the $(N^2 - 1)$ -dimensional set \mathcal{M}_N of density matrices of size N with respect to the Bures measure and show that it is equal to that of an $(N^2 - 1)$ -dimensional hyper-hemisphere of radius $1/2$. For $N = 2$ we obtain the volume of the Uhlmann hemisphere, $\frac{1}{2}\mathbf{S}^3 \subset \mathbb{R}^4$. We find also the area of the boundary of the set \mathcal{M}_N and obtain analogous results for the smaller set of all real density matrices. An explicit formula for the Bures–Hall normalization constants is derived for an arbitrary N .

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1. Introduction

Modern applications of quantum mechanics renewed interest in the properties of the set of density matrices of finite size. Its geometry depends on the metric used [1, 2]. However, the simplest possible choices exhibit some drawbacks: the trace metric, defined by the trace distance

$$D_{\text{Tr}}(\rho, \sigma) = \|\rho - \sigma\|_1 := \text{Tr}|\rho - \sigma| = \text{Tr}\sqrt{(\rho - \sigma)^2} \quad (1.1)$$

is monotone [3], but not Riemannian, while the Hilbert–Schmidt metric, induced by the Hilbert–Schmidt scalar product, $\langle A|B \rangle = \text{Tr} A^\dagger B$ and related to the H–S distance,

$$D_{\text{HS}}(\rho, \sigma) = \|\rho - \sigma\|_2 := \sqrt{\text{Tr}[(\rho - \sigma)^2]} \quad (1.2)$$

is Riemannian but not monotone [4]. This fact provides an additional motivation to investigate other possible metrics and distances in the space of mixed quantum states.

Nowadays it is widely accepted that the Bures metric [5, 6] is distinguished by its rather special properties: it is a Riemannian, monotone metric, which is Fisher adjusted [1]: in the subspace of diagonal matrices it induces the statistical distance [7]. Moreover, it is also

Fubini–Study adjusted, since it agrees with this metric at the space of pure states [8]. The Bures distance between any two mixed states is a function of their fidelity [6, 9] and various properties of this distance are a subject of considerable interest (see [8, 10–16]).

A given distance between density matrices induces a certain measure in this space. The probability measure in the space of mixed quantum states induced by the Bures metric was defined by Hall [17]. He demonstrated that the eigenvectors of a random state of size N generated according to this measure are distributed according to the Haar measure on $U(N)$, derived an explicit expression for the joint probability density for eigenvalues of a random state generated according to this measure and found for $N = 2$ the normalization constant C_N for the joint probability density of the eigenvalues. Further Bures–Hall normalization constants C_3 and C_4 were calculated by Slater [18], but the problem of finding the constants C_N for arbitrary N remained unsolved.

The aim of this work is to compute the volume of the set \mathcal{M}_N of all density matrices of size N and the hyperarea of its boundary according to the Bures measure. This work is complementary to our parallel paper [19], in which the volume was computed according to the Hilbert–Schmidt measure, but the notation and the structure of both papers are not exactly the same. In this work we treat in parallel two different cases: of complex density matrices, and its particular subset, of real density matrices. Both cases are labelled by the ‘repulsion exponent’ $\beta = 2$ for the complex case and $\beta = 1$ for the real case.

The paper is organized as follows. In section 2 the Bures distance is defined and its remarkable properties are reviewed. In section 3 we derive the Bures measure and express the volume and the surface of the space of mixed states as a function of the Hall normalization constants. Key results of the paper are presented in section 4, in which we compute the normalization constants C_N for arbitrary N (see (4.11)) and calculate explicitly the Bures volume of \mathcal{M}_N (see equation (4.12)). In section 5 we perform a similar analysis of the space of real density matrices. A concise presentation of the results obtained is provided by equation (5.15), from which one may read out the volume of the sets of complex and real density matrices, the surface of their boundaries and their ‘edges’.

2. Bures metric

We shall start the discussion considering the set of pure states $|\psi\rangle$ belonging to an N -dimensional Hilbert space \mathcal{H}_N . This set has the structure of a complex projective space, $\mathbb{C}P^{N-1}$, and there exists a distinguished, unitarily invariant measure, which corresponds to the geodesic distance on this manifold. It is called the Fubini–Study distance [20, 21],

$$D_{\text{FS}}(|\varphi_A\rangle, |\varphi_B\rangle) = \frac{1}{2} \arccos(2\kappa - 1) = 1 \arccos(\sqrt{\kappa}) \quad (2.1)$$

where $\kappa = |\langle \varphi_A | \varphi_B \rangle|^2$ denotes the transition probability. This quantity was generalized for an arbitrary pair of mixed quantum states by Uhlmann [6]

$$F(\rho_A, \rho_B) = [\text{Tr}(\sqrt{\sqrt{\rho_A} \rho_B \sqrt{\rho_A}})^{1/2}]^2 = \|\sqrt{\rho_A} \sqrt{\rho_B}\|_1^2 \quad (2.2)$$

and its remarkable properties were studied by Jozsa [9] who called it *fidelity*⁴. It is a symmetric, non-negative, continuous, concave function of both states and is unitarily invariant. For any pair of pure states the fidelity reduces to their overlap, $F = \text{Tr} \rho_A \rho_B = |\langle \psi_A | \psi_B \rangle|^2 = \kappa$. Hence a function of fidelity, called *Bures length* [8] or *angle* [22],

$$D_A(\rho_A, \rho_B) := \arccos \sqrt{F(\rho_A, \rho_B)} = \frac{1}{2} \arccos(2F(\rho_A, \rho_B) - 1) \quad (2.3)$$

coincides for any pair of pure states with their Fubini–Study distance (2.1).

⁴ Although this was the original definition of Jozsa, some authors use this name for \sqrt{F} .

Fidelity may also be defined [9] as the maximal overlap between the purifications of two mixed states, $|\langle \Phi_A | \Phi_B \rangle|^2$, where $|\Phi_i\rangle \in \mathcal{H}_{N^2} = \mathcal{H}_N \otimes \mathcal{H}_N$ and both mixed states are obtained by partial tracing over the auxiliary subsystem E , $\rho_i = \text{Tr}_E |\Phi_i\rangle \langle \Phi_i|$. Fidelity allows one to characterize the ‘closeness’ of a pair of mixed states: it is equal to unity only if both states coincide. Another function of fidelity,

$$D_B(\rho_A, \rho_B) = (2 - 2\sqrt{F(\rho_A, \rho_B)})^{1/2} = \sqrt{2 - 2 \text{Tr} \sqrt{\sqrt{\rho_A} \rho_B \sqrt{\rho_A}}} \quad (2.4)$$

satisfies all axioms of a distance and is called *Bures distance* [5]. Hence Bures metric is Fubini–Study adjusted, since for pure states it induces the same geometry. Several relevant papers on this subject are due to Uhlmann [6, 8, 10], who showed that the topological metric of Bures is Riemannian. Hübner provided a detailed analysis of the $N = 2$ [11] and $N = 3$ case [13], while Dittmann analysed differential geometric properties of the Bures metric [12]. Relations of the Bures metric to information theory can be seen in papers by Fuchs and Caves [23], Vedral and Plenio [24] while the closely related fidelity is often used in the comprehensive book by Nielsen and Chuang [22]. It was shown by Braunstein and Caves [7] that for neighbouring density matrices the Bures distance is proportional to the statistical distance introduced by Wootters [25] in the context of measurements which optimally resolve neighbouring quantum states.

For diagonal matrices, $\rho_A = \text{diag}(\vec{a})$ and $\rho_B = \text{diag}(\vec{b})$, the expression for the Bures distance simplifies and becomes a function of the *Bhattacharyya coefficient* [26], $B(\vec{a}, \vec{b})$,

$$D_B^2(\rho_A, \rho_B) = 2 - 2 \sum_{i=1}^N \sqrt{a_i b_i} = 2 - 2B(\vec{a}, \vec{b}). \quad (2.5)$$

This is the Euclidean distance between two points on a unit circle, the corresponding vectors form the angle θ such that $\cos \theta = \vec{a} \cdot \vec{b}$. The geodesic distance along the circle $\vartheta = 2 \arccos(1 - D_B^2/2) = 2D_A$, is called in this case the *statistical distance*, since it provides a measure of distinguishability between both probability distributions by statistical sampling. Another function is called the *Hellinger distance* [27]

$$D_H(\vec{a}, \vec{b}) = \sqrt{\sum_{i=1}^N (\sqrt{a_i} - \sqrt{b_i})^2} = \sqrt{2 - 2B(\vec{a}, \vec{b})}. \quad (2.6)$$

It is clear that for any two diagonal density matrices their fidelity reduces to the squared Bhattacharyya coefficient, $F(\rho, \sigma) = B^2(\vec{a}, \vec{b})$, while the Bures distance between both states coincides with the Hellinger distance between both vectors of eigenvalues, $D_B(\rho, \sigma) = D_H(\vec{a}, \vec{b})$.

Let us write the Bures distance for infinitesimally closed diagonal states defined by the vectors \vec{a} and $\vec{a}' = \vec{a} + d\vec{a}$,

$$ds_B^2 = (D_B(\rho_A, \rho'_A))^2 = 2 - 2 \sum_{i=1}^N a_i \sqrt{1 + \frac{da_i}{a_i}}. \quad (2.7)$$

Since $\sum_{i=1}^N a_i = 1$ and $\sum_{i=1}^N da_i = 0$, so computing the Bures line element ds_B^2 we need to expand the square root up to second order, and obtain

$$ds_B^2 = \frac{1}{4} \sum_{i=1}^N \frac{da_i da_i}{a_i} = \text{Tr}(d\sqrt{\rho})^2 \quad (2.8)$$

precisely the metric on a sphere, or also, the statistical metric on the simplex, also called the *Fisher–Rao* metric [28]. Hence the Bures metric is *Fisher adjusted*—restricted to the simplex

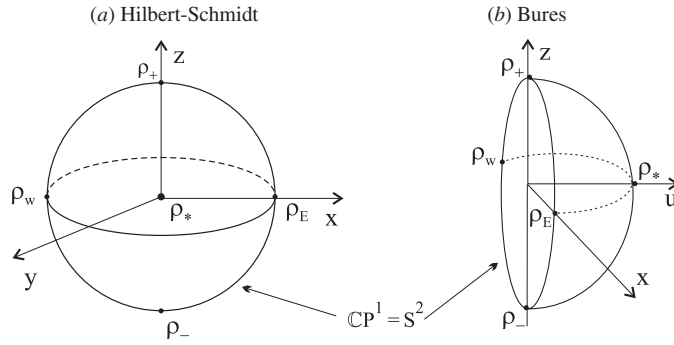


Figure 1. Geometry of the set of mixed states for $N = 2$: (a) the 3-ball embedded in \mathbb{R}^3 induced by the Hilbert–Schmidt distance, (b) hemisphere of \mathbf{S}^3 embedded in \mathbb{R}^4 (shown as a cross-section of R^4 taken at $y = 0$) induced by the Bures distance. The maximally mixed state ρ_* is located at the centre of the ball (a), and at the hyper-pole of \mathbf{S}^3 (b). The set of pure states is represented by the Bloch sphere \mathbf{S}^2 (a) and by the Uhlmann equator $\mathbf{S}^2 \in \mathbf{S}^3$ (b). The cross-section of \mathcal{M}_2 with the plane $z = 0$ produces a full circle in the equatorial plane (a), or half of a hyper-meridian joining the states ρ_w and ρ_E (b).

of diagonal matrices it agrees with this metric. For $N = 2$ the simplex of diagonal matrices is one-dimensional, and from the point of view of Bures metric it forms a semicircle.

It is instructive to compare the geometry induced by the Bures (2.4) and the Hilbert–Schmidt metrics (1.2). Any $N = 2$ density matrix ρ may be expressed in the Bloch representation

$$\rho = \frac{1}{2}(\mathbb{I} + \vec{\tau} \cdot \vec{\sigma}) \tag{2.9}$$

where $\vec{\sigma}$ denotes a vector of three Pauli matrices, $\{\sigma_x, \sigma_y, \sigma_z\}$, while the Bloch vector $\vec{\tau} = \{x, y, z\}$ belongs to \mathbb{R}^3 . With respect to the H–S metric the set of mixed states \mathcal{M}_2 forms the Bloch ball B^3 with the set of all pure states at its boundary, called the *Bloch sphere*. The H–S distance between any mixed states of a qubit is proportional to the Euclidean distance inside the ball, so the H–S metric induces the flat geometry in \mathcal{M}_2 . The radius of the Bloch ball depends on the normalization of the Bloch vector, and is equal to unity while using the definition (2.9).

Working in a Cartesian coordinate system we may rewrite (2.9) as

$$\rho = \frac{1}{2} \begin{pmatrix} 1+z & x-iy \\ x+iy & 1-z \end{pmatrix} \quad x^2 + y^2 + z^2 \leq 1. \tag{2.10}$$

Setting $\rho_A = \rho, \rho_B = \rho + d\rho$ in the expression for the Bures distance (2.4) and expanding to second order we obtain a quarter of the round metric on the 3-sphere,

$$ds_B^2 = \frac{1}{4} \left(dx^2 + dy^2 + dz^2 + \frac{(x dx + y dy + z dz)^2}{1 - x^2 - y^2 - z^2} \right). \tag{2.11}$$

Uhlmann noted this fact in [10] and suggested embedding the three-dimensional space of the $N = 2$ mixed states in \mathbb{R}^4 . The transformation

$$\rho(x, y, z) \rightarrow \frac{1}{2}(x, y, z, u := \sqrt{1 - x^2 - y^2 - z^2}) \tag{2.12}$$

blows up the 3-ball into the Uhlmann hyper-hemisphere of \mathbf{S}^3 of radius $R_2 = 1/2$. The maximally mixed state ρ_* , mapped into a hyper-pole, is equally distant from all pure states located at the hyper-equator (see figure 1). The hyper-equator is equivalent to an ordinary two-dimensional sphere and hence isometric to $\mathbb{C}P^1$. The comparison between both metrics

is very transparent for real density matrices: the space of all rebits, which in the H–S metric has the structure of the 2-ball, in the Bures metric has the form of a hemisphere of \mathbf{S}^2 .

Since the radius R_B of the Uhlmann hemisphere is equal to $1/2$ we obtain immediately the Bures volume V and the Bures area S for $N = 2$

$$V_2^{(2)} = \text{vol}_B(\mathcal{M}_2) = \frac{1}{2} S_3 R_B^3 = \frac{\pi^2}{8} \quad S_2^{(2)} = \text{vol}_B(\partial\mathcal{M}_2) = S_2 R_B^2 = \pi \quad (2.13)$$

where S_k denotes the volume of the unit sphere \mathbf{S}^k . This result was obtained by Caves [29], who also expressed the Bures volume of the set of mixed states in the form of an integral. In the further sections of our work we are going to compute such integrals to derive an explicit result for the Bures volume for an arbitrary matrix size N .

The last property of the Bures metric we are going to review, concerns monotonicity. In the classical case of commuting diagonal density matrices, one studies the space of probability vectors $\vec{a} = \{a_1, \dots, a_N\}$, where $a_i \geq 0$ and $\sum_{i=1}^N a_i = 1$. This space is isomorphic with an $(N - 1)$ -dimensional simplex Δ_{N-1} . A discrete dynamics in this space, $\vec{a}' = T\vec{a}$, is given by an arbitrary stochastic matrix T of size N . This matrix contains non-negative entries, $T_{ij} \geq 0$, and the stochasticity condition, $\sum_{j=1}^N T_{ji} = 1$ for $i = 1, \dots, N$ assures that the output vector \vec{a}' is normalized. A distance in the space Δ_{N-1} of N -dimensional probability vectors is called *monotone* if it does not increase under the action of any stochastic matrix T ,

$$D_{\text{mon}}(\vec{a}, \vec{b}) \geq D_{\text{mon}}(T\vec{a}, T\vec{b}). \quad (2.14)$$

If a geodesic distance in the probability simplex is monotone, the corresponding Riemannian metric is called monotone. Chentsov showed [30] that every monotone Riemannian distance in this space is a function of the Fisher statistical distance [28], or the Bhattacharyya coefficient B defined in (2.5).

The quantum case is more complicated. Any discrete dynamics may be described by a quantum operation, $\Phi : \mathcal{M}_N \rightarrow \mathcal{M}_N$, which is trace preserving, $\text{Tr } \Phi(\rho) = \text{Tr } \rho = 1$, and completely positive. Positivity means that $\Phi(\rho) \geq 0$, i.e. Φ sends positive operators into positive operators. From a physical point of view it is necessary to assure that an operation is well defined on the system coupled to an ancilla—an auxiliary system which describes the environment. Hence one requires that Φ is *completely positive*, which means that any extension of the map by an identity operator, $\Phi \otimes \mathbb{I}$, is positive [31]. Completely positive trace-preserving maps play the role of stochastic matrices T in the quantum case, and are thus called *stochastic maps*. In full analogy to (2.14) any distance D in the space of mixed quantum states $\mathcal{M}^{(N)}$ is called *monotone* if it does not grow under the action of a stochastic map,

$$D_{\text{mon}}(\rho, \sigma) \geq D_{\text{mon}}(\Phi(\rho), \Phi(\sigma)). \quad (2.15)$$

If a monotone distance is geodesic the corresponding metric on \mathcal{M}_N is called monotone.

In contrast to the classical case, there exist infinitely many monotone Riemannian metrics on the space of mixed quantum states. However, as shown by Morozova and Chentsov [32] and Petz and Sudár [1], they may be characterized by a symmetric function $c(x, y)$. In general, the length of a vector (matrix) B_{ij} may be position dependent; at a diagonal point $A = \text{diag}(a_1, a_2, \dots, a_N)$ the squared length of B is given by [1]

$$\|B\|_A^2 = \sum_{j=1}^N \frac{B_{jj}}{a_j} + 2 \sum_{j < k=1}^N c(a_j, a_k) |B_{jk}|^2. \quad (2.16)$$

For a diagonal matrix B the second term vanishes and the first term gives back the unique statistical metric on the simplex. The off-diagonal elements, which enter the second term in (2.16), allow for more freedom in the choice of a monotone Riemannian metric.

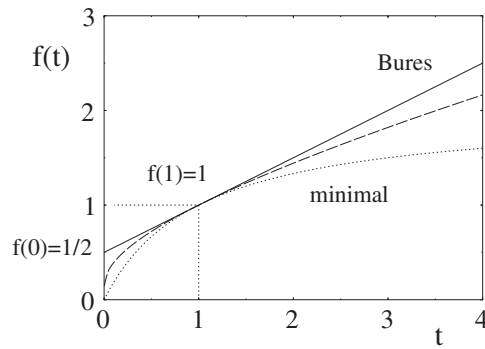


Figure 2. Morozova–Chentsov functions $f(t)$: minimal function for maximal metric (dotted line), Kubo–Mori metric (dashed line), and maximal function for the minimal Bures metric (upper line). These metrics are Fisher adjusted, $f(1) = 1$, while the Bures metric is also Fubini–Study adjusted, $f(0) = 1/2$.

The Morozova–Chentsov function satisfies $c(sx, sy) = s^{-1}c(x, y)$. The symmetry of this two-argument function c enables us to express it as a function of a single parameter, $c(x, y) = f(x/y)/y$, such that $f(1/t) = f(t)/t$.

A function f is called *operator monotone*, if for any matrices G, H the relation $0 \leq G \leq H$ implies $0 \leq f(G) \leq f(H)$. Here $G \leq H$ denotes that their difference is semi-positive, $H - G \geq 0$. Taking for G and H real numbers we see that operator monotonicity implies that f maps $\mathbb{R}_+ \rightarrow \mathbb{R}_+$ and is concave. The result of Morozova and Chentsov [32], completed and extended by Petz and Sudár [1, 33], states that every monotone metric may be written in the form (2.16) up a proportionality constant. Conversely, this equation determines a monotone Riemannian metric, if the function $f(t) = 1/c(t, 1)$ is: (a) operator monotone and (b) self-transposed, $f(1/t) = f(t)/t$. Such functions f are called Morozova–Chentsov functions. Comparison of different metrics is meaningful under a certain normalization. Usually one requires: (c) $f(1) = 1$, since for diagonal matrices such a metric agrees with the statistical (Fisher) metric, and is called *Fisher adjusted*. There exist infinitely many functions f satisfying all three conditions (a)–(c), and leading to Fisher adjusted metrics [1]. Let us mention three examples here:

$$f_{\min}(t) = \frac{2t}{t+1} \quad f_{\text{KM}}(t) = \frac{t-1}{\ln t} \quad f_{\max}(t) = \frac{1+t}{2} \quad (2.17)$$

containing both extremal cases and the intermediate Kubo–Mori (KM) (Bogolioubov) metric used in quantum statistical mechanics [34] and distinguished by the fact that both affine connections with respect to this metric are mutually dual [35]. These functions, plotted in figure 2, correspond to

$$c_{\min}(x, y) = \frac{x+y}{2xy} \quad c_{\text{KM}}(x, y) = \frac{\ln x - \ln y}{x-y} \quad c_{\max}(x, y) = \frac{2}{x+y} \quad (2.18)$$

so the inverse, $1/c$, is equal to the harmonic, logarithmic and arithmetic mean, respectively. It is known that among all normalized, self-transposed, operator monotone functions f there is a minimal one and a maximal one [36]. They are distinguished above by the appropriate labels. The maximal concave function $f_{\max}(t)$, the straight line $t/2 + 1/2$, induces the Bures metric and the Bures distance [1, 37].

If $f(0) = 1/2$ the metric induces the natural Riemannian metric on the subspace $\mathbb{C}P^{N-1}$ of pure states and is called *Fubini–Study adjusted* [1, 8]. The Bures metric is the only

monotone metric which is simultaneously Fisher adjusted and Fubini–Study adjusted. This property, valid for any matrix size N , is easiest to discuss for $N = 2$. All metrics defined by (2.16) are rotationally invariant, i.e. the uniform angular distribution (of eigenvectors of the density matrix) is independent of the radial distribution (of its eigenvalues). In the one-qubit case the metric depends only on the radius $r = \sqrt{x^2 + y^2 + z^2}$ in the unit Bloch ball, and may be divided into the radial and the normal (tangential) components [33],

$$ds^2 = \frac{1}{1-r^2} dr^2 + \frac{1}{1+r} g\left(\frac{1-r}{1+r}\right) dn^2 \quad \text{with} \quad g(t) = \frac{1}{f(t)}. \quad (2.19)$$

The radial component is independent of the function f . It is easy to see that the value of $f(t)$ at $t = 0$ determines the metric at the subspace of pure states, $r = 1$. If $f(0) = 0$, then the metric diverges at the manifold of pure states, which is the case for f_{KM} and f_{min} .

The relation between the Morozova–Chentsov function and the metric $g = 1/f$ shows that the larger the (normalized) function f , the smaller the metric and the corresponding distance. The Bures metric given by the *maximal* function $f_{\text{max}}(t)$, is therefore the *minimal* Fisher adjusted, monotone Riemannian metric. These properties single out the Bures metric and provide an additional motivation to study the geometry it induces in the set of mixed quantum states.

3. Bures measure

3.1. Infinitesimal distance

We are going to compute the Bures distance (2.4) between two infinitesimally close density matrices of size N . Let us set $\rho_A = \rho$, $\rho_B = \rho + \delta\rho$:

$$\sqrt{\rho_A^{1/2} \rho_B \rho_A^{1/2}} = \rho + X + Y \quad (3.1)$$

where the matrix X is of order 1 in $\delta\rho$, while Y is of order 2. Squaring this equation we obtain to first and second order

$$\rho^{1/2} \delta\rho \rho^{1/2} = X\rho + \rho X \quad -X^2 = Y\rho + \rho Y \quad (3.2)$$

or in the basis in which ρ is diagonal with eigenvalues $\rho_\nu > 0$

$$X_{\nu\mu} = \delta\rho_{\nu\mu} \frac{\rho_\nu^{1/2} \rho_\mu^{1/2}}{\rho_\nu + \rho_\mu} \quad Y_{\nu\mu} = -(X^2)_{\nu\mu} \frac{1}{\rho_\nu + \rho_\mu}. \quad (3.3)$$

Since $\text{Tr} \rho = 1$, hence $\text{Tr} \delta\rho = 0$ and $\text{Tr} X = \text{Tr} \delta\rho/2 = 0$, while

$$\text{Tr} Y = - \sum_{\nu\mu} \frac{1}{2\rho_\nu} |X_{\nu\mu}|^2 = - \sum_{\nu\mu} \frac{1}{4} \frac{|\delta\rho_{\nu\mu}|^2}{\rho_\nu + \rho_\mu}. \quad (3.4)$$

Thus we arrive at the result of Hübner [11] for the Bures metric

$$(ds)_B^2 = (D(\rho, \rho + \delta\rho))^2 = \frac{1}{2} \sum_{\nu\mu} \frac{|\delta\rho_{\nu\mu}|^2}{\rho_\nu + \rho_\mu}. \quad (3.5)$$

Note, that if $\rho_\nu = 0$ and $\rho_\mu = 0$, $\delta\rho_{\nu\mu}$ does not appear and therefore terms where the denominator vanishes have to be excluded.

3.2. The volume

Let us rewrite the metric (3.5) distinguishing the diagonal elements

$$(\mathrm{d}s)_B^2 = \sum_{v=1}^N \frac{|\delta\rho_{vv}|^2}{4\rho_v} + \sum_{v<\mu} \frac{|\delta\rho_{v\mu}|^2}{\rho_v + \rho_\mu}. \quad (3.6)$$

For diagonal matrices the second term vanishes and the above expression reduces to (2.8). Since $\mathrm{Tr} \rho = 1$ so $\sum_{v=1}^N \delta\rho_{vv} = 0$ and not all $\delta\rho_{vv}$ are independent. Eliminating $\delta\rho_{NN}$ we obtain

$$\sum_{v=1}^N \frac{(\delta\rho_{vv})^2}{\rho_v} = \sum_{v=1}^{N-1} \frac{(\delta\rho_{vv})^2}{\rho_v} + \left(\sum_{v=1}^{N-1} \delta\rho_{vv} \right)^2 \frac{1}{\rho_N}. \quad (3.7)$$

The metric (3.7) in the $(N-1)$ -dimensional subspace is of the form $g_{ik} = (\delta_{ik}/\rho_i + 1/\rho_N)$ with determinant $\det g = (\rho_1 + \rho_2 + \dots + \rho_N)/(\rho_1\rho_2 \dots \rho_N) = 1/\det \rho$ using $\mathrm{Tr} \rho = 1$. Thus the volume element gains a factor $\sqrt{\det g} = (\det \rho)^{-1/2}$:

$$\mathrm{d}V_B = \frac{1}{2^{N^2-1}} (\det \rho)^{-1/2} \prod_{v=1}^{N-1} \mathrm{d}\rho_{vv} \prod_{v<\mu} \frac{2}{\rho_v + \rho_\mu} \prod_{v<\mu} (\sqrt{2} \mathrm{d} \mathrm{Re}(\rho_{v\mu}) \sqrt{2} \mathrm{d} \mathrm{Im}(\rho_{v\mu})). \quad (3.8)$$

The total volume of the set \mathcal{M}_N is given by

$$V_B = 2^{1-N^2} \int D\rho \frac{\delta(\mathrm{Tr} \rho - 1)}{\det \rho^{1/2}} \theta(\rho) \prod_{v<\mu} \frac{2}{\rho_v + \rho_\mu} \quad (3.9)$$

with $\theta(\rho) = \theta(\rho_1) \dots \theta(\rho_N)$ a step function that restricts integration to non-negative ρ . We introduced the volume element

$$D\rho = \prod_{v=1}^N \mathrm{d}\rho_{vv} \prod_{v<\mu} (\sqrt{2} \mathrm{d} \mathrm{Re}(\rho_{v\mu}) \sqrt{2} \mathrm{d} \mathrm{Im}(\rho_{v\mu})) \quad (3.10)$$

which differs from the usual definition by a factor $2^{N(N-1)/2}$. It follows from the metric for unrestricted Hermitian matrices:

$$(\mathrm{d}s)^2 = \sum_{v=1}^N (\delta\rho_{vv})^2 + 2 \sum_{v<\mu} |\delta\rho_{v\mu}|^2. \quad (3.11)$$

Above we considered the case of Hermitian density matrices ($\beta = 2$). In the case of real density matrices ($\beta = 1$) there are no imaginary parts $\mathrm{Im} \rho_{v\mu}$.

3.3. Radial coordinates

Let us diagonalize the matrices ρ

$$\rho = U \Lambda U^{-1} \quad \text{or} \quad \rho = O \Lambda O^{-1} \quad (3.12)$$

with U unitary for $\beta = 2$, O orthogonal for $\beta = 1$, $\Lambda = \mathrm{diag}(\rho_1, \rho_2, \dots, \rho_N)$. Then we have

$$\mathrm{d}\rho = U[\mathrm{d}\Lambda + U^{-1} \mathrm{d}U \Lambda - \Lambda U^{-1} \mathrm{d}U]U^{-1} \quad (3.13)$$

or

$$\mathrm{d}\rho = O[\mathrm{d}\Lambda + O^{-1} \mathrm{d}O \Lambda - \Lambda O^{-1} \mathrm{d}O]O^{-1}.$$

Let us first rewrite the Bures metric in a basis independent way,

$$(\mathrm{d}s)_B^2 = \frac{1}{2} \int_0^\infty \mathrm{d}t \mathrm{Tr}(\mathrm{d}\rho e^{-\rho t} \mathrm{d}\rho e^{-\rho t}). \quad (3.14)$$

This means it contains left and right multiplications with ρ . Inserting now the expressions for $d\rho$ we see that again we can go to the representation where ρ is diagonal and obtain metrics in the cases of complex density matrices,

$$(ds)^2 = \sum_{v=1}^N \frac{(d\rho_v)^2}{4\rho_v} + \sum_{v<\mu} \frac{(\rho_v - \rho_\mu)^2}{\rho_v + \rho_\mu} |(U^{-1}dU)_{v\mu}|^2 \tag{3.15}$$

and real density matrices

$$(ds)^2 = \sum_{v=1}^N \frac{(d\rho_v)^2}{4\rho_v} + \sum_{v<\mu} \frac{(\rho_v - \rho_\mu)^2}{\rho_v + \rho_\mu} |(O^{-1}dO)_{v\mu}|^2. \tag{3.16}$$

In both cases the Bures measure has the following product form

$$dV_B^{(\beta)} = d\mu^{(\beta)}(\rho_1, \rho_2, \dots, \rho_N) \times dv_\beta. \tag{3.17}$$

The first factor depends only on the eigenvalues ρ_i , while the latter, determining the distribution of the eigenvectors of the density matrix, is the unique, unitarily invariant, Haar measure on $U(N)$ for $\beta = 2$ or on $O(N)$ for $\beta = 1$. In the general case of complex density matrices ($\beta = 2$), the Bures measure in the simplex of eigenvalues reads

$$P_B(\Lambda) = P_B(\rho_1, \rho_2, \dots, \rho_N) = C_N \frac{\delta(\rho_1 + \rho_2 + \dots + \rho_N - 1)}{\sqrt{\rho_1 \rho_2 \dots \rho_N}} \prod_{v<\mu} \frac{(\rho_v - \rho_\mu)^2}{\rho_v + \rho_\mu} \tag{3.18}$$

where the normalization constant C_N assures that the integral of P over all eigenvalues is equal to unity. The measure was derived by Hall [17], and was later analysed in [38, 39]. To compute the area of the surface of the set of complex density matrices, and to find the volume of the set of real density matrices, we will need a family of generalized constants $C_N(\alpha, \beta)$ defined by

$$\frac{1}{C_N(\alpha, \beta)} = \int_0^\infty \prod_{v=1}^N \frac{d\rho_v}{\rho_v^{1/2}} \delta(\rho_1 + \dots + \rho_N - 1) \left[\prod_{v<\mu} \frac{(\rho_v - \rho_\mu)^2}{\rho_v + \rho_\mu} \right]^{\beta/2} \prod_{\kappa=1}^N \rho_\kappa^{\alpha-1}. \tag{3.19}$$

The standard Hall constants entering (3.18) become a special case of this definition, $C_N = C_N(1, 2)$. They will be needed to compute the Bures volume of \mathcal{M}_N .

Integrating the Bures measure over the eigenvectors distributed according to the Haar measure on $U(N)$ or $O(N)$ we obtain

$$dV_B^{(\beta)} = 2^{1-N[1+(N-1)\beta/2]} \det \rho^{-1/2} \prod_{v=1}^{N-1} d\rho_v \prod_{v<\mu} \left[\frac{2(\rho_v - \rho_\mu)^2}{\rho_v + \rho_\mu} \right]^{\beta/2} V_{\text{Flag}}^{(\beta)}(N) \tag{3.20}$$

where $V_{\text{Flag}}^{(\beta)}(N)$ denotes the volume of the flag manifold, $Fl_N^{\mathbb{C}} = U(N)/U(1)^N$ or $Fl_N^{\mathbb{R}} = O(N)/O(1)^N$ for $\beta = 2, 1$. Although these volumes

$$V_{\text{Flag}}^{(2)}(N) = \text{Vol}(Fl_N^{\mathbb{C}}) = \frac{(2\pi)^{N(N-1)/2}}{\Gamma(1)\Gamma(2) \dots \Gamma(N)} \tag{3.21}$$

and

$$V_{\text{Flag}}^{(1)}(N) = \text{Vol}(Fl_N^{\mathbb{R}}) = \frac{(2\pi)^{N(N-1)/4} \pi^{N/2}}{\Gamma(1/2)\Gamma(2/2) \dots \Gamma(N/2)}$$

were computed by Hua several years ago [40], we provide their short derivation in [19] and show that various results for the volumes of the unitary groups and flag manifolds present

in the literature [29, 41–43] are due to different choices of normalization. Formally we may write the volumes in the form

$$V_{\text{Flag}}^{(\beta)}(N) = \prod_{j=1}^N (2\pi)^{(j-1)\beta/2} \frac{\Gamma(\beta/2)}{\Gamma(j\beta/2)} \quad (3.22)$$

which shows that it is the product of the volumes of projective spaces with increasing dimension $j - 1$, real for $\beta = 1$, complex for $\beta = 2$, and the radius rescaled by a factor $\sqrt{2}$ coming from the factor $2^{\beta N(N-1)/4}$ (see the appendix of [19]).

Since the unitary or orthogonal rotations produce all permutations, in (3.20) we have to restrict to a certain order of eigenvalues, $\rho_1 < \rho_2 < \dots < \rho_N$. In order to lift this condition we need to divide the result by the number of permutations, equal to $N!$,

$$V_B^{(\beta)} = 2^{1-N[1+(N-1)\beta/2]} \int_0^\infty \frac{d\rho_1 \dots d\rho_N}{\det \rho^{1/2}} \delta(\text{Tr } \rho - 1) \prod_{\nu < \mu} \left[\frac{2(\rho_\nu - \rho_\mu)^2}{\rho_\nu + \rho_\mu} \right]^{\beta/2} \frac{V_{\text{Flag}}^{(\beta)}(N)}{N!}. \quad (3.23)$$

3.4. The surface

The surface consists of the N pieces with one eigenvalue = 0. To calculate the metric on the surface (with $\rho_1 = 0$) we put first $d\rho_1 = 0$ and then $\rho_1 = 0$ (remember that terms with vanishing denominator have to be excluded):

$$(ds)^2 = \sum_{\nu=2}^N \frac{(d\rho_\nu)^2}{4\rho_\nu} + \sum_{\nu < \mu}^{2\dots N} \frac{(\rho_\nu - \rho_\mu)^2}{\rho_\nu + \rho_\mu} |(U^{-1} dU)_{\nu\mu}|^2 + \sum_{\mu=2}^N \rho_\mu |(U^{-1} dU)_{1\mu}|^2. \quad (3.24)$$

Then with the same reasoning as above the surface element is given by

$$dS = 2^{1-(N-1)(1+N\beta/2)} \prod_{\nu=2}^{N-1} \frac{d\rho_\nu}{\rho_\nu^{1/2}} \left[\prod_{\nu < \mu}^{2\dots N} \frac{2(\rho_\nu - \rho_\mu)^2}{\rho_\nu + \rho_\mu} \prod_{\kappa=2}^N 2\rho_\kappa \right]^{\beta/2} V_{\text{Flag}}^{(\beta)}(N) \quad (3.25)$$

and the total surface

$$S_N^{(\beta)} = S_{N,1}^{(\beta)} = 2^{1-(N-1)(1+N\beta/2)} \int \prod_{\nu=2}^N \frac{d\rho_\nu}{\rho_\nu^{1/2}} \frac{\delta(\rho_2 + \dots + \rho_N - 1)}{(N-1)!} \times \left[\prod_{\nu < \mu}^{2\dots N} \frac{2(\rho_\nu - \rho_\mu)^2}{\rho_\nu + \rho_\mu} \prod_{\kappa=2}^N 2\rho_\kappa \right]^{\beta/2} V_{\text{Flag}}^{(\beta)}(N) \quad (3.26)$$

where we have taken into account all permutations of the $N - 1$ non-zero eigenvalues.

3.5. The edges and hyperedges

There are $N(N-1)/2$ edges which correspond to two vanishing eigenvalues. Hence there are $(N-2)!$ different permutations of positive, generically different eigenvalues which form the edges. To calculate the metric on the edges we put first $d\rho_1 = d\rho_2 = 0$ and then $\rho_1 = \rho_2 = 0$:

$$(ds)^2 = \sum_{\nu=3}^N \frac{(d\rho_\nu)^2}{4\rho_\nu} + \sum_{\nu < \mu}^{3\dots N} \frac{(\rho_\nu - \rho_\mu)^2}{\rho_\nu + \rho_\mu} |(U^{-1} dU)_{\nu\mu}|^2 + \sum_{\mu=3}^N \rho_\mu (|(U^{-1} dU)_{1\mu}|^2 + |(U^{-1} dU)_{2\mu}|^2). \quad (3.27)$$

We see that there do not appear terms $(U^{-1} dU)_{\nu\mu}$ with $\nu, \mu = 1, 2$. Thus the corresponding coset space which has to be integrated over is the flag manifold $U(N)/[U(2) \times U(1)^{N-2}]$ for $\beta = 2$ or $O(N)/[O(2) \times O(1)^{N-2}]$ for $\beta = 1$. Since their volume is equal to the ratio $\text{Vol}(Fl_N)/\text{Vol}(Fl_2)$, the edge element is then given by

$$dS_{N,2}^{(\beta)} = 2^{-d_2} \prod_{\nu=3}^{N-1} \frac{d\rho_\nu}{\rho_\nu^{1/2}} \left[\prod_{\nu<\mu}^{3\dots N} \frac{2(\rho_\nu - \rho_\mu)^2}{\rho_\nu + \rho_\mu} \prod_{\kappa=3}^N (2\rho_\kappa)^2 \right]^{\beta/2} \frac{V_{\text{Flag}}^{(\beta)}(N)}{V_{\text{Flag}}^{(\beta)}(2)} \quad (3.28)$$

with the dimension d_n

$$d_n = (N - n)(1 + (N + n - 1)\beta/2) - 1. \quad (3.29)$$

The total area of the edges is

$$S_{N,2}^{(\beta)} = 2^{-d_2} \int_0^\infty \prod_{\nu=3}^N \frac{d\rho_\nu}{\rho_\nu^{1/2}} \frac{\delta(\rho_3 + \dots + \rho_N - 1)}{(N - 2)!} \left[\prod_{\nu<\mu}^{3\dots N} \frac{2(\rho_\nu - \rho_\mu)^2}{\rho_\nu + \rho_\mu} \prod_{\kappa=3}^N (2\rho_\kappa)^2 \right]^{\beta/2} \frac{V_{\text{Flag}}^{(\beta)}(N)}{V_{\text{Flag}}^{(\beta)}(2)}. \quad (3.30)$$

It is straightforward to generalize this to hyperedges: the manifold of states of rank $N - n$ with $n = 0, 1, \dots, N - 1$ has the volume

$$S_{N,n}^{(\beta)} = 2^{-d_n} \int_0^\infty \prod_{\nu=n+1}^N \frac{d\rho_\nu}{\rho_\nu^{1/2}} \frac{\delta(\rho_{n+1} + \dots + \rho_N - 1)}{(N - n)!} \times \left[\prod_{\nu<\mu}^{n+1,\dots,N} \frac{2(\rho_\nu - \rho_\mu)^2}{\rho_\nu + \rho_\mu} \prod_{\kappa=n+1}^N (2\rho_\kappa)^n \right]^{\beta/2} \frac{V_{\text{Flag}}^{(\beta)}(N)}{V_{\text{Flag}}^{(\beta)}(n)}. \quad (3.31)$$

4. Bures volume

4.1. Normalization constants

The above formulae for the volumes of manifolds of states of rank $N - n$ may be expressed in a compact way with use of the generalized Hall constants (3.19)

$$S_{N,n}^{(\beta)} = \frac{2^{-d_n+(N-n)(N+n-1)\beta/4}}{(N - n)! C_{N-n}(1 + n\beta/2, \beta)} \frac{V_{\text{Flag}}^{(\beta)}(N)}{V_{\text{Flag}}^{(\beta)}(n)}. \quad (4.1)$$

We are going to compute the constants $C_N(\alpha, \beta)$ for integer α, β and then continue analytically to general positive α and β . Let us go to variables $\rho_i = t_i^2$. Then the integral (3.19) is an integral over the full sphere $R^2 = t_1^2 + t_2^2 + \dots + t_N^2 = 1$ with a homogeneous function in R of order $\beta N(N - 1)/2 + 2N(\alpha - 1)$ as integrand. The radial integral may be replaced by a Γ function, which amounts to replacing $\delta(R^2 - 1)$ by e^{-R^2} . The result is the same up to a factor. Afterwards we may go back to the variables ρ_i and obtain

$$\frac{\Gamma[N(2\alpha + (N - 1)\beta/2 - 1)/2]}{C_N(\alpha, \beta)} = \int_0^\infty \prod_{\nu=1}^N \frac{d\rho_\nu}{\rho_\nu^{1/2}} e^{-(\rho_1+\dots+\rho_N)} \left[\prod_{\nu<\mu}^{1\dots N} \frac{(\rho_\nu - \rho_\mu)^2}{\rho_\nu + \rho_\mu} \right]^{\beta/2} \prod_{\kappa=1}^N \rho_\kappa^{\alpha-1}. \quad (4.2)$$

In the next step we want to eliminate the denominators in (4.2). In this section we discuss the case $\beta = 2$ of complex density matrices,

$$\frac{1}{(\rho_1 \dots \rho_N)^{1/2}} \prod_{\nu<\mu} \frac{1}{\rho_\nu + \rho_\mu} = \int e^{-\sum \rho_i X_{ii}^2 - \sum_{i<j} |X_{ij}|^2 (\rho_i + \rho_j)} \prod_{i=1}^N \frac{dX_{ii}}{\sqrt{\pi}} \prod_{i<j} \frac{d\text{Re } X_{ij} d\text{Im } X_{ij}}{\pi}. \quad (4.3)$$

Using the volume element DX of a Hermitian matrix X (3.10) we may rewrite this as

$$\frac{1}{(\rho_1 \dots \rho_N)^{1/2}} \prod_{v < \mu} \frac{1}{\rho_v + \rho_\mu} = \pi^{-N^2/2} 2^{-N(N-1)/2} \int DX e^{-\text{Tr} \rho X^2}. \quad (4.4)$$

This expression is basis independent and provides a way to describe the Bures probability distribution in a random matrix description. With this we may write for $\beta = 2$

$$\frac{\Gamma(N^2/2 + N(\alpha - 1))}{C_N(\alpha, 2)} = \pi^{-N^2/2} 2^{-N(N-1)/2} \frac{N!}{V_{\text{Flag}}^{(2)}(N)} \int D\rho \theta(\rho) \det \rho^{\alpha-1} \int DX e^{-\text{Tr} \rho(1+X^2)}. \quad (4.5)$$

Now we use a formula which is an extension of the Ingham–Siegel integral [45]

$$\left[\det \left(\frac{\delta}{\delta \rho} + \epsilon \right) \right]^{-N} \delta(\rho) = A_N \theta(\rho) e^{-\text{Tr} \epsilon \rho} \quad (4.6)$$

valid for a positive Hermitian matrix ϵ and with a constant A_N . Let us derive this formula

$$\left[\det \left(\frac{\delta}{\delta \rho} + \epsilon \right) \right]^{-N} \delta(\rho) = \pi^{-N^2} \int d\psi_1 \dots d\psi_N e^{-[\psi_1^\dagger (\delta/\delta \rho + \epsilon) \psi_1 + \dots + \psi_N^\dagger (\delta/\delta \rho + \epsilon) \psi_N]} \delta(\rho) \quad (4.7)$$

with N -dimensional complex vectors ψ_1, \dots, ψ_N . The translation operator shifts the argument ρ of the δ function by the matrix $\psi_1 \otimes \psi_1^\dagger + \dots + \psi_N \otimes \psi_N^\dagger$. Then the integration can be done and yields

$$\left[\det \left(\frac{\delta}{\delta \rho} + \epsilon \right) \right]^{-N} \delta(\rho) = e^{-\text{Tr} \epsilon \rho} \pi^{-N^2} \int d\psi_1 \dots d\psi_N \delta(\rho - (\psi_1 \otimes \psi_1^\dagger + \dots + \psi_N \otimes \psi_N^\dagger)).$$

For $\rho > 0$ we may rescale $\psi \rightarrow \sqrt{\rho} \psi$. The Jacobian cancels out and the result is equation (4.6). The constant A_N can be calculated from integrating this equation (4.6) over ρ . With partial integration we find

$$\frac{2^{N(N-1)/2}}{\det \epsilon^N} = A_N \int D\rho \theta(\rho) e^{-\text{Tr} \epsilon \rho}.$$

This is valid for any Hermitian matrix $\epsilon > 0$. The coefficient A_N is independent of the matrix ϵ . To calculate A_N we put $\epsilon = \mathbb{I}$. The integral can again be done using the Laguerre ensemble:

$$\frac{1}{A_N} = \frac{V_{\text{Flag}}^{(2)}(N)}{2^{N(N-1)/2} N!} \prod_{j=1}^N \Gamma(1+j) \Gamma(j) = \pi^{N(N-1)/2} \Gamma(1) \dots \Gamma(N). \quad (4.8)$$

4.2. Main results

Using equations (4.5), (4.6) and (4.8) we may write

$$\frac{\Gamma(N^2/2 + N(\alpha - 1))}{C_N(\alpha, 2)} = \frac{\pi^{-N^2/2} 2^{-N(N-1)/2} N!}{A_N V_{\text{Flag}}^{(2)}(N)} \times \int D\rho \int DA \det \rho^{\alpha-1} \left[\det \left(\frac{\delta}{\delta \rho} + 1 + A^2 \right) \right]^{-N} \delta(\rho). \quad (4.9)$$

For $\alpha = 1$ we obtain immediately by partial integration

$$\frac{\Gamma(N^2/2)}{C_N(1, 2)} = \frac{\pi^{-N^2/2} N!}{A_N V_{\text{Flag}}^{(2)}(N)} \int \frac{DA}{\det(1 + A^2)^N} = \frac{\pi^{-N^2/2}}{A_N} \int \prod_{i=1}^N \frac{da_i}{(1 + a_i^2)^N} \prod_{i < j} (a_i - a_j)^2. \quad (4.10)$$

The last integral may be calculated in the complex plane and yields: $(2\pi)^N N! 2^{-N^2}$, such that the Bures–Hall constants are given by

$$C_N = C_N(1, 2) = \frac{2^{N^2-N} \Gamma(N^2/2)}{\pi^{N/2} \Gamma(1) \dots \Gamma(N+1)}. \tag{4.11}$$

This coincides with the known values for the Bures–Hall constants, $C_2 = 2/\pi$, $C_3 = 35/\pi$ and $C_4 = 2^{11} 35/\pi^2$ and confirms some conjectures of Slater concerning C_5 and C_6 [18]. The Bures volume of the set of complex density matrices of size N is now given by

$$V_N^{(2)} = \frac{2^{1-N(N+1)/2} V_{\text{Flag}}^{(2)}(N)}{C_N(1, 2) N!} = 2^{1-N^2} \frac{\pi^{N^2/2}}{\Gamma(N^2/2)} \tag{4.12}$$

and for $N = 2$ reduces to (2.13). Note that the factor 2^{1-N^2} enters from the beginning in the definition. It disappears if we increase ds (3.6) by a factor of 2. The Bures volume is exactly equal to the $(N^2 - 1)$ -dimensional volume of an $(N^2 - 1)$ -dimensional hemisphere with radius $1/2$. Equations (4.11) and (4.12) constitute the central results of this work.

4.3. Area of surface and edges

For the surface and the edges of the Bures manifold we need $\alpha \neq 1$. Scaling $\rho \rightarrow \epsilon^{-1/2} \rho \epsilon^{-1/2}$ for ϵ any Hermitian matrix > 0 shows that the integral (4.9) can be obtained from

$$\int D\rho \det \rho^{\alpha-1} \left[\det \left(\frac{\delta}{\delta\rho} + \epsilon \right) \right]^{-N} \delta(\rho) = B_N \det \epsilon^{1-N-\alpha} \tag{4.13}$$

with B_N independent of ϵ . To compute B_N we put $\epsilon = \mathbb{I}$ and go back using equation (4.6). This again leads to an integral over the Laguerre ensemble and we obtain

$$B_N = A_N \frac{V_{\text{Flag}}^{(2)}(N)}{N!} \prod_{j=1}^N \Gamma(1+j) \Gamma(\alpha+j-1) = 2^{N(N-1)/2} \prod_{j=1}^N \frac{\Gamma(\alpha+j-1)}{\Gamma(j)}. \tag{4.14}$$

Such an integral has already appeared for the H–S metric [19]. Thus we have

$$\begin{aligned} \frac{\Gamma[N^2/2 + N(\alpha - 1)]}{C_N(\alpha, 2)} &= \frac{\pi^{-N^2/2} N!}{A_N V_{\text{Flag}}^{(2)}(N)} \int \frac{DX}{\det(1 + X^2)^{N+\alpha-1}} \\ &= \prod_{j=1}^N \frac{\Gamma(\alpha + j - 1)}{\Gamma(1/2)} \int_{-\infty}^{+\infty} \prod_{i=1}^N \frac{dx_i}{(1 + x_i^2)^{N-1+\alpha}} \prod_{j < k} (x_j - x_k)^2. \end{aligned} \tag{4.15}$$

Thus the ensemble is reduced to a kind of Lorentz ensemble. The last integral can be found in the book by Mehta [44], (p 350) following from Selberg’s integral:

$$J(1, 1, N + \alpha - 1, N + \alpha - 1, 1, N) = \pi^N 2^{-N^2+N-2N(\alpha-1)} \prod_{j=1}^N \frac{\Gamma(1+j) \Gamma(N + 2\alpha - 1 - j)}{\Gamma(N + \alpha - j)^2}. \tag{4.16}$$

As a result we obtain

$$\frac{\Gamma(N^2/2 + N(\alpha - 1))}{C_N(\alpha, 2)} = \pi^{N/2} 2^{-N^2+N-2N(\alpha-1)} \prod_{j=1}^N \frac{\Gamma(1+j) \Gamma(2\alpha - 2 + j)}{\Gamma(\alpha + j - 1)}. \tag{4.17}$$

From equation (4.1) we obtain for the volumes of submanifolds of rank $N - n$ of the space of complex density matrices

$$S_{N,n}^{(2)} = \frac{2^{-d_n+(N-n)(N+n-1)/2} V_{\text{Flag}}^{(2)}(N)}{C_{N-n}(1+n, 2)(N-n)! V_{\text{Flag}}^{(2)}(n)}. \tag{4.18}$$

The result is rather simple

$$S_{N,n}^{(2)} = 2^{-d_n} \frac{\pi^{(d_n+1)/2}}{\Gamma[(d_n+1)/2]} \binom{N+n-1}{n} \quad (4.19)$$

and reduces to (4.12) for $n = 0$. Here $d_n = N^2 - n^2 - 1$ denotes the dimensionality of each submanifold.

These volumes are equal to the volume of a d_n -dimensional hyper-hemisphere with radius $1/2$ times a factor obtained from Bose statistics, which is equal to the number of possibilities of putting n identical balls into N boxes. Note that this is not equal to the number of equal pieces of edges, which is obtained from Fermi statistics where only one ball fits into one box: $\binom{N}{n}$. There is no difference for $n = 1$. Thus the surface to volume ratio γ is given by

$$\gamma_B = \frac{S_{N,1}^{(2)}}{S_{N,0}^{(2)}} = \frac{2}{\sqrt{\pi}} \frac{\Gamma(N^2/2)}{\Gamma(N^2/2 - 1/2)} N \quad (4.20)$$

which behaves as N^2 , so in the limit of large matrix size N it grows proportionally to the dimensionality $N^2 - 1$ of the space of mixed states. Note that such a ratio for the hemispheres of dimensionality N^2 is proportional to N . For pure states $n = N - 1$ we obtain the volume

$$S_{N,N-1}^{(2)} = \text{Vol}(\mathbb{C}P^{N-1}) = \frac{\pi^{N-1}}{(N-1)!} \quad (4.21)$$

which is equal to the volume of a $2(N-1)$ -dimensional real ball of radius 1 and this equals the volume of an $(N-1)$ -dimensional complex projective space, which is a correct consequence of the Bures metric for pure states. By the way, up to a scale factor this is the same for the Hilbert–Schmidt metric [19]. Differences come only for mixed states.

5. Real density matrices and Lorentz-type ensemble

To compute the volume of the set of real density matrices we need to find the generalized Hall constants (3.19) for $\beta = 1$. To do so we write

$$\frac{1}{(\rho_1 \dots \rho_N)^{1/2}} \prod_{v < \mu} \frac{1}{(\rho_v + \rho_\mu)^{1/2}} = \int e^{-\sum \rho_i X_{ii}^2 - \sum_{i < j} X_{ij}^2 (\rho_i + \rho_j)} \prod_{i=1}^N \frac{dX_{ii}}{\sqrt{\pi}} \prod_{i < j} \frac{dX_{ij}}{\sqrt{\pi}}. \quad (5.1)$$

Let us introduce the volume element of a real symmetric matrix X with the metric

$$(ds)^2 = \text{Tr}(dX)^2 = \sum_{i=1}^N (dX_{ii})^2 + 2 \sum_{i < j} dX_{ij}^2 \quad (5.2)$$

$$DX = \prod_i dX_{ii} \prod_{j < k} (dX_{jk} \sqrt{2}). \quad (5.3)$$

Then we have

$$\frac{1}{(\rho_1 \dots \rho_N)^{1/2}} \prod_{v < \mu} \frac{1}{(\rho_v + \rho_\mu)^{1/2}} = \pi^{-N(N+1)/4} 2^{-N(N-1)/4} \int DX e^{-\text{Tr} \rho X^2}. \quad (5.4)$$

With this we may write the formula for $\beta = 1$

$$\frac{\Gamma(N(\alpha - 1/2 + (N-1)/2))}{C_N(\alpha, 1)} = (2\pi)^{-N(N+1)/4} 2^{N/2} \times \int_0^\infty d\rho_1 \dots d\rho_N \prod_{v < \mu} |\rho_v - \rho_\mu| \det \rho^{\alpha-1} \int DA e^{-\text{Tr}(\rho(1+A^2))}. \quad (5.5)$$

Now with ϵ a real symmetric positive matrix we want to calculate for real symmetric ρ :

$$\begin{aligned} \left[\det \left(\frac{\delta}{\delta\rho} + \epsilon \right) \right]^{-N/2} \delta(\rho) &= \pi^{-N^2/2} \int d\psi_1 \dots d\psi_N e^{-[\psi_1^\top (\delta/\delta\rho + \epsilon) \psi_1 + \dots + \psi_N^\top (\delta/\delta\rho + \epsilon) \psi_N]} \delta(\rho) \\ &= e^{-\text{Tr} \epsilon \rho} \pi^{-N^2} \int d\psi_1 \dots d\psi_N \delta(\rho - (\psi_1 \otimes \psi_1^\top + \dots + \psi_N \otimes \psi_N^\top)) \end{aligned} \tag{5.6}$$

with real vectors ψ_1, \dots, ψ_N . For $\rho > 0$ we may rescale $\psi \rightarrow \sqrt{\rho} \psi$, then the volume element is $\propto \det \rho^{N/2}$ and the δ -function $\propto \det \rho^{-(N+1)/2}$. This implies

$$\left[\det \left(\frac{\delta}{\delta\rho} + \epsilon \right) \right]^{-N/2} \delta(\rho) = K_N \theta(\rho) e^{-\text{Tr} \epsilon \rho} \det \rho^{-1/2} \tag{5.7}$$

with K_N a constant independent of ϵ . With partial integration we find

$$\frac{2^{N(N-1)/4}}{\det \epsilon^{N/2}} = K_N \int D\rho \theta(\rho) e^{-\text{Tr} \epsilon \rho} \det \rho^{-1/2}.$$

To calculate K_N we put $\epsilon = \mathbb{I}$ and find again with the help of the Laguerre ensemble [44] (p 354)

$$\frac{1}{K_N} = \frac{V_{\text{Flag}}^{(1)}(N)}{2^{N(N-1)/4} N!} \prod_{j=1}^N \frac{\Gamma(1 + j\beta/2) \Gamma[1/2 + (j-1)\beta/2]}{\Gamma(1 + \beta/2)}. \tag{5.8}$$

To obtain the generalized normalization constants for $\beta = 1$ and arbitrary α we may write

$$\begin{aligned} \frac{\Gamma[N(2\alpha - 1 + (N-1)/2)/2]}{C_N(\alpha, 1)} &= \frac{(2\pi)^{-N(N-1)/4} 2^{N/2} N!}{K_N V_{\text{Flag}}^{(1)}(N)} \\ &\times \int D\rho \int DX \det \rho^{\alpha-1/2} \left[\det \left(\frac{\delta}{\delta\rho} + 1 + X^2 \right) \right]^{-N/2} \delta(\rho). \end{aligned} \tag{5.9}$$

Scaling $\rho \rightarrow \epsilon^{-1/2} \rho \epsilon^{-1/2}$ for ϵ any real symmetric matrix > 0 shows the identity

$$\int D\rho \det \rho^{\alpha-1} \left[\det \left(\frac{\delta}{\delta\rho} + \epsilon \right) \right]^{-N/2} \delta(\rho) = L_N \det \epsilon^{(1-N-2\alpha)/2} \tag{5.10}$$

with L_N a constant independent of the matrix ϵ . To compute L_N we put $\epsilon = \mathbb{I}$ and go back. Again we obtain an integral over the Laguerre ensemble with the result

$$L_N = 2^{N(N-1)/4} \prod_{j=1}^N \frac{\Gamma[\alpha + (j-1)/2]}{\Gamma[1/2 + (j-1)/2]}. \tag{5.11}$$

This formula is very similar to (4.14) for the constant B_N in the complex case. In fact it is not difficult to rewrite both results in one expression as a function of β . This allows us to write down an equation which is valid in the complex as well as in the real case, for $\beta = 2$ and $\beta = 1$, respectively,

$$\begin{aligned} \frac{\Gamma[N(2\alpha - 1 + (N-1)\beta/2)/2]}{C_N(\alpha, \beta)} &= \prod_{j=1}^N \frac{\Gamma[\alpha + (j-1)\beta/2]}{\Gamma(1/2)} \\ &\times \int_{-\infty}^{+\infty} \prod_{i=1}^N \frac{dx_i}{(1+x_i^2)^{(N-1)\beta/2+\alpha}} \prod_{j<k} |x_j - x_k|^\beta. \end{aligned} \tag{5.12}$$

As result we have a Lorentz-type ensemble. The last integral can be found in the book by Mehta (p 350) with $\gamma = (N - 1)\beta/2 + \alpha$:

$$J(1, 1, \gamma, \gamma, \beta/2, N) = \pi^N 2^{N((N-1)\beta/2+2-2\gamma)} \times \prod_{j=0}^{N-1} \frac{\Gamma[1 + (j+1)\beta/2]\Gamma[2\gamma - (N+j-1)\beta/2 - 1]}{\Gamma(1 + \beta/2)[\Gamma(\gamma - j\beta/2)]^2}. \quad (5.13)$$

Inserting this into equation (5.12) we obtain

$$\frac{\Gamma[N(2\alpha - 1 + (N - 1)\beta/2)/2]}{C_N(\alpha, \beta)} = \frac{\pi^{N/2}}{2^{N((N-1)\beta/2+2(\alpha-1))}} \times \prod_{j=1}^N \frac{\Gamma(1 + j\beta/2)\Gamma[(N - j)\beta/2 + 2\alpha - 1]}{\Gamma(1 + \beta/2)\Gamma[(N - j)\beta/2 + \alpha]}. \quad (5.14)$$

From the above equality we may read out the explicit form of the generalized Hall constants $C_N(\alpha, \beta)$. They allow us to obtain a fairly general expression for the Bures volume of the submanifold of the states of rank $N - n$ of the set of complex ($\beta = 2$) or real ($\beta = 1$) density matrices

$$S_{N,n}^{(\beta)} = 2^{-d_n} \frac{\pi^{(d_n+1)/2}}{\Gamma((d_n+1)/2)} \prod_{j=1}^{N-n} \frac{\Gamma(j\beta/2)\Gamma[1 + (2n+j-1)\beta/2]}{\Gamma[(n+j)\beta/2]\Gamma[1 + (n+j-1)\beta/2]} \quad (5.15)$$

where $d_n = (N - n)[1 + (N + n - 1)\beta/2] - 1$ represents the dimensionality of the manifold. In a sense, this formula may be considered as a brief summary of the paper: for $n = 0$ the last factor simply equals unity and (5.15) gives the Bures volume of the entire space of density matrices, equal to that of a d_0 -dimensional hyper-hemisphere with radius $1/2$. In the case $n = 1$ we obtain the volume of the surface of this set, while for $n = N - 1$ we get the volume of the set of pure states

$$S_{N,N-1}^{(\beta)} = \frac{\pi^{(N-1)\beta/2}\Gamma(\beta/2)}{\Gamma(N\beta/2)} \quad (5.16)$$

which for $\beta = 1(2)$ gives correctly the volume of the real (complex) projective space of dimension $N - 1$. This result can be seen directly from equations (3.31) and (3.22). In the case of a real projective space the volume is equal to that of a hemisphere of dimension $N - 1$ and radius 1: $\pi^{N/2}/\Gamma(N/2)$. The final formulae are probably correctly continued to general positive β , though we have strictly proved them only for $\beta = 1, 2$.

6. Concluding remarks

In this work we have computed the volume of the set of complex (real) density matrices with respect to the Bures measure. Interestingly, this volume is equal to that of a hyper-hemisphere of radius $1/2$ and the same dimensionality. However, this fact does not mean that the geometry of the set of complex density matrices induced by the Bures metric is identical with the geometry of a hemisphere of dimensionality $N^2 - 1$ embedded in \mathbb{R}^{N^2} . This is the case only for $N = 2$, for which the set \mathcal{M}_2 is isomorphic with the Uhlmann hemisphere $\frac{1}{2}\mathbf{S}^3$, of a constant positive curvature, embedded in \mathbb{R}^4 .

On the other hand, in the general case, $N \geq 3$, the curvature of the set \mathcal{M}_2 induced by the Bures metric is not constant. To explain this fact, rigorously analysed by Dittmann [46], consider the set of pure states for $N = 3$. This manifold forms a complex projective space, $\mathbb{C}P^2$, and contains, on one hand, the sphere $\mathbf{S}^2 = \mathbb{C}P^1$ and on the other, the real projective

space $\mathbb{R}P^2$. The latter is equivalent to a hemisphere (with all antipodal points identified), so it has a different geodesic length and curvature different from $\mathbb{C}P^1$. Hence the set of mixed states for $N > 2$ analysed with respect to the Bures metric, which preserves the geometry of the manifold of pure states, cannot have a constant curvature. Note that the Hilbert–Schmidt distance induces a flat geometry of the space of mixed states, (i.e. with the curvature equal to zero), for an arbitrary dimensionality N .

The Bures measure, related to statistical distance, Fisher information and Jeffreys' prior, is often used to define and compute the probability that a random density matrix satisfies a certain condition. For instance, such an approach was applied to find the probability that a random state acting on a given composed Hilbert space is separable [47–49]. In this work we computed the Bures–Hall normalization constants, which may be useful to extend such calculations for higher-dimensional problems.

Results presented in this work may also be considered as a contribution to the theory of random matrices. The closest work in this field is due to Eynard and Kristjansen [50], who analysed the $O(n)$ model on a random lattice. We introduced a different class of ensembles of random matrices defined by the joint probability density of eigenvalues

$$P^{(\beta)}(\rho_1, \rho_2, \dots, \rho_N) = C_N(1, \beta) \frac{\delta(\rho_1 + \rho_2 + \dots + \rho_N - 1)}{\sqrt{\rho_1 \rho_2 \dots \rho_N}} \prod_{\nu < \mu} \frac{|\rho_\nu - \rho_\mu|^\beta}{(\rho_\nu + \rho_\mu)^{\beta/2}} \quad (6.1)$$

with normalization constants computed in (5.14), which for $\beta = 2$ and $\beta = 1$ give the Bures measure on the sets of complex and real density matrices, respectively. The density of eigenvalues for these ensembles will be studied in a forthcoming publication [51]. It might be also instructive to analyse a family of such ensembles by allowing the parameter β to admit arbitrary real values. In the limit $\beta \rightarrow 0$ this distribution tends to the Dirichlet distribution of order $1/2$. It describes the distribution of squared components of a real random vector, i.e. a column (or a row) of a random orthogonal matrix generated according to the Haar measure on $O(N)$ [39, 52].

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References

- [1] Petz D and Sudár C 1996 *J. Math. Phys.* **37** 2662
- [2] Życzkowski K and Słomczyński W 2001 *J. Phys. A: Math. Gen.* **34** 6689
- [3] Ruskai M B 1994 *Rev. Math. Phys.* **5** 1147
- [4] Ozawa M 2001 *Phys. Lett. A* **268** 158
- [5] Bures D J C 1969 *Trans. Am. Math. Soc.* **135** 199
- [6] Uhlmann A 1976 *Rep. Math. Phys.* **9** 273
- [7] Braunstein S L and Caves C M 1994 *Phys. Rev. Lett.* **72** 3439
- [8] Uhlmann A 1995 *Rep. Math. Phys.* **36** 461
- [9] Jozsa R 1994 *J. Mod. Opt.* **41** 2315
- [10] Uhlmann A 1992 *Groups and Related Topics* ed R Gierelak *et al* (Dordrecht: Kluwer)
- [11] Hübner M 1992 *Phys. Lett. A* **163** 239
- [12] Dittmann J 1993 *Sem. S. Lie* **3** 73
- [13] Hübner M 1993 *Phys. Lett. A* **179** 226

- [14] Uhlmann A 1996 *J. Geom. Phys.* **18** 76
- [15] Dittmann J 1995 *Rep. Math. Phys.* **36** 309
- [16] Dittmann J 1999 *J. Phys. A: Math. Gen.* **32** 2663
- [17] Hall M J W 1998 *Phys. Lett. A* **242** 123
- [18] Slater P B 1999 *J. Phys. A: Math. Gen.* **32** 8231
- [19] Życzkowski K and Sommers H-J 2003 Hilbert–Schmidt volume of the set of mixed quantum states *J. Phys. A: Math. Gen.* **36** 10115
- [20] Fubini G 1903 *Atti Inst. Veneto* **6** 501
- [21] Study E 1905 *Math. Ann.* **60** 321
- [22] Nielsen M A and Chuang I L 2000 *Quantum Computation and Quantum Information* (Cambridge: Cambridge University Press)
- [23] Fuchs C A and Caves C M 1995 *Open Sys. Inf. Dyn.* **3** 1
- [24] Vedral V and Plenio M B 1998 *Phys. Rev. A* **57** 1619
- [25] Wootters W K 1981 *Phys. Rev. D* **23** 357
- [26] Bhattacharyya A 1943 On a measure of divergence between two statistical populations defined by their probability distributions *Bull. Calcutta Math. Soc.* **35** 99
- [27] Liese F and Vajda I 1987 *Convex Statistical Distances* (Leipzig: Teubner)
- [28] Fisher R A 1925 *Proc. Camb. Phil. Soc.* **22** 700
- [29] Caves C 2002 Measures and volumes for spheres, the probability simplex, projective Hilbert space and density operators, unpublished notes, see webpage <http://info.phys.unm.edu/caves/reports/reports.html>
- [30] Cencov N N 1982 *Statistical Decision Rules and Optimal Inference (Translation of Math. Monogr. vol 53)* (Providence, RI: American Mathematical Society)
- [31] Ohya M and Petz D 1993 *Quantum Entropy and Its Use* (Berlin: Springer)
- [32] Morozova E A and Chentsov N N 1990 *Izvestiya Akad. Nauk SSSR Tekhn. Kibernet.* **36** 135
- [33] Petz D 1996 *Linear Algebr. Appl.* **244** 81
- [34] Balian R, Alhassid Y and Reinhardt H 1986 *Phys. Rep.* **131** 1
- [35] Grasselli M R and Streater R F 2001 *Inf. Dim. Anal., Quantum Prob.* **4** 173–82
- [36] Kubo F and Ando T 1980 *Math. Ann.* **246** 205
- [37] Lesniewski A and Ruskai M B 1999 *J. Math. Phys.* **40** 5702
- [38] Byrd M S and Slater P B 2001 *Phys. Lett. A* **283** 152
- [39] Życzkowski K and Sommers H-J 2001 *J. Phys. A: Math. Gen.* **34** 7111
- [40] Hua L K 1963 *Harmonic Analysis of Functions of Several Variables in the Classical Domains* (Providence, RI: American Mathematical Society) Chinese original 1958, Russian translation, Moskva 1959
- [41] Fuiji K 2002 *J. Appl. Math.* **2** 371
- [42] Boya L J, Sudarshan E C G and Tilma T 2002 Volumes of compact manifolds *Preprint math-ph/0210033*
- [43] Tilma T and Sudarshan E C G 2002 *J. Phys. A: Math. Gen.* **35** 10467
- [44] Mehta M L 1991 *Random Matrices* 2nd edn (New York: Academic)
- [45] Fyodorov Y V 2002 *Nucl. Phys. B* **621** 643
- [46] Dittmann J 1999 *J. Geom. Phys.* **31** 16
- [47] Slater P B 1999 *J. Phys. A: Math. Gen.* **32** 5261
- [48] Slater P B 2002 *Quantum Inf. Proc.* **1** 397
- [49] Slater P B 2003 *Preprint quant-ph/0306132*
- [50] Eynard B and Kristjansen C 1995 *Nucl. Phys. B* **455** 577
- [51] Sommers H-J and Życzkowski K 2003 in preparation
- [52] Życzkowski K 1999 *Phys. Rev. A* **60** 3496