Invariance of separability probability over reduced states in 4×4 bipartite systems *

Attila Lovas[†], Attila Andai[‡], Department for Mathematical Analysis, Budapest University of Technology and Economics, Stoczek u. 2, Budapest, H-1521, Hungary

January 5, 2017

Abstract

The geometric separability probability of the composite quantum systems has been extensively studied in the recent decades. One of the simplest but strikingly difficult problem is to compute the separability probability of qubit-qubit and rebit-rebit quantum states with respect to the Hilbert-Schmidt measure. A lot of numerical simulations confirm the $P_{\text{rebit-rebit}} = \frac{29}{64}$ and $P_{\text{qubit-qubit}} = \frac{8}{33}$ conjectured probabilities. Milz and Strunz studied the separability probability with respect to given subsystems. They conjectured that the separability probability of qubit-qubit qubit (and qubit-qutrit) states of the form of $\begin{pmatrix} D_1 & C \\ C^* & D_2 \end{pmatrix}$ depends on $D = D_1 + D_2$ (on single qubit subsystems), moreover it depends only on the Bloch radii (r) of D and it is constant in r. Using the Peres-Horodecki criterion for separability we give mathematical proof for the $\frac{29}{64}$ probability, and we present an integral formula for the complex case which hopefully will help to prove the $\frac{8}{33}$ probability, too. We prove Milz and Strunz's conjecture for rebit-rebit and qubit-qubit states. The case, when the state space is endowed with the volume form generated by the operator monotone function $f(x) = \sqrt{x}$ is also studied in detail. We show that even in this setting the Milz and Strunz's conjecture holds true and we give an integral formula for separability probability according to this measure.

1 Introduction

Since entanglement is one of the most striking features of composite quantum systems, it is natural to ask what the probability is that a given quantum state is entangled (or separable). "Is the world more classical or more quantum? Does it contain more quantum correlated (entangled) states than classically correlated ones?" These questions were addressed to physicists in 1998 by Zyczkowski, Horodecki, Sanpera and Lewenstein [6]. The first question is a rather philosophical one, the second is easier to formulate mathematically, although more specification is needed. It has turned out during the recent years that even in the simplest quantum case, when one considers only qubit-qubit states over real or complex Hilbert-space, to determine the separability probability of a given state is a highly nontrivial problem. Many researchers agree and emphasize the philosophical and experimental

^{*}keywords: Entanglement, Peres-Horodecki condition, Separability probability, Hilbert-Schmidt measure, Monotone metrics; MSC: 81P16, 81P40, 81P45

[†]lovas@math.bme.hu

[‡]andaia@math.bme.hu, Phone.: +36-1-4633127, Fax.:+36-1-633172

interest of the separability probability. First, one should specify a natural measure on the state space and then should compute somehow the volume of the separable states and the volume of the state space. In this paper we endow the state space with Hilbert-Schmidt measure which is induced by the Hilbert-Schmidt metric. We note here that other measures are also relevant, as it was pointed out by Slater [11], mainly those which are generated by monotone metrics [10]. The volume of the state space with respect to the Hilbert-Schmidt measure was computed by Zyczkowski [16] and Andai [1]. There are several good separability criteria, we use the Peres–Horodecki criterion [5] which is a simple necessary and sufficient condition for separability of qubit-qubit states. To compute the volume of separable states is a much more complicated task.

So far only extensive numerical studies and some related conjectures have existed for the separability probability. Numerical simulations give rise to an intriguing formula for separability probability, presented in 2013 by Slater [12], which was tested in real, complex and even in quaternionic Hilbert-spaces [14, 13, 4]. Based on this formula and on numerical simulations the separability probability for real qubit-qubit state is $\frac{29}{64}$ and for complex state is $\frac{8}{33}$. Now we give mathematical proof for the $\frac{29}{64}$ probability and we present an integral formula for the complex case which hopefully will help to prove the $\frac{8}{33}$ probability, too. One of the most useful conjecture about separability probability was presented by Milz and Strunz in 2015 [7]. They conjectured that the separability probability of qubit-qubit (and qubit-qutrit) states of the form of $\begin{pmatrix} D_1 & C \\ C^* & D_2 \end{pmatrix}$ depends on $D = D_1 + D_2$ (on single qubit subsystems), moreover it depends only on the Bloch radii (r) of D and it is constant in r. In this paper we prove this conjecture for real and complex qubit-qubit states.

We study the case in detail when the state space is endowed with the volume form generated by the operator monotone function $f(x) = \sqrt{x}$. We show that the volume of rebit-rebit and qubitqubit states are infinite, although there is a simple and reasonable method to define the separability probabilities. We present integral formulas for separability probabilities in this setting, too. We argue that from the separability probability point of view, the main difference between the Hilbert-Schmidt measure and the volume form generated by the operator monotone function $x \mapsto \sqrt{x}$ is a special distribution on the unit ball in operator norm of 2×2 matrices, more precisely in the Hilbert-Schmidt case one faces with a uniform distribution on the whole unit ball and for monotone volume forms one gets uniform distribution on the surface of the unit ball.

The paper is organized as follows. In Section 2, we fix the notations for further computations and we mention some elementary lemmas which will be used in the sequel. In Section 3, we present our main results, namely an explicit integral formula for the volume of separable qubit-qubit states over real and complex Hilbert-space, a proof for Milz and Strunz's conjecture [7] and an analytical proof for the rebit-rebit separability probability. In Section 4 we endow the state space with the volume measure which induced by the operator monotone function $f(x) = \sqrt{x}$, and we show, that even in this setting the Milz and Strunz's conjecture holds and we give an integral formula for separability probability according to this measure. As a kind of checking, in Section 5, we compute the volume of the real and complex qubit-qubit state space with methods introduced in Section 3 and we compare our results to the previously published ones. In the second part of Section 5 we prove that the volume of the qubit-qubit state space is infinite if the volume measure comes from the function $f(x) = \sqrt{x}$, but still there is a natural way to define the separability probability.

2 Basic lemmas and notations

The quantum mechanical state space consists of real and complex self-adjoint positive matrices with trace 1. We consider only the set of faithful states with real and complex entries. In our notation the state space is

$$\mathcal{D}_{n,\mathbb{K}} = \{ D \in \mathbb{K}^{n \times n} | D = D^*, D > 0, \operatorname{Tr}(D) = 1 \} \quad \mathbb{K} = \mathbb{R}, \mathbb{C}.$$
(1)

The space of $n \times n$ self-adjoint matrices is denoted by $\mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}}$ ($\mathbb{K} = \mathbb{R}, \mathbb{C}$). Let us introduce the notation $\mathcal{E}_{\mathbb{K}}$ for the operator interval

$$\mathcal{E}_{n,\mathbb{K}} = \left\{ Y \in \mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}} \middle| -I < Y < I \right\}$$
(2)

where "<" denotes the partial ordering of self-adjoint matrices defined by the cone of positive matrices. The following lemma is an essential ingredient of the proof of our main theorem. It gives a characterization of positive definite matrices in terms of their Schur complement.

Lemma 1. For any symmetric matrix, D, of the form

$$D = \left(\begin{array}{cc} D_1 & C \\ C^* & D_2 \end{array}\right),$$

if D_2 is invertible then D > 0 if and only if $D_2 > 0$ and $D_1 - CD_2^{-1}C^* > 0$. Similarly, if D_1 is invertible then D > 0 if and only if $D_1 > 0$ and $D_2 - C^*D_1^{-1}C > 0$.

Proof. The statement is well-known in linear algebra. For the proof see for example p. 34 in [15]. \Box

Lemma 2. For every matrix $V \in \mathbb{K}^{n \times n}$ there exists a factorization, called a singular value decomposition of the form

$$V = U_1 \Sigma U_2,\tag{3}$$

where $U_1, U_2 \in \mathbb{K}^{n \times n}$ are unitary matrices and $\Sigma \in \mathbb{K}^{n \times n}$ is a diagonal matrix with real non-negative entries.

Proof. The proof can be found for example in Bathia's book (See p. 6 in [2]). \Box

Lemma 3. Let $X \in \mathbb{K}^{n \times n}$ be an arbitrary matrix. The matrix X^*X is positive semidefinite and the following equivalence holds

$$X^*X < I \Leftrightarrow \|X\| < 1,\tag{4}$$

where $\|\cdot\|$ denotes the usual operator norm i.e. the largest singular value or Schatten- ∞ norm.

Proof. The inequality $\langle v, X^*Xv \rangle = ||Xv||^2 \ge 0$ holds for all $v \in \mathbb{K}^n$ which proves the first part of the statement. By the definition of operator norm, we can write

$$||X||^{2} = \sup\left\{ ||Xv||^{2} | v \in \mathbb{K}^{n}, ||v|| = 1 \right\} \le 1$$

because $||Xv||^2 = \langle v, X^*Xv \rangle \le ||v||^2 = 1$ for every vector v of length 1.

To a matrix $D \in \mathbb{K}^n$, one can associate the left and right multiplication operators L_D, R_D : $\mathbb{K}^{n \times n} \to \mathbb{K}^{n \times n}$ that acts like

$$A \mapsto L_D(A) = DA$$
$$A \mapsto R_D(A) = AD.$$

It is obvious that L_D and R_D are invertible if and only if $D \in Gl(n, \mathbb{K})$. By a straightforward computation, one can show that

$$\det(L_D) = \det(R_D) = \det(D)^n$$

In integral transformations, the $n \times n$ complex matrix D is regarded as a $2n \times 2n$ real matrix that acts on $\mathbb{R}^{2n} \cong \mathbb{C}^n$ therefore the Jacobian of L_D and R_D is $\det(D)^{2n}$ in the complex case.

The vector space of $n \times n$ matrices is the direct sum of the space of $n \times n$ self-adjoint matrices and $n \times n$ anti self-adjoint matrices

$$\mathbb{K}^{n \times n} = \mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}} \oplus \widetilde{\mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}}}.$$

For any self-adjoint matrix $D \in \mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}}$, the map $L_D \circ R_D : \mathbb{K}^n \times \mathbb{K}^n$ preserves the direct sum decomposition i.e. $L_D \circ R_D \left(\mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}} \right) \subset \mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}}$ and $L_D \circ R_D \left(\widetilde{\mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}}} \right) \subset \widetilde{\mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}}}$. Consequently, $L_D \circ R_D = (L_D \circ R_D)|_{\mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}}} \oplus (L_D \circ R_D)|_{\widetilde{\mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}}}}$ holds which implies that

$$\det \left(L_D \circ R_D \right) = \det \left(\left(L_D \circ R_D \right) |_{\mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}}} \right) \times \det \left(\left(L_D \circ R_D \right) |_{\widetilde{\mathcal{M}_{n,\mathbb{K}}^{\mathrm{sa}}}} \right).$$
(5)

This observation lead us to the following lemma.

Lemma 4. Let $D \in \mathcal{M}_{2,\mathbb{K}}^{sa}$ be an arbitrary positive definite matrix. The determinant of the restricted map $(L_{D^{1/2}} \circ R_{D^{1/2}})|_{\mathcal{M}_{2,\mathbb{K}}^{sa}}$ is

$$\det\left(\left.\left(L_{D^{1/2}}\circ R_{D^{1/2}}\right)\right|_{\mathcal{M}^{sa}_{2,\mathbb{K}}}\right) = \det(D)^{2-\frac{d}{2}}$$

where $d = \dim_{\mathbb{R}} \mathbb{K} = 1, 2$.

Proof. In the real case, $\widetilde{\mathcal{M}_{2,\mathbb{R}}^{\mathrm{sa}}} = \mathbb{R} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$. One can verify that

$$L_{D^{1/2}} \circ R_{D^{1/2}} = \det(D)^{1/2} \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$$

hence

$$\det\left(\left(L_{D^{1/2}} \circ R_{D^{1/2}}\right)|_{\mathcal{M}_{2,\mathbb{R}}^{\mathrm{sa}}}\right) = \frac{\det\left(L_{D^{1/2}} \circ R_{D^{1/2}}\right)}{\det\left(\left(L_{D^{1/2}} \circ R_{D^{1/2}}\right)|_{\widetilde{\mathcal{M}_{2,\mathbb{R}}^{\mathrm{sa}}}}\right)}$$
$$= \frac{\det(D)^2}{\det(D)^{1/2}} = \det(D)^{3/2}.$$

In the complex case, we have an isomorphism $\widetilde{\mathcal{M}^{sa}_{2,\mathbb{C}}} = i \, \mathcal{M}^{sa}_{2,\mathbb{C}}$ and thus

$$\det\left(\left(L_{D^{1/2}} \circ R_{D^{1/2}}\right)|_{\mathcal{M}_{2,\mathbb{R}}^{\mathrm{sa}}}\right) = \sqrt{\det\left(L_{D^{1/2}} \circ R_{D^{1/2}}\right)} = \det(D)$$

which completes the proof.

Note that the Jacobian of the transformation

$$(L_{D^{1/2}} \circ R_{D^{1/2}})|_{\mathcal{M}^{\mathrm{sa}}_{2,\mathbb{K}}} : \mathcal{M}^{\mathrm{sa}}_{2,\mathbb{K}} \to \mathcal{M}^{\mathrm{sa}}_{2,\mathbb{K}}$$

$$\tag{6}$$

is $\det(D)^{2d-d^2/2}$ because D is regarded in integral transformations as a 4×4 real matrix that acts on $\mathbb{R}^4 \cong \mathbb{C}^2$.

Lemma 5. Let A be a 2 × 2 invertible matrix with singular values $\sigma_1 > \sigma_2 > 0$. The operator norm and the singular value ratio of A, which is defined as $\sigma(A) := \sigma_2/\sigma_1$, can be expressed as follows

$$||A|| = \sqrt{|\det(A)|} e^{\frac{1}{2}\cosh^{-1}\left(\frac{1}{2}\frac{||A||_{HS}^2}{|\det(A)|}\right)}$$
$$\sigma(A) = \frac{\sigma_2}{\sigma_1} = e^{-\cosh^{-1}\left(\frac{1}{2}\frac{||A||_{HS}^2}{|\det(A)|}\right)},$$

where $\|\cdot\|_{HS}$ denotes the Hilbert-Schmidt norm.

Proof. By definition, singular values of A are the eigenvalues of $\sqrt{A^*A}$ that are

$$\sigma_{1,2} = \sqrt{|\det(A)|} \left(\frac{\|A\|_{\mathrm{HS}}^2}{2|\det(A)|} \pm \sqrt{\left(\frac{\|A\|_{\mathrm{HS}}^2}{2|\det(A)|}\right)^2 - 1} \right)^{1/2}$$
$$= \sqrt{|\det(A)|} e^{\pm \frac{1}{2} \cosh^{-1} \left(\frac{1}{2} \frac{\|A\|_{\mathrm{HS}}^2}{|\det(A)|}\right)}$$

which completes the proof.

The standard unit ball in the normed vector space of 2×2 matrices is denoted by $\mathcal{B}_1(\mathbb{K}^{2\times 2})$ and the notation $\partial \mathcal{B}_1(\mathbb{K}^{2\times 2})$ stands for the surface of the unit ball. We set the notation $\mathbf{1}_A$ for the indicator function of the set $A \subseteq \mathbb{K}^{2\times 2}$.

Definition 1. The functions $\chi_d, \eta_d : [0, \infty) \to [0, \infty)$ are defined by the following formulas

$$\chi_d(\varepsilon) = \int_{\mathcal{B}_1(\mathbb{K}^{2\times 2})} \mathbf{1}_{\|V_{\varepsilon}^{-1}XV_{\varepsilon}\| < 1} \, \mathrm{d}\lambda_{4d}(X), \tag{7}$$

$$\eta_d(\varepsilon) = \int_{\mathcal{B}_1(\mathbb{K}^{2\times 2})} \det(I - XX^*)^{-\frac{3d}{4} - \frac{1}{2}} \mathbf{1}_{\|V_\varepsilon^{-1}XV_\varepsilon\| < 1} \, \mathrm{d}\lambda_{4d}(X), \tag{8}$$

where $V_{\varepsilon} = \begin{pmatrix} 1 & 0 \\ 0 & \varepsilon \end{pmatrix}$ and $d = \dim_{\mathbb{R}}(\mathbb{K})$.

Clearly, these functions are reciprocal symmetric i.e. $\chi_d(1/\varepsilon) = \chi_d(\varepsilon)$ and $\eta_d(1/\varepsilon) = \eta_d(\varepsilon)$ holds for $\varepsilon > 0$. The normalized χ_d -function $\tilde{\chi}_d(\varepsilon) = \chi_d(\varepsilon)/\chi_d(1)$ measures the probability that a uniformly distributed matrix in $\mathcal{B}_1(\mathbb{K}^{2\times 2})$ is mapped in $\mathcal{B}_1(\mathbb{K}^{2\times 2})$ by the similarity transformation $V_{\varepsilon}^{-1}(.)V_{\varepsilon}$. The normalized $\tilde{\eta}_d(\varepsilon) = \eta_d(\varepsilon)/\eta_d(1)$ function would have a similar probabilistic meaning, but we will see that $\eta_d(1) = \infty$ therefore we should find an other way to calculate $\tilde{\eta}_d(\varepsilon)$.

Lemma 6. The function $\tilde{\chi}_1(\varepsilon) : [0,1] \to [0,1]$ can be expressed as follows

$$\tilde{\chi}_{1}(\varepsilon) = 1 - \frac{4}{\pi^{2}} \int_{\varepsilon}^{1} \left(s + \frac{1}{s} - \frac{1}{2} \left(s - \frac{1}{s} \right)^{2} \log \left(\frac{1+s}{1-s} \right) \right) \frac{1}{s} \, \mathrm{d}s \\
= \frac{4}{\pi^{2}} \int_{0}^{\varepsilon} \left(s + \frac{1}{s} - \frac{1}{2} \left(s - \frac{1}{s} \right)^{2} \log \left(\frac{1+s}{1-s} \right) \right) \frac{1}{s} \, \mathrm{d}s.$$
(9)

Proof. The proof, which is elementary but somewhat lengthy, can be found in Appendix A. \Box



Figure 1: Graph of the function $\varepsilon \mapsto \tilde{\chi}_1(\varepsilon) - \varepsilon$.

The function $\tilde{\chi}_1(\varepsilon)$ can be written in a closed form using polylogarithmic functions but this is unnecessary for our purposes. It is somewhat interesting, that the identity function approximates well $\tilde{\chi}_1(\varepsilon)$ (See Fig. 2).

Recall that Pauli matrices $\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ with $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ form an orthogonal basis of the space of 2 × 2 self-adjoint matrices. We parametrize the spaces $\mathcal{M}_{2,\mathbb{R}}^{\mathrm{sa}}$ and $\mathcal{M}_{2,\mathbb{C}}^{\mathrm{sa}}$ in the following way

$$R(\theta, x, y) = \frac{x+y}{2}I + \frac{x-y}{2}(\cos(\theta)\sigma_1 + \sin(\theta)\sigma_3),$$

$$0 < \theta < 2\pi, x, y \in \mathbb{R}$$
(10)

$$R(\theta, \phi, x, y) = \frac{x+y}{2}I + \frac{x-y}{2}(\cos(\theta)\sin(\phi)\sigma_1 + \sin(\theta)\sin(\phi)\sigma_2 + \cos(\phi)\sigma_3), \qquad (11)$$
$$0 < \theta < 2\pi, \ 0 < \phi < \pi, \ x, y \in \mathbb{R}.$$

This parametrization is very convenient because eigenvalues of $R(\theta, x, y)$ and $R(\theta, \phi, x, y)$ can be directly read out from the parametrization.

We introduce the notation $O(\phi)$ for the standard 2×2 rotation matrix that rotates points counterclockwise through an angle ϕ about the origin. Let us denote by $\Lambda(x, y)$ the 2×2 diagonal matrix that contains x, y in its diagonal.

Let us introduce the parametrization of U(2) (12) that can be found in Mirman's book (See p.

284-285 in [8]).

$$U(\Theta, \Phi, \omega, \tau) = e^{i\Theta} \times \begin{pmatrix} e^{\frac{i(\omega+\tau)}{2}} \cos \frac{\Phi}{2} & i e^{\frac{i(\omega-\tau)}{2}} \sin \frac{\Phi}{2} \\ i e^{-\frac{i(\omega-\tau)}{2}} \sin \frac{\Phi}{2} & e^{-\frac{i(\omega+\tau)}{2}} \cos \frac{\Phi}{2} \end{pmatrix}$$
(12)
$$0 < \Phi < \pi, 0 < \Theta < 2\pi, 0 < \omega, \tau < 4\pi$$

Polar decomposition will be utilized to parametrize the space of 2×2 complex matrices. The space of 2×2 real and complex density matrices will be parametrized by the canonical Bloch sphere parametrization as follows.

$$D(\theta, r) = \frac{1}{2} (I + r(\cos(\theta)\sigma_1 + \sin(\theta)\sigma_3)),$$

$$0 < \theta < 2\pi, \ 0 < r < 1$$
(13)

$$D(\theta, \phi, r) = \frac{1}{2} (I + r(\cos(\theta)\sin(\phi)\sigma_1 + \sin(\theta)\sin(\phi)\sigma_2 + \cos(\phi)\sigma_3)), \qquad (14)$$
$$0 < \theta < 2\pi, \ 0 < \phi < \pi, \ 0 < r < 1$$

In Table 2, we collected the parameterizations of manifolds $\mathbb{R}^{2\times 2}$, $\mathbb{C}^{2\times 2}$, $\mathcal{M}_{2,\mathbb{R}}^{\mathrm{sa}}$, $\mathcal{M}_{2,\mathbb{C}}^{\mathrm{sa}}$, $\mathcal{D}_{2,\mathbb{R}}$, $\mathcal{D}_{2,\mathbb{C}}$, and volume forms corresponding to the considered parametrization. These formulas will be applied in the sequel without mentioning.

Manifold	Parametrization	Volume form
$\mathbb{R}^{2 \times 2}$	$O(\phi)\Lambda(x,y)O(\theta), \ 0 < \phi, \theta < 2\pi, \ 0 < x, y$	$\frac{ x^2 - y^2 }{2}$
$\mathbb{C}^{2 \times 2}$	$R(\theta, \phi, x, y)U(\Theta, \Phi, \omega, \tau)$, where $0 < x, y$ (See Equations (11) and (12).)	$\frac{xy(x^2-y^2)^2}{64}\sin\phi\sin\Phi$
$\mathcal{M}^{\mathrm{sa}}_{2,\mathbb{R}}$	$R(\theta, x, y)$ (See Equation (10))	$\frac{ x-y }{\sqrt{2}}$
$\mathcal{M}^{\mathrm{sa}}_{2,\mathbb{C}}$	$R(\theta, \phi, x, y)$ (See Equation (11).)	$\frac{(x-y)^2}{2}\sin\phi$
$\mathcal{D}_{2,\mathbb{R}}$	$D(\theta, r)$ (See Equation (13).)	$\frac{r}{2}$
$\overline{\mathcal{D}}_{2,\mathbb{C}}$	$R(\theta, \phi, x, y)$ (See Equation (14).)	$\frac{r^2 \sin \phi}{2\sqrt{2}}$

Table 1: Parametrization of manifolds $\mathbb{R}^{2\times 2}$, $\mathbb{C}^{2\times 2}$, $\mathcal{M}_{2,\mathbb{R}}^{sa}$, $\mathcal{M}_{2,\mathbb{C}}^{sa}$ and the corresponding volume forms.

In Table 2, we summarize the normalization constants corresponding to χ_d and η_d d = 1, 2.

	d = 1	d = 2
$\chi_d(1) =$	$\frac{2}{3}\pi^2$	$\frac{\pi^4}{6}$
$\eta_d(1) =$	∞	∞

Table 2: Normalization constants corresponding to χ_d and η_d d = 1, 2.

As an example, we calculate here $\chi_2(1)$. By definition, we can write

$$\chi_{2}(1) = \int_{\mathcal{B}_{1}(\mathbb{C}^{2\times 2})} \mathbf{1}_{\|V_{1}^{-1}X} \underbrace{V_{1}}_{=\operatorname{id}_{\mathbb{C}^{2}}} \|<1 \, \mathrm{d}\lambda_{4d}(X) = \int_{\mathcal{B}_{1}(\mathbb{C}^{2\times 2})} 1 \, \mathrm{d}\lambda_{4d}(X).$$

Now we apply the parametrization and volume form presented in Table 2 and we obtain

$$\chi_2(1) = \int_{\mathcal{B}_1(\mathbb{C}^{2\times 2})} 1 \, \mathrm{d}\lambda_{4d}(X)$$

= $4^3 \pi^4 \int_0^1 \int_0^1 \int_0^\pi \int_0^\pi \frac{xy(x^2 - y^2)^2}{64} \sin \phi \sin \Phi \, \mathrm{d}\phi \, \mathrm{d}\Phi \, \mathrm{d}y \, \mathrm{d}x$
= $4\pi^4 \int_0^1 \int_0^1 xy(x^2 - y^2)^2 \, \mathrm{d}y \, \mathrm{d}x = \frac{\pi^4}{6}.$

To make the explanation precise, we define $\tilde{\eta}_d(\varepsilon)$ as

$$\tilde{\eta}_d(\varepsilon) = \lim_{\delta \to 1-0} \frac{\int\limits_{\mathcal{B}_1(\mathbb{K}^{2\times 2})} \det(I - XX^*)^{-\left(\frac{3d}{4} - \frac{1}{2}\right)\delta} \mathbf{1}_{\|V_{\varepsilon}^{-1}XV_{\varepsilon}\| < 1} \, \mathrm{d}\lambda_{4d}(X)}{\int\limits_{\mathcal{B}_1(\mathbb{K}^{2\times 2})} \det(I - XX^*)^{-\left(\frac{3d}{4} - \frac{1}{2}\right)\delta} \, \mathrm{d}\lambda_{4d}(X)}$$

which limit exists because the measures

$$\frac{\left((1-x^2)(1-y^2)\right)^{-\frac{5\delta}{4}}\left|x^2-y^2\right|}{\int\limits_{0}^{1}\int\limits_{0}^{1}\left((1-t^2)(1-s^2)\right)^{-\frac{5\delta}{4}}\left|t^2-s^2\right|\,\mathrm{d}\lambda_2(t,s)}\frac{\left((1-x^2)(1-y^2)\right)^{-2\delta}xy(x^2-y^2)^2}{\int\limits_{0}^{1}\int\limits_{0}^{1}\left((1-t^2)(1-s^2)\right)^{-2\delta}st(s^2-t^2)^2\,\mathrm{d}\lambda_2(t,s)}\,\mathrm{d}\lambda_2(x,y)$$

converge in weak-* topology to a measure concentrated on $\{(x, y) \in [0, 1] \mid x = 1 \lor y = 1\}$ as $\delta \to 1-0$. By the unitary symmetry, we can conclude that the measure

$$\frac{\det(I - XX^*)^{-\left(\frac{3d}{4} - \frac{1}{2}\right)\delta}}{\int\limits_{\mathcal{B}_1(\mathbb{K}^{2\times 2})} \det(I - XX^*)^{-\left(\frac{3d}{4} - \frac{1}{2}\right)\delta} \,\mathrm{d}\lambda_{4d}(X)} \,\mathrm{d}\lambda_{4d}(X)$$

converges in weak-* topology to the uniform distribution on $\partial \mathcal{B}_1(\mathbb{K}^{2\times 2})$ as $\delta \to 1-0$. The next lemma states that with this definition we get back $\tilde{\chi}_1$. We conjecture that this identity also holds true for $\tilde{\chi}_2$ and $\tilde{\eta}_2$.

Lemma 7. The functions $\tilde{\chi}_1$ and $\tilde{\eta}_1$ are equals to each other.

$$\tilde{\chi}_1(\varepsilon) = \tilde{\eta}_1(\varepsilon) \quad \varepsilon \in [0,1]$$

Proof. The proof of this theorem is provided in Appendix B.

Definition 2. The polylogarithmic function is defined by the infinite sum

$$\operatorname{Li}_s(z) = \sum_{k=1}^{\infty} \frac{z^k}{k^s}.$$

for arbitrary complex s and for all complex arguments z with |z| < 1.

3 The main result

We parametrize the space of 4×4 density matrices $(\mathcal{D}_{4,\mathbb{K}})$ in the following way

$$\rho(D_1, D_2, C) = \begin{pmatrix} D_1 & C \\ C^* & D_2 \end{pmatrix}$$

where $D_1, D_2 > 0, D_1 + D_2 \in \mathcal{D}_{2,\mathbb{K}}$ and $C \in \mathbb{K}^{2 \times 2}$. Note that, with this parametrization

$$Tr_2(\rho(D_1, D_2, C)) = D_1 + D_2.$$
(15)

For a given state $D \in \mathcal{D}_{2,\mathbb{K}}$ we define

$$\mathcal{D}_{4,\mathbb{K}}(D) = \left\{ \rho \in \mathcal{D}_{4,\mathbb{K}} | \operatorname{Tr}_2(\rho) = D \right\},\tag{16}$$

that is the set of those states, which partial trace with respect to the system 2, respectively yield the matrix $D \in \mathcal{D}_{2,\mathbb{K}}$.

Let us introduce the involution

$$\rho(D_1, D_2, C) \mapsto T(\rho(D_1, D_2, C)) = \rho(D_1, D_2, C^*)$$
(17)

that is just the composition of partial transpose and element-wise conjugation which is a positive map. Consequently, the aforementioned Peres–Horodecki positive partial transpose criterion can be reformulated as

$$\mathcal{D}_{4,\mathbb{K}}^{s} = T\left(\mathcal{D}_{4,\mathbb{K}}\right) \cap \mathcal{D}_{4,\mathbb{K}}.$$
(18)

Now we are in the position to state one of our main results.

Theorem 1. Let $D \in \mathcal{D}_{2,\mathbb{K}}$ be a fixed density matrix. The Hilbert-Schmidt measure of $\mathcal{D}_{4,\mathbb{K}}^s(D)$ is

$$Vol\left(\mathcal{D}_{4,\mathbb{K}}^{s}(D)\right) = \frac{\det(D)^{4d-\frac{d^{2}}{2}}}{2^{6d}}$$
$$\times \int_{\mathcal{E}_{2,\mathbb{K}}} \det(I-Y^{2})^{d} \times \chi_{d} \circ \sigma\left(\sqrt{\frac{I-Y}{I+Y}}\right) \, \mathrm{d}\lambda_{d+2}(Y)$$
(19)

and the volume of the space $\mathcal{D}^s_{4,\mathbb{K}}$ can be expressed as

$$Vol\left(\mathcal{D}_{4,\mathbb{K}}^{s}\right) = \int_{\mathcal{D}_{2,\mathbb{K}}} Vol\left(\mathcal{D}_{4,\mathbb{K}}^{s}(D)\right) \, \mathrm{d}\lambda_{d+1}(D), \tag{20}$$

where $d = \dim_{\mathbb{R}}(\mathbb{K}) = 1, 2.$

Proof. For fixed $D_1, D_2 \in \mathcal{M}_{2,\mathbb{K}}^{\mathrm{sa}}$, we set

$$\mathcal{C}(D_1, D_2) = \left\{ C \in \mathbb{K}^{2 \times 2} \middle| \rho(D_1, D_2, C) > 0, \ \rho(D_1, D_2, C^*) > 0 \right\}.$$

By Fubini's theorem, we have

$$\operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{K}}^{s}\right) = \lambda_{6d+3} \left(T\left(\mathcal{D}_{4,\mathbb{K}}\right) \cap \mathcal{D}_{4,\mathbb{K}}\right)$$
$$= \int_{\begin{array}{c}D_{1}, D_{2} > 0\\\operatorname{Tr}(D_{1} + D_{2}) = 1\end{array}} \int_{C \in \mathcal{C}(D_{1}, D_{2})} 1 \, \mathrm{d}\lambda_{4d}(C) \, \mathrm{d}\lambda_{2d+3}(D_{1}, D_{2}).$$
(21)

If $D_1, D_2 > 0$ and $\operatorname{Tr}(D_1 + D_2) = 1$ fixed, then a matrix $C \in \mathbb{K}^{2 \times 2}$ belongs to the set $\mathcal{C}(D_1, D_2)$ if and only if $\begin{pmatrix} D_1 & C \\ C^* & D_2 \end{pmatrix} > 0$ and $\begin{pmatrix} D_1 & C^* \\ C & D_2 \end{pmatrix} > 0$ holds. This condition can be reformulated by Lemma 1. as

$$I > \left(D_1^{-1/2} C D_2^{-1/2}\right)^* D_1^{-1/2} C D_2^{-1/2} \Leftrightarrow \left\|D_1^{-1/2} C D_2^{-1/2}\right\| < 1$$
$$I > \left(D_2^{-1/2} C D_1^{-1/2}\right)^* D_2^{-1/2} C D_1^{-1/2} \Leftrightarrow \left\|D_2^{-1/2} C D_1^{-1/2}\right\| < 1,$$

where $\|\cdot\|$ denotes the usual operator norm.

To compute the inner integral, we substitute

$$X = D_1^{-1/2} C D_2^{-1/2} = \left(L_{D_1^{-1/2}} \circ R_{D_2^{-1/2}} \right) (C).$$

The Jacobian of this transform is det $\left(L_{D_1^{-1/2}} \circ R_{D_2^{-1/2}}\right)^{-1} = \det(D_1)^d \det(D_2)^d$ and the inner integral of (21) can be written as

$$\int_{C \in \mathcal{C}(D_1, D_2)} 1 \, \mathrm{d}\lambda_{4d}(C) = \det(D_1 D_2)^d \int_{\mathcal{B}_1(\mathbb{K}^{2 \times 2})} \mathbf{1}_{\|(V^*)^{-1} X V\| < 1} \, \mathrm{d}\lambda_{4d}(X),$$

where $V = D_2^{1/2} D_1^{-1/2}$. Observe that the last term depends only on the singular value ratio of V, because taking the singular value decomposition of V: $V = U_1 \Sigma U_2$, we have

$$\|(V^*)^{-1}XV\| = \|U_1\Sigma^{-1}U_2XU_1\Sigma U_2\| = \|\Sigma^{-1}U_2XU_1\Sigma\|$$

and the transformation $X \mapsto U_2 X U_1$ is isometric with respect to the Hilbert-Schmidt norm. It means that

$$\chi_d(\sigma(V)) = \int_{\mathcal{B}_1(\mathbb{K}^{2\times 2})} \mathbf{1}_{\|(V^*)^{-1}XV\| < 1} \, \mathrm{d}\lambda_{4d}(X)$$

holds. By Lemma 5, the singular value ratio of V is

$$\sigma(V) = e^{-\cosh^{-1}\left(\frac{\|V\|_{\text{HS}}^2}{2|\det(V)|}\right)} = e^{-\cosh^{-1}\left(\frac{1}{2}\sqrt{\frac{\det(D_1)}{\det(D_2)}}\operatorname{Tr}(D_2D_1^{-1})\right)}$$

hence for the volume of separable states (21) we obtain

$$\operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{K}}^{s}\right) = \int_{\substack{D_{1}, D_{2} > 0 \\ \operatorname{Tr}(D_{1} + D_{2}) = 1}} \det(D_{1}D_{2})^{d} f(D_{2}D_{1}^{-1}) \, \mathrm{d}\lambda_{2d+3}(D_{1}, D_{2}),$$

where

$$f(D_2 D_1^{-1}) = \chi_d \circ \exp\left(-\cosh^{-1}\left(\frac{1}{2}\sqrt{\frac{\det(D_1)}{\det(D_2)}} \operatorname{Tr}\left(D_2 D_1^{-1}\right)\right)\right).$$

We introduce the parametrization

$$D_{1} = \frac{1}{2}(D+A)$$

$$D_{2} = \frac{1}{2}(D-A),$$
(22)

where D takes values in $\mathcal{D}_{2,\mathbb{K}}$ and A runs on self-adjoint 2×2 matrices that satisfy the condition -D < A < D.

By the invariance of trace under cyclic permutations, the previous integral can be written as

$$\operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{K}}^{s}\right) = \int_{\mathcal{D}_{2,\mathbb{K}}} \operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{K}}^{s}(D)\right) \, \mathrm{d}\lambda_{d+1}(D),$$

where

$$\operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{K}}^{s}(D)\right) = \frac{\det(D)^{2d}}{2^{6d}} \times \int_{\substack{A \in \mathcal{M}_{2,\mathbb{K}}^{\mathrm{sa}} \\ -D < A < D}} \det(I - (D^{-1/2}AD^{-1/2})^{2})^{d} f\left(\frac{I - D^{-1/2}AD^{-1/2}}{I + D^{-1/2}AD^{-1/2}}\right) d\lambda_{d+2}(A).$$

We substitute $Y = D^{-1/2}AD^{-1/2} = (L_{D^{-1/2}} \circ R_{D^{-1/2}})(A)$. According to the remark after Lemma 4, the Jacobian of this transformation is

$$\det \left(L_{D^{-1/2}} \circ R_{D^{-1/2}} \right)^{-1} = \det(D)^{2d - d^2/2}.$$

Observe that $f\left(\frac{I-Y}{I+Y}\right) = \chi_d \circ \sigma\left(\sqrt{\frac{I-Y}{I+Y}}\right)$ and thus $\operatorname{Vol}\left(\mathcal{D}^s_{4,\mathbb{K}}(D)\right) = \frac{\det(D)^{4d-\frac{d^2}{2}}}{2^{6d}} \int_{\mathcal{E}_{2,\mathbb{K}}} \det(I-Y^2)^d \times (\chi_d \circ \sigma)\left(\sqrt{\frac{I-Y}{I+Y}}\right) \, \mathrm{d}\lambda_{d+2}(Y)$

which completes the proof.

The next Corollary proves Milz and Strunz's conjecture on the behavior of the conditioned volume over reduced states (See equation (23) in [7]).

Corollary 1. In the complex case, the conditioned volume can be expressed as

$$Vol\left(\mathcal{D}_{4,\mathbb{K}}^{s}(D)\right) = K_{1} \times \det(D)^{6} = K_{2} \times (1 - r^{2})^{6},$$

where K_1, K_2 are constants and r is the radius of D in the Bloch sphere.

Proof. We set d = 2 in (19) and obtain the first equality. According to the parametrization of $\mathcal{D}_{2,\mathbb{C}}$ (14), det $(D) = \frac{1}{4}(1-r^2)$ which proves the second equality.

Corollary 2. If $D \in \mathcal{D}_{2,\mathbb{K}}$ is a fixed density matrix, then the probability to find a separable state in $\mathcal{D}_{4,\mathbb{K}}(D)$ can be written as

$$\mathcal{P}_{sep}(\mathbb{K}) = \int_{\mathcal{E}_{2,\mathbb{K}}} \tilde{\chi}_d \circ \sigma\left(\sqrt{\frac{I-Y}{I+Y}}\right) d\mu_{d+2}(Y), \tag{23}$$

where

$$d\mu_{d+2}(Y) = \frac{\det(I-Y^2)^d}{\int\limits_{\mathcal{E}_{2,\mathbb{K}}} \det(I-Z^2)^d \, d\lambda_{d+2}(Z)} \, d\lambda_{d+2}(Y).$$

It is apparent that this probability is not depend on D that proves the conjecture of Milz and Strunz [7].

Proof. In a similar way, we can calculate the volume of the whole space

$$\operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{K}}(D)\right) = \chi_d(1) \frac{\det(D)^{4d-\frac{d^2}{2}}}{2^{6d}} \int_{\mathcal{E}_{2,\mathbb{K}}} \det(I-Y^2)^d \, \mathrm{d}\lambda_{d+2}(Y)$$

and thus we have

$$\frac{\operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{K}}^{s}(D)\right)}{\operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{K}}(D)\right)} = \frac{\int\limits_{\mathcal{E}_{2,\mathbb{K}}} \det(I-Y^{2})^{d} \chi_{d} \circ \sigma\left(\sqrt{\frac{I-Y}{I+Y}}\right) d\lambda_{d+2}(Y)}{\chi_{d}(1) \int\limits_{\mathcal{E}_{2,\mathbb{K}}} \det(I-Y^{2})^{d} d\lambda_{d+2}(Y)}$$

which completes the proof.

Using the fact that μ_{d+2} and $\sigma\left(\sqrt{\frac{I-Y}{I+Y}}\right)$ are invariant under orthogonal (unitary) transformation, we can simplify (23) and we obtain the following theorem.

Theorem 2. The separability probability in the rebit-rebit system with respect to the Hilbert–Schmidt measure is

$$\mathcal{P}_{sep}(\mathbb{R}) = \frac{29}{64}.$$
(24)

Proof. According to Equation (23) and the above mentioned unitary invariance, we can write

$$\mathcal{P}_{sep}(\mathbb{R}) = \frac{\int\limits_{-1}^{1} \int\limits_{-1}^{x} \tilde{\chi}_1\left(\sqrt{\frac{1-x}{1+x}} \times \sqrt{\frac{1+y}{1-y}}\right) (1-x^2)(1-y^2)(x-y) \,\mathrm{d}y \,\mathrm{d}x}{\int\limits_{-1}^{1} \int\limits_{-1}^{x} (1-x^2)(1-y^2)(x-y) \,\mathrm{d}y \,\mathrm{d}x},$$

where the denominator is equal to $\frac{16}{35}$. In the numerator, we substitute $u = \frac{1-x}{1+x}$, $v = \frac{1-y}{1+y}$. The Jacobian of this transformation is $\frac{4}{(1+u)^2(1+v)^2}$. Not that, the map $z \mapsto \frac{1-z}{1+z}$ is a monotone decreasing involution that maps (-1, 1) onto $(0, \infty)$. After substitution, the numerator gains the following form

$$\int_{0}^{\infty} \int_{0}^{v} \tilde{\chi}_{1}\left(\sqrt{\frac{u}{v}}\right) \frac{128uv(v-u)}{(1+u)^{5}(1+v)^{5}} \,\mathrm{d}u \,\mathrm{d}v.$$

We substitute again. Let u = ts and $v = \frac{s}{t}$. The Jacobian of this substitution is $\frac{2s}{t}$ and the domain of integration is $0 < s < \infty$, 0 < t < 1. So, we have

$$\int_{0}^{\infty} \int_{0}^{v} \tilde{\chi}_{1}\left(\sqrt{\frac{u}{v}}\right) \frac{128uv(v-u)}{(1+u)^{5}(1+v)^{5}} \,\mathrm{d}u \,\mathrm{d}v = \int_{0}^{\infty} \int_{0}^{1} \tilde{\chi}_{1}(t) \frac{256s^{4}t^{3}(1-t^{2})}{(s+t)^{5}(1+st)^{5}} \,\mathrm{d}t \,\mathrm{d}s.$$

Now we integrate by parts in the inner integral and we get

$$\int_{0}^{1} \tilde{\chi}_{1}(t) \frac{256s^{4}t^{3}(1-t^{2})}{(s+t)^{5}(1+st)^{5}} \, \mathrm{d}t = \frac{64s^{3}}{(s+1)^{8}} - \int_{0}^{1} \frac{64s^{3}t^{4} \left(\tilde{\chi}_{1}\right)'(t)}{(s+t)^{4}(1+st)^{4}} \, \mathrm{d}t.$$

With this, the numerator can be written as

$$\int_{0}^{\infty} \frac{64s^{3}}{(s+1)^{8}} \,\mathrm{d}s - \int_{0}^{1} \int_{0}^{\infty} \frac{64s^{3}t^{4} \left(\tilde{\chi}_{1}\right)'(t)}{(s+t)^{4}(1+st)^{4}} \,\mathrm{d}s \,\mathrm{d}t$$
$$= \frac{16}{35} - \frac{64}{3} \int_{0}^{1} \frac{11(1-t^{6}) + 27t^{2}(1-t^{2}) + 6(1+t^{2})(1+8t^{2}+t^{4})\log(t)}{(t^{2}-1)^{7}} \left(\tilde{\chi}_{1}\right)'(t) \,\mathrm{d}t,$$

where we have interchanged the order of integration in the last term.

One can check that

$$\begin{aligned} \frac{64}{3} \int \frac{11(1-t^6) + 27t^2(1-t^2) + 6(1+t^2)(1+8t^2+t^4)\log(t)}{(t^2-1)^7} \left(\tilde{\chi}_1\right)'(t) \, \mathrm{d}t &= \\ &= -\frac{1}{9\pi^2 \left(t^2-1\right)^6} \left[9 \left(t^2-1\right)^6 \mathrm{Li}_2(1-t) + 9 \left(t^2-1\right)^6 \mathrm{Li}_2(-t) + \\ &+ 96 \left(t^2+1\right) \left(t^4+28t^2+1\right) \left(t^2-1\right)^3 \tanh^{-1}(t) + \\ &+ 9 \left(t^8-132t^6-378t^4-132t^2+1\right) \left(t^2-1\right)^2 \log(t)\log(t+1) + \\ &+ 2t \left(-57t^{10}-1211t^8+78t^6-78t^4+1211t^2\right) + \\ &+ 6t \left(\left(-3t^{10}+401t^8+882t^6+882t^4+401t^2+192+ \\ &+ \left(t^9+t^7-4t^5+t^3+t\right)\log(1-t)-3\right)\log(t)+57\right)\right] + \mathrm{const}, \end{aligned}$$

where we applied Lemma 6. Using this, one can conclude that

$$\frac{64}{3} \int_{0}^{1} \frac{11(1-t^{6}) + 27t^{2}(1-t^{2}) + 6(1+t^{2})(1+8t^{2}+t^{4})\log(t)}{(t^{2}-1)^{7}} \left(\tilde{\chi}_{1}\right)'(t) dt = \frac{1}{4}$$

and thus we have

$$\mathcal{P}_{sep}(\mathbb{R}) = \frac{\frac{16}{35} - \frac{1}{4}}{\frac{16}{35}} = \frac{29}{64}$$

which completes the proof.

4 Generalization to $\left(\mathcal{D}_{4,\mathbb{K}},g_{\sqrt{x}} ight)$

The operator monotone function $f : \mathbb{R}^+ \to R$ is said to be symmetric and normalized if $f(x) = xf(x^{-1})$ holds for every positive argument x and f(1) = 1. The set of symmetric and normalized operator monotone functions plays an important role in quantum information geometry [9, 3]. Petz's classification theorem states that there exists a bijective correspondence between the set of symmetric and normalized operator monotone functions and the family of monotone metrics [10]. The metric associated to the operator monotone function f is given by

$$g_f(D)(X,Y) = \text{Tr}\left(X\left(R_D^{\frac{1}{2}}f\left(L_D R_D^{-1}\right)R_D^{\frac{1}{2}}\right)^{-1}(Y)\right)$$
(25)

for all $n \in \mathbb{N}^+$, $D \in \mathcal{D}_{n,\mathbb{K}}$ and $X, Y \in T_D \mathcal{D}_{n,\mathbb{K}}$. The space of $n \times n$ density matrices endowed with the accompanying monotone metric of the operator monotone function f is denoted by $(\mathcal{D}_{n,\mathbb{K}}, g_f)$.

In this point, we generalize our results to the space $(\mathcal{D}_{4,\mathbb{K}}, g_{\sqrt{x}})$. According to theorem 6 in [1], the volume form of $(\mathcal{D}_{n,\mathbb{K}}, g_f)$ can be expressed as

$$\sqrt{\det(g_f(D))} = \frac{1}{\sqrt{\det(D)}} \left(2^{\binom{n}{2}} \prod_{1 \le i < j \le n} c_f(\mu_i, \mu_j) \right)^{d/2},$$
(26)

where $d = \dim_{\mathbb{R}} \mathbb{K}$, μ_i -s are the eigenvalues of D and $c_f(x, y) = \frac{1}{yf(x/y)}$ is the Čenzov-Morozova function associated to f. For n = 4 and $f(x) = \sqrt{x}$, we have

$$\sqrt{\det(g_f(D))} = \frac{2^{3d}}{\det(D)^{\frac{3d}{4} + \frac{1}{2}}} \quad d = 1, 2.$$
(27)

A slight modification of the previous proofs gives the following Theorem.

Theorem 3. Let $D \in \mathcal{D}_{2,\mathbb{K}}$ be a fixed density matrix. The volume of the submanifold $(\mathcal{D}_{4,\mathbb{K}}^s(D), g_{\sqrt{x}})$ can be formally written as

$$Vol_{\sqrt{x}}\left(\mathcal{D}_{4,\mathbb{K}}^{s}(D)\right) = 4\det(D)^{\frac{5}{2}d - \frac{d^{2}}{2} - 1}$$
$$\times \int_{\mathcal{E}_{2,\mathbb{K}}} \det(I - Y^{2})^{\frac{d-2}{4}} \eta_{d} \circ \sigma\left(\sqrt{\frac{I-Y}{I+Y}}\right) \, \mathrm{d}\lambda_{d+2}(Y)$$

and the volume of the space $\left(\mathcal{D}_{4,\mathbb{K}}^s,g_{\sqrt{x}}\right)$ can be formally expressed as

$$\operatorname{Vol}_{\sqrt{x}}\left(\mathcal{D}_{4,\mathbb{K}}^{s}\right) = \int_{\mathcal{D}_{2,\mathbb{K}}} \operatorname{Vol}_{\sqrt{x}}\left(\mathcal{D}_{4,\mathbb{K}}^{s}(D)\right) \, \mathrm{d}\lambda_{d+1}(D),$$

where $d = \dim_{\mathbb{R}}(\mathbb{K}) = 1, 2.$

Proof. By the factorization $\det(D) = \det(D_1 D_2) \det(I - D_1^{-1/2} C D_2^{-1} C^* D_1^{-1/2})$, we can write

$$\operatorname{Vol}_{\sqrt{x}}\left(\mathcal{D}_{4,\mathbb{K}}^{s}\right) = 2^{3d} \int \det(D_{1}D_{2})^{-\frac{3d}{4} - \frac{1}{2}}$$
(28)
$$\operatorname{Tr}(D_{1} + D_{2}) = 1$$

$$\times \int_{C \in \mathcal{C}(D_{1}, D_{2})} \det(I - D_{1}^{-1/2}CD_{2}^{-1}C^{*}D_{1}^{-1/2})^{-\frac{3d}{4} - \frac{1}{2}} d\lambda_{4d}(C) d\lambda_{2d+3}(D_{1}, D_{2}),$$
(29)

where $C(D_1, D_2)$ is the same as in Theorem 1. Using the substitution $X = D_1^{-1/2} C D_2^{-1/2}$, the inner integral can be written in the following form

$$\det(D_1 D_2)^d \int_{\mathcal{B}_1(\mathbb{K}^{2\times 2})} \det(I - XX^*)^{-\frac{3d}{4} - \frac{1}{2}} \mathbf{1}_{\|(V^*)^{-1}XV\| < 1} \, \mathrm{d}\lambda_{4d}(X),$$

where $V = D_2^{1/2} D_1^{-1/2}$. By a similar argument, the last term depends only on the singular value ratio of V hence it can be written as $\eta_d \circ \sigma(V)$. As a result, for the volume we get

$$\operatorname{Vol}_{\sqrt{x}}\left(\mathcal{D}_{4,\mathbb{K}}^{s}\right) = \int_{\substack{D_{1}, D_{2} > 0\\\operatorname{Tr}(D_{1} + D_{2}) = 1}} 2^{3d} \det(D_{1}D_{2})^{\frac{d-2}{4}} \eta_{d} \circ \sigma(D_{2}^{1/2}D_{1}^{-1/2}) \, \mathrm{d}\lambda_{2d+3}(D_{1}, D_{2}).$$

Using the parametrization (22) and the substitution $Y = D^{-1/2}AD^{-1/2}$, we obtain

$$\operatorname{Vol}_{\sqrt{x}}\left(\mathcal{D}_{4,\mathbb{K}}^{s}\right) = \int_{\mathcal{D}_{2,\mathbb{K}}} \operatorname{Vol}_{\sqrt{x}}\left(\mathcal{D}_{4,\mathbb{K}}^{s}(D)\right) \, \mathrm{d}\lambda_{d+1}(D),$$

where

$$\operatorname{Vol}_{\sqrt{x}}\left(\mathcal{D}_{4,\mathbb{K}}^{s}(D)\right) = 4\det(D)^{\frac{5}{2}d - \frac{d^{2}}{2} - 1} \int_{\mathcal{E}_{2,\mathbb{K}}} \det(I - Y^{2})^{\frac{d-2}{4}} \eta_{d} \circ \sigma\left(\sqrt{\frac{I - Y}{I + Y}}\right) \, \mathrm{d}\lambda_{d+2}(Y).$$

Corollary 3. For a fixed density matrix $D \in (\mathcal{D}_{2,\mathbb{K}}, g_{\sqrt{x}})$ the probability to find a separable state in $\mathcal{D}_{4,\mathbb{K}}(D)$ is

$$\mathcal{P}_{sep,\sqrt{x}}(\mathbb{K}) = \int_{\mathcal{E}_{2,\mathbb{K}}} \tilde{\eta}_d \circ \sigma\left(\sqrt{\frac{I-Y}{I+Y}}\right) \, \mathrm{d}\nu_{d+2}(Y),\tag{30}$$

where

$$d\nu_{d+2}(Y) = \frac{\det(I - Y^2)^{\frac{d-2}{4}}}{\int\limits_{\mathcal{E}_{2,\mathbb{K}}} \det(I - Z^2)^{\frac{d-2}{4}} d\lambda_{d+2}(Z)} d\lambda_{d+2}(Y).$$

This probability is also independent from D which means that the conjecture of Milz and Strunz holds true for the statistical manifold $(\mathcal{D}_{4,\mathbb{K}}, g_{\sqrt{x}})$.

Proof. Similarly, one can show that

$$\operatorname{Vol}_{\sqrt{x}}\left(\mathcal{D}_{4,\mathbb{K}}(D)\right) = 4\eta_d(1)\det(D)^{\frac{5}{2}d - \frac{d^2}{2} - 1} \times \int_{\mathcal{E}_{2,\mathbb{K}}} \det(I - Y^2)^{\frac{d-2}{4}} d\lambda_{d+2}(Y)$$
(31)

then we take the ratio

$$\mathcal{P}_{sep,\sqrt{x}}(\mathbb{K}) = \frac{\operatorname{Vol}_{\sqrt{x}} \left(\mathcal{D}_{4,\mathbb{K}}^{s}(D) \right)}{\operatorname{Vol}_{\sqrt{x}} \left(\mathcal{D}_{4,\mathbb{K}}(D) \right)}$$

and we get the desired result.

Now, we are in the position to calculate the separability probability for rebit-rebit systems in this setting.

Theorem 4. The separability probability in the statistical manifold $(\mathcal{D}_{4,\mathbb{R}}, g_{\sqrt{x}})$ is

$$\mathcal{P}_{sep,\sqrt{x}}(\mathbb{R}) = \int_{0}^{1} \frac{8\left(8\left(t^{4}+t^{2}\right) E\left(1-\frac{1}{t^{2}}\right)-\left(t^{2}+3\right)\left(3t^{2}+1\right) K\left(1-\frac{1}{t^{2}}\right)\right)}{\pi\sqrt{t}\left(t^{2}-1\right)^{3}} \tilde{\chi}_{1}(t) \,\mathrm{d}t \approx 0.26223,$$

where K is the complete elliptic integral of the first kind and E is the elliptic integral of the second kind, that is

$$K(k) = \int_0^1 \frac{1}{\sqrt{1 - t^2}\sqrt{1 - k^2 t^2}} \, \mathrm{d}t \qquad and \qquad E(k) = \int_0^1 \frac{\sqrt{1 - k^2 t^2}}{\sqrt{1 - t^2}} \, \mathrm{d}t.$$

Proof. Due to the fact that $\tilde{\eta}_1 = \tilde{\chi}_1$ (See Lemma 7 and Appendix B.) and by the unitary invariance, we can write

$$\mathcal{P}_{sep,\sqrt{x}}(\mathbb{R}) = \frac{\int\limits_{-1}^{1} \int\limits_{-1}^{x} \tilde{\chi}_1\left(\sqrt{\frac{1-x}{1+x}} \times \sqrt{\frac{1+y}{1-y}}\right) (1-x^2)^{-\frac{1}{4}} (1-y^2)^{-\frac{1}{4}} (x-y) \,\mathrm{d}y \,\mathrm{d}x}{\int\limits_{-1}^{1} \int\limits_{-1}^{x} (1-x^2)^{-\frac{1}{4}} (1-y^2)^{-\frac{1}{4}} (x-y) \,\mathrm{d}y \,\mathrm{d}x},$$

where the denominator is equal to $\frac{2\pi}{3}$. To evaluate the numerator, we use the same strategy that we have applied in the Hilbert–Schmidt case. After the first substitution, the numerator gains the following form

$$\int_{0}^{\infty} \int_{0}^{v} \tilde{\chi}_{1}\left(\sqrt{\frac{u}{v}}\right) \frac{4(v-u)}{(uv)^{\frac{1}{4}}(1+u)^{\frac{5}{2}}(1+v)^{\frac{5}{2}}} \,\mathrm{d}u \,\mathrm{d}v.$$

After the second substitution, we have

$$\int_{0}^{\infty} \int_{0}^{v} \tilde{\chi}_{1}\left(\sqrt{\frac{u}{v}}\right) \frac{4(v-u)}{(uv)^{\frac{1}{4}}(1+u)^{\frac{5}{2}}(1+v)^{\frac{5}{2}}} \,\mathrm{d}u \,\mathrm{d}v = \int_{0}^{\infty} \int_{0}^{1} \frac{8s^{\frac{3}{2}}\sqrt{t}(1-t^{2})\tilde{\chi}_{1}(t)}{(s+t)^{\frac{5}{2}}(1+ts)^{\frac{5}{2}}} \,\mathrm{d}t \,\mathrm{d}s.$$

We interchange the order of integration and obtain

$$\int_{0}^{1} \frac{16\left(8\left(t^{4}+t^{2}\right) E\left(1-\frac{1}{t^{2}}\right)-\left(t^{2}+3\right)\left(3t^{2}+1\right) K\left(1-\frac{1}{t^{2}}\right)\right)}{3\sqrt{t}\left(t^{2}-1\right)^{3}}\tilde{\chi}_{1}(t) \,\mathrm{d}t \approx 0.549213$$

that can be evaluate only numerically. For the separability probability, we have

$$\mathcal{P}_{sep,\sqrt{x}}(\mathbb{R}) = \int_{0}^{1} \frac{8\left(8\left(t^{4}+t^{2}\right) E\left(1-\frac{1}{t^{2}}\right)-\left(t^{2}+3\right)\left(3t^{2}+1\right) K\left(1-\frac{1}{t^{2}}\right)\right)}{\pi\sqrt{t}\left(t^{2}-1\right)^{3}} \tilde{\chi}_{1}(t) \,\mathrm{d}t \approx 0.26223$$

which completes the proof.

5 Examples

To verify the results, first we calculate the volume of 4×4 density matrices with respect to the standard Lebesgue measure. As we mentioned in the proof of Corollary 2, the volume of $\mathcal{D}_{4,\mathbb{K}}$ can be expressed as

$$\operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{K}}\right) = \int_{\mathcal{D}_{2,\mathbb{K}}} \operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{K}}(D)\right) \, \mathrm{d}\lambda_{d+1}(D) \tag{32}$$

which can be written in the following product form

$$\operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{K}}\right) = \frac{\chi_d(1)}{2^{6d}} \times \int_{\mathcal{D}_{2,\mathbb{K}}} \det(D)^{4d - \frac{d^2}{2}} d\lambda_{d+1}(D) \times \int_{\mathcal{E}_{2,\mathbb{K}}} \det(I - Y^2)^d d\lambda_{d+2}(Y).$$
(33)

In the real case we have

$$\chi_1(1) = \frac{2}{3}\pi^2$$
$$\int_{\mathcal{D}_{2,\mathbb{R}}} \det(D)^{\frac{7}{2}} d\lambda_2(D) = \frac{\pi}{2^{7}3^2}$$
$$\int_{\mathcal{E}_{2,\mathbb{R}}} \det(I - Y^2) d\lambda_3(Y) = \frac{2^5\sqrt{2}\pi}{35}.$$

In the complex case we have

$$\chi_2(1) = \frac{\pi^4}{6}$$
$$\int_{\mathcal{D}_{2,\mathbb{C}}} \det(D)^6 \, \mathrm{d}\lambda_3(D) = \frac{\pi}{2 \times 3^2 \times 5 \times 7 \times 11 \times 13 \times \sqrt{2}}$$
$$\int_{\mathcal{E}_{2,\mathbb{C}}} \det(I - Y^2)^2 \, \mathrm{d}\lambda_4(Y) = \frac{2^{10}\pi}{3^2 \times 5^2 \times 7}.$$

If we put all together, we get

$$\operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{R}}\right) = \frac{\pi^4}{\sqrt{2} \times 2^6 \times 3^3 \times 35}$$
$$\operatorname{Vol}\left(\mathcal{D}_{4,\mathbb{C}}\right) = \frac{\pi^6}{\sqrt{2} \times 2^{14} \times 3^4 \times 5^3 \times 7^2 \times 11 \times 13}$$

which is equal to the volume obtained by Życzkowski and Sommers [16] and Andai (See Theorem 1 and 2 in [1]) up to a factor that comes from the difference between the Lebesgue measure and the Hilbert–Schmidt measure. Contrary to the 2×2 case (See Corollary 1 in [1]), the volume of the statistical manifold $(\mathcal{D}_{4,\mathbb{K}}, g_{\sqrt{x}})$ is infinite in both of the real and complex cases because $\eta_d(1) = \infty$ (See Table 2.) and the volume admits the following factorization

$$\operatorname{Vol}_{\sqrt{x}}\left(\mathcal{D}_{4,\mathbb{K}}\right) = 4\eta_{d}(1) \times \int_{\mathcal{D}_{2,\mathbb{K}}} \det(D)^{\frac{5}{2}d - \frac{d^{2}}{2} - 1} d\lambda_{d+1}(D) \times \int_{\mathcal{E}_{2,\mathbb{K}}} \det(I - Y^{2})^{\frac{d-2}{4}} d\lambda_{d+2}(Y).$$

6 Conclusion

The structure of the unit ball in operator norm of 2×2 matrices plays a critical role in separability probability of qubit-qubit and rebit-rebit quantum systems. It is quite surprising that the space of 2×2 real or complex matrices seems simple, but to compute the volume of the set

$$\left\{ \begin{pmatrix} a & b \\ c & d \end{pmatrix} \middle| \quad \left\| \begin{pmatrix} a & b \\ c & d \end{pmatrix} \right\| < 1, \quad \left\| \begin{pmatrix} a & \varepsilon b \\ \frac{c}{\varepsilon} & d \end{pmatrix} \right\| < 1 \right\}$$

for a given parameter $\varepsilon \in [0, 1]$, which is the value of the function $\chi_d(\varepsilon)$, is a very challenging problem. The gist of our considerations is that the behavior of the function $\chi_d(\varepsilon)$ determines the separability probabilities with respect to the Hilbert-Schmidt measure. When the volume form generated by the operator monotone function $x \mapsto \sqrt{x}$, a reasonable normalization can be given to define the separability probability and in this case the probability is determined by the structure of the surface of the unit ball.

References

- A. Andai. Volume of the quantum mechanical state space. Journal of Physics A: Mathematical and Theoretical, 39:13641–13657, 2006.
- [2] R. Bhatia. Matrix analysis, volume 169 of Graduate Texts in Mathematics. Springer-Verlag, New York, 1997.
- [3] J. Dittmann. On the Riemannian metric on the space of density matrices. *Rep. Math. Phys.*, 36(2-3):309-315, 1995.
- [4] J. Fei and R. Joynt. Numerical Computations of Separability Probabilities. ArXiv e-prints, September 2014.
- [5] M. Horodecki, P. Horodecki, and R. Horodecki. Separability of mixed states: necessary and sufficient conditions. *Phys. Lett.*, A, 223(1-2):1–8, 1996.
- [6] K. Zyczkowski, P. Horodecki, A. Sanpera, and M. Lewenstein. Volume of the set of separable states. *Phys. Rev. A*, 58:883–892, Aug 1998.
- [7] S. Milz and W. T. Strunz. Volumes of conditioned bipartite state spaces. J. Phys. A, 48(3):035306, 16, 2015.
- [8] R. Mirman. Group theory: An intuitive approach. World Scientific, 1995.
- [9] D. Petz. Quantum Information Theory and Quantum Statistics. Springer, Berlin-Heidelberg, 2008.
- [10] D. Petz and Cs. Sudár. Geometries of quantum states. J. Math. Phys., 37(6):2662–2673, 1996.
- P. B. Slater. Sensitivity of estimates of the volume of the set of separable states to the choice of "uniform" distributions. *eprint arXiv:quant-ph/9809042*, September 1998.
- [12] P. B. Slater. A concise formula for generalized two-qubit Hilbert–Schmidt separability probabilities. Journal of Physics A: Mathematical and Theoretical, 46(44):445302, 2013.
- [13] Paul B. Slater and Charles F. Dunkl. Moment-based evidence for simple rational-valued Hilbert-Schmidt generic 2 × 2 separability probabilities. J. Phys. A, 45(9):095305, 33, 2012.
- [14] Paul B. Slater and Charles F. Dunkl. Generalized two-qubit whole and half Hilbert-Schmidt separability probabilities. J. Geom. Phys., 90:42–54, 2015.
- [15] F. Zhang. The Schur Complement and Its Applications. Springer, New York, 2005.
- [16] K. Życzkowski and H.-J. Sommers. Hilbert-Schmidt volume of the set of mixed quantum states. J. Phys. A, 36(39):10115–10130, 2003.

A Proof of Lemma 6

For local usage, we redefine the matrix $\Lambda_{\delta} = \begin{pmatrix} 1 & 0 \\ 0 & e^{-\delta} \end{pmatrix}$, where $\delta > 0$. Let us introduce the function $\Delta(\delta) = \operatorname{Vol}(\mathcal{B}_1(\mathbb{R}^{2\times 2})) - \chi_1(e^{-\delta})$ to which we will refer as a *defect function*. In terms of Δ , the statement of Lemma 6 can be reformulated as follows for every positive δ

$$\Delta(\delta) = \frac{16}{3} \int_{0}^{\delta} \cosh t - \sinh^2 t \log\left(\frac{e^t + 1}{e^t - 1}\right) \, \mathrm{d}t.$$

First we fix $\delta > 0$ and we cover the space of 2×2 real matrices with the following atlas

$$\mathcal{A} = \{ X_{\pm}(r, t, \rho, \phi), X_{\pm}(r, t, \rho, \phi)\sigma_3 \},$$
(34)

where

$$X_{\pm}(r,t,\rho,\phi) = rY_{\pm}(t,\rho,\phi) Y_{\pm}(t,\rho,\phi) = \begin{pmatrix} \sqrt{\rho}\cos\phi & \pm \frac{\frac{\rho}{2}\sin 2\phi - 1}{\sqrt{|\frac{\rho}{2}\sin 2\phi - 1|}}e^t \\ \pm \sqrt{|\frac{\rho}{2}\sin 2\phi - 1|}e^{-t} & \sqrt{\rho}\sin\phi \end{pmatrix},$$
(35)

 $t \in \mathbb{R}, r, \rho > 0$ and $\phi \in [0, 2\pi[$. This parametrization is very convenient because the similarity transformation by Λ_{δ} is just a translation

$$(r,t,\rho,\phi) \stackrel{\Lambda_{\delta}^{-1}(.)\Lambda_{\delta}}{\Longrightarrow} (r,t-\delta,\rho,\phi).$$

The metric tensor (g) corresponding to this parametrization (X_{\pm}) has 10 independent components.

$$\begin{split} g_{rr} &= \rho + 2\cosh(2t) \left| \frac{\rho}{2} \sin(2\phi) - 1 \right| \\ g_{rt} &= 2r \sinh(2t) \left| \frac{\rho}{2} \sin(2\phi) - 1 \right| \\ g_{r\rho} &= \frac{r}{2} \left(1 + \sin(2\phi) \cosh(2t) \operatorname{sgn} \left(\frac{\rho}{2} \sin(2\phi) - 1 \right) \right) \\ g_{r\phi} &= r\rho \cos(2\phi) \cosh(2t) \operatorname{sgn} \left(\frac{\rho}{2} \sin(2\phi) - 1 \right) \\ g_{tt} &= 2r^2 \cosh(2t) \left| \frac{\rho}{2} \sin(2\phi) - 1 \right| \\ g_{t\rho} &= \frac{r^2}{4} \sin(2\phi) \cosh(2t) \operatorname{sgn} \left(\frac{\rho}{2} \sin(2\phi) - 1 \right) \\ g_{t\phi} &= -r^2 \rho \cos(2\phi) \sinh(2t) \operatorname{sgn} \left(\frac{\rho}{2} \sin(2\phi) - 1 \right) \\ g_{\rho\rho} &= \frac{r^2}{4} \left(\frac{1}{\rho} + \frac{\cosh(2t) \sin^2(2\phi)}{2 \left| \frac{\rho}{2} \sin(2\phi) - 1 \right|} \right) \\ g_{\rho\phi} &= \frac{r^2 \rho \cosh(2t) \sin(4\phi)}{8 \left| \frac{\rho}{2} \sin(2\phi) - 1 \right|} \\ g_{\phi\phi} &= r^2 \rho \left(1 + \frac{\rho \cosh(2t) \cos^2(2\phi)}{\left| \frac{\rho}{2} \sin(2\phi) - 1 \right|} \right) \end{split}$$

Although the metric tensor has a complicated form, the volume form is quite simple

$$\sqrt{\det(g(r,t,\rho,\phi))} = r^3.$$

We can write

$$\begin{split} \chi_1(e^{-\delta}) &= \lambda_4 \left(\mathcal{B}_1 \left(\mathbb{R}^{2\times 2} \right) \cap \Lambda_{\delta}^{-1} \mathcal{B}_1 \left(\mathbb{R}^{2\times 2} \right) \Lambda_{\delta} \right) \\ &= \int_{\mathbb{R}^{2\times 2}} \mathbf{1}_{\{ \|X\| < 1 \& \| \Lambda_{\delta}^{-1} X \Lambda_{\delta} \| < 1 \}} \, \mathrm{d}\lambda_4(X) \\ &= 2 \int_{-\infty}^{\infty} \int_{0}^{2\pi} \int_{0}^{\infty} \int_{0}^{\infty} \mathbf{1}_{r < \min\left(\frac{1}{\|Y_+(t,\rho,\phi)\|}, \frac{1}{\|Y_+(t-\delta,\rho,\phi)\|} \right)} r^3 \, \mathrm{d}r \, \mathrm{d}\rho \, \mathrm{d}\phi \, \mathrm{d}t \\ &+ 2 \int_{-\infty}^{\infty} \int_{0}^{2\pi} \int_{0}^{\infty} \int_{0}^{\infty} \mathbf{1}_{r < \min\left(\frac{1}{\|Y_-(t,\rho,\phi)\|}, \frac{1}{\|Y_-(t-\delta,\rho,\phi)\|} \right)} r^3 \, \mathrm{d}r \, \mathrm{d}\rho \, \mathrm{d}\phi \, \mathrm{d}t. \end{split}$$

Note that $Y_{\pm}(t,\rho,\phi) \in \mathrm{SL}_2(\mathbb{R})$ and by Lemma 5, we have

$$||Y_{\pm}(t,\rho,\phi)|| = \exp\left(\frac{1}{2}\cosh^{-1}\left(\frac{||Y_{\pm}(t,\rho,\phi)||^2_{\mathrm{HS}}}{2}\right)\right),$$

where

$$\|Y_{\pm}(t,\rho,\phi)\|_{\mathrm{HS}}^2 = 2\left(\frac{\rho}{2} + \left|\frac{\rho}{2}\sin(2\phi) - 1\right|\cosh(2t)\right)$$

which means

$$\|Y_{\pm}(t-\delta,\rho,\phi)\|_{\mathrm{HS}}^2 > \|Y_{\pm}(t,\rho,\phi)\|_{\mathrm{HS}}^2 \quad \text{if and only if} \quad |t-\delta| > |t| \Leftrightarrow t < \delta/2.$$

With this observation, the previous integral can be written as

$$\begin{split} & \int_{-\infty}^{\infty} \int_{0}^{\pi} \int_{0}^{\infty} \int_{0}^{\infty} \mathbf{1} \left(r < e^{-\frac{1}{2} \cosh^{-1} \max\left(\frac{\|Y_{\pm}(t,\rho,\phi)\|_{\mathrm{HS}}^{2}}{2}, \frac{\|Y_{\pm}(t-\delta,\rho,\phi)\|_{\mathrm{HS}}^{2}}{2}\right)} \right) 4r^{3} \, \mathrm{d}r \, \mathrm{d}\rho \, \mathrm{d}\phi \, \mathrm{d}t \\ &= \int_{-\infty}^{\infty} \int_{0}^{\pi} \int_{0}^{\pi} e^{-2 \cosh^{-1} \max\left(\frac{\|Y_{\pm}(t,\rho,\phi)\|_{\mathrm{HS}}^{2}}{2}\right)} \, \mathrm{d}\rho \, \mathrm{d}\phi \, \mathrm{d}t \\ &= \int_{-\infty}^{\frac{\delta}{2}} \int_{0}^{\pi} \int_{0}^{\infty} e^{-2 \cosh^{-1} \left(\frac{\|Y_{\pm}(t-\delta,\rho,\phi)\|_{\mathrm{HS}}^{2}}{2}\right)} \, \mathrm{d}\rho \, \mathrm{d}\phi \, \mathrm{d}t + \int_{\frac{\delta}{2}}^{\infty} \int_{0}^{\pi} \int_{0}^{\infty} e^{-2 \cosh^{-1} \left(\frac{\|Y_{\pm}(t,\rho,\phi)\|_{\mathrm{HS}}^{2}}{2}\right)} \, \mathrm{d}\rho \, \mathrm{d}\phi \, \mathrm{d}t \\ &= \int_{-\infty}^{\infty} \int_{0}^{\pi} \int_{0}^{\infty} e^{-2 \cosh^{-1} \left(\frac{\|Y_{\pm}(t,\rho,\phi)\|_{\mathrm{HS}}^{2}}{2}\right)} \, \mathrm{d}\rho \, \mathrm{d}\phi \, \mathrm{d}t - \int_{\frac{\delta}{2}}^{\frac{\delta}{2}} \int_{0}^{\pi} \int_{0}^{\infty} e^{-2 \cosh^{-1} \left(\frac{\|Y_{\pm}(t,\rho,\phi)\|_{\mathrm{HS}}^{2}}{2}\right)} \, \mathrm{d}\rho \, \mathrm{d}\phi \, \mathrm{d}t \\ &= \int_{-\infty}^{\infty} \int_{0}^{\pi} \int_{0}^{\infty} e^{-2 \cosh^{-1} \left(\frac{\|Y_{\pm}(t,\rho,\phi)\|_{\mathrm{HS}}^{2}}{2}\right)} \, \mathrm{d}\rho \, \mathrm{d}\phi \, \mathrm{d}t - \int_{0}^{\frac{\delta}{2}} \int_{0}^{\pi} \int_{0}^{\infty} e^{-2 \cosh^{-1} \left(\frac{\|Y_{\pm}(t,\rho,\phi)\|_{\mathrm{HS}}^{2}}{2}\right)} \, \mathrm{d}\rho \, \mathrm{d}\phi \, \mathrm{d}t, \end{split}$$

where the last term can be written as

$$\frac{1}{2}\Delta(\delta) = \int_{-\frac{\delta}{2}}^{\frac{\delta}{2}} \int_{0}^{\pi} \int_{0}^{\infty} e^{-2\cosh^{-1}\left(\frac{\|Y_{\pm}(t,\rho,\phi)\|_{HS}^{2}}{2}\right)} d\rho d\phi dt$$

$$= \int_{-\frac{\delta}{2}}^{\frac{\delta}{2}} \int_{0}^{2\pi} \int_{0}^{\infty} e^{-2\cosh^{-1}(\rho+|\rho\sin\phi-1|\cosh(2t))} d\rho d\phi dt \qquad (36)$$

$$= \int_{0}^{\delta} \int_{0}^{2\pi} \int_{0}^{\infty} e^{-2\cosh^{-1}(\rho+|\rho\sin\phi-1|\cosh t)} d\rho d\phi dt.$$

We decompose the inner double integral in the following way

$$\int_{0}^{2\pi} \int_{0}^{\infty} e^{-2\cosh^{-1}(\rho+|\rho\sin\phi-1|\cosh t)} d\rho d\phi = \int_{0}^{\pi} \int_{0}^{\infty} e^{-2\cosh^{-1}(\rho+(\rho\sin\phi+1)\cosh t)} d\rho d\phi + \int_{0}^{\pi} \left(\int_{0}^{\frac{1}{\sin\phi}} e^{-2\cosh^{-1}(\rho-(\rho\sin\phi-1)\cosh t)} d\rho + \int_{\frac{1}{\sin\phi}}^{\infty} e^{-2\cosh^{-1}(\rho+(\rho\sin\phi-1)\cosh t)} d\rho \right) d\phi.$$

After some manipulation with the inner integrals we have

$$\begin{split} &\int_{0}^{2\pi} \int_{0}^{\infty} e^{-2\cosh^{-1}(\rho+|\rho\sin\phi-1|\cosh t)} \,\mathrm{d}\rho \,\mathrm{d}\phi = \int_{0}^{\pi} \frac{1}{1+\cosh t\sin\phi} \int_{t}^{\infty} e^{-2u}\sinh u \,\mathrm{d}u \,\mathrm{d}\phi \\ &+ \int_{0}^{\pi} \left(\frac{1}{1-\cosh t\sin\phi} \int_{t}^{\cosh^{-1}\left(\frac{1}{\sin\phi}\right)} e^{-2u}\sinh u \,\mathrm{d}u + \frac{1}{1+\cosh t\sin\phi} \int_{\cosh^{-1}\left(\frac{1}{\sin\phi}\right)}^{\infty} e^{-2u}\sinh u \,\mathrm{d}u \right) \,\mathrm{d}\phi \\ &= 2\int_{0}^{\frac{\pi}{2}} \left(e^{-t} - \frac{e^{-3t}}{3} - \left(\tan\frac{\phi}{2} - \frac{1}{3}\tan^{3}\frac{\phi}{2}\right)\cosh t\sin\phi \right) \frac{1}{1-\cosh^{2}t\sin^{2}\phi} \,\mathrm{d}\phi, \end{split}$$

where we applied the identity $\exp\left(-\cosh^{-1}\left(\frac{1}{\sin\phi}\right)\right) = \tan\frac{\phi}{2}$. Now we substitute $\tan\frac{\phi}{2} = e^{-s}$ and we get

$$2\int_{0}^{\infty} \left(e^{-t} - \frac{e^{-3t}}{3} - \left(e^{-s} - \frac{e^{-3s}}{3}\right)\frac{\cosh t}{\cosh s}\right)\frac{1}{1 - \left(\frac{\cosh t}{\cosh s}\right)^{2}}\frac{1}{\cosh s}\,\mathrm{d}s$$
$$= \frac{8}{3}\int_{0}^{\infty} e^{-t}\cosh s - \frac{\sinh^{2} s}{\sinh(t+s)}\,\mathrm{d}s = \frac{8}{3}\left(\cosh t - \sinh^{2} t\log\left(\frac{e^{t}+1}{e^{t}-1}\right)\right).$$

For the defect function, we gain the following formula

$$\Delta(\delta) = \frac{16}{3} \int_{0}^{\delta} \cosh t - \left(\sinh^2 t\right) \log\left(\frac{e^t + 1}{e^t - 1}\right) \,\mathrm{d}t \tag{37}$$

which completes the proof.

B Proof of Lemma 7

We cover the manifold $\partial \mathcal{B}_1(\mathbb{R}^{2\times 2})$ with the following atlas

$$\mathcal{A} = \left(\frac{Y_{\pm}(t,\rho,\phi)}{\|Y_{\pm}(t,\rho,\phi)\|}, \frac{Y_{\pm}(t,\rho,\phi)\sigma_3}{\|Y_{\pm}(t,\rho,\phi)\sigma_3\|}\right),\tag{38}$$

where $Y_{\pm}(r, t, \rho, \phi)$ is given by (35) and $\|\cdot\|$ denotes the usual operator norm. Direct computation of the volume form from this parametrization would be a cumbersome task even for computer algebra systems.

It is obvious that the metric tensor has the same form on every element of \mathcal{A} hence it is enough to deal with the parametrization

$$X(t,\rho,\phi) = \frac{Y(t,\rho,\phi)}{\|Y(t,\rho,\phi)\|},$$

where $Y(t, \rho, \phi) := Y_+(t, \rho, \phi)$. Recall the fact that $Y(t, \rho, \phi) \in SL_2(\mathbb{R})$ and by Lemma 5, we have

$$X(t,\rho,\phi) = f(t,\rho,\phi)Y(t,\rho,\phi),$$
(39)

where

$$f(t,\rho,\phi) = \exp\left(-\frac{1}{2}\cosh^{-1}\left(\frac{\|Y(t,\rho,\phi)\|_{\rm HS}^2}{2}\right)\right).$$
(40)

The metric tensor (g) corresponding to this parametrization can be written as

$$\frac{1}{f^2}g_{ij} = \frac{1}{f^2} \langle \partial_i X, \partial_j X \rangle = (\partial_i \log(f)) (\partial_j \log(f)) \|Y\|_{\mathrm{HS}}^2 + \frac{1}{2} \left((\partial_i \log(f)) \left(\partial_j \|Y\|_{\mathrm{HS}}^2 \right) + (\partial_j \log(f)) \left(\partial_i \|Y\|_{\mathrm{HS}}^2 \right) \right) + \langle \partial_i Y, \partial_j Y \rangle,$$

where \langle , \rangle denotes the usual Hilbert–Schmidt scalar product. By the chain rule, the metric tensor can be written in the following convenient form

$$g = f^{2} \left(G + \left(\|Y\|_{\mathrm{HS}}^{2} \left(h' \left(\|Y\|_{\mathrm{HS}}^{2} \right) \right)^{2} + h' \left(\|Y\|_{\mathrm{HS}}^{2} \right) \right) \times \nabla \left(\|Y\|_{\mathrm{HS}}^{2} \right) \nabla \left(\|Y\|_{\mathrm{HS}}^{2} \right)^{T} \right), \quad (41)$$

where $G_{ij} = \langle \partial_i Y, \partial_j Y \rangle$ and $h(r) = -\frac{1}{2} \cosh^{-1} \left(\frac{r}{2} \right)$.

According to the matrix determinant lemma, we have

$$\det(g) = f^{6} \det(G) \times \left(1 + \left(\|Y\|_{\mathrm{HS}}^{2} \left(h'\left(\|Y\|_{\mathrm{HS}}^{2} \right) \right)^{2} + h'\left(\|Y\|_{\mathrm{HS}}^{2} \right) \right) \nabla \left(\|Y\|_{\mathrm{HS}}^{2} \right)^{T} G^{-1} \nabla \left(\|Y\|_{\mathrm{HS}}^{2} \right) \right)$$

where all the factors can be directly evaluated. We obtain the following nice form for the volume form

$$\sqrt{\det(g)} = f^4 = \exp\left(-2\cosh^{-1}\left(\frac{\|Y\|_{\mathrm{HS}}^2}{2}\right)\right). \tag{42}$$

Using the notations introduced in Appendix A, we can write

$$\begin{split} \tilde{\eta}_{1}(e^{-\delta}) &= 4 \int_{-\infty}^{\infty} \int_{0}^{2\pi} \int_{0}^{\infty} \frac{e^{-2\cosh^{-1}\left(\frac{\|Y(t,\rho,\phi)\|_{\mathrm{HS}}^{2}}{2}\right)}}{\operatorname{Vol}(\partial\mathcal{B}_{1}\left(\mathbb{R}^{2\times2}\right))} \mathbf{1}_{\|Y(t-\delta,\rho,\phi)\|<\|Y(t,\rho,\phi)\|} \,\mathrm{d}\rho \,\mathrm{d}\phi \,\mathrm{d}t \\ &= \frac{4}{\operatorname{Vol}(\partial\mathcal{B}_{1}\left(\mathbb{R}^{2\times2}\right))} \int_{\frac{\delta}{2}}^{\infty} \int_{0}^{2\pi} \int_{0}^{\infty} e^{-2\cosh^{-1}\left(\frac{\|Y(t,\rho,\phi)\|_{\mathrm{HS}}^{2}}{2}\right)} \,\mathrm{d}\rho \,\mathrm{d}\phi \,\mathrm{d}t \\ &= 1 - \frac{4}{\operatorname{Vol}(\partial\mathcal{B}_{1}\left(\mathbb{R}^{2\times2}\right))} \underbrace{\int_{0}^{\delta} \int_{0}^{2\pi} \int_{0}^{\infty} e^{-2\cosh^{-1}\left(\rho+|\rho\sin\phi-1|\cosh t\right)} \,\mathrm{d}\rho \,\mathrm{d}\phi \,\mathrm{d}t, \\ &\frac{1}{2}\Delta(\delta) \text{ (See (36).)} \end{split}$$

where we applied the following identities

$$\Lambda_{\delta}^{-1}Y(t,\rho,\phi)\Lambda_{\delta} = Y(t-\delta,\rho,\phi)$$
$$\|Y(t-\delta,\rho,\phi)\| < \|Y(t,\rho,\phi)\| \Leftrightarrow t > \delta/2.$$

So, we have

$$\tilde{\eta}_1(\varepsilon) = 1 - \frac{2\operatorname{Vol}(\mathcal{B}_1(\mathbb{R}^{2\times 2}))}{\operatorname{Vol}(\partial \mathcal{B}_1(\mathbb{R}^{2\times 2}))} \left(1 - \tilde{\chi}_1(\varepsilon)\right)$$

which implies $\tilde{\eta}_1(\varepsilon) = \tilde{\chi}_1(\varepsilon)$ for $\varepsilon \in [0,1]$ because $\tilde{\eta}_1(0) = \tilde{\chi}_1(0) = 0$ and $\tilde{\eta}_1(1) = \tilde{\chi}_1(1) = 1$.