On the Bures Volume of Separable Quantum States *

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Abstract

We obtain two sided estimates for the Bures volume of an arbitrary subset of the set of $N \times N$ density matrices, in terms of the Hilbert-Schmidt volume of that subset. For general subsets, our results are essentially optimal (for large $N$). As applications, we derive in particular nontrivial lower and upper bounds for the Bures volume of sets of separable states and for sets of states with positive partial transpose.

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1 Introduction

Quantum entanglement was discovered in 1930’s [10, 28] and is now at the heart of quantum computation and quantum information. The key ingredients in quantum algorithms such as Shor’s algorithm for integer factorization [29] or Deutsch-Jozsa

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algorithm (see e.g. [24]), are entangled quantum states, i.e., those states which cannot be represented as a mixture of tensor products of states on subsystems. Following [43], states that can be so represented are called separable states. Since determining whether a state is entangled or separable is in general a difficult problem [11], sufficient and/or necessary conditions for separability are very important in quantum computation and quantum information theory, and have been studied extensively in the literature (see e.g. [14, 15, 16, 17, 18, 19, 25]). One well-known tool is the Peres’ positive partial transpose (PPT) criterion [25], that is, if a state on $\mathcal{H} = \mathbb{C}^{D_1} \otimes \mathbb{C}^{D_2} \cdots \otimes \mathbb{C}^{D_n}$ is separable then its partial transpose must be positive. Equivalently, if a state on $\mathcal{H}$ does not have positive partial transpose, it must be entangled. This criterion works perfectly, namely, the set of separable states $\mathcal{S} = \mathcal{S}(\mathcal{H})$ equals to the set of states with positive partial transpose $\mathcal{PPT} = \mathcal{PPT}(\mathcal{H})$ for $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$ (two-qubits), $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^3$ (qubit-qutrit), and $\mathcal{H} = \mathbb{C}^3 \otimes \mathbb{C}^2$ (qutrit-qubit) [14, 37, 44]. However, entangled states with positive partial transpose appear in the composite Hilbert space $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^4$ and $\mathcal{H} = \mathbb{C}^3 \otimes \mathbb{C}^3$ [15] (and of course in all “larger” composite spaces; see also [4] discussing the three-qubit case). One striking result is that, by some measures, the positive partial transpose criterion becomes less and less precise as $N = \prod_{i=1}^{n} D_i$ grows to infinity [2, 38]. This is inferred by comparing the Hilbert-Schmidt volumes of $\mathcal{S}$ and $\mathcal{PPT}$, the estimates which rely on the special geometric properties of the Hilbert-Schmidt metric and were obtained by using tools of classical convexity, high dimensional probability, and geometry of Banach spaces.

The same method can also be employed to derive tight estimates for the Hilbert-Schmidt volume of $\mathcal{D} = \mathcal{D}(\mathcal{H})$ (the set of all states on $\mathcal{H}$). However, a closed expression for the exact value of this volume is known; it was found in [45] via the random matrix theory and calculating some nontrivial multivariate integrals.
Compared with the Hilbert-Schmidt metric, the Bures metric on $\mathcal{D}$ [5, 42] is, in some measures, more natural and has attracted considerable attention (see e.g. [7, 8, 9, 20, 21, 39, 40, 41]). The Bures metric is Riemannian but not flat. It is monotone [26], i.e., it does not increase under the action of any completely positive, trace preserving maps. It induces the Bures measure [3, 12, 36], which has singularities on the boundary of $\mathcal{D}$. The Bures volume of $\mathcal{D}$ has been calculated exactly in [36] and happens to be equal to the volume of an $(N^2 - 1)$-dimensional hemisphere of radius $\frac{1}{2}$ [3, 36]. (This mysterious fact does not seem to have a satisfactory explanation.) On the other hand, the precise Bures (or Hilbert-Schmidt) volumes of $\mathcal{S}$ and $\mathcal{PPT}$ are rather difficult to calculate since the geometry of these sets is not very well understood and the relevant integrals seem quite intractable. These quantities can be used to measure the priori Bures probabilities of separability and of positive partial transpose within the set of all quantum states. (Here priori means that the state is selected randomly according to the Bures measure and no further information about it is available.) For small $N$, e.g., $N = 2 \times 2$ and $N = 2 \times 3$, the Bures volume of $\mathcal{S}$ (hence of $\mathcal{PPT}$) has been extensively studied by numerical methods in [30, 31, 32, 33, 34, 35]. For large $N$, the asymptotic behavior of the Hilbert-Schmidt volume of $\mathcal{S}$ and $\mathcal{PPT}$ was successfully studied in [2, 38]. Based on that work, we shall derive in this paper qualitatively similar “large $N$” results for the Bures volume. In summary, our results state that the relative size of $\mathcal{S}$ within $\mathcal{D}$ is extremely small for large $N$ (see Corollaries 1 and 2 for detail). On the other hand, the corresponding relative size for $\mathcal{PPT}$ within $\mathcal{D}$ is, in the Bures volume radius sense (see section 2 for a precise definition), bounded from below by a universal (independent of $N$) positive constant (see Corollary 3). The conclusion is that when $N$ is large, the priori Bures probability of finding a separable state within $\mathcal{PPT}$ is exceedingly small. In other
words, we have shown that, as a tool to detect separability, the positive partial transpose
criterion for large $N$ is not precise in the priori Bures probability sense. Its effectiveness
to detect entanglement is less clear (see the comments following Corollary 3).

This paper is organized as follows. In section 2, we review some necessary
mathematical background, particularly the background for the Hilbert-Schmidt volume
and the Bures volume. Precise statements of our main results can be found in section
3. Section 4 explains why our estimates are essentially optimal for general subsets of
quantum states. Section 5 contains conclusions, comments and final remarks.

2 Notation and Mathematical Preliminaries

2.1 Mathematical framework

We now introduce the mathematical framework and some notation. Let $\mathcal{H}$ be the
(complex) Hilbert space $\mathbb{C}^{D_1} \otimes \mathbb{C}^{D_2} \cdots \otimes \mathbb{C}^{D_n}$ with (complex) dimension $N = D_1D_2 \cdots D_n$.
Here we always assume $n \geq 2$ and $D_i \geq 2$ for all $i = 1, 2, \cdots, n$. Recall that $D_i = 2$ for all
$i$ corresponds to $n$-qubits, and $D_i = 3$ for all $i$ corresponds to $n$-qutrits. $n = 2$ corresponds
to bipartite quantum systems and $n > 2$ corresponds to multipartite quantum systems.
Denote by $\mathcal{B}(\mathcal{H})$ the space of linear maps on $\mathcal{H}$. Define the Hilbert-Schmidt inner product
on space $\mathcal{B}(\mathcal{H})$ as $\langle A, B \rangle_{HS} = \text{tr}(A^\dagger B)$. The subspace of $\mathcal{B}(\mathcal{H})$ consisting of all self-adjoint
operators is $\mathcal{B}_{sa}(\mathcal{H})$. It inherits a (real) Euclidean structure from the scalar product
$\langle \cdot, \cdot \rangle_{HS}$ on $\mathcal{B}(\mathcal{H})$. (This is because if $A, B \in \mathcal{B}_{sa}(\mathcal{H})$, then $\langle A, B \rangle_{HS}$ must be a real
number.) $\mathcal{D}$ denotes the set of all states on $\mathcal{H}$ (more precisely, states on $\mathcal{B}(\mathcal{H})$), i.e.,
positive (semi) definite trace one operator in $\mathcal{B}_{sa}(\mathcal{H})$:

$$\mathcal{D} = \mathcal{D}(\mathcal{H}) := \{\rho \in \mathcal{B}_{sa}(\mathcal{H}), \rho \geq 0, \text{tr}\rho = 1\}. $$

A state in $\mathcal{D}$ is said to be separable if it is a convex combination of tensor products of $n$ states (otherwise, it is called entangled). Denote the set of separable states by $\mathcal{S}$, then

$$\mathcal{S} = \mathcal{S}(\mathcal{H}) := \text{conv}\{\rho_1 \otimes \cdots \otimes \rho_n, \rho_i \in \mathcal{D}(\mathbb{C}^{D_i})\}. $$

Both $\mathcal{D}$ and $\mathcal{S}$ are convex subsets of $\mathcal{B}_{sa}(\mathcal{H})$ of (real) dimension $d = N^2 - 1$.

Indent: The notation $\mathcal{S}(\mathcal{H})$ is in principle ambiguous: separability of a state on $\mathcal{B}(\mathcal{H})$ is not an intrinsic property of the Hilbert space $\mathcal{H}$ nor of the algebra $\mathcal{B}(\mathcal{H})$; it depends on the particular decomposition of $\mathcal{H}$ as a tensor product of (smaller) Hilbert spaces. However, this will not be an issue here since our study focuses on fixed decompositions.

### 2.2 Hilbert-Schmidt and Bures Measures on $\mathcal{D}$

Any quantum state on $\mathcal{H}$ can be represented as a density matrix, i.e., the $N \times N$ positive (semi) definite matrix whose diagonal elements sum up to 1. Therefore, any quantum state $\rho \in \mathcal{D}$ has eigenvalue decomposition $\rho = U\Lambda U^\dagger$ for some unitary matrix $U \in \mathcal{U}(N)$ and some diagonal matrix $\Lambda = \text{diag}(\lambda_1, \cdots, \lambda_N)$ with $(\lambda_1, \cdots, \lambda_N) \in \Delta$. Hereafter, $\text{Id}_N$ is the $N \times N$ identity matrix and $U \in \mathcal{U}(N)$ means that $U$ is an $N \times N$ matrix with $UU^\dagger = U^\dagger U = \text{Id}_N$. We denote by $\Delta$ the regular simplex in $\mathbb{R}^N$, i.e.,

$$\Delta = \left\{(\lambda_1, \cdots, \lambda_N) \in \mathbb{R}^N : \lambda_i \geq 0, \sum_{i=1}^{N} \lambda_i = 1\right\}. $$

The Weyl chamber of $\Delta$ defined by the constraint $\lambda_1 \geq \cdots \geq \lambda_N$ is denoted by $\Delta_1$. Clearly, for any $\rho = U\Lambda U^\dagger$ as above and for any diagonal matrix $B \in \mathcal{U}(N)$, we
have \( U \Lambda U^\dagger = U B \Lambda B^\dagger U \). Thus, to have unique parametrization of generic states \( \rho = U \Lambda U^\dagger \in \mathcal{D} \), we have to restrict \((\lambda_1, \cdots, \lambda_N)\), for instance, to \( \Delta_1 \) and select one specific point in the coset space \( \mathcal{F}^N = \mathcal{U}(N)/[\mathcal{U}(1)]^N \) (the flag manifold).

We will be interested in various measures on \( \mathcal{D} \). A natural restriction is to require invariance with respect to unitary rotations. For most problems, the interesting class of measures are those that are invariant under conjugation by a unitary matrix. Such measures can normally be represented as the product of some measure on \( \Delta_1 \) and the invariant measure on \( \mathcal{F}^N \) (see [3, 13] for more on this and for the background on the discussion that follows). The unique (up to a multiplicative constant) invariant measure \( \gamma \) on \( \mathcal{F}^N \) is induced by the Haar measure on the unitary group \( \mathcal{U}(N) \) and has the form

\[
d\gamma = \prod_{1 \leq i < j \leq N} 2 \text{Re}(U^{-1}dU)_{ij} \text{Im}(U^{-1}dU)_{ij},
\]

where \( U \in \mathcal{U}(N) \) and \( dU \) is the variation of \( U \) such that \( U + dU \in \mathcal{U}(N) \). The total \( \gamma \) measure of \( \mathcal{F}^N \) is known to be (see [45])

\[
Z_N = \frac{(2\pi)^{N(N-1)/2}}{E(N)}, \quad \text{where } E(N) = \prod_{j=1}^{N} \Gamma(j).
\]

(1)

Here \( \Gamma(x) = \int_{0}^{\infty} t^{x-1} e^{-t} \, dt \) is the Gamma function.

The Hilbert-Schmidt measure \( V_{HS}(\cdot) \) on \( \mathcal{D} \), induced by the Hilbert-Schmidt metric, may be expressed as [45]

\[
dV_{HS} = \sqrt{N} \prod_{1 \leq i < j \leq N} (\lambda_i - \lambda_j)^2 \prod_{i=1}^{N-1} d\lambda_i \, d\gamma,
\]

(2)

where \( (\lambda_1, \cdots, \lambda_N) \in \Delta_1 \). (This is just a different name for the canonical \( d \)-dimensional Lebesgue measure on \( \mathcal{D} \)\.) Therefore, to obtain the Hilbert-Schmidt volume of \( \mathcal{D} \), one has
to calculate the following integral [45]:

\[
V_{HS}(\mathcal{D}) = \int_{\Delta_1 \times \mathcal{F}^N} \sqrt{N} \prod_{1 \leq i < j \leq N} (\lambda_i - \lambda_j)^2 \prod_{i=1}^{N-1} d\lambda_i d\gamma
\]

\[
= (2\pi)^{\frac{N(N-1)}{2}} \sqrt{N} \frac{E(N)}{\Gamma(N^2)}.
\]

We define \(v_{rad_{HS}}(\mathcal{K})\), the Hilbert-Schmidt volume radius of \(\mathcal{K} \subset \mathcal{D}\), to be the radius of \(d\)-dimensional Euclidean ball which has the same volume as the Hilbert-Schmidt volume of \(\mathcal{K}\). In other words,

\[
v_{rad_{HS}}(\mathcal{K}) = \left( \frac{V_{HS}(\mathcal{K})}{\sigma_d} \right)^{\frac{1}{d}},
\]

where \(\sigma_d = \frac{\pi^{d/2}}{\Gamma(1+d/2)}\) is the volume of \(d = N^2 - 1\) dimensional Euclidean ball. For later convenience, we also denote \(VR_{HS}(\mathcal{K}, \mathcal{L})\) as \(VR_{HS}(\mathcal{K}, \mathcal{L}) = \left( \frac{V_{HS}(\mathcal{K})}{V_{HS}(\mathcal{L})} \right)^{1/d} = \frac{v_{rad_{HS}}(\mathcal{K})}{v_{rad_{HS}}(\mathcal{L})}\). It amounts to comparing the Hilbert-Schmidt volume radii of \(\mathcal{K}\) and \(\mathcal{L}\).

It is known that \(v_{rad_{HS}}(\mathcal{D}) \sim e^{-\frac{1}{4}d^{-\frac{1}{2}}} [38]\) by Stirling approximation

\[
\Gamma(z) = \sqrt{2\pi} \left( \frac{z}{e} \right)^z \left( 1 + O\left( \frac{1}{z} \right) \right).
\]

Stirling approximation (4) also implies that \((\sigma_d)^{\frac{1}{2}} \sim \sqrt{2\pi} d^{-\frac{1}{2}}\) and therefore

\[
(V_{HS}(\mathcal{D}))^{\frac{1}{2}} \sim (4\pi^2 e)^{\frac{1}{4}} d^{-\frac{1}{2}}.
\]

Here \(a(n) \sim b(n)\) means \(\lim_{n \to \infty} a(n)/b(n) = 1\).

An arguably more important measure in the present context is the Bures measure (or Bures volume) \(V_B(\cdot)\), which can be written as [36]

\[
dV_B = \frac{2^{2-N-N^2}}{\sqrt{\lambda_1 \cdots \lambda_N}} \prod_{1 \leq i < j \leq N} (\lambda_i - \lambda_j)^2 \prod_{i=1}^{N-1} d\lambda_i d\gamma,
\]
where \((\lambda_1, \cdots, \lambda_N) \in \Delta_1\). The Bures measure is induced by the Bures distance \(d_B(\cdot, \cdot)\), which may be defined via \(d_B(\rho_1, \rho_2) = \sqrt{2 - 2\text{tr}\sqrt{\rho_1} \sqrt{\rho_2} \sqrt{\rho_1}}\) for any states \(\rho_1, \rho_2 \in \mathcal{D}\).

The Bures measure has singularities (with respect to the Hilbert-Schmidt measure) on the boundary of \(\mathcal{D}\). (The boundary corresponds to at least one of the \(\lambda_i\)'s being 0, and if two or more of them are 0, then some denominators in (6) vanish.) Thanks to the work of Sommers and Zyczkowski [36], we know the precise value of the Bures volume of \(\mathcal{D}\), that is

\[
V_B(\mathcal{D}) = \int_{\Delta_1 \times \mathbb{R}^N} \frac{2^{2-N^2} \prod_{1 \leq i < j \leq N} (\lambda_i - \lambda_j)^2 \prod_{i=1}^{N-1} \lambda_i + \lambda_j}{\sqrt{\lambda_1 \cdots \lambda_N}} \prod_{i} d\lambda_i d\gamma
\]

As mentioned earlier, this value happens to be the \(d\)-dimensional volume of the \(d\)-dimensional hemisphere with radius \(\frac{1}{2}\). We define \(v_{rad_B}(\mathcal{K})\), the Bures volume radius of \(\mathcal{K} \subset \mathcal{D}\), to be

\[
v_{rad_B}(\mathcal{K}) = \left(\frac{V_B(\mathcal{K})}{\sigma_d}\right)^{\frac{1}{d}}.
\]

While comparing the Bures volume of \(\mathcal{K}\) with the Hilbert-Schmidt volume of the Euclidean ball does not have immediate geometric meaning, we find this way of describing the size of \(\mathcal{K}\) in the Bures volume sense convenient in our calculations.

By formulas (4) and (7), one has \(v_{rad_B}(\mathcal{D}) \sim \frac{1}{2}\) and hence

\[
(V_B(\mathcal{D}))^{\frac{1}{d}} \sim \sqrt{\frac{e\pi}{2}} \cdot d^{-\frac{1}{2}}.
\]

For later convenience, we also define the (relative) Bures volume radii ratio of \(\mathcal{K}\) to \(\mathcal{L}\) as

\[
VR_B(\mathcal{K}, \mathcal{L}) = \left(\frac{V_B(\mathcal{K})}{V_B(\mathcal{L})}\right)^{1/d} = \frac{v_{rad_B}(\mathcal{K})}{v_{rad_B}(\mathcal{L})}.\]

This can be used as a measure of the relative size of \(\mathcal{K}\) to \(\mathcal{L}\) in the Bures volume sense, and clearly does have geometric meaning.
We refer the reader to the references [3, 12, 13, 36, 45] for more detailed background and for motivation. In the following sections, we are interested in the (asymptotical) behavior of $\text{VR}_B(\mathcal{K}, \mathcal{D})$ in terms of its relative $\text{VR}_{\text{HS}}(\mathcal{K}, \mathcal{D})$.

## 3 Main Results

In this section, $\mathcal{K}$ will be an arbitrary (Borel) subset of $\mathcal{D}$. We will estimate the Bures volume of $\mathcal{K}$, in terms of the Hilbert-Schmidt volume of $\mathcal{K}$, both from below and from above. The following lemma is our main tool to study the asymptotical behavior of $\text{VR}_B(\mathcal{K}, \mathcal{D})$. We point out that these estimates are independent of the possible tensor product structure of $\mathcal{H}$.

**Lemma 1** For any subset $\mathcal{K}$ in $\mathcal{D}$ and any $p > 1$, one has

$$2^{-\frac{N-N^2}{2}} N^{-\frac{N^2-1}{2}} \text{V}_{\text{HS}}(\mathcal{K}) \leq 2^{-\frac{N^2-N-2}{2}} \text{V}_B(\mathcal{K}) \leq \left( \frac{\text{V}_{\text{HS}}(\mathcal{K})}{\sqrt{N}} \right)^{\frac{1}{2p}} I(p) \frac{2p-1}{2^p},$$

where $I(p)$ is defined as

$$I(p) := \frac{1}{N!} \frac{1}{\Gamma \left( \frac{(p-1)N^2}{2p-1} \right)} \prod_{j=1}^{N} \frac{1}{\Gamma \left( \frac{3p-2}{2p-1} \right)} \left( 1 + \frac{j(p-1)}{2p-1} \right)^{\frac{j(p-1)\Gamma \left( \frac{3p-2}{2p-1} \right)}{\Gamma \left( \frac{3p-2}{2p-1} \right)}} \left( \frac{2\pi}{E(N)} \right)^{\frac{N(N-1)}{2}}. \quad (9)$$

**Remark.** $I(p)$ can be defined for all $p \notin [\frac{1}{2}, 1]$ (irrespective of $N$; since the Gamma function has poles at nonpositive integers, there are singularities in $[\frac{1}{2}, 1]$ whose exact locations depend on $N$.) In particular, $I(0) = \frac{\text{V}_{\text{HS}}(\mathcal{D})}{\sqrt{N}}$. The quantity $E(N)$ was defined in (1).

**Proof.** First of all, we estimate $V_B(\mathcal{K})$ from below. To that end, define $h : \Delta \to \mathbb{R}$ as

$$h(\lambda_1, \cdots, \lambda_N) = \prod_{i=1}^{N} \lambda_i \prod_{1 \leq i < j \leq N} (\lambda_i + \lambda_j)^2.$$
Lagrange multiplier method implies that $(1/N, \cdots, 1/N)$ is the only critical point of $h(\lambda_1, \cdots, \lambda_N)$ in the interior of simplex $\Delta$. Clearly $h(\lambda_1, \cdots, \lambda_N)$ is always 0 on the boundary of the simplex $\Delta$, which consists of sequences for which one or more of the $\lambda_i$'s equal to 0, and strictly positive in the interior of the simplex $\Delta$. By compactness, $h(\lambda_1, \cdots, \lambda_N)$ must have a maximum inside, and the critical point $(1/N, \cdots, 1/N)$ must be the (only) maximizer of $h(\lambda_1, \cdots, \lambda_N)$ on $\Delta$. Therefore,

$$
\frac{1}{\sqrt{h(\lambda_1, \cdots, \lambda_N)}} = \frac{1}{\sqrt{\lambda_1 \cdots \lambda_N}} \prod_{1 \leq i < j \leq N} \frac{1}{\lambda_i + \lambda_j} \geq 2^{\frac{N^2}{2}} N^{-\frac{N^2}{2}}. \tag{10}
$$

By formula (6), the Bures volume of $\mathcal{K}$ equals to $\int_{\mathcal{K}} dV_B$, i.e.,

$$
V_B(\mathcal{K}) = \int_{\mathcal{K}} 2^{\frac{N^2}{2}} N^{-\frac{N^2}{2}} \prod_{1 \leq i < j \leq N} (\frac{\lambda_i - \lambda_j}{\lambda_i + \lambda_j})^2 \prod_{i=1}^{N-1} d\lambda_i d\gamma.
$$

Considering inequality (10) and formula (2), one gets

$$
V_B(\mathcal{K}) \geq 2^{1-N^2} N^{\frac{N^2}{2}} \int_{\mathcal{K}} \prod_{1 \leq i < j \leq N} (\lambda_i - \lambda_j)^2 \prod_{i=1}^{N-1} d\lambda_i d\gamma = 2^{1-N^2} N^{\frac{N^2}{2}-1} V_{HS}(\mathcal{K}).
$$

Next, we will derive the upper bound, which is more involved (and more important for our results). The subset $\partial \Delta$, the boundary of $\Delta$, consists of sequences for which some $\lambda_i = 0$ and has zero $N - 1$ dimensional measure. Thus, without loss of generality, we can assume $\lambda_i > 0$ for all $i = 1, \cdots, N$ and, in particular, $\left| \frac{\lambda_i - \lambda_j}{\lambda_i + \lambda_j} \right| < 1$ for all $i \neq j$. This
implies

\[ 2^{N^2+1} V_B(K) = \int_K \frac{1}{\sqrt{\lambda_1 \cdots \lambda_N}} \prod_{1 \leq i < j \leq N} \frac{(\lambda_i - \lambda_j)^2}{\lambda_i + \lambda_j} \prod_{i=1}^{N-1} d\lambda_i \, d\gamma \]

\[ < \int_K \frac{1}{\sqrt{\lambda_1 \cdots \lambda_N}} \prod_{1 \leq i < j \leq N} |\lambda_i - \lambda_j| \prod_{i=1}^{N-1} d\lambda_i \, d\gamma \]

\[ = \int_K f \prod_{i=1}^{N-1} d\lambda_i \, d\gamma \]  

(11)

where, to reduce the clutter, we denoted

\[ g(\lambda_1, \cdots, \lambda_N) = \frac{1}{\sqrt{\lambda_1 \cdots \lambda_N}} \prod_{1 \leq i < j \leq N} |\lambda_i - \lambda_j|^{1-\frac{1}{2p}}, \]

\[ f(\lambda_1, \cdots, \lambda_N) = \prod_{1 \leq i < j \leq N} |\lambda_i - \lambda_j|^\frac{1}{p}. \]

For any \( p > \frac{1}{2} \) (so that \( 2p > 1 \)), we employ the Hölder inequality to (11) and get

\[ 2^{N^2+1} V_B(K) \leq \left( \int_K f^{2p} \prod_{i=1}^{N-1} d\lambda_i \, d\gamma \right)^{\frac{1}{2p}} \left( \int_K g^{2p-1} \prod_{i=1}^{N-1} d\lambda_i \, d\gamma \right)^{\frac{2p-1}{2p}}. \]  

(12)

Substituting \( f \) into the first integral of (12) and by (2), one has

\[ \left( \int_K f^{2p} \prod_{i=1}^{N-1} d\lambda_i \, d\gamma \right)^{\frac{1}{2p}} = \left( \int_K \prod_{1 \leq i < j \leq N} (\lambda_i - \lambda_j)^2 \prod_{i=1}^{N-1} d\lambda_i \, d\gamma \right)^{\frac{1}{2p}} = \left( \frac{V_{HS}(K)}{\sqrt{N}} \right)^{\frac{1}{2p}}. \]  

(13)

Substituting \( g \) into the second integral of (12) leads to

\[ \int_K g^{2p-1} \prod_{i=1}^{N-1} d\lambda_i \, d\gamma = \int_K \prod_{1 \leq i < j \leq N} |\lambda_i - \lambda_j|^{2p-2} \prod_{i=1}^{N} \prod_{i=1}^{N} (\frac{p-1}{2p-1}) \prod_{i=1}^{N-1} d\lambda_i \, d\gamma \]

\[ \leq \int_D \prod_{1 \leq i < j \leq N} |\lambda_i - \lambda_j|^{\frac{2p-2}{2p-1}} \prod_{i=1}^{N} \prod_{i=1}^{N} (\frac{p-1}{2p-1}) \prod_{i=1}^{N-1} d\lambda_i \, d\gamma, \]  

(14)

the inequality following just from \( K \subset D \). By (1) and the Fubini’s theorem, the last integral in (14) equals to

\[ \frac{(2\pi)^{N(N-1)/2}}{E(N)} \prod_{1 \leq i < j \leq N} |\lambda_i - \lambda_j|^{\frac{2p-2}{2p-1}} \prod_{i=1}^{N} \prod_{i=1}^{N} (\frac{p-1}{2p-1}) \prod_{i=1}^{N-1} d\lambda_i. \]  

(15)
Under the condition $\frac{p-1}{2p-1} > 0$ (i.e., $p > 1$ or $p < 1/2$), one has (see e.g. [22, 45])

$$\int_\Delta \prod_{1 \leq i < j \leq N} |\lambda_i - \lambda_j|^{\frac{2p-2}{2p-1}} \prod_{i=1}^{N} \lambda_i^{\frac{p-1}{2p-1} - 1} d\lambda_i = \frac{1}{\Gamma\left(\frac{(p-1)N^2}{2p-1}\right)} \left( \prod_{j=1}^{N} \Gamma\left(1 + \frac{j(p-1)}{2p-1}\right) \right).$$

Taking into account that $\Delta$ consists of $N!$ Weyl chambers, we conclude that the expression in (15) is then equal to $I(p)$. In other words, we have shown that

$$I(p) = \int_{\mathcal{D}} \prod_{1 \leq i < j \leq N} |\lambda_i - \lambda_j|^{\frac{2p-2}{2p-1}} \prod_{i=1}^{N} \lambda_i^{\frac{p-1}{2p-1} - 1} \prod_{i=1}^{N-1} d\lambda_i d\gamma.$$

Combining this with (12), (13), and (14), we conclude that if $p > 1$, then

$$2^{\frac{n^2 + N - 2}{2}} V_B(K) \leq \left( \frac{V_{HS}(K)}{V_{HS}(D)} \right)^{\frac{1}{d}} I(p)^{\frac{2p-1}{2p}},$$

which is the upper estimate from Lemma 1.

**Theorem 1** There is a universal computable constant $c_1 > 0$, such that for any Hilbert space $\mathcal{H}$ and any subset $K \subset \mathcal{D}$,

$$c_1 \text{VR}_{HS}(K, \mathcal{D}) \leq \text{VR}_{B}(K, \mathcal{D}).$$

**Proof.** Recall $d = N^2 - 1$. From the lower bound of Lemma 1, one has

$$V_B(K)^{\frac{1}{d}} \geq \frac{1}{2} (d + 1)^{\frac{1}{d}} V_{HS}(K)^{\frac{1}{d}} > \frac{1}{2} d^{\frac{1}{d}} V_{HS}(K)^{\frac{1}{d}}.$$

Dividing both sides by $V_B(D)^{\frac{1}{d}}$, one obtains

$$\left( \frac{V_B(K)}{V_B(D)} \right)^{\frac{1}{d}} > \frac{1}{2} d^{\frac{1}{d}} \left( \frac{V_{HS}(K)}{V_{HS}(D)} \right)^{\frac{1}{d}} \left( \frac{V_B(D)}{V_B(D)} \right)^{\frac{1}{d}} = \frac{1}{2} d^{\frac{1}{d}} \left( \frac{\text{vrad}_{HS}(D)}{\text{vrad}_{B}(D)} \right) \left( \frac{V_{HS}(K)}{V_{HS}(D)} \right)^{\frac{1}{d}}.$$

(16)
Formulas (5) and (8) imply that \( d^{\frac{1}{2}} \operatorname{vrad}_{HS}(D) \sim 2e^{-\frac{1}{4}}\operatorname{vrad}_B(D) \), i.e.,

\[
\lim_{d \to \infty} \frac{1}{2} d^{\frac{1}{2}} \left( \frac{\operatorname{vrad}_{HS}(D)}{\operatorname{vrad}_B(D)} \right) = e^{-\frac{1}{4}}.
\]

Therefore, there is a (computable) universal constant \( c_1 > 0 \), such that, for any \( N \),

\[
\frac{1}{2} d^{\frac{1}{2}} \frac{\operatorname{vrad}_{HS}(D)}{\operatorname{vrad}_B(D)} \geq c_1.
\]

Together with (16), this shows that for any \( \mathcal{K} \subset D \) and for any \( N \),

\[
\operatorname{VR}_B(\mathcal{K}, D) \geq c_1 \operatorname{VR}_{HS}(\mathcal{K}, D).
\]

Remark. If \( N \) is relatively large, the optimal constant \( c_1 = c_1(N) \) is close to \( e^{-1/4} \) because \( c_1(N) = \frac{d^{\frac{1}{2}} \operatorname{vrad}_{HS}(D)}{2 \operatorname{vrad}_B(D)} \to e^{-1/4} \) as \( N \to \infty \). For specific values of \( N \), one can compute \( c_1 \) precisely. For instance, \( c_1(4) \approx 0.7572 \). Actually, \( c_1(6) \approx 0.7686, c_1(8) \approx 0.7728 \) and \( c_1(10) \approx 0.7748 \) which are very close to the \( e^{-1/4} \approx 0.7788 \). It appears that the sequence \( c_1(N) \) is increasing and so \( c_1 = c_1(4) \) should work for all \( N \), however, we do not have a rigorous proof.

Theorem 2. There is a universal computable constant \( C_1 > 0 \) such that, for any Hilbert space \( \mathcal{H} \) and any \( \mathcal{K} \subset D \),

\[
\operatorname{VR}_B(\mathcal{K}, D) \leq C_1 \sqrt{\alpha} \exp \left( \frac{\ln \ln(e/\alpha)}{2N} \right)
\]

where \( \alpha = \operatorname{VR}_{HS}(\mathcal{K}, D) \).

Proof. Recall \( N = D_1 D_2 \cdots D_n \) and \( d = N^2 - 1 \). For any \( p > 1 \), Lemma 1 implies that

\[
2^d V_B(\mathcal{K}) \leq 2^{\frac{N^2 + N - 2}{2}} V_B(\mathcal{K}) \leq \alpha \frac{d}{2p} (V_{HS}(D))^\frac{1}{2p} I(p)^\frac{2p-1}{2p}.
\]
Let $\beta = \frac{p-1}{2p-1}$. Replacing $V_{HS}(\mathcal{D})$ and $I(p)$ by formula (3) and formula (9), one has

$$2^d V_B(\mathcal{K}) \leq \alpha \frac{d}{2p} \pi^{\frac{d}{2p}} \frac{[E(N)]^{\frac{1}{p}} N^{\frac{1}{2p}}}{[N!]^{\frac{1}{2p}}} \left[ \frac{\prod_{j=1}^{\beta} \left( \Gamma(\beta j) \Gamma(1+\beta j) \right)^{1-\frac{j}{p}}}{\Gamma(\beta N^2)^{\frac{1}{2p}}} \right].$$

Clearly $[E(N)]^{\frac{1}{p}} \leq 1$ and $N^{\frac{1}{2p}} (N!)^{\frac{1}{2p}} \leq 1$ if $p > 1$. Hence,

$$V_B(\mathcal{K}) \leq \alpha \frac{d}{2p} \pi^{\frac{d}{2p}} \frac{\prod_{j=1}^{\beta} \left( \Gamma(\beta j) \Gamma(1+\beta j) \right)^{1-\frac{j}{p}}}{\Gamma(\beta N^2)^{\frac{1}{2p}}} \left[ \Gamma(\beta N^2)^{\frac{1}{2p}} \right].$$

(17)

Since $x \Gamma(x) = \Gamma(x+1)$, it is easy to see that for all $x \in (0,1)$ the upper estimate of $\Gamma(x)$ is $\frac{1}{x}$ and (somewhat less easy that) the lower estimate of $\Gamma(x)$ is $\frac{1}{\vartheta x}$, where $\vartheta \approx 1.12917$ [6]. That is

$$\frac{1}{\vartheta x} \leq \Gamma(x) \leq \frac{1}{x}, \text{ or } \frac{1}{\vartheta} \leq \Gamma(1+x) \leq 1, \text{ for all } x \in (0,1).$$

(18)

Pick $p = p(N, \alpha) := \frac{N^2 \ln(e/\alpha)-1}{N^2 \ln(e/\alpha)-2}$ as a function of $N$ and $\alpha$, so that $\beta = \frac{p-1}{2p-1} = \frac{1}{N^2 \ln(e/\alpha)}$.

Equivalently, $\beta N^2 = \frac{1}{\ln(e/\alpha)}$. Since $\alpha \leq 1$ for all $\mathcal{K} \subset \mathcal{D}$, then $\beta N^2 < 1$ and hence $\beta j \leq 1$ for all $j = 1, 2, \cdots N^2$. Taking inequality (18) into account, one has

$$\left[ \frac{\Gamma(1+\beta j)}{\Gamma(1+\beta)} \right]^{1-\frac{j}{p}} \leq \vartheta, \text{ for all } j = 1, 2, \cdots N.$$  

(19)

Consequently, again by inequality (18), and $N \geq 4$,

$$\left[ \prod_{j=1}^{\beta} \Gamma(\beta j) \right]^{1-\frac{1}{p}} \leq \left( \frac{\vartheta N}{(N-1)!} \right)^{1-\frac{1}{p}} \beta^{(1-N)(1-\frac{1}{p})} \leq \beta^{(1-N)(1-\frac{1}{p})}.$$  

(20)

Combining inequality (17) with inequalities (19) and (20), one has

$$V_B(\mathcal{K}) \leq \alpha \frac{d}{2p} \pi^{\frac{d}{2p}} \vartheta^N \beta^{(1-N)(1-\frac{1}{p})} \left[ \Gamma(\beta N^2)^{\frac{1}{2p}} \right].$$

Equivalently, taking $d$-th root from both sides,

$$\left( V_B(\mathcal{K}) \right)^{\frac{1}{d}} \leq \alpha \frac{1}{2p} \pi^{\frac{1}{2}} \vartheta^{N \frac{1}{d}} \beta^{(1-N)(1-\frac{1}{p})} \left[ \Gamma(\beta N^2)^{\frac{1}{2pd}} \right].$$

(21)
Note \( N \geq 4 \), and hence \( \vartheta^{\frac{1}{N-1}} \leq \vartheta^{\frac{1}{3}} = 1.0413 \). Now dividing \( V_B(D)\frac{1}{3} \) from both sides of the above inequality, one gets

\[
VR_B(K, D) \leq 2\vartheta^{\frac{1}{3}} \alpha^{\frac{1}{2}} [N^2 \ln(e/\alpha)]^{\frac{1}{2}(1-\frac{1}{N})} [\Gamma \left( \frac{N^2}{2} \right)]^{\frac{1}{2}} [\Gamma(N^2)]^{\frac{1}{2N}}. \tag{21}
\]

It is easy to verify that

\[
[N^2 \ln(e/\alpha)]^{\frac{1}{2(N+1)}} \leq \exp \left( \frac{\ln N}{N} \right) \exp \left( \frac{\ln \ln(e/\alpha)}{2N} \right) \leq \sqrt{2} \exp \left( \frac{\ln \ln(e/\alpha)}{2N} \right),
\]

\[
[N^2 \ln(e/\alpha)]^{\frac{1}{2(N+1)}(1-\frac{1}{N})} = \exp \left( \frac{\ln(N^2 \ln(e/\alpha))}{2(N+1)(N^2 \ln(e/\alpha) - 1)} \right) \leq \exp \left( \frac{1}{N} \right) \leq e^{\frac{1}{N}}.
\]

Therefore,

\[
[N^2 \ln(e/\alpha)]^{\frac{1}{2(N+1)}(1-\frac{1}{N})} \leq \sqrt{2} e^{\frac{1}{N}} \exp \left( \frac{\ln \ln(e/\alpha)}{2N} \right) \tag{22}
\]

Also, we can verify that

\[
\alpha^{\frac{1}{2p}} = \alpha^{\frac{1}{2}} \exp \left( \frac{\ln(1/\alpha)}{2\left[ N^2(1 + \ln(1/\alpha)) - 1 \right] } \right) \leq \alpha^{\frac{1}{2}} \exp \left( \frac{1}{2N^2} \right) \leq e^{\frac{1}{2N}} \sqrt{\alpha}. \tag{23}
\]

Since \( \Gamma(N^2) \leq (N^2)! \leq \exp(N^2 \ln N^2) \), one has

\[
\Gamma(N^2)^{\frac{1}{2(N+1)}} = \exp \left( \frac{\ln(\Gamma(N^2))}{2(N^2 - 1) (N^2 \ln(e/\alpha) - 1)} \right) \leq \exp \left( \frac{2 \ln N}{N^2 \ln(e/\alpha)} \right) \leq \exp \left( \frac{2}{N} \right) \leq e^{\frac{1}{N}}. \tag{24}
\]

Stirling approximation formula (4) implies that

\[
\lim_{N \to \infty} \frac{\Gamma(N^2/2)^{\frac{1}{2}}}{\Gamma(N^2)^{\frac{1}{2}}} = \frac{1}{\sqrt{2}} \tag{25}
\]

Together with inequalities (21), (22), (23), and (24), there exists a universal (independent of \( N, \alpha \)) constant \( C_1 > 0 \), such that, \( VR_B(K, D) \leq C_1 \sqrt{\alpha} \exp \left( \frac{\ln \ln(e/\alpha)}{2N} \right) \).
Remark. A slightly more precise calculation shows that

\[ VR_B(\mathcal{K}, \mathcal{D}) \leq \sqrt{2\alpha} \exp \left( \frac{\ln \ln(e/\alpha)}{2N} \right) \left[ 1 + O \left( \frac{\ln N}{N} \right) \right]. \]

The calculation yields explicit (not necessarily optimal) values of \( C_1 \) in the theorem. For small dimensions, our proof yields \( C_1(4) \approx 2.5164 \) if \( N = 4 \), \( C_1(6) \approx 2.2137 \), and \( C_1(8) \approx 2.0478 \). As the dimension \( N \) becomes large, the value of \( C_1 \) given by the argument tends to \( \sqrt{2} \approx 1.4142 \). On the other hand, the Legendre duplication formula (see [1]) says that

\[ \Gamma(z) \Gamma(z + 1/2) = 2^{1-2z} \sqrt{\pi} \Gamma(2z). \]

By taking \( z = N^2/2 \), one can rewrite the expression in (25) as

\[ \left( \frac{\Gamma(N^2/2)}{\Gamma(N^2)} \right)^{\frac{1}{2(N^2-1)}} = \frac{1}{\sqrt{2}} \left( \frac{\sqrt{\pi} \Gamma(N^2/2)}{\Gamma(N^2/2 + 1/2)} \right)^{\frac{1}{2(N^2-1)}}. \] (26)

Gamma function is log-convex [23], and hence

\[ \Gamma(N^2/2)^2 \leq \Gamma(N^2/2 - 1/2)\Gamma(N^2/2 + 1/2) = \frac{\Gamma(N^2/2 + 1/2)^2}{N^2/2 - 1/2}. \]

Equivalently

\[ \frac{\Gamma(N^2/2 + 1/2)}{\Gamma(N^2/2)} \geq \sqrt{\frac{N^2 - 1}{2}}, \]

which is greater than \( \sqrt{\pi} \) iff \( N > \sqrt{2\pi + 1} \approx 2.7 \). Together with formula (26), this shows that the asymptotic relation (25) is in fact an upper bound for all \( N \geq 3 \). It follows that \( C_1 \approx 2.5164 \) works for all \( N \geq 4 \), \( C_1 \approx 2.2137 \) works for all \( N \geq 6 \), etc.

Remark. In most cases of interest \( \alpha \) is such that the factor \( \exp \left( \frac{\ln \ln(e/\alpha)}{2N} \right) \) is bounded by a universal numerical constant. For instance, if \( \ln(1/\alpha) \leq a_1 e^{a_2 N} \) for some constants \( a_1 > 0, a_2 > 0 \), then

\[ VR_B(\mathcal{K}, \mathcal{D}) \leq \sqrt{2e^{a_2}} \sqrt{VR_{HS}(\mathcal{K}, \mathcal{D})} \left[ 1 + O \left( \frac{\ln N}{N} \right) \right]. \]
While our argument doesn’t give similar estimates for general $\alpha$, other ways of writing the estimates in more transparent ways are possible. For example, for any fixed $p > 1$ there is a constant $C_p > 0$ depending on $p$ (but independent of $N$ and $\alpha$), such that
\[
VR_B(K, D) \leq C_p \left( VR_{HS}(K, D) \right)^{1/p}.
\]

In the cases of $S$ and $\mathcal{PPT}$, $\frac{1}{\alpha}$ is bounded from above by $N^k$ for some (fixed) integer $k$ [2, 38]. Therefore, $VR_B(S, D) \leq \tilde{C}_1 \sqrt{VR_{HS}(S, D)}$ where $\tilde{C}_1 > 0$ is a universal constant independent of $N$. Similarly, $VR_B(\mathcal{PPT}, D) \leq \tilde{C}_1 \sqrt{VR_{HS}(\mathcal{PPT}, D)}$ where $\tilde{C}_1 > 0$ is a universal constant independent of $N$.

**Remark.** We point out that there is a lot of flexibility in the choice of $\beta = \frac{1}{N^2 \ln(e/\alpha)}$ (hence the choice of $p(N, \alpha)$). For example, one can choose $\beta = \frac{1}{e^N \ln(e/\alpha)}$, and proves Theorem 2 with different (larger) constants. However, formula (23) does suggest that the factor $\ln(e/\alpha)$ in $\beta$ is essentially optimal in general.

As applications of Theorems 1 and 2, and the estimates for $VR_{HS}(S, D)$ implicit in [2], one immediately has the following corollaries.

**Corollary 1 (Large number of small subsystems)** For system $\mathcal{H} = (\mathbb{C}^D)^{\otimes n}$, there exist universal computable constants $c_2, C_2 > 0$, such that for all $D, n \geq 2$,
\[
\frac{c_2}{N^{1/2+\alpha_D}} \leq VR_B(S, D) \leq C_2 \sqrt{\frac{(Dn \ln n)^{1/2}}{N^{1/2+\alpha_D}}},
\]
where $\alpha_D = \frac{1}{2} \log_D(1 + \frac{1}{D}) - \frac{1}{2D^2} \log_D(D + 1)$.

**Corollary 2 (Small number of large subsystems)** For system $\mathcal{H} = (\mathbb{C}^D)^{\otimes n}$, there exist universal computable constants $c_3, C_3 > 0$, such that for all $D, n \geq 2$,
\[
\frac{c_3}{N^{1/2-1/(2n)}} \leq VR_B(S, D) \leq C_3 \sqrt{\frac{(n \ln n)^{1/2}}{N^{1/2-1/(2n)}}}.
\]
Remark. Recall that if $\mathcal{H} = (\mathbb{C}^D)^\otimes n$, then the dimension of $\mathcal{H}$ is $N = D^n$ and so the expressions in the numerators of the estimates in the Corollaries above are of smaller order than the denominators. Hence, for any fixed small $D$, Corollary 1 shows that $\text{VR}_B(S, D)$ goes to 0 exponentially as $n \to \infty$. On the other hand, for $\mathcal{H} = (\mathbb{C}^D)^\otimes n$ and for fixed small $n$, Corollary 2 shows that “the order of decay” of $\text{VR}_B(S, D)$ is between $D^{\frac{1}{2} - \frac{n}{2}}$ and $D^{\frac{1}{4} - \frac{n}{4}}$ as $D \to \infty$. In both cases, the \textit{priori} Bures probability of separability is extremely small for large (and even for moderate) $N$. It is possible to provide (not necessarily optimal) estimates on the constants appearing in both corollaries. For instance, in Corollary 1, one can take $c_2(4) = 0.2272$, $C_2(4) = \sqrt{4.4}$, $C_1(4) = 5.2785$ if $N = 4$, $c_2(6) = 0.2306$, $C_2(6) = \sqrt{4.4}$, $C_1(6) = 4.6436$, and $c_2(8) = 0.2318$, $C_2(8) = \sqrt{4.4}$, $C_1(8) = 4.2955$. If the dimension $N$ is large (particularly for large $n$), the relevant asymptotic behaviors of $c_2$ and $C_2$ given by the proofs are: $c_2$ tends to $\frac{\sqrt{2}}{2\pi} \approx 0.6577$, and $C_2$ tends to $2^{3/4}e^{1/8} \approx 1.9057$. In Corollary 2, $c_3$ can be taken as $c_3 = e^{-1/4}/\sqrt{6} \approx 0.3179$ and $C_3 = C_2$. We refer the readers to [2] for the constants in terms of the Hilbert-Schmidt volume.

In the rest of this section, we will discuss the Bures volume of PPT. For a bipartite system $\mathcal{H} = \mathbb{C}^{D_1} \otimes \mathbb{C}^{D_2}$, any state $\rho$ on $\mathcal{H}$ can be expressed uniquely as

$$\rho = \sum_{i,j}^{D_1} \sum_{\alpha,\beta}^{D_2} \rho_{\alpha,i\beta} |e_i \otimes f_\alpha \rangle \langle e_j \otimes f_\beta|$$

where $\{e_i\}_{i=1}^{D_1}$ and $\{f_\alpha\}_{\alpha=1}^{D_2}$ are the canonical bases of $\mathbb{C}^{D_1}$ and $\mathbb{C}^{D_2}$ respectively. Define the partial transpose $T(\rho)$ with respect to the first subsystem as

$$T(\rho) = \sum_{i,j}^{D_1} \sum_{\alpha,\beta}^{D_2} \rho_{j\alpha,i\beta} |e_i \otimes f_\alpha \rangle \langle e_j \otimes f_\beta|.$$
We write $PPT$ for the set of states $\rho$ such that $T(\rho)$ is also positive. (Note that $PPT$ is basis-independent because eigenvalues do not depend on a basis [25].) The Peres criterion asserts: *every separable state has a positive partial transpose* [25]. That is, $S \subset PPT \subset D$. For qubit-qubit system $\mathbb{C}^2 \otimes \mathbb{C}^2$ and qubit-qutrit (or qutrit-qubit) system $\mathbb{C}^2 \otimes \mathbb{C}^3$ (or $\mathbb{C}^3 \otimes \mathbb{C}^2$), the positive partial transpose criterion gives a sufficient and necessary condition for separability, i.e., $S = PPT$ [14, 37, 44]. The following corollary, which is a direct consequence of Theorems 1, 2, and of Theorem 4 of [2], gives the estimation of the Bures volume of $PPT$.

**Corollary 3 (Bures Volume of $PPT$):** There exists an absolute computable constant $c_0 > 0$, such that, for any bipartite system $\mathcal{H} = \mathbb{C}^D \otimes \mathbb{C}^D$, $c_0 \leq VR_B(PPT, D) \leq 1$.

Indent: An unsolved question is: *does there exist a universal constant $0 < C_0 < 1$ such that $VR_B(PPT, D) \leq C_0 < 1$?* Answering this question would help us understand the effectiveness of positive partial transpose criterion as a tool to detect quantum entanglement for all $D \geq 3$. (The answer to the analogous question about $VR_{HS}$ is not known, either.)

An immediate consequence of Corollaries 2 and 3 is that, for $\mathcal{H} = \mathbb{C}^D \otimes \mathbb{C}^D$ and large $D$, there exist universal constants $c_4, C_4 > 0$ (independent of $D$), such that, $c_4D^{-\frac{1}{2}} \leq VR_B(S, PPT) \leq C_4D^{-\frac{1}{4}}$. The upper bound decreases to 0 as $D \to \infty$. In other word, the conditional *priori* Bures probability of separability given positive partial transpose condition is exceedingly small. Hence, for large $N$, the PPT criterion is not precise as a tool to detect separability.
4 Optimality of the bounds

In this section, we will prove that, in general, the bounds in Theorems 1 and 2 are essentially optimal. The Bures volume has singularities close to the boundary of $\mathcal{D}$, so the optimal upper bound is intuitively attained by the subsets close to the boundary of $\mathcal{D}$. On the other hand, for the subsets located near the maximal state $\rho_{\text{max}} = \frac{\text{Id}_N}{N}$, we can achieve the lower bound (this is really a simple consequence of the proof of Lemma 1).

4.1 Optimality of the lower bound

For $0 < t < 1$, let $\mathcal{K}_t = t\mathcal{D} + (1-t)\rho_{\text{max}}$, i.e.,

$$\mathcal{K}_t = \left\{ UXU^\dagger : X = \text{diag} \left( \frac{1-t}{N} + t\lambda_1, \cdots, \frac{1-t}{N} + t\lambda_N \right), (\lambda_1, \cdots, \lambda_N) \in \Delta \text{ and } U \in \mathcal{U}(N) \right\}.$$

Let $Z_N$ be as in (1).

We now estimate $V_B(\mathcal{K}_t)$ from above. By formula (6),

$$2 \frac{N^2 + N - 2}{2} V_B(\mathcal{K}_t) = \int_{\Delta_1} \frac{Z_N}{\prod_{i=1}^N (t\lambda_i + \frac{1-t}{N})} \prod_{1 \leq i < j \leq N} \frac{(\lambda_i - \lambda_j)^2}{(\frac{2}{N} - t\lambda_i + t\lambda_j)} \prod_{i=1}^{N-1} d\lambda_i.$$

As $\frac{1-t}{N} + t\lambda_i \geq \frac{1-t}{N}$ for all $i$, one obtains

$$2 \frac{N^2 + N - 2}{2} V_B(\mathcal{K}_t) \leq Z_N \frac{t^{N^2-1} N^{N^2/2}}{2(N^2-N)/2 (1-t)^{N^2/2}} \int_{\Delta_1} \prod_{1 \leq i < j \leq N} (\lambda_i - \lambda_j)^2 \prod_{i=1}^{N-1} d\lambda_i

= \frac{t^{N^2-1} N(N^2-1)/2}{2(N^2-N)/2 (1-t)^{N^2/2}} V_{HS}(\mathcal{D}),$$

where the equality follows the formula (2). By Lemma 1, one gets

$$V_B(\mathcal{K}_t) \leq \frac{t^{N^2-1}}{(1-t)^{N^2/2}} V_B(\mathcal{D}) \leq \frac{t^{N^2-1}}{(1-t)^{N^2-1}} V_B(\mathcal{D}).$$
Hence, \( \text{VR}_B(\mathcal{K}_t, \mathcal{D}) \leq \frac{4}{t} \leq 4t \) for all \( t \leq \frac{3}{4} \). On the other hand, \( \text{VR}_{HS}(\mathcal{K}_t, \mathcal{D}) = t \) holds trivially because of the homogeneity of the Hilbert-Schmidt measure. We have proved that \( \text{VR}_B(\mathcal{K}_t, \mathcal{D}) \leq 4 \text{VR}_{HS}(\mathcal{K}_t, \mathcal{D}) \) for all \( \mathcal{K}_t \) such that \( \text{VR}_{HS}(\mathcal{K}_t, \mathcal{D}) \leq \frac{3}{4} \).

Theorem 1 guarantees that the lower bound of \( \text{VR}_B(\mathcal{K}_t, \mathcal{D}) \) is at least (up to a multiplicative constant) \( \text{VR}_{HS}(\mathcal{K}_t, \mathcal{D}) \). So the lower bound of \( \text{VR}_B(\mathcal{K}_t, \mathcal{D}) \) in Theorem 1 can be obtained, and hence is optimal in general.

### 4.2 Optimality of the upper bound

For \( 0 < t < 1 \), we consider \( \mathcal{K}_t \) as

\[
\mathcal{K}_t = \{ UXU^\dagger : X = \text{diag}(1 - t + t\lambda_1, t\lambda_2, \ldots, t\lambda_N), (\lambda_1, \ldots, \lambda_N) \in \Delta_1 \text{ and } U \in \mathcal{U}(N)\}.
\]

Recall \( \Delta_1 \) is the chamber of \( \Delta \) with order \( \lambda_1 \geq \cdots \geq \lambda_N \).

The Hilbert-Schmidt volume of \( \mathcal{K}_t \) can be calculated by the following integral

\[
\text{V}_{HS}(\mathcal{K}_t) = Z_N \ t^{(N-1)^2} \sqrt{N} \int_{\Delta_1} \prod_{2 \leq i < j \leq N} (\lambda_i - \lambda_j)^2 \prod_{k=2}^N (t\lambda_1 - t\lambda_k + 1 - t)^2 \prod_{i=1}^{N-1} d\lambda_i.
\]

As \( 0 \leq t\lambda_1 - t\lambda_k + 1 - t \leq 1 \), one has

\[
\text{V}_{HS}(\mathcal{K}_t) \leq Z_N \ t^{(N-1)^2} \sqrt{N} \int_{\Delta_1} \prod_{2 \leq i < j \leq N} (\lambda_i - \lambda_j)^2 \prod_{i=1}^{N-1} d\lambda_i
\]

\[
= \frac{Z_N}{Z_{N-1}} \ t^{(N-1)^2} \sqrt{\frac{N}{N-1}} \text{V}_{HS}(\mathcal{D}_{N-1}) \int_{0}^{1} (1 - \lambda_1)^{N^2 - 2N} d\lambda_1
\]

\[
\leq \sqrt{2} \ \frac{Z_N}{Z_{N-1}} \ t^{(N-1)^2} \text{V}_{HS}(\mathcal{D}_{N-1}). \quad (27)
\]

By Stirling approximation (4), \( \text{V}_{HS}(\mathcal{K}_t, \mathcal{D}) \leq C_4 \ t \ t^{\frac{2}{N+1}} \) holds for some universal constant \( C_4 > 0 \). If \( t^{\frac{2}{N+1}} \) is bounded from above, e.g., \( t > e^{C_4(-1-N)} \) for some constant
\(c_4 > 0\), then
\[
\text{VR}_{HS}(\mathcal{K}', \mathcal{D}) \leq C_5 t
\] (28)
holds for a new universal constant \(C_5 > 0\).

Next, we estimate the Bures volume of \(\mathcal{K}'\) from below. By formula (6),
\[
2^{\frac{N^2 + N - 2}{2}} V_B(\mathcal{K}')
= \int_{\Delta_1} \frac{Z_N t^{\frac{(N-1)^2}{2}}}{\sqrt{(t\lambda_1 + 1 - t)\lambda_2 \cdots \lambda_N}} \prod_{2 \leq i < j \leq N} \frac{(\lambda_i - \lambda_j)^2}{\lambda_i + \lambda_j} \prod_{k=2}^{N-1} \frac{(t\lambda_1 + t\lambda_k + 1 - t)^2}{t\lambda_1 + t\lambda_k + 1 - t} \prod_{i=1}^{N-1} d\lambda_i
\geq Z_N \int_{\Delta_1} \frac{(1-t)^{2N-2} t^{\frac{(N-1)^2}{2}}}{\sqrt{\lambda_2 \cdots \lambda_N}} \prod_{2 \leq i < j \leq N} \frac{(\lambda_i - \lambda_j)^2}{\lambda_i + \lambda_j} \prod_{i=1}^{N-1} d\lambda_i,
\]
where the inequality is because of \(0 \leq t\lambda_1 + 1 - t \leq 1, 0 \leq t\lambda_1 + t\lambda_k + 1 - t \leq 1\) and \(t\lambda_1 - t\lambda_k + 1 - t \geq 1 - t\). The last integral can be computed as in (27) and leads to
\[
2^{\frac{N^2 + N - 2}{2}} V_B(\mathcal{K}')
\geq \frac{Z_N}{Z_{N-1}} (1-t)^{2N-2} t^{\frac{(N-1)^2}{2}} \prod_{2 \leq i < j \leq N} \frac{(\lambda_i - \lambda_j)^2}{\lambda_i + \lambda_j} \int_0^1 (1 - \lambda_1)^{\frac{N^2 - 2N - 1}{2}} d\lambda_1
= \frac{Z_N}{Z_{N-1}} \frac{2^{N^2 - N - 2}}{(N-1)^2} (1-t)^{2N-2} t^{\frac{(N-1)^2}{2}} V_B(\mathcal{D}_{N-1}).
\]
Employing the Stirling approximation (4) one gets \(\text{VR}_B(\mathcal{K}', \mathcal{D}) \geq c_5 \sqrt{t}\) for some universal constant \(c_5 > 0\) if, say, \(t < \frac{4}{9}\). Together with (28), we have thus proved
\[
\text{VR}_B(\mathcal{K}', \mathcal{D}) \geq \bar{c}_5 \sqrt{\text{VR}_{HS}(\mathcal{K}', \mathcal{D})}
\]
for some universal constant \(\bar{c}_5 > 0\), if \(t < \frac{4}{9}\) and \(t > e^{c_4(-1-N)}\). Theorem 2 guarantees that \(\text{VR}_B(\mathcal{K}', \mathcal{D}) \leq C_1 \sqrt{\text{VR}_{HS}(\mathcal{K}', \mathcal{D})}\). Therefore, the upper bound in Theorem 2 can also be achieved, and is optimal in general.
5 Conclusion and Comments

In summary, we proved that if $\mathcal{K}$ is a Borel subset of $\mathcal{D}$, then the \textit{priori} Bures probability of $\mathcal{K}$ can be estimated from above and from below in terms of the \textit{priori} Hilbert-Schmidt probability of $\mathcal{K}$. Specifically, under some mild conditions on $\mathcal{K}$ the relative Bures volume radius $\text{VR}_B(\mathcal{K}, \mathcal{D})$ can be (approximately) bounded from below by the relative Hilbert-Schmidt volume radius $\text{VR}_{HS}(\mathcal{K}, \mathcal{D})$, and from above by $\sqrt{\text{VR}_{HS}(\mathcal{K}, \mathcal{D})}$. We employ these results to estimate the Bures volume of $\mathcal{S}$ and \textit{PPT} and the relevant \textit{priori} Bures probabilities. We deduce that positive partial transpose criterion becomes less and less precise as the dimension of $\mathcal{H}$ becomes larger and larger, at least if the goal is to detect separability. We also give examples showing that, for general subsets, our bounds are essentially optimal.

When $N$ is small, for instance when $N = 4$ or 6, our estimates for $V_B(\mathcal{S})$ are less precise than Slater’s numerical results. However, our methods overcome the big disadvantage of the numerical approach, which works only for small $N$. Moreover, our results are independent of the structure of $\mathcal{H}$. (In applications, of course, the information on the structure of $\mathcal{H}$ will be hidden in the calculation of $\text{VR}_{HS}(\mathcal{K}, \mathcal{D})$.) Proceeding along similar lines one can obtain similar results for real Hilbert spaces, and then estimate the Bures volume of $\mathcal{S}$ or \textit{PPT} on a real Hilbert space.

As is well known, for sets in a Euclidean space (in particular, for sets of matrices endowed with the Hilbert-Schmidt metric) the volumetric information is roughly equivalent to the metric entropy information such as covering and packing numbers (see, e.g., [27]). However, for the Bures geometry the parallels are not so immediate. Consequently, further work is required to answer (even approximately) questions of the
Given \( \varepsilon > 0 \), what is the maximal cardinality of a subset of \( D \) (or \( S \)), every two elements of which are at least \( \varepsilon \) apart in the Bures metric?

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