Relative volume of separable bipartite states

Rajeev Singh,[1,2] Ravi Kunjwal,[1] and R. Simon[1]

[1]*Optics & Quantum Information Group, The Institute of Mathematical Sciences, CIT Campus, Taramani, Chennai 600113, India*
[2]*Max-Planck-Institut für Physik komplexer Systeme, 01187 Dresden, Germany*

Every choice of an orthonormal frame in the d-dimensional Hilbert space of a system corresponds to one set of all mutually commuting density matrices or, equivalently, to the classical statistical state space of the system; the quantum state space itself can thus be profitably viewed as an SU(d) orbit of classical state spaces, one for each orthonormal frame. We exploit this connection to study the relative volume of separable states of a bipartite quantum system. While the two-qubit case is studied in considerable analytic detail, for higher-dimensional systems we fall back on Monte Carlo. Several insights seem to emerge from our study.

I. INTRODUCTION

States of a quantum system are represented by density operators (positive-semidefinite unit-trace operators acting on a d-dimensional Hilbert space $\mathcal{H}_d$). The set of all density operators of such a d-dimensional (d-level) system constitutes a convex subset of $\mathbb{R}^{d^2-1}$; this is the *state space* (*generalized Bloch sphere*) Ω_d of the quantum system. An understanding of the geometry of the state space is of fundamental importance [1,2]. The state space of a two-level system or qubit is the well-known Bloch (or Poincaré) sphere, while the generalized Bloch sphere of higher-dimensional system is much richer, and more complex to visualize and analyze. Recently, a limited analysis of the cross sections of the state space of the three-level system (qutrit) has been performed [3,4].

When d is nonprime, it is possible that the system is composite, i.e., made up of two or more subsystems. For example, a four-dimensional system could be a single quantum system with four levels or a pair of two-level systems or qubits. In the latter case of composite system, the issue of separability becomes important, entanglement being a characteristic feature of quantum theory of composite systems, and a key resource in quantum information processing [5]. An understanding of the separability property of states is therefore important from both foundational and application perspectives. We would like to understand the geometry of separable states and know how much of the state space is entangled.

The issue regarding the relative volume of the set of all separable states was considered in the seminal work of Życzkowski *et al.* [6]. It was not only shown that the set of separable states has nonzero volume, but also analytical lower and upper bounds were obtained for the two-qubit and the qubit-qutrit cases. They also argued that all states in a sufficiently small neighborhood of the maximally mixed state are separable, and conjectured that the volume of the separable region decreases exponentially with Hilbert space dimension. Different aspects of this issue have been addressed by other authors [7–9]. Vidal and Tarrach [10] generalized the result to obtain an analytical lower bound on this volume for multipartite systems, showing that it is nonzero. Verstraete *et al.* [11] gave an improved lower bound on the volume of the separable region for the two-qubit system. More recently,

significant contribution has been made to the understanding of the generalized two-qubit Hilbert-Schmidt separability probabilities by Slater [12,13]. In similar work on pure states it was shown that typical or generic pure states of multiple-qubit systems are highly entangled, while having low amounts of pairwise entanglement [14]. Regarding the issue of geometry of state space, the geometry of Bell-diagonal states for two-qubit systems in the context of quantum discord has been addressed recently [15].

The genesis of this work is the following. During a recent reading of the seminal work of Życzkowski *et al.* [6] (a paper we had indeed read more than once earlier), the following observation by these authors somehow captured our attention: "Our numerical results agree with these bounds, but to our surprise the probability that a mixed state $\rho \in \mathcal{H}_2 \otimes \mathcal{H}_2$ is separable exceeds 50%". Their paper established an interesting analytical lower bound of 0.302 for the probability of separability (fractional volume of separable states) of a two-qubit system (and an analytical upper bound of 0.863), but on numerical (Monte Carlo) estimation they found it to actually exceed 50% and assume 0.632. We could not resist asking ourselves the following question: Could there be a ground to "anticipate" this value in excess of 50%? It is this question that marked the beginning of this work.

The quantum (statistical) state space of a two-state system or qubit is simply the Bloch (Poincaré) sphere, a unit ball $B_3 \subset \mathbb{R}^3$ centered at the origin; but, for $d \geqslant 3$ the generalized Bloch "sphere" has a much richer structure. It is a convex body $\Omega_d \subset \mathbb{R}^{d^2-1}$ determined by CP^{d-1} worth of pure states as extremals, this $2(d-1)$-parameter family of pure states being "sprinkled over" the (d^2-2)-dimensional boundary of Ω_d. In contrast, the classical (statistical) state space of a d-state system is extremely simple, for all d. Indeed, it is the regular simplex $\Delta_{d-1} \subset \mathbb{R}^{d-1}$, the convex body defined by d equidistant vertices or extremals (the classical pure states). The quantum state space itself can be profitably viewed, for all d, as the union of the SU(d) orbit Γ of simplices (classical state spaces) Δ_{d-1}. This fact is fundamental to both our point of view and analysis in this work. Every set of all mutually commuting $d \times d$ density matrices constitutes one classical state space or simplex Δ_{d-1}, a point in the orbit, and choice of a set or frame of orthonormal unit

vectors (more properly, unit rays) labels different points on the orbit. Thus, the orbit Γ is exactly as large as the coset space $U(d)/[U(1) \times U(1) \times \ldots \times U(1)]$, a particular case of (complex) Stiefel manifold. The volume of Ω_d is thus the product of the volume of the simplex Δ_{d-1} and the volume of the $(d^2 - d)$-dimensional orbit $U(d)/[U(1) \times U(1) \times \ldots \times U(1)]$, the latter volume being determined by the measure inherited from the Haar (uniform) measure on the unitary group $SU(d)$.

Our interest here is the $d_1 \times d_2$ bipartite system, and therefore the relevant simplex is $\Delta_{d_1 d_2 - 1}$ and the dimension of the orbit Γ of orthonormal frames is $d_1 d_2 (d_1 d_2 - 1)$. *Separability issues are invariant under local unitaries $U_{d_1} \otimes U_{d_2}$*, so it is sufficient to restrict attention to the local unitarily inequivalent frames. This removes $d_1^2 + d_2^2 - 2$ parameters, and so we are left with $(d_1^2 - 1)(d_2^2 - 1) - d_1 d_2 + 1$ parameters needed to label points on the orbit of local-unitarily inequivalent orthonormal frames or simplices $\Delta_{d_1 d_2 - 1}$, this number evaluating to 6 for the two-qubit systems and to 56 for the two-qutrit systems.

We now have all the ingredients to describe our approach to the problem of (fractional) volume of separable states in more precise terms. Considering the full state space $\Omega_{d_1 d_2}$ of the $d_1 \times d_2$ bipartite system as an orbit Γ of simplices $\Delta_{d_1 d_2 - 1}$, let ξ denote the collection of variables, say k in number, needed to label points on the orbit or manifold Γ, i.e., for each $\xi \in \Gamma$ we have an orthonormal basis of $d_1 d_2$-dimensional vectors and an associated simplex $\Delta_{d_1 d_2 - 1}(\xi)$ of mutually commuting density operators. The volume of simplex $\Delta_{d_1 d_2 - 1}(\xi)$ is independent of ξ; this fact is trivially obvious, but proves important for our present purpose. For each ξ, a convex subset of $\Delta_{d_1 d_2 - 1}(\xi)$, whose volume is not independent of ξ, is separable. Let $f(\xi)$ represent the fractional $(d_1 d_2 - 1)$-dimensional volume of this convex subset of $\Delta_{d_1 d_2 - 1}(\xi)$. The uniform Haar measure on the unitary group $SU(d_1 d_2)$ induces a measure or probability $p(\xi)$ on the orbit Γ. Clearly, the fractional volume of separable states for the full space is given by

$$V^{\text{sep}}/V^{\text{tot}} \equiv v^{\text{sep}} = \int d^k \xi \, p(\xi) f(\xi). \tag{1}$$

An immediate and important implication of this rendering of relative volume of separable states is this: Should it turn out that $f(\xi) \geqslant a > 0, \forall \, \xi \in \Gamma$, then v^{sep} is trivially bounded from below by a. For the two-qubit system we shall indeed show that $a = 0.5$, thus reconciling the "surprise" element which acted as the "seed" for this work, as noted earlier.

Two remarks are in order in respect of our analysis leading to Eq. (1): one in respect of choice of measure over the simplex and the other regarding the fact that the simplices corresponding to two distinct points of the orbit Γ are not necessarily disjoint.

Remark 1. There exists a natural volume measure for Γ arising from the very fact that it is an $SU(d_1 d_2)$ orbit. But, the situation in respect of the simplex $\Delta_{d_1 d_2 - 1}$ is quite different. There seems to exist no fundamental mathematical principle to pick one unique or distinguished measure on $\Delta_{d_1 d_2 - 1}$, and therefore the choice seems to be ultimately a matter of taste or point of view. However, the action of the permutation

group $S_{d_1 d_2}$ on the simplex $\Delta_{d_1 d_2 - 1}$, through permutation of its vertices, renders $\Delta_{d_1 d_2 - 1}$ the union of $(d_1 d_2)!$ mutually equivalent fundamental domains. Thus, the complete freedom in choice of measure applies to one fundamental domain, of fractional volume $1/(d_1 d_2)!$. The measure is transferred to the other copies of the fundamental domain by the natural action of the permutation group $S_{d_1 d_2}$. The choice of Życzkowski *et al.* is the uniform measure, the one inherited by embedding $\Delta_{d_1 d_2 - 1}$ in the Euclidean space $\mathbb{R}^{d_1 d_2 - 1}$. Other measures have been motivated and used in [7,8]. Since this work was inspired by that of Życzkowski *et al.*, we stick to their measure.

Remark 2. The different simplices on the orbit Γ are not necessarily disjoint. As is readily seen, the intersection is, however, restricted to those points of the simplex which correspond to density matrices with degenerate spectrum. For instance, in the case of a qutrit, such points correspond precisely to the bisectors of the equilateral triangle, the 2-simplex Δ_2. Since such points of zero measure contribute neither to the total volume of the simplex nor to that of its separable convex subset, the fact that the simplices are not disjoint affects in no way the development leading to Eq. (1).

The content of the paper is organized as follows. In Sec. II, we present details of the two-qubit system, and this is followed by numerical Monte Carlo analysis for higher-dimensional systems in Sec. III. In Sec. IV, we make a few observations on the separable volume for the qubit-qutrit system. Section V concludes with a comment on the volume and "effective radius" of the separable region for higher-dimensional quantum systems. The final Sec. VI summarizes our results.

II. TWO-QUBIT SYSTEM

The state space of a two-qubit system Ω_4 corresponds to positive-semidefinite unit-trace operators on the four-dimensional Hilbert space, and in the present scheme can be symbolically expressed as $\Omega_4 \sim \Gamma_{22} \times \Delta_3$. But, this 15-parameter convex set Ω_4 should not be viewed as the Cartesian product of the two sets Γ_{22} and Δ_3, but rather as the union of 3-simplices (tetrahedra) Δ_3 parametrized by the 12-parameter manifold of frames $\Gamma_{22} = U(4)/[U(1) \times U(1) \times U(1) \times U(1)]$. We first describe the 3-simplex Δ_3 comprising probabilities $\{p_j\}$, $\sum_{j=1}^4 p_j = 1, p_j \geqslant 0, j = 1, \ldots, 4$. Since Δ_3 resides in a three-dimensional Cartesian real space, it is both desirable and instructive to pictorially visualize this simplex along with its convex subset of separable states. We can explicitly picture the separable set corresponding to any selected frame using the following change of variables from the four p_j's *constrained* by $\sum p_j = 1$ to three *independent* Cartesian variables x, y, z:

$$
\begin{aligned}
p_1 &= (1 + x + y + z)/4, \\
p_2 &= (1 + x - y - z)/4, \\
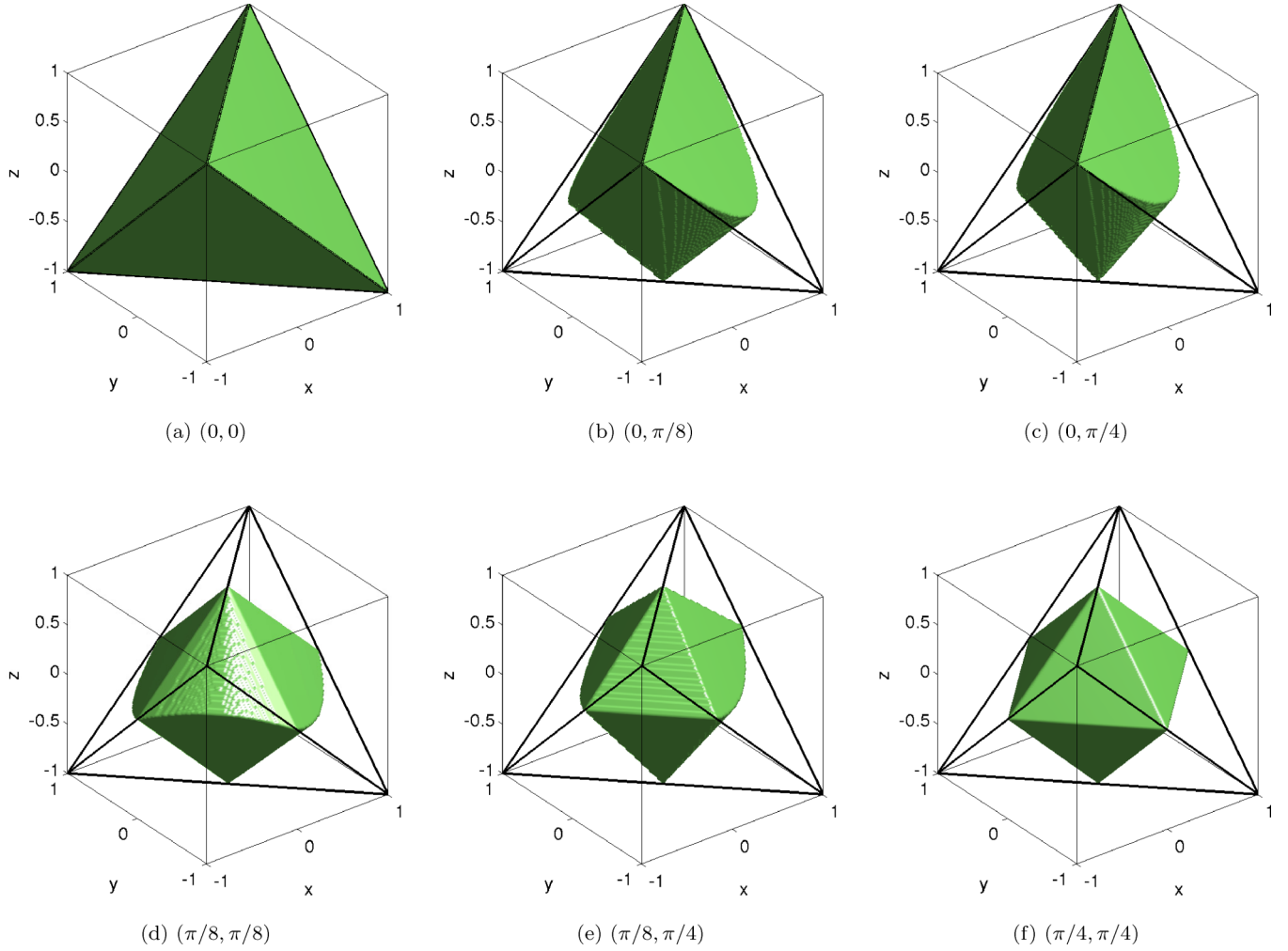p_3 &= (1 - x + y - z)/4, \\
p_4 &= (1 - x - y + z)/4.
\end{aligned}
\tag{2}
$$

(a) $(0,0)$ (b) $(0,\pi/8)$ (c) $(0,\pi/4)$

(d) $(\pi/8,\pi/8)$ (e) $(\pi/8,\pi/4)$ (f) $(\pi/4,\pi/4)$

FIG. 1. (Color online) Separable regions for different values of (θ,α). Each tetrahedron represents a set of all density matrices with common eigenvectors. The volume enclosed by the shaded surface shows the separable region for the given frame. We find that the separable set is the entire tetrahedron for $(\theta,\alpha) = (0,0)$ and is an octahedron for $(\theta,\alpha) = (\pi/4,\pi/4)$ as expected. For other values of (θ,α), we find the separable set to be the tetrahedron limited by planes and conic surfaces.

The situation where one particular $p_j = 0, j = 1, \ldots, 4$, is seen to correspond to one of the four faces of the tetrahedron or 3-simplex Δ_3 in the three-dimensional xyz space with vertices at $(1,1,1)$, $(1,-1,-1)$, $(-1,1,-1)$, and $(-1,-1,1)$ (see Fig. 1). The six edges correspond to pairs of p_j's vanishing, and the vertices to only one nonvanishing p_j. In this way, we associate a tetrahedron with *every* set of all mutually commuting density matrices determined by choice of a frame of four orthonormal pure states $\{|\Psi_k\rangle\}$, $\langle \Psi_j|\Psi_k\rangle = \delta_{jk}$.

A. A special two-parameter family of frames

Before we discuss the general parametrization of the 12-parameter manifold Γ_{22} of two-qubit frames, for clarity of presentation we consider first a special two-parameter family of locally inequivalent frames which are obtained as two orthonormal linear combinations within the computational basis pair $\{|00\rangle,|11\rangle\}$ and two within the pair

$\{|01\rangle,|10\rangle\}$:

$$
\begin{aligned}
|\Psi_1\rangle &= \cos\theta \, |00\rangle + \sin\theta \, |11\rangle, \\
|\Psi_2\rangle &= \sin\theta \, |00\rangle - \cos\theta \, |11\rangle, \\
|\Psi_3\rangle &= \cos\alpha \, |01\rangle + \sin\alpha \, |10\rangle, \\
|\Psi_4\rangle &= \sin\alpha \, |01\rangle - \cos\alpha \, |10\rangle.
\end{aligned}
\tag{3}
$$

These frames can be viewed, in an obvious manner, as a two-parameter generalization of the Bell or magic frame of maximally entangled states. Indeed, the Bell basis corresponds to $\theta = \pi/4 = \alpha$. The entanglement of the first two states is determined by $\sin(2\theta)$ while that of the next two by $\sin(2\alpha)$. That there are only two parameters is an immediate consequence of our forbidding superposition across the two pairs of vectors $\{|00\rangle,|11\rangle\}$ and $\{|01\rangle,|10\rangle\}$. It is readily verified that if one constructs any orthonormal pair of vectors as linear combinations of $|00\rangle$ and $|11\rangle$, both would have one and the same measure of entanglement; the same is true of $|01\rangle$ and $|10\rangle$ as well. For this special parametrization, the density

matrix corresponding to a given point $\{p_j\}$ in Δ_3 is

$$\rho(\{p_i\}) = \sum_{j=1}^{4} p_j \, |\Psi_j\rangle\langle\Psi_j|$$

$$= \begin{pmatrix} p_1 \cos^2\theta + p_2 \sin^2\theta & 0 & 0 & (p_1 - p_2)\sin\theta\cos\theta \\ 0 & p_3 \cos^2\alpha + p_4 \sin^2\alpha & (p_3 - p_4)\sin\alpha\cos\alpha & 0 \\ 0 & (p_3 - p_4)\sin\alpha\cos\alpha & p_3 \sin^2\alpha + p_4 \cos^2\alpha & 0 \\ (p_1 - p_2)\sin\theta\cos\theta & 0 & 0 & p_1 \sin^2\theta + p_2 \cos^2\theta \end{pmatrix}. \quad (4)$$

It is well known that positivity under partial transpose (PPT) is both a necessary and sufficient condition for separability of the qubit-qubit system [16,17]. Since the partial transpose of the above matrix is a direct sum of 2×2 matrices, the condition for separability attains a simple (quadratic) form in $\{p_j\}$ (or x,y,z):

$$\left(p_1^2 + p_2^2\right) \sin^2\theta \cos^2\theta + p_1 p_2(\sin^4\theta + \cos^4\theta)$$
$$- (p_3 - p_4)^2 \sin^2\alpha \cos^2\alpha \geqslant 0,$$
$$\left(p_3^2 + p_4^2\right) \sin^2\alpha \cos^2\alpha + p_3 p_4(\sin^4\alpha + \cos^4\alpha)$$
$$- (p_1 - p_2)^2 \sin^2\theta \cos^2\theta \geqslant 0. \quad (5)$$

It is clear that (saturation of) these separability inequalities, for a given numerical pair (θ,α), corresponds to surfaces that are quadratic in the xyz space. For special values of the parameters, one or both of these quadratic surfaces might factorize to give planes. Thus, the boundaries of the separable region of Δ_3, for any choice of (θ,α), consist entirely of quadratic and planar surfaces.

In Fig. 1, we picture the separable region (inside the tetrahedron) for a few selected values of (θ,α). The Bell or magic frame which corresponds to $\theta = \alpha = \pi/4$ is shown as the last and sixth (as is well known, the separable region is an octahedron in this case). We numerically estimate the volume of the separable region for each value of (θ,α), and the result is pictured in Fig. 2 in the $(\sin 2\theta, \sin 2\alpha)$ plane. Clearly, the volume decreases with increasing "entanglement of the frame". Since the volume of the octahedron is exactly half the volume of the tetrahedron of which it is a convex subset, the ratio of the volume of separable states to the total volume $V^{\text{sep}}/V^{\text{tot}} = 0.5$ for the Bell frame. For every other frame in this two-parameter family, this ratio is larger, as is evident from Fig. 2.

B. Parametrization of Γ_{22}

Having looked at a special two-parameter family of frames in some detail, now we move on to parametrization of the full orbit Γ_{22} of two-qubit frames, *modulo local unitaries*. To this end, we expand a generic set of orthonormal two-qubit vectors $\{|\Psi_k\rangle\}$ in the computational basis:

$$|\Psi_k\rangle = \sum_{a,b=1}^{2} C_{ab}^{(k)} |a\rangle_A \otimes |b\rangle_B, \quad k = 1,2,3,4. \quad (6)$$

Orthonormality of the set $\{|\Psi_k\rangle\}$ reads as the trace-orthonormality condition

$$\langle\Psi_j|\Psi_k\rangle = \text{Tr}(C^{(j)\dagger} C^{(k)}) = \delta_{jk} \quad (7)$$

on the corresponding set of 2×2 matrices $\{C^{(k)}\}$ of expansion coefficients. Clearly, quadruples of complex 2×2 matrices $\{C^{(k)}\}$ meeting the requirement (7) are in one-to-one correspondence with ONB's or frames in a two-qubit Hilbert space.

Under the six-parameter local unitaries $U_A, U_B \in \text{SU}(2)$, these coefficient matrices undergo the change $C^{(k)} \to \widetilde{C}^{(k)} = U_A C^{(k)} U_B^T, k = 1,2,3,4$. We begin by using this local freedom to first bring $C^{(1)}$ to the canonical form

$$\widetilde{C}^{(1)} = \begin{pmatrix} \cos\theta_1 & 0 \\ 0 & \sin\theta_1 \end{pmatrix}, \quad 0 \leqslant \theta_1 \leqslant \pi/4 \quad (8)$$

$\cos\theta_1$ and $\sin\theta_1$ being, respectively, the larger and smaller singular values of $C^{(1)}$. In this process, we have already used up all local unitary freedom except conjugation by diagonal $\text{SU}(2)$ matrices: $U_A = \text{diag}(e^{-i\eta}, e^{i\eta})$, $U_B = U_A^\star$. (Just as we are free to multiply every $|\Psi_k\rangle$ of a frame by a phase factor $e^{i\eta_k}$, so also we can multiply every coefficient matrix by a unimodular scalar $e^{i\eta_k}$.)

To obtain the canonical form for the second vector, note that any normalized matrix orthogonal to $\widetilde{C}^{(1)}$ is necessarily of the form

$$\begin{pmatrix} \alpha \sin\theta_1 & \sqrt{1 - \alpha^2} e^{i\phi} \sin\theta_2 \\ \sqrt{1 - \alpha^2} e^{i\phi'} \cos\theta_2 & -\alpha \cos\theta_1 \end{pmatrix}, \quad 0 \leqslant \alpha \leqslant 1. \quad (9)$$
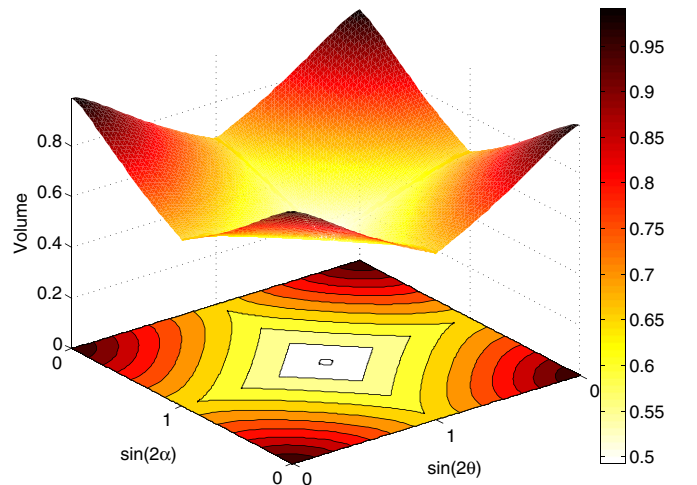

FIG. 2. (Color online) Volume of separable states as a function of the two entanglement parameters $\sin 2\theta$, $\sin 2\alpha$ in the case of the two-parameter family of frames. It is seen that the volume is minimum for $(\pi/4, \pi/4)$ which corresponds to the Bell or magic frame.

Now, we may use up the sixth and last local freedom to render the phases of the off-diagonal elements equal. Thus, the canonical form for the second matrix is

$$\widetilde{C}^{(2)} = \begin{pmatrix} \alpha \sin\theta_1 & \sqrt{1-\alpha^2}e^{i\phi}\sin\theta_2 \\ \sqrt{1-\alpha^2}e^{i\phi}\cos\theta_2 & -\alpha\cos\theta_1 \end{pmatrix}. \quad (10)$$

With the local unitary freedom having been thus fully exhausted, $\widetilde{C}^{(3)}$ has the canonical form

$$\widetilde{C}^{(3)} = \begin{pmatrix} \beta\sin\theta_1 & \sqrt{1-\beta^2}e^{i\phi_3}\cos\theta_3 \\ -\sqrt{1-\beta^2}e^{i\phi_3'}\sin\theta_3 & -\beta\cos\theta_1 \end{pmatrix}. \quad (11)$$

It should be noted that the four (real) parameters β, θ_3, ϕ_3, ϕ_3' of $\widetilde{C}^{(3)}$ are not arbitrary. While $\widetilde{C}^{(3)}$ is manifestly orthogonal to $\widetilde{C}^{(1)}$, the orthogonality requirement $\mathrm{Tr}(\widetilde{C}^{(3)\dagger}\widetilde{C}^{(2)}) = 0$ when enforced would determine these four parameters in terms of two independent parameters. Finally, $\widetilde{C}^{(4)}$ has the canonical form

$$\widetilde{C}^{(4)} = \begin{pmatrix} \gamma\sin\theta_1 & \sqrt{1-\gamma^2}e^{i\phi_4}\cos\theta_4 \\ -\sqrt{1-\gamma^2}e^{i\phi_4'}\sin\theta_4 & -\gamma\cos\theta_1 \end{pmatrix}, \quad (12)$$

but it is clear that none of γ, θ_4, ϕ_4, ϕ_4' is a free (continuous) parameter: they get fixed by the two complex-valued conditions $\mathrm{Tr}(\widetilde{C}^{(4)\dagger}\widetilde{C}^{(2)}) = 0 = \mathrm{Tr}(\widetilde{C}^{(4)\dagger}\widetilde{C}^{(3)})$.

Returning to $\widetilde{C}^{(3)}$, the complex-valued condition $\mathrm{Tr}(\widetilde{C}^{(3)\dagger}\widetilde{C}^{(2)}) = 0$, when written out in detail, reads as

$$\alpha\beta + \sqrt{(1-\alpha^2)(1-\beta^2)}[e^{i(\phi-\phi_3)}\sin\theta_2\cos\theta_3 \\ -e^{i(\phi-\phi_3')}\cos\theta_2\sin\theta_3] = 0. \quad (13)$$

The imaginary part of this equation leads to the restriction

$$\phi_3' = \phi - \sin^{-1}\left[\frac{\tan\theta_2}{\tan\theta_3}\sin(\phi-\phi_3)\right], \quad (14)$$

while the real part requires

$$\beta = \sqrt{\frac{(1-\alpha^2)\Gamma^2}{\alpha^2 + (1-\alpha^2)\Gamma^2}}, \quad (15)$$

where $\Gamma = \sin\theta_2\cos\theta_3\cos(\phi-\phi_3) - \cos\theta_2\sin\theta_3\cos(\phi-\phi_3')$. Thus, in the present scheme we may choose the following six as free parameters: $0 \leqslant \alpha \leqslant 1, 0 \leqslant \theta_1 \leqslant \pi/4, 0 \leqslant \theta_2, \theta_3 \leqslant \pi/2$, and $0 \leqslant \phi, \phi_3 < 2\pi$. In terms of these six parameters, the other two parameters for $|\psi_3\rangle$ or $\widetilde{C}^{(3)}$, namely ϕ_3', β, can be determined through Eqs. (14) and (15). Note that the allowed ranges for angles are not completely free and have to satisfy constraints such that the argument of $\sin^{-1}$ in Eq. (14) has magnitude less than or equal to 1, and $\Gamma \leqslant 0$ since $\alpha, \beta \geqslant 0$ by assumption.

Let us quickly do a parameter counting to check the reasonableness of this parametrization. A generic orthonormal frame in the two-qubit Hilbert space would be expected to be parametrized by 12 parameters: 6 (real, continuous) parameters for the first vector (a generic element of CP^3), 4 for the second (an element of the orthogonal CP^2), 2 for the third (the $CP^1 \sim S^2$ orthogonal to the first two vectors), and none for the fourth. We have thus "efficiently" used the $3+3 = 6$-parameter local unitary freedom to maximal effect

to go from 12 to 6: $|\psi_1\rangle$ is left with one parameter (θ_1) with five local unitary parameters used up, $|\psi_2\rangle$ has three parameters (α, θ_2, ϕ) with the sixth and last local parameter used up, $\langle\psi_1|\psi_3\rangle = \langle\psi_2|\psi_3\rangle = 0$ implies just two residual (continuous) parameters for $|\psi_3\rangle$, namely, (θ_3, ϕ_3). And, $|\psi_4\rangle$ is automatically fixed by the requirement that this four-dimensional vector is orthogonal to $|\psi_1\rangle, |\psi_2\rangle, |\psi_3\rangle$.

Note that the special two-parameter family of frames or tetrahedra discussed earlier corresponds to the choice $\alpha = 1$, which immediately renders $\beta = 0 = \gamma$. Unlike the case of this special two-parameter family, the condition for separability in the general case of six canonical parameters does not break into direct sum of a pair of 2×2 matrices. And hence the resulting separable subsets of the associated tetrahedra can have boundaries considerably more complex than quadratic and planar surfaces of the earlier two-parameter case: they can be up to quadric surfaces.

For each $\xi \in \Gamma_{22}$ we have numerically evaluated the fractional volume $f(\xi)$ of the convex subset of separable states in $\Delta_3(\xi)$, and using this result in Eq. (1), we find the following:

(i) $f(\xi) \geqslant 0.5$ for every $\xi \in \Gamma_{22}$, the inequality saturating only for the Bell or magic frame (modulo local unitaries);

(ii) the integral in Eq. (1) for v^{sep} actually evaluates to the value 0.632, consistent with the earlier result of Ref. [6].

III. MONTE CARLO SAMPLING: HIGHER-DIMENSIONAL SYSTEMS

To gain quick insight into the situation in respect of higher-dimensional systems, we perform Monte Carlo sampling of the sets Γ_{AB} and $\Delta_{d_A d_B - 1}$ following the scheme in [6]. However, instead of sampling from the joint distribution we estimate the relative separable volume for each frame. The relative separable volume in the full space is simply the average over frames, as expressed in Eq. (1). For most systems, $2^{15} \approx 3 \times 10^4$ frames were sampled from Γ_{AB} using Haar measure, and for each frame 10^6 points were sampled from the corresponding simplex $\Delta_{d_A d_B - 1}$ uniformly. Although the Haar measure for the orbit Γ_{AB} is the natural one, there is no "unique" measure to sample the simplex $\Delta_{d_A d_B - 1}$, and indeed different measures have been motivated and used in [7,8]. However, we have used the uniform measure, in order to be consistent with the work of Życzkowski *et al.* [6] which motivated this work. Figure 3 shows the distribution of relative separable volume and *frame entanglement*, the average entanglement of the orthonormal pure states ($d_A d_B$ in number) defining the frame. It also shows the joint distribution of these two quantities as well as their scatter plots. We observe that for a 2×2 system the separable volume distribution becomes narrow as the frame entanglement approaches 1, which does not happen for other cases. This is possibly a consequence of the fact that for a 2×2 system there exists only one maximally entangled frame modulo local unitary, whereas for higher-dimensional systems there are many locally inequivalent maximally entangled frames [18,19]. We show in Fig. 4 the mean and minimum separable volume and frame entanglement as a function of Hilbert space dimension. Consistent with earlier work [6], we find that the separable volume decreases exponentially with Hilbert space dimension. Systems with the same total or composite Hilbert space dimension but different
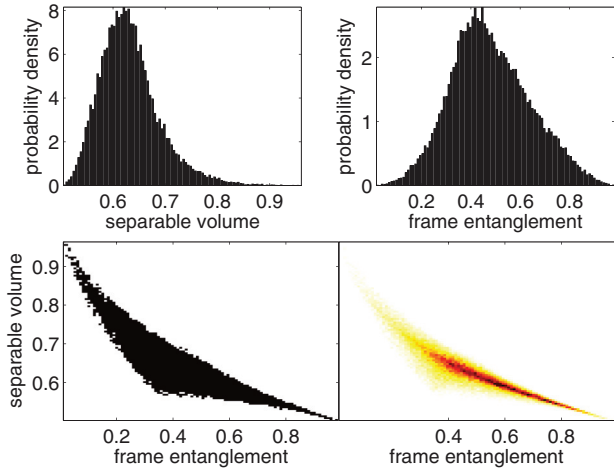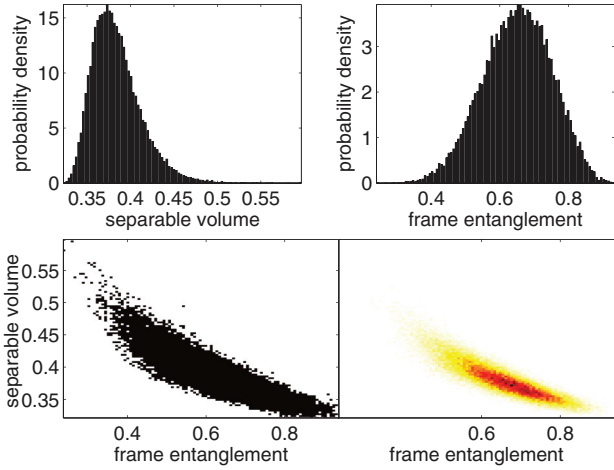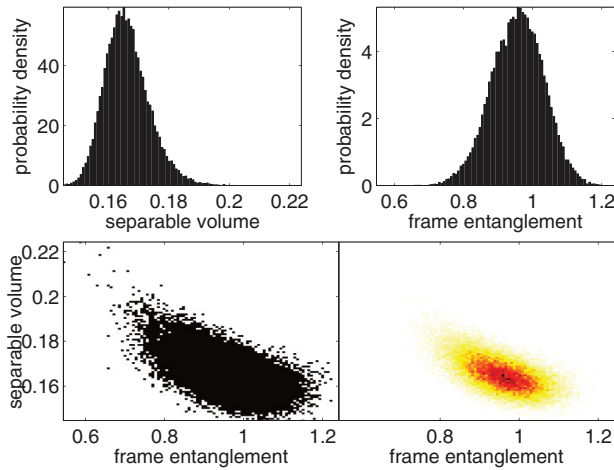
(a) 2 × 2 system

(b) 2 × 3 system

(c) 3 × 3 system

FIG. 3. (Color online) Distribution of separable volume and frame entanglement over the orbit of frames. In each subfigure, the top-left plot shows the distribution of (fractional) separable volume, the top-right plot shows the distribution of frame entanglement, the bottom-left plot shows the scatter plot of all pairs of separable volume and frame entanglement, and the bottom-right plot shows the two-dimensional histogram corresponding to the joint distribution of separable volume and frame entanglement.
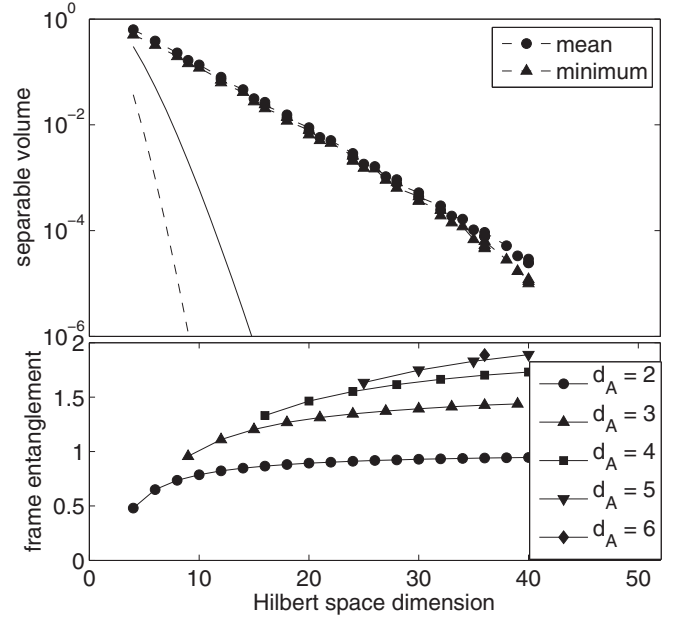

FIG. 4. Top panel shows mean and minimum of separable volume over frames as a function of Hilbert space dimension, showing an exponential decrease. It also shows the lower bounds given by [6] as a solid line, and the one given by [10] as a dashed line. Bottom panel shows the corresponding mean frame entanglement with different symbols for different d_A, for fixed $d_A d_B$.

subsystem dimensions have only slightly different separable volume which is not prominently visible in Fig. 4, and so has been detailed in Table I.

Our approach generalizes to higher-dimensional systems, wherein qualitatively different additional features emerge. For instance, for the qutrit-qutrit systems, not all frames of maximally entangled states are local unitarily equivalent and, consequently, they lead to unequal fractional volume of separable states and, perhaps surprisingly, the "Bell frame" *is not* the one to result in minimum separable volume. This result is significant should it possibly imply that for higher-dimensional $d \times d$ systems, the Bell frame is not the most robust one among the maximally entangled frames.

TABLE I. Relative separable volume for bipartite systems with fixed total Hilbert space dimensions $d_A d_B$ that can be decomposed as $\mathcal{H}_A \otimes \mathcal{H}_B$ in more ways than one.

$d_A d_B$	$d_A \times d_B$	Mean	Minimum
12	2 × 6	0.0796	0.0708
	3 × 4	0.0724	0.0631
16	2 × 8	0.0268	0.0242
	4 × 4	0.0233	0.0204
18	2 × 9	0.0154	0.0140
	3 × 6	0.0135	0.0118
20	2 × 10	0.0088	0.0080
	4 × 5	0.0075	0.0065
24	2 × 12	0.0029	0.0026
	3 × 8	0.0025	0.0021
	4 × 6	0.0024	0.0021

To indicate what we mean by Bell frame for a $d \times d$ system, define a pair of $d \times d$ matrices X, Y through $X = \mathrm{diag}\,(1, \omega_d, \omega_d^2, \ldots, \omega_d^{d-1})$, $Y_{jk} = \delta_{j+1,k}$ where $\omega_d = \exp(-i2\pi/d)$ and $j + 1 = k$ is to be understood in the mod d sense. It is clear that the d^2 matrices $C^{\alpha\beta} = d^{-1/2} X^\alpha Y^\beta$, $\alpha, \beta = 1, 2, \ldots, d$, viewed as coefficient matrices in the computational product basis correspond to maximally entangled orthonormal vectors. For brevity, we call this basis of maximally entangled states "the Bell frame".

IV. QUBIT-QUTRIT SYSTEM

Analogous to the special two-parameter family of the two-qubit frames considered earlier, we now consider a special three-parameter family of orthogonal frames for the 2×3 system representing a qubit-qutrit system:

$$C_{|\psi_1\rangle} = \begin{pmatrix} \cos\theta & 0 & 0 \\ 0 & \sin\theta & 0 \end{pmatrix}, \quad C_{|\psi_2\rangle} = \begin{pmatrix} \sin\theta & 0 & 0 \\ 0 & -\cos\theta & 0 \end{pmatrix},$$

$$C_{|\psi_3\rangle} = \begin{pmatrix} 0 & \cos\alpha & 0 \\ 0 & 0 & \sin\alpha \end{pmatrix}, \quad C_{|\psi_4\rangle} = \begin{pmatrix} 0 & \sin\alpha & 0 \\ 0 & 0 & -\cos\alpha \end{pmatrix},$$

$$C_{|\psi_5\rangle} = \begin{pmatrix} 0 & 0 & \cos\beta \\ \sin\beta & 0 & 0 \end{pmatrix}, \quad C_{|\psi_6\rangle} = \begin{pmatrix} 0 & 0 & \sin\beta \\ -\cos\beta & 0 & 0 \end{pmatrix}.$$

(16)

The particular case $\theta = \alpha = \beta = \pi/4$ may be called the Bell basis for the 2×3 system. We find using Monte Carlo sampling that the relative separable volume is approximately 0.377. We find numerically that there are other maximally entangled frames which do not belong to this special parametrization *that have lower separable volume than the Bell-diagonal frame.*

V. VOLUME OF HYPERSPHERES

In this section, we suggest that an exponential decrease in the volume of separable states with increasing Hilbert space dimension implies an *increase* in "effective radius" for separable states [6,10,20]. To gain some perspective, let us discuss the effect of Hilbert space dimension on the ratio of volumes of hyperspheres (in the state space) with constant ratio of radii. Let r_{sep} and r_{tot} be the radii of the inner (separable) and outer (total) hyperspheres, respectively ($r_{\text{sep}} < r_{\text{tot}}$). The ratio of the volumes of these hyperspheres in n dimensions is $V^{\text{sep}}/V^{\text{tot}} = (r_{\text{sep}}/r_{\text{tot}})^n$. Thus, the ratio of the volumes decreases exponentially with the dimension n even if the ratio of the radii is constant. For a quantum system represented by a d-dimensional Hilbert space, the state space, i.e., the space of density matrices, is $d^2 - 1$ dimensional. Thus, in the hypothetical case in which the set of all states and the set of separable states were (concentric) hyperspheres with ratio of radii independent of d, the ratio of the volume would have decreased as $(r_{\text{sep}}/r_{\text{tot}})^{(d^2-1)}$, which is faster than exponential in Hilbert space dimension d. Thus, if one observes no-stronger-than exponential decrease ($e^{-\alpha d}$) in the actual ratio of volumes, then the ratio ($r_{\text{sep}}/r_{\text{tot}}$) ought to increase with d as $e^{-\alpha d/(d^2-1)}$, and approach 1 asymptotically (see Fig. 5). Thus, it follows that a no-faster-than exponential decrease
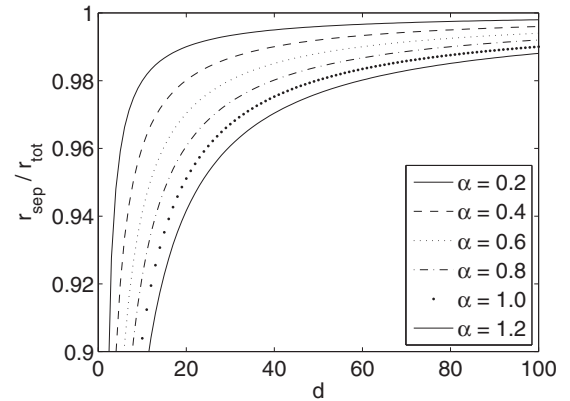

FIG. 5. Behavior of the ratio of radii for hyperspheres in state space Ω_d with Hilbert space dimension d, assuming exponential decrease $e^{-\alpha d}$ in the ratio of volumes.

in relative separable volume with Hilbert space dimension implies that the "effective" relative radius of the separable region must actually *increase* with dimension. This seems to be a new insight, as earlier results have claimed a decreasing lower bound on this effective radius [20]. More importantly, there exists one claim that *an upper bound* on this effective radius too decreases with increasing Hilbert space dimension [20] for the case of quantum systems composed of many qubits.

VI. SUMMARY AND CONCLUSIONS

In this paper, we have analyzed in some detail the geometry of separable states in some three sections of the 15-parameter two-qubit state space Ω_4, and some of these sections are pictured in Fig. 1. This hopefully gives some insight into the geometry of separable sets for two-qubits. We have also given a general parametrization for the state space of two-qubit system. We believe our analysis shows why the surprising result of Ref. [6] could indeed have been "anticipated". Using Monte Carlo sampling of the state space of the higher-dimensional system, we have explored the relation between separable volume and frame entanglement. One of the major surprising results is that for higher-dimensional systems, the Bell frame is not the one having minimum separable volume. This result could possibly have important consequences for generating robust entangled states. We have also pointed out that a no-stronger-than exponential decrease in relative separable volume with Hilbert space dimension actually implies an increase in the "effective radius" of the separable set, contrary to earlier claims.

Although we have considered the uniform measure on the simplex, other measures can also be considered. As an example, we find that with Dirichlet measure ($\nu = \frac{1}{2}$) the separable volumes are 0.350 (2×2), 0.122 (2×3), and 0.022 (3×3) consistent with earlier results [7,8]. The computational cost of our approach appears to grow as $\sim d^{5/2}$ with Hilbert space dimension $d (= d_A d_B)$, which makes it possible to go to even bigger systems if sufficient computational resources are available. Since the Monte Carlo method

employed is embarrassingly parallel, the performance of simulation should increase linearly with the number of available processors.

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