

To: *J. Renes and K. Manne*

From: *C. M. Caves*

Subject: **Measures and volumes for spheres, the probability simplex, projective Hilbert space, and density operators**

2001 February 10; modified 2001 February 22 and 2001 March 9 to correct volume of $SU(D)$

I. The unit sphere

The unit sphere S_{L-1} in L dimensions—i.e., the unit $(L - 1)$ -sphere—is defined by

$$1 = \sum_{j=1}^L x_j^2 . \quad (1)$$

A. Metric and volume element on the unit sphere

The Euclidean metric in L dimensions has the line element

$$ds^2 = \sum_{j=1}^L dx_j^2 . \quad (2)$$

Defining a radial coordinate r by

$$r^2 = \sum_{j=1}^L x_j^2 , \quad (3)$$

one can write the line element as

$$ds^2 = dr^2 + r^2 d\Omega_{L-1}^2 , \quad (4)$$

where $d\Omega_{L-1}^2$ is the line element on the unit $(L - 1)$ -sphere.

Picking a “polar axis” along x_1 , we can define a cylindrical radial coordinate ρ by

$$\rho^2 = \sum_{j=2}^L x_j^2 . \quad (5)$$

The surface generated by holding both x_1 and ρ constant is a $(L - 2)$ -dimensional sphere of radius ρ . Thus we can write the line element as

$$ds^2 = dx_1^2 + d\rho^2 + \rho^2 d\Omega_{L-2}^2 . \quad (6)$$

We can also use a “polar angle” θ defined by

$$x_1 = r \cos \theta \quad \text{and} \quad \rho = r \sin \theta , \quad (7)$$

where $0 \leq \theta \leq \pi$, in terms of which the line element takes the form

$$ds^2 = dr^2 + r^2 d\theta^2 + r^2 \sin^2 \theta d\Omega_{L-2}^2 . \quad (8)$$

We can conclude that

$$d\Omega_{L-1}^2 = d\theta^2 + \sin^2 \theta d\Omega_{L-2}^2 . \quad (9)$$

The L -dimensional Euclidean volume element is

$$dx_1 \cdots dx_L = r^{L-1} dr d\mathcal{S}_{L-1} , \quad (10)$$

where $d\mathcal{S}_{L-1}$ is the volume element on the unit $(L-1)$ -sphere. We can also write

$$dx_1 \cdots dx_L = \rho^{L-2} dx_1 d\rho d\mathcal{S}_{L-2} = r^{L-1} \sin^{L-2} \theta dr d\theta d\mathcal{S}_{L-2} . \quad (11)$$

Combining Eqs. (10) and (11) or using Eq. (9) gives

$$d\mathcal{S}_{L-1} = \sin^{L-2} \theta d\theta d\mathcal{S}_{L-2} . \quad (12)$$

We can also introduce nearly global angular coördinates on the unit sphere in the following way:

$$\begin{aligned} x_1 &= \cos \theta_1 , \\ x_2 &= \sin \theta_1 \cos \theta_2 , \\ x_3 &= \sin \theta_1 \sin \theta_2 \cos \theta_3 , \\ &\vdots \\ x_{L-1} &= \sin \theta_1 \cdots \sin \theta_{L-2} \cos \theta_{L-1} , \\ x_L &= \sin \theta_1 \cdots \sin \theta_{L-2} \sin \theta_{L-1} . \end{aligned} \quad (13)$$

These relations can be summarized by

$$x_j = \begin{cases} \cos \theta_1 , & j = 1, \\ \sin \theta_1 \cdots \sin \theta_{j-1} \cos \theta_j , & j = 2, \dots, L-1, \\ \sin \theta_1 \cdots \sin \theta_{L-1} , & j = L. \end{cases} \quad (14)$$

To cover the unit sphere, the angular coördinates range over the values

$$\begin{aligned} 0 \leq \theta_j \leq \pi , & \quad j = 1, \dots, L-2, \\ 0 \leq \theta_{L-1} \leq 2\pi , & \quad j = L-1. \end{aligned} \quad (15)$$

Notice that

$$\sum_{j=L-k}^L x_j^2 = \begin{cases} \sin^2 \theta_1 \cdots \sin^2 \theta_{L-k-1} , & k = 1, \dots, L-2, \\ 1 , & k = L-1. \end{cases} \quad (16)$$

This means that for constant values of $\theta_1, \dots, \theta_{L-k-1}$, where $k = 1, \dots, L-2$, the coördinates x_{L-k}, \dots, x_L range over a k -sphere of radius $\sin \theta_1 \cdots \sin \theta_{L-k-1}$.

These facts allow us to write the line element on the unit $(L - 1)$ -sphere as

$$\begin{aligned}
d\Omega_{L-1}^2 &= ds_{r=1}^2 \\
&= d\theta_1^2 + \sin^2\theta_1 \left(d\theta_2^2 + \sin^2\theta_2 \left(d\theta_3^2 + \cdots + \sin^2\theta_{L-3} (d\theta_{L-2}^2 + \sin^2\theta_{L-2} d\theta_{L-1}^2) \right) \right) \\
&= d\theta_1^2 + \sin^2\theta_1 d\theta_2^2 + \sin^2\theta_1 \sin^2\theta_2 d\theta_3^2 + \cdots + \sin^2\theta_1 \cdots \sin^2\theta_{L-2} d\theta_{L-1}^2 .
\end{aligned} \tag{17}$$

The corresponding volume element is

$$d\mathcal{S}_{L-1} = \sin^{L-2}\theta_1 \sin^{L-3}\theta_2 \cdots \sin\theta_{L-2} d\theta_1 \cdots d\theta_{L-1} . \tag{18}$$

B. Volume \mathcal{S}_{L-1} of the unit sphere S_{L-1}

1. The Gaussian method

The easiest method for calculating the volume of a sphere is to use a trick involving Gaussian integrals:

$$\begin{aligned}
\frac{1}{2}\mathcal{S}_{L-1} \Gamma(L/2) &= \frac{1}{2}\mathcal{S}_{L-1} \int_0^\infty dw w^{L/2-1} e^{-w} \\
&= \mathcal{S}_{L-1} \int_0^\infty dr r^{L-1} e^{-r^2} \quad (w = r^2) \\
&= \int r^{L-1} dr d\mathcal{S}_{L-1} e^{-r^2} \\
&= \int dx_1 \cdots dx_L e^{-(x_1^2 + \cdots + x_L^2)} \\
&= \left(\int_{-\infty}^\infty dx e^{-x^2} \right)^L \\
&= \pi^{L/2} .
\end{aligned} \tag{19}$$

The result is

$$\mathcal{S}_{L-1} = \frac{2\pi^{L/2}}{\Gamma(L/2)} = \begin{cases} \frac{2(2\pi)^{(L-1)/2}}{(L-2)!!} , & L \text{ odd,} \\ \frac{(2\pi)^{L/2}}{(L-2)!!} , & L \text{ even,} \end{cases} \tag{20}$$

where we use

$$\Gamma(n+1) = n! \quad \text{and} \quad \Gamma(n + \frac{1}{2}) = \frac{(2n-1)!!}{2^n} \sqrt{\pi} . \tag{21}$$

2. An iterative method

Using Eq. (12), we get a recursion relation for $L - 1 \geq 2$,

$$\mathcal{S}_{L-1} = \int d\mathcal{S}_{L-1} = \int \sin^{L-2}\theta d\theta \mathcal{S}_{L-2} = \mathcal{S}_{L-2} I_{L-2} , \tag{22}$$

where

$$I_L \equiv \int_0^\pi d\theta \sin^L \theta . \quad (23)$$

The recursion relation gives

$$\mathcal{S}_{L-1} = \mathcal{S}_1 \prod_{l=1}^{L-2} I_l = 2\pi \prod_{l=1}^{L-2} I_l . \quad (24)$$

Integrating by parts, for $L > 1$, we find

$$\begin{aligned} I_L &= \int_0^\pi d\theta \sin^{L-1} \theta \sin \theta \\ &= \underbrace{-\sin^{L-1} \theta \cos \theta \Big|_0^\pi}_{=0} + (L-1) \underbrace{\int_0^\pi d\theta \sin^{L-2} \theta \cos^2 \theta}_{= I_{L-2} - I_L} \\ &= (L-1)(I_{L-2} - I_L) . \end{aligned} \quad (25)$$

The resulting recursion relation for I_L , valid for $L \geq 2$, is

$$I_L = \frac{L-1}{L} I_{L-2} . \quad (26)$$

Using $I_0 = \pi$ and $I_1 = 2$, we find

$$I_L = \frac{(L-1)!!}{L!!} \begin{cases} 2 , & L \text{ odd,} \\ \pi , & L \text{ even,} \end{cases} \quad (27)$$

which gives

$$\prod_{l=1}^L I_l = \begin{cases} \frac{2(2\pi)^{(L-1)/2}}{L!!} , & L \text{ odd,} \\ \frac{(2\pi)^{L/2}}{L!!} , & L \text{ even.} \end{cases} \quad (28)$$

Plugging this result into Eq. (24) gives

$$\mathcal{S}_{L-1} = \begin{cases} \frac{2(2\pi)^{(L-1)/2}}{(L-2)!!} , & L \text{ odd,} \\ \frac{(2\pi)^{L/2}}{(L-2)!!} , & L \text{ even,} \end{cases} \quad (29)$$

in agreement with the Eq. (20).

3. Direct integration

Using Eq. (18), we can integrate directly to find the volume of S_{L-1} ,

$$\mathcal{S}_{L-1} = \int_0^\pi d\theta_1 \sin^{L-2}\theta_1 \int_0^\pi d\theta_2 \sin^{L-3}\theta_2 \cdots \int_0^\pi d\theta_{L-2} \sin\theta_{L-2} \int_0^{2\pi} d\theta_{L-1} = 2\pi \prod_{l=1}^{L-2} I_l, \quad (30)$$

thus giving the same volume as in Eq. (24).

4. Related results

The volume *interior* to a $(L-1)$ -sphere of radius R is

$$\int r^{L-1} dr d\mathcal{S}_{L-1} = \mathcal{S}_{L-1} \int_0^R dr r^{L-1} = \frac{1}{L} \mathcal{S}_{L-1} R^L; \quad (31)$$

II. The probability simplex

For L alternatives, the probability simplex is defined by

$$1 = \sum_{j=1}^L p_j \quad \text{and} \quad p_j \geq 0, \quad j = 1, \dots, L. \quad (32)$$

A. Euclidean metric

1. Line element and volume element on the probability simplex

If we regard the probabilities as Cartesian coördinates, the corresponding Euclidean line element,

$$ds^2 = \sum_{j=1}^L dp_j^2, \quad (33)$$

induces a flat geometry on the probability simplex.

The unit vector orthogonal to the simplex is given by

$$\mathbf{n} \equiv \frac{\nabla \left(\sum_{j=1}^L p_j \right)}{\left| \nabla \left(\sum_{j=1}^L p_j \right) \right|} = \frac{1}{\sqrt{L}} \sum_{j=1}^L \mathbf{e}_j. \quad (34)$$

We can define a coördinate v that measures distance orthogonal to the simplex:

$$v = \mathbf{n} \cdot \sum_{j=1}^L p_j \mathbf{e}_j = \frac{1}{\sqrt{L}} \sum_{j=1}^L p_j. \quad (35)$$

Notice that the simplex is defined by $v = 1/\sqrt{L}$. The Euclidean line element can be written as

$$ds^2 = dv^2 + (\sqrt{L}v)^2 d\mu_{L-1}^2, \quad (36)$$

where $d\mu_{L-1}^2$ is the line element on the simplex.

The L -dimensional Euclidean volume element is

$$dp_1 \cdots dp_L = (\sqrt{L}v)^{L-1} dv d\mathcal{A}_{L-1}, \quad (37)$$

where $d\mathcal{A}_{L-1}$ is the volume element on the simplex. This allows us to write

$$d\mathcal{A}_{L-1} = \delta\left(v - \frac{1}{\sqrt{L}}\right) dp_1 \cdots dp_L = \delta\left(1 - \sum_{j=1}^L p_j\right) \sqrt{L} dp_1 \cdots dp_L = \sqrt{L} dp_1 \cdots dp_{L-1}. \quad (38)$$

In the last form the δ function has been used to do the integral over p_L ; the result is an integral over the region \mathcal{R} defined by

$$\sum_{j=1}^{L-1} p_j \leq 1 \quad \text{and} \quad p_j \geq 0, \quad j = 1, \dots, L-1, \quad \text{with} \quad p_L = 1 - \sum_{j=1}^{L-1} p_j. \quad (39)$$

The factor of \sqrt{L} in Eq. (38) is the inverse of a direction cosine that comes from projecting volumes on the simplex onto the region (39).

2. Volume \mathcal{A}_{L-1} of the probability simplex

a. The exponential method

The easiest way to calculate the volume of the probability simplex is to use a trick involving integrals over exponentials:

$$\begin{aligned} \frac{1}{\sqrt{L}} \mathcal{A}_{L-1} \Gamma(L) &= \frac{1}{\sqrt{L}} \mathcal{A}_{L-1} \int_0^\infty dw w^{L-1} e^{-w} \\ &= \mathcal{A}_{L-1} \int_0^\infty dv (\sqrt{L}v)^{L-1} e^{-\sqrt{L}v} \quad (w = \sqrt{L}v) \\ &= \int (\sqrt{L}v)^{L-1} dv d\mathcal{A}_{L-1} e^{-\sqrt{L}v} \\ &= \int dp_1 \cdots dp_L e^{-(p_1 + \cdots + p_L)} \\ &= \left(\int_0^\infty dp e^{-p} \right)^L \\ &= 1. \end{aligned} \quad (40)$$

The result is

$$\mathcal{A}_{L-1} = \frac{\sqrt{L}}{\Gamma(L)} = \frac{\sqrt{L}}{(L-1)!}. \quad (41)$$

b. Explicit integration

Using Eqs. (38) and (39), we can write \mathcal{A}_{L-1} as

$$\begin{aligned} \mathcal{A}_{L-1} &= \sqrt{L} \int_{\mathcal{R}} dp_1 \cdots dp_{L-1} \\ &= \sqrt{L} \int_0^1 dp_1 \int_0^{1-p_1} dp_2 \int_0^{1-(p_1+p_2)} dp_3 \\ &\quad \cdots \int_0^{1-(p_1+\cdots+p_{L-3})} dp_{L-2} \int_0^{1-(p_1+\cdots+p_{L-2})} dp_{L-1} . \end{aligned} \quad (42)$$

New integration variables, defined by

$$q_j = 1 - (p_1 + \cdots + p_{L-j}) , \quad j = 1, \dots, L-1, \quad (43)$$

satisfy

$$q_j = \begin{cases} q_{j+1} - p_{L-j} , & j = 1, \dots, L-2, \\ 1 - p_1 , & j = L-1, \end{cases} \quad (44)$$

which allows us to write the integral as

$$\mathcal{A}_{L-1} = \sqrt{L} \int_0^1 dq_{L-1} \int_0^{q_{L-1}} dq_{L-2} \cdots \int_0^{q_3} dq_2 \int_0^{q_2} dq_1 = \frac{\sqrt{L}}{(L-1)!} . \quad (45)$$

Though it is easy to evaluate directly the integral

$$I_{L-1} \equiv \int_0^1 dq_{L-1} \int_0^{q_{L-1}} dq_{L-2} \cdots \int_0^{q_3} dq_2 \int_0^{q_2} dq_1 , \quad (46)$$

there is a clever way to determine the value without doing any integrations at all. Notice that for each of the $(L-1)!$ permutations of the integration variables, the integration region defines a subset of the unit hypercube in $L-1$ dimensions. These regions are disjoint and equivalent, and their union is the entire hypercube. Thus we have immediately that

$$(L-1)! I_{L-1} = 1 . \quad (47)$$

3. Properties of regular polyhedra

The simplex is an $(L-1)$ -dimensional regular polyhedron with sides of length $\sqrt{2}$. The volume of the regular polyhedron is $\mathcal{A}_{L-1} = \sqrt{L}/(L-1)!$. Other properties of regular polyhedra and of hypercubes can be found in the attached notes entitled ‘‘Number of probability distributions.’’

B. Wootters metric

1. Line element and volume element on the probability simplex

In terms of the coördinates

$$r_j = \sqrt{p_j}, \quad (48)$$

the probability simplex is the all positive 2^L -ant of a unit sphere, i.e., the portion of the unit sphere for which all the coördinates are positive:

$$1 = \sum_{j=1}^L p_j = \sum_{j=1}^L r_j^2 \quad \text{and} \quad r_j \geq 0, \quad j = 1, \dots, L. \quad (49)$$

If we regard the coördinates r_j as Cartesian coördinates, the Euclidean line element is

$$ds^2 = \sum_{j=1}^L dr_j^2 = \frac{1}{4} \sum_{j=1}^L \frac{dp_j^2}{p_j}. \quad (50)$$

With this line element, the metric on the probability simplex, called the Wootters metric, is the standard metric of a unit sphere. The Wootters metric defines distances in terms of the statistical distinguishability of neighboring probability distributions. The standard radial coördinate r measures distance orthogonal to the simplex. The line element can be written as

$$ds^2 = dr^2 + r^2 d\Omega_{L-1}^2, \quad (51)$$

where $d\Omega_{L-1}^2$, the line element on the unit $(L-1)$ -sphere, is the Wootters line element on the simplex.

The L -dimensional Euclidean volume element is

$$dr_1 \cdots dr_L = \frac{1}{2^L} \frac{dp_1 \cdots dp_L}{\sqrt{p_1 \cdots p_L}} = r^{L-1} dr d\mathcal{S}_{L-1}. \quad (52)$$

This allows us to write

$$d\mathcal{S}_{L-1} = \delta(r-1) dr_1 \cdots dr_L = \delta(r-1) \frac{1}{2^L} \frac{dp_1 \cdots dp_L}{\sqrt{p_1 \cdots p_L}}. \quad (53)$$

By rewriting the δ function as

$$\delta(r-1) = 2\delta(r^2-1) = 2\delta\left(1 - \sum_{j=1}^L r_j^2\right) = 2\delta\left(1 - \sum_{j=1}^L p_j\right), \quad (54)$$

we obtain the more useful forms

$$\begin{aligned}
d\mathcal{S}_{L-1} &= 2 \delta \left(1 - \sum_{j=1}^L r_j^2 \right) dr_1 \cdots dr_L \\
&= \delta \left(1 - \sum_{j=1}^L p_j \right) \frac{1}{2^{L-1}} \frac{dp_1 \cdots dp_L}{\sqrt{p_1 \cdots p_L}} \\
&= \frac{1}{2^{L-1}} \frac{dp_1 \cdots dp_{L-1}}{\sqrt{p_1 \cdots p_{L-1}}} \\
&= \frac{1}{2^{L-1} \sqrt{L}} \frac{d\mathcal{A}_{L-1}}{\sqrt{p_1 \cdots p_L}} .
\end{aligned} \tag{55}$$

2. Volume $\mathcal{S}_{L-1}^{(W)}$ of the probability simplex

Since the all-positive 2^L -ant is one of 2^L equivalent portions of the unit $(L-1)$ -sphere, the volume of the probability simplex with respect to the Wootters metric is

$$\mathcal{S}_{L-1}^{(W)} = \frac{\mathcal{S}_{L-1}}{2^L} = \frac{\pi^{L/2}}{2^{L-1} \Gamma(L/2)} = \begin{cases} \frac{\pi^{(L-1)/2}}{2^{(L-1)/2} (L-2)!!} , & L \text{ odd,} \\ \frac{\pi^{L/2}}{2^{L/2} (L-2)!!} , & L \text{ even.} \end{cases} \tag{56}$$

This volume can also be written as the integral

$$\mathcal{S}_{L-1} = \int d\mathcal{S}_{L-1} = \frac{1}{2^{L-1}} \int_{\mathcal{R}} \frac{dp_1 \cdots dp_{L-1}}{\sqrt{p_1 \cdots p_L}} . \tag{57}$$

III. Projective Hilbert space

Projective Hilbert space is the space of rays in a D -dimensional complex vector space. It is equivalent to the space of normalized pure states $|\phi\rangle$, i.e.,

$$\langle \phi | \phi \rangle = 1 , \tag{58}$$

with states that differ only by a phase identified, i.e.,

$$|\phi\rangle \iff e^{i\delta} |\phi\rangle . \tag{59}$$

A general vector in the Hilbert space can be written as

$$|\tilde{\psi}\rangle = r e^{i\delta} |\phi\rangle , \quad 0 \leq r \leq \infty , \quad 0 \leq \delta < 2\pi . \tag{60}$$

where $|\phi\rangle$ is an element of projective Hilbert space. In practice, what this means is that for each ray in Hilbert space, we make a particular choice of phase for $|\phi\rangle$.

A. Fubini-Studi metric and associated volume element

The Euclidean line element on a complex vector space is

$$ds^2 = \langle d\tilde{\psi} | d\tilde{\psi} \rangle . \quad (61)$$

If we introduce an orthonormal basis $|e_j\rangle$ and expand an arbitrary vector in terms of it,

$$|\tilde{\psi}\rangle = \sum_{j=1}^D c_j |e_j\rangle , \quad (62)$$

we can write the line element (61) as

$$ds^2 = \sum_{j=1}^D |dc_j|^2 = \sum_{j=1}^D (dx_j^2 + dy_j^2) = \sum_{j=1}^D (dr_j^2 + r_j^2 d\phi_j^2) = \sum_{j=1}^D \left(\frac{dp_j^2}{4p_j} + p_j d\phi_j^2 \right) , \quad (63)$$

where we have defined

$$c_j = x_j + iy_j = r_j e^{i\phi_j} = \sqrt{p_j} e^{i\phi_j} . \quad (64)$$

Notice that the squared magnitude of $|\tilde{\psi}\rangle$ has the forms

$$r^2 = \langle \tilde{\psi} | \tilde{\psi} \rangle = \sum_{j=1}^D |c_j|^2 = \sum_{j=1}^D (x_j^2 + y_j^2) = \sum_{j=1}^D r_j^2 = \sum_{j=1}^D p_j . \quad (65)$$

The difficulty in dealing with projective Hilbert space is that there is no way to define a satisfactory global overall-phase coordinate. Thus, in contrast to Eq. (60), it is best to write a general vector as

$$|\tilde{\psi}\rangle = r |\psi\rangle , \quad (66)$$

where $|\psi\rangle$ is normalized, but can have an arbitrary phase. A small displacement in $|\tilde{\psi}\rangle$ can be written as

$$|d\tilde{\psi}\rangle = dr |\psi\rangle + r |d\psi\rangle . \quad (67)$$

Preservation of the normalization of $|\psi\rangle$ requires that

$$0 = d(\langle \psi | \psi \rangle) = \langle d\psi | \psi \rangle + \langle \psi | d\psi \rangle + \langle d\psi | d\psi \rangle = 2\text{Re}(\langle \psi | d\psi \rangle) + \langle d\psi | d\psi \rangle , \quad (68)$$

which implies that

$$\text{Re}(\langle \psi | d\psi \rangle) = -\frac{1}{2} \langle d\psi | d\psi \rangle = 0 , \quad (69)$$

where the last equality is good to first order in small displacements. The Euclidean line element (61) takes on the standard form for spherical coordinates,

$$ds^2 = dr^2 + 2rdr \text{Re}(\langle \psi | d\psi \rangle) + r^2 \langle d\psi | d\psi \rangle = dr^2 + r^2 \underbrace{\langle d\psi | d\psi \rangle}_{= d\Omega_{2D-1}^2} , \quad (70)$$

with the normalized vectors $|\psi\rangle$ describing a unit $(2D - 1)$ -sphere.

The line element on projective Hilbert space, called the *Fubini-Studi metric*, is given by the Hilbert-space angle $d\gamma_D$ between neighboring vectors:

$$\cos d\gamma_D = |\langle\psi|\psi'\rangle| = |1 + \langle\psi|d\psi\rangle|, \quad |\psi'\rangle = |\psi\rangle + |d\psi\rangle. \quad (71)$$

The line element is given by

$$d\gamma_D^2 = \sin^2 d\gamma_D = 1 - \cos^2 d\gamma_D = -2\text{Re}(\langle\psi|d\psi\rangle) - |\langle\psi|d\psi\rangle|^2, \quad (72)$$

which becomes

$$d\gamma_D^2 = \langle d\psi|d\psi\rangle - |\langle\psi|d\psi\rangle|^2 = \langle d\psi_\perp|d\psi_\perp\rangle, \quad (73)$$

where

$$|d\psi_\perp\rangle \equiv |d\psi\rangle - |\psi\rangle\langle\psi|d\psi\rangle \quad (74)$$

is the projection of $|d\psi\rangle$ orthogonal to $|\psi\rangle$. The imaginary quantity $\langle\psi|d\psi\rangle$ describes an infinitesimal phase change of $|\psi\rangle$ and is thus subtracted out of the line element on projective Hilbert space, which is insensitive to phase changes.

If we fix a phase for each ray in Hilbert space and write

$$|\psi\rangle = e^{i\delta}|\phi\rangle, \quad (75)$$

a small displacement in $|\psi\rangle$ becomes

$$|d\psi\rangle = id\delta|\psi\rangle + e^{i\delta}|d\phi\rangle, \quad (76)$$

which gives

$$\langle\psi|d\psi\rangle = id\delta + \langle\phi|d\phi\rangle \implies |d\psi_\perp\rangle = e^{i\delta}(|d\phi\rangle - |\phi\rangle\langle\phi|d\phi\rangle) = e^{i\delta}|d\phi_\perp\rangle \quad (77)$$

and

$$d\gamma_D^2 = \langle d\psi_\perp|d\psi_\perp\rangle = \langle d\phi_\perp|d\phi_\perp\rangle = \langle d\phi|d\phi\rangle - |\langle\phi|d\phi\rangle|^2. \quad (78)$$

It would be nice if one could choose a particular phase for each ray and introduce a global overall phase in such a way that $\langle\phi|d\phi\rangle$ vanished everywhere. Unfortunately, it is impossible to do this, for if $\langle\phi|d\phi\rangle$ vanished everywhere, then from Eq. (77), $\langle\psi|d\psi\rangle$ would also be a perfect differential, satisfying

$$0 = id^2\delta = d(\langle\psi|d\psi\rangle) = \langle d\psi|d\psi\rangle, \quad (79)$$

but this is impossible. Thus one is forced always to use Eq. (73) for the Fubini-Studi line element, explicitly removing the infinitesimal phase displacement.

A useful set of coördinates comes from picking a “polar axis” along $|e_1\rangle$ and defining a “polar angle” θ by

$$c_1 \equiv r e^{i\phi_1} \cos \theta, \quad 0 \leq \theta \leq \pi/2. \quad (80)$$

Writing the other complex amplitudes in terms of these coördinates, we have

$$c_j = r e^{i\phi_1} \sin \theta b_j, \quad j = 2, \dots, D, \quad (81)$$

where the reduced expansion coefficients $b_j = (r_j/r \sin \theta) e^{i(\phi_j - \phi_1)}$, $j = 2, \dots, D$, are normalized to unity, i.e.,

$$\sum_{j=2}^D |b_j|^2 = \frac{1}{r^2 \sin^2 \theta} \sum_{j=2}^D r_j^2 = \frac{r^2 - r_1^2}{r^2 \sin^2 \theta} = 1. \quad (82)$$

Thus we can define a normalized vector in the subspace orthogonal to $|e_1\rangle$,

$$|\eta\rangle \equiv \sum_{j=2}^D b_j |e_j\rangle, \quad (83)$$

and write $|\psi\rangle$ as

$$|\psi\rangle = e^{i\phi_1} (\cos \theta |e_1\rangle + \sin \theta |\eta\rangle). \quad (84)$$

A small displacement in $|\psi\rangle$ takes the form

$$|d\psi\rangle = id\phi_1 |\psi\rangle + e^{i\phi_1} (d\theta (-\sin \theta |e_1\rangle + \cos \theta |\eta\rangle) + \sin \theta |d\eta\rangle), \quad (85)$$

where $\text{Re}(\langle \eta | d\eta \rangle) = 0$ for the same reasons as in Eq. (69). We can now calculate

$$\langle \psi | d\psi \rangle = id\phi_1 + \sin^2 \theta \langle \eta | d\eta \rangle. \quad (86)$$

Projective Hilbert space is defined by $r = 1$ and $\phi_1 = \text{constant}$, corresponding to a particular phase choice for each Hilbert space ray. Though this is a reasonable choice, we are still left with a nonzero value of $\langle \psi | d\psi \rangle = \sin^2 \theta \langle \eta | d\eta \rangle$, in accordance with the preceding discussion.

Given a particular vector $|\psi_0\rangle$, we can always choose our basis such that $|e_1\rangle = |\psi_0\rangle$ and use “polar” coördinates relative to this basis. Near $|\psi_0\rangle$, the polar angle θ is an infinitesimal quantity, so locally we have

$$\langle \psi | d\psi \rangle = id\phi_1, \quad (87)$$

which means that locally $\phi_1 = \delta$ describes overall phase changes. We also have

$$d\Omega_{2D-1}^2 = \langle d\psi | d\psi \rangle = \langle d\psi_\perp | d\psi_\perp \rangle + |\langle \psi | d\psi \rangle|^2 = d\gamma_D^2 + d\delta^2. \quad (88)$$

Thus, at each point in projective Hilbert space, the overall phase changes produce displacements that are orthogonal to projective Hilbert space. Adding the overall phase changes to projective Hilbert space gives the metric on a unit $(2D - 1)$ -sphere. The volume element on the unit $(2D - 1)$ -sphere is

$$d\mathcal{S}_{2D-1} = d\delta d\Gamma_D, \quad (89)$$

where $d\Gamma_D$ is the volume element on projective Hilbert space. Though this is a local relation—i.e., there is no global overall phase δ such that the line element has the form (88)—we can use the volume element (89) in integrals by patching together local volume elements. As a result, we can turn an integral over projective Hilbert space into an integral over the unit $(2D - 1)$ -sphere simply by appending at each point an integral over a phase δ that runs from 0 to 2π .

The coordinates in Eq. (63) yield a variety of forms for the Euclidean volume element on Hilbert space,

$$dx_1 \cdots dx_D dy_1 \cdots dy_D = r_1 \cdots r_D dr_1 \cdots dr_D d\phi_1 \cdots d\phi_D = \frac{1}{2^D} dp_1 \cdots dp_D d\phi_1 \cdots d\phi_D, \quad (90)$$

and Eq. (70) gives

$$dx_1 \cdots dx_D dy_1 \cdots dy_D = r^{2D-1} dr d\mathcal{S}_{2D-1}. \quad (91)$$

Combining Eqs. (89), (90), (91), and (38), we get another useful form:

$$\begin{aligned} d\delta d\Gamma_D &= d\mathcal{S}_{2D-1} \\ &= \underbrace{\delta(r-1)}_{2\delta(r^2-1)} \frac{1}{2^D} dp_1 \cdots dp_D d\phi_1 \cdots d\phi_D \\ &= \delta \left(1 - \sum_{j=1}^D p_j \right) \frac{1}{2^{D-1}} dp_1 \cdots dp_D d\phi_1 \cdots d\phi_D \\ &= \frac{1}{2^{D-1} \sqrt{D}} d\mathcal{A}_{D-1} d\phi_1 \cdots d\phi_D. \end{aligned} \quad (92)$$

This form illustrates the important result that after integrating over the phases in a particular basis, the resulting measure on the probability simplex is, aside from constants, the Euclidean measure of Sec. II.A.

Another set of useful relations comes from setting $\phi_1 = 0$, thus working in projective Hilbert space by making a particular phase choice. With this choice, Eq. (85) becomes

$$|d\psi\rangle = d\theta(-\sin\theta|e_1\rangle + \cos\theta|\eta\rangle) + \sin\theta|d\eta\rangle, \quad (93)$$

and Eq. (86) becomes

$$\langle\psi|d\psi\rangle = \sin^2\theta\langle\eta|d\eta\rangle. \quad (94)$$

Thus we have

$$\langle d\psi|d\psi\rangle = d\theta^2 + \sin^2\theta\langle d\eta|d\eta\rangle \quad (95)$$

and

$$\begin{aligned} d\gamma_D^2 &= \langle d\psi|d\psi\rangle - |\langle\psi|d\psi\rangle|^2 \\ &= d\theta^2 + \sin^2\theta\langle d\eta|d\eta\rangle - \sin^4\theta|\langle\eta|d\eta\rangle|^2 \\ &= d\theta^2 + \sin^2\theta(\langle d\eta_\perp|d\eta_\perp\rangle + \cos^2\theta|\langle\eta|d\eta\rangle|^2). \end{aligned} \quad (96)$$

There is an apparent puzzle here, because the normalization constraint on changes in $|\eta\rangle$ implies

$$0 = 2\text{Re}(\langle\eta|d\eta\rangle) + \langle d\eta|d\eta\rangle, \quad (97)$$

in analogy to Eq. (68), but then Eqs. (68), (95), and (96) say

$$0 = 2\text{Re}(\langle\psi|d\psi\rangle) + \langle d\psi|d\psi\rangle = d\theta^2 + \sin^2\theta(2\text{Re}(\langle\eta|d\eta\rangle) + \langle d\eta|d\eta\rangle) = d\theta^2, \quad (98)$$

which can't be right. The puzzle is resolved by noting that in the normalization constraints, we have to evaluate the small changes to second order. Thus we have to write

$$\begin{aligned} |\psi'\rangle &= |\psi\rangle + |d\psi\rangle \\ &= \cos(\theta + d\theta)|e_1\rangle + \sin(\theta + d\theta)(|\eta\rangle + |d\eta\rangle) \\ &= |\psi\rangle + d\theta(-\sin\theta|e_1\rangle + \cos\theta|\eta\rangle) + \sin\theta|d\eta\rangle - \frac{1}{2}d\theta^2|\psi\rangle + \cos\theta d\theta|d\eta\rangle, \end{aligned} \quad (99)$$

which gives

$$\langle\psi|d\psi\rangle = (\sin^2\theta + \cos\theta\sin\theta d\theta)\langle\eta|d\eta\rangle - \frac{1}{2}d\theta^2 \quad (100)$$

and

$$\begin{aligned} 2\text{Re}(\langle\psi|d\psi\rangle) + \langle d\psi|d\psi\rangle &= (\sin^2\theta + \cos\theta\sin\theta d\theta)2\text{Re}(\langle\eta|d\eta\rangle) - d\theta^2 + d\theta^2 + \sin^2\theta\langle d\eta|d\eta\rangle \\ &= -(\sin^2\theta + \cos\theta\sin\theta d\theta)\langle d\eta|d\eta\rangle + \sin^2\theta\langle d\eta|d\eta\rangle \\ &= 0 \end{aligned} \quad (101)$$

to second order in small quantities.

In Eq. (96) the line element

$$\langle d\eta_\perp|d\eta_\perp\rangle + \cos^2\theta|\langle\eta|d\eta\rangle|^2 \quad (102)$$

is that of a projective Hilbert space in $D-1$ dimensions plus overall phase changes whose associated length is scaled by a factor $\cos\theta$. The corresponding volume element, $\cos\theta d\mathcal{S}_{2D-3}$, is that of a unit $(2D-3)$ -sphere with lengths in one dimension scaled by the factor $\cos\theta$. Thus for the volume element on projective Hilbert space, we have

$$d\Gamma_D = \sin^{2D-3}\theta \cos\theta d\theta d\mathcal{S}_{2D-3}. \quad (103)$$

This form is useful for doing integrals over projective Hilbert space where the integrand depends only on the polar angle θ .

We can also define nearly global coordinates on projective Hilbert space in the following way. For normalized vectors the coordinates r_j define the all-positive 2^D -ant of the unit $(D-1)$ -sphere. Thus we can introduce angular coordinates as in Eq. (14):

$$r_j = \begin{cases} \cos\theta_1, & j = 1, \\ \sin\theta_1 \cdots \sin\theta_{j-1} \cos\theta_j, & j = 2, \dots, D-1, \\ \sin\theta_1 \cdots \sin\theta_{D-1}, & j = D. \end{cases} \quad (104)$$

Since the coördinates r_j are all positive, the angular coördinates are all restricted to the same range:

$$0 \leq \theta_j \leq \pi/2, \quad j = 1, \dots, D-1. \quad (105)$$

To fix a phase—and thus work in projective Hilbert space—we choose $\phi_1 = 0$. With these choices, the state vector $|\psi\rangle$ becomes

$$|\psi\rangle = \sum_{j=1}^D r_j e^{i\phi_j} |e_j\rangle \quad (\phi_1 = 0), \quad (106)$$

and a small displacement takes the form

$$|d\psi\rangle = \sum_{j=1}^D e^{i\phi_j} (dr_j + ir_j d\phi_j) |e_j\rangle. \quad (107)$$

With these choices we have

$$\langle d\psi | d\psi \rangle = \sum_{j=1}^D dr_j^2 + \sum_{j=2}^D r_j^2 d\phi_j^2 \quad (108)$$

and

$$\langle \psi | d\psi \rangle = \sum_{j=1}^D r_j dr_j + i \sum_{j=2}^D r_j^2 d\phi_j = i \sum_{j=2}^D r_j^2 d\phi_j, \quad (109)$$

where we use

$$\sum_{j=1}^D r_j dr_j = \frac{1}{2} d \left(\underbrace{\sum_{j=1}^D r_j^2}_{=1} \right) = 0. \quad (110)$$

Thus the line element on projective Hilbert space is given by

$$d\gamma_D^2 = \langle d\psi | d\psi \rangle - |\langle \psi | d\psi \rangle|^2 = \sum_{j=1}^D dr_j^2 + \sum_{j=2}^D r_j^2 d\phi_j^2 - \sum_{j,k=2}^D r_j^2 r_k^2 d\phi_j d\phi_k, \quad (111)$$

where in terms of the angular coördinates, the first term is given by Eq. (17):

$$\sum_{j=1}^D dr_j^2 = d\theta_1^2 + \sin^2 \theta_1 d\theta_2^2 + \sin^2 \theta_1 \sin^2 \theta_2 d\theta_3^2 + \dots + \sin^2 \theta_1 \dots \sin^2 \theta_{D-2} d\theta_{D-1}^2. \quad (112)$$

In terms of these coördinates, the volume element on projective Hilbert space is given by

$$d\Gamma_D = \sin^{D-2} \theta_1 \sin^{D-3} \theta_2 \dots \sin \theta_{D-2} d\theta_1 \dots d\theta_{D-1} \sqrt{\det \mathbf{M}} d\phi_2 \dots d\phi_D, \quad (113)$$

where \mathbf{M} is the matrix whose elements are given by

$$M_{jk} = r_j^2 \delta_{jk} - r_j^2 r_k^2, \quad j, k = 2, \dots, D. \quad (114)$$

We can calculate the determinant of \mathbf{M} from

$$\begin{aligned} \det \mathbf{M} &= \sum_{j_1, \dots, j_D} \epsilon_{j_2 \dots j_D} M_{2j_2} \cdots M_{Dj_D} \\ &= \sum_{j_1, \dots, j_D} \epsilon_{j_2 \dots j_D} (r_2^2 \delta_{2j_2} - r_2^2 r_{j_2}^2) \cdots (r_D^2 \delta_{Dj_D} - r_D^2 r_{j_D}^2) \\ &= r_2^2 \cdots r_D^2 \sum_{j_1, \dots, j_D} \epsilon_{j_2 \dots j_D} (\delta_{2j_2} - r_{j_2}^2) \cdots (\delta_{Dj_D} - r_{j_D}^2) \\ &= r_2^2 \cdots r_D^2 \left(1 - \sum_{j=2}^D r_j^2 \right) \\ &= r_1^2 r_2^2 \cdots r_D^2, \end{aligned} \quad (115)$$

where $\epsilon_{j_2 \dots j_D}$ is the completely antisymmetric symbol. This gives us

$$\sqrt{\det \mathbf{M}} = r_1 \cdots r_D = \sin^{D-1} \theta_1 \sin^{D-2} \theta_2 \cdots \sin^2 \theta_{D-2} \sin \theta_{D-1} \cos \theta_1 \cdots \cos \theta_{D-1}. \quad (116)$$

The final result for the volume element on projective Hilbert space is

$$\begin{aligned} d\Gamma_D &= \sin^{2D-3} \theta_1 \sin^{2D-5} \theta_2 \cdots \sin^3 \theta_{D-2} \sin \theta_{D-1} \cos \theta_1 \cdots \cos \theta_{D-1} d\theta_1 \cdots d\theta_{D-1} \\ &\quad \times d\phi_2 \cdots d\phi_D. \end{aligned} \quad (117)$$

B. Volume of projective Hilbert space

1. Projecting down from the unit $(2D - 1)$ -sphere

The simplest method for getting the volume of projective Hilbert space is to use Eq. (89):

$$\mathcal{S}_{2D-1} = \int_0^{2\pi} d\delta \int d\Gamma_D = 2\pi \Gamma_D. \quad (118)$$

The result is

$$\Gamma_D = \frac{\mathcal{S}_{2D-1}}{2\pi} = \frac{(2\pi)^{D-1}}{(2D-2)!!} = \frac{\pi^{D-1}}{(D-1)!}. \quad (119)$$

2. Integrating up from the unit $(2D - 3)$ -sphere

Equation (103) gives

$$\begin{aligned}
\Gamma_D &= \int d\Gamma_D \\
&= \int_0^{\pi/2} d\theta \sin^{2D-3}\theta \cos\theta \int d\mathcal{S}_{2D-3} \\
&= \frac{\mathcal{S}_{2D-3}}{2(D-1)} \\
&= \frac{(2\pi)^{D-1}}{2(D-1)(2D-4)!!} \\
&= \frac{\pi^{D-1}}{(D-1)!} .
\end{aligned} \tag{120}$$

3. Integration over phases and the probability simplex

Using Eq. (92), we can also proceed through direct integration over phases and then over the probability simplex:

$$2\pi\Gamma_D = \frac{1}{2^{D-1}\sqrt{D}} \int d\mathcal{A}_{D-1} \underbrace{\int d\phi_1 \cdots d\phi_D}_{=(2\pi)^D} . \tag{121}$$

The result is

$$\Gamma_D = \pi^{D-1} \frac{\mathcal{A}_{D-1}}{\sqrt{D}} = \frac{\pi^{D-1}}{(D-1)!} . \tag{122}$$

4. Direct integration

Using Eq. (117), we can evaluate the volume of projective Hilbert space as follows:

$$\begin{aligned}
\Gamma_D &= \int_0^{\pi/2} d\theta_1 \sin^{2D-3}\theta_1 \cos\theta_1 \int_0^{\pi/2} d\theta_2 \sin^{2D-5}\theta_2 \cos\theta_2 \cdots \\
&\quad \times \int_0^{\pi/2} d\theta_{D-2} \sin^3\theta_{D-2} \cos\theta_{D-2} \int_0^{\pi/2} d\theta_{D-1} \sin\theta_{D-1} \cos\theta_{D-1} \\
&\quad \times \int_0^{2\pi} d\phi_2 \cdots \int_0^{2\pi} d\phi_D \\
&= (2\pi)^{D-1} \int_0^1 du_1 u_1^{2D-3} \int_0^1 du_2 u_2^{2D-5} \cdots \int_0^1 du_{D-2} u_{D-2}^3 \int_0^1 du_{D-1} u_{D-1} \\
&= \frac{(2\pi)^{D-1}}{(2D-2)!!} \\
&= \frac{\pi^{D-1}}{(D-1)!} .
\end{aligned} \tag{123}$$

IV. Density-operator space

The space of density operators consists of positive, trace-one operators ρ , i.e.,

$$\rho \geq 0, \quad \text{tr}(\rho) = 1. \quad (124)$$

The main difficulty in dealing with density-operator space is knowing where the boundary is. If one introduces coordinates based on the matrix elements of ρ in some fixed orthonormal basis, then there is no simple test for determining when ρ is on the boundary—i.e., has one or more zero eigenvalues—or outside the space—i.e., has one or more negative eigenvalues. We get around this difficulty by using the eigendecomposition to specify ρ :

$$\rho = \sum_{j=1}^D \lambda_j |e_j\rangle\langle e_j|. \quad (125)$$

Thus a density operator is specified by a set of eigenvalues λ_j , which lie in the probability simplex, and by an associated orthonormal set of eigenvectors $|e_j\rangle$, each of which is determined up to a phase.

Notice that if we permute simultaneously the eigenvalues and eigenvectors, the density operator remains unchanged. Thus, in general, when doing integrals over density operators, we must restrict the integrals to run over distinct (unordered) *sets* of bases or over distinct (unordered) *sets* of eigenvalues. If we allow the integral to run over the entire eigenvalue simplex *and* over all *ordered* sets of orthonormal eigenvectors, we will include each density operator $D!$ times. One way to handle this would be to integrate over all ordered sets of eigenvectors, but to restrict the integral over the eigenvalue simplex to one of the $D!$ regions that are equivalent under permutation. Usually, however, we are interested in integrals whose integrand depends only on the eigenvalues. Then it is easiest to integrate over the entire eigenvalue simplex and over all ordered sets of eigenvectors and to divide by $D!$ to remove the resulting overcounting of density operators.

A small displacement in the density operator takes the form

$$d\rho = \sum_{j=1}^D d\lambda_j |e_j\rangle\langle e_j| + \sum_{j=1}^D \lambda_j (|e_j\rangle\langle de_j| + |de_j\rangle\langle e_j|). \quad (126)$$

The displacement must preserve orthonormality, so we have

$$0 = d\delta_{jk} = d\langle e_j|e_k\rangle = \langle de_j|e_k\rangle + \langle e_j|de_k\rangle. \quad (127)$$

When $j = k$, this simplifies to the requirement that the displaced eigenvectors remain normalized:

$$0 = 2\text{Re}(\langle e_j|de_j\rangle). \quad (128)$$

The imaginary part of $\langle e_j|de_j\rangle$ describes a change in the phase of $|e_j\rangle$. Such a phase change has no effect on $d\rho$. Indeed, if we define

$$|de_{j\perp}\rangle = |de_j\rangle - |e_j\rangle\langle e_j|de_j\rangle, \quad (129)$$

the part of $d\rho$ having to do with changes in the eigenvectors becomes

$$\begin{aligned} |e_j\rangle\langle de_j| + |de_j\rangle\langle e_j| &= |e_j\rangle\langle de_{j\perp}| + |de_{j\perp}\rangle\langle e_j| + 2|e_j\rangle\langle e_j| \underbrace{\operatorname{Re}(\langle e_j|de_j\rangle)}_{=0} \\ &= |e_j\rangle\langle de_{j\perp}| + |de_{j\perp}\rangle\langle e_j|. \end{aligned} \quad (130)$$

The matrix elements of $d\rho$ in the local eigenbasis are given by

$$\langle e_j|d\rho|e_k\rangle = d\lambda_j\delta_{jk} + (\lambda_k - \lambda_j)\langle e_j|de_k\rangle = \begin{cases} d\lambda_j, & j = k, \\ (\lambda_k - \lambda_j)\langle e_j|de_k\rangle, & j \neq k. \end{cases} \quad (131)$$

A. Haar metric and volume of projective $U(D)$

Any *ordered* eigenbasis $|e_j\rangle$ is related to a fiducial orthonormal basis $|e_j^{(0)}\rangle$ by a unique unitary operator U defined by

$$U|e_j^{(0)}\rangle = |e_j\rangle. \quad (132)$$

Thus there is a one-to-one correspondence between unitary operators in $U(D)$ and *ordered* eigenbases. The matrix elements of U relative to the fiducial basis are

$$U_{jk} = \langle e_j^{(0)}|U|e_k^{(0)}\rangle = \langle e_j^{(0)}|e_k\rangle. \quad (133)$$

In this section matrix elements written like U_{jk} refer to the fiducial basis. Matrix elements with respect to a local eigenbasis are written out explicitly, as in Eq. (131).

A small displacement dU produces a change in the eigenbasis given by

$$dU|e_j^{(0)}\rangle = |de_j\rangle. \quad (134)$$

The matrix elements of dU ,

$$dU_{jk} = \langle e_j^{(0)}|dU|e_k^{(0)}\rangle = \langle e_j^{(0)}|de_k\rangle, \quad (135)$$

are important, but more useful are the matrix elements of $U^\dagger dU$,

$$(U^\dagger dU)_{jk} = \langle e_j^{(0)}|U^\dagger dU|e_k^{(0)}\rangle = \langle e_j|de_k\rangle. \quad (136)$$

Preservation of unitarity means that the displacements dU satisfy

$$0 = d1 = d(U^\dagger U) = dU^\dagger U + U^\dagger dU. \quad (137)$$

The matrix elements of this relation,

$$0 = \langle e_j^{(0)}|(dU^\dagger U + U^\dagger dU)|e_k^{(0)}\rangle = \langle de_j|e_k\rangle + \langle e_j|de_k\rangle, \quad (138)$$

are identical, as they should be, to the requirements (127) set by the orthonormality of the eigenbases.

There is a natural metric on $U(D)$, the group of unitary matrices. This metric, called the *Haar metric*, has a line element

$$ds^2 = \sum_{j,k} |dU_{jk}|^2 = \text{tr}(dU^\dagger dU). \quad (139)$$

There being a one-to-one correspondence between unitary operators and ordered eigenbases, the Haar metric induces a metric on orthonormal bases:

$$ds^2 = \sum_j \langle e_j^{(0)} | dU^\dagger dU | e_j^{(0)} \rangle = \sum_j \langle de_j | de_j \rangle. \quad (140)$$

Our objective is to use the Haar metric to provide a measure for a part of density-operator space, the part corresponding to changes in eigenbasis. Since a change in the phases of the eigenvectors has no effect on the density operator, we are really interested in a *projective* version of $U(D)$, where we identify unitary operators that produce the same eigenbasis up to phase changes of the eigenvectors. In practice, this means that we choose a particular set of phases for each eigenbasis. Looking at the matrix elements U_{jk} in Eq. (133), we could fix the phases of the eigenbasis, for example, by choosing $U_{jj} = \langle e_j^{(0)} | e_j \rangle$ to be real and positive or by choosing $U_{1j} = \langle e_1^{(0)} | e_j \rangle$ to be real and positive. In terms of the line element, we want to use a projective version of Eq. (140); since $\langle e_j | de_j \rangle$ describes phase changes of $|e_j\rangle$, the appropriate line element is

$$du_D^2 = \sum_j \langle de_{j\perp} | de_{j\perp} \rangle = \sum_j \langle de_j | de_j \rangle - |\langle e_j | de_j \rangle|^2 = \sum_{j,k} |\langle e_k | de_j \rangle|^2 - \sum_j |\langle e_j | de_j \rangle|^2. \quad (141)$$

By writing

$$|de_{j\perp}\rangle = |de_j\rangle - |e_j\rangle \langle e_j | de_j \rangle = dU |e_j^{(0)}\rangle - U |e_j^{(0)}\rangle \langle e_j^{(0)} | U^\dagger dU |e_j^{(0)}\rangle = dU_\perp |e_j^{(0)}\rangle, \quad (142)$$

where

$$dU_\perp \equiv dU - \sum_j U |e_j^{(0)}\rangle \langle e_j^{(0)} | U^\dagger dU |e_j^{(0)}\rangle \langle e_j^{(0)} |, \quad (143)$$

we can write the line element on projective $U(D)$ formally as

$$du_D^2 = \text{tr}(dU_\perp^\dagger dU_\perp), \quad (144)$$

although we have little occasion to use this form.

The most useful way to think about projective $U(D)$ is the following. The elements of projective $U(D)$ are in one-to-one correspondence with ordered eigenbases determined up to phase changes of the eigenvectors. An ordered eigenbasis can be specified by first picking an arbitrary vector and fixing its phase, then picking an arbitrary vector in the subspace orthogonal to the first and fixing its phase, and so forth. Moreover, the line element (141) can be written as

$$du_D^2 = 2 \sum_{k>j} |\langle e_k | de_j \rangle|^2 = 2 \sum_j \langle de_j^\perp | de_j^\perp \rangle, \quad (145)$$

where

$$|de_j^\rangle \equiv \sum_{k>j} |e_k\rangle \langle e_k| de_j \rangle \quad (146)$$

is the displacement $|de_j\rangle$ projected onto the subspace spanned by subsequent vectors in the basis. The j th term in the line element (145) is the line element on a projective Hilbert space of dimension $D - j + 1$. Thus we can write the volume element on projective $U(D)$ as

$$\begin{aligned} d\Upsilon_D &= (\sqrt{2})^{2(D-1)} d\Gamma_D (\sqrt{2})^{2(D-2)} d\Gamma_{D-1} \cdots (\sqrt{2})^{2(3-1)} d\Gamma_3 (\sqrt{2})^{2(2-1)} d\Gamma_2 \\ &= 2^{D(D-1)/2} d\Gamma_D \cdots d\Gamma_2 . \end{aligned} \quad (147)$$

The volume of projective $U(D)$ is obtained by integrating over the entirety of each of the projective Hilbert spaces:

$$\Upsilon_D = 2^{D(D-1)/2} \Gamma_D \cdots \Gamma_2 = \frac{(2\pi)^{D(D-1)/2}}{\prod_{d=1}^{D-1} d!} . \quad (148)$$

Notice that had we dealt with $U(D)$ instead of projective $U(D)$, we would have had the line element (140):

$$ds^2 = \sum_j \langle de_j | de_j \rangle = du_D^2 + \sum_j |\langle e_j | de_j \rangle|^2 = \sum_j 2 \langle de_j^\rangle | de_j^\rangle + |\langle e_j | de_j \rangle|^2 . \quad (149)$$

This line element differs from the line element on projective $U(D)$ by additional terms that describe the phase changes of each basis vector; i.e., if we used a fiducial basis vector $|e'_j\rangle$ in projective $U(D)$, then we must consider all basis vectors $|e_j\rangle = e^{i\delta_j} |e'_j\rangle$ in $U(D)$, thus giving $|\langle e_j | de_j \rangle|^2 = d\delta_j^2$. The corresponding volume of $U(D)$ is bigger than that of Eq. (148) by a factor of 2π for each dimension, thus giving

$$\left(\begin{array}{c} \text{volume of} \\ U(D) \end{array} \right) = \frac{(2\pi)^{D(D+1)/2}}{\prod_{d=1}^{D-1} d!} . \quad (150)$$

For $D = 2$ this gives a volume of $8\pi^3$, which agrees with a direct calculation.

What if we are interested in the volume of $SU(D)$? Choosing the phases of the fiducial basis vectors $|e'_j\rangle$ so as to make the determinant of U equal to 1, we see that the additional phases $e^{i\delta_j}$ change the determinant to $e^{i(\delta_1 + \cdots + \delta_D)}$. To maintain a unit determinant, we must choose

$$\delta_1 = - \sum_{j=2}^D \delta_j . \quad (151)$$

Each of the phases δ_j for $j = 2, \dots, D$, runs from 0 to 2π , because every choice of these phases corresponds to a different basis and thus to a different unitary operator U . The phase δ_1 tracks the other phases according to the unit-determinant condition (151); other choices of δ_1 , differing by multiples of 2π , do not lead to a different unitary operator and thus can be ignored. As a consequence of these considerations, the local line element for the additional phase changes becomes

$$\sum_{j=1}^D |\langle e_j | de_j \rangle|^2 = \sum_{j=1}^D d\delta_j^2 = \sum_{j=2}^D d\delta_j^2 + \sum_{j,k=2}^D d\delta_j d\delta_k. \quad (152)$$

The phase part of the volume element is given by $\sqrt{\det \mathbf{M}} d\delta_2 \cdots d\delta_D$, where \mathbf{M} has matrix elements $M_{jk} = 1 + \delta_{jk}$, $j, k = 2, \dots, D$. Writing

$$\mathbf{M} = \mathbf{I} + (D-1)|e\rangle\langle e|, \quad (153)$$

where

$$|e\rangle = \frac{1}{\sqrt{D-1}} \sum_{j=2}^D |j\rangle \quad (154)$$

is a normalized vector, we find that $\det \mathbf{M} = D$. The result is that, relative to the volume element on projective $U(D)$, there is an additional phase volume element $\sqrt{D} d\delta_2 \cdots d\delta_D$ at each fiducial basis, which contributes an additional volume factor $\sqrt{D}(2\pi)^{D-1}$. (The need for this calculation, instead of just including $D-1$ factors of 2π , was pointed out to me by Mark S. Byrd.) The result is

$$\left(\text{volume of } \text{SU}(D) \right) = \frac{\sqrt{D}(2\pi)^{(D+2)(D-1)/2}}{\prod_{d=1}^{D-1} d!}. \quad (155)$$

For $D = 2$ this gives a volume $4\sqrt{2}\pi^2$, which agrees with a direct calculation.

The above measures and volumes were founded on the line element (139). It is sometimes more convenient to begin with the line element

$$(ds')^2 = \frac{1}{2} ds^2 = \frac{1}{2} \text{tr}(dU^\dagger dU). \quad (156)$$

With this choice the volume of projective $U(D)$ becomes

$$\Upsilon'_D = \frac{\Upsilon_D}{(\sqrt{2})^{D(D-1)}} = \frac{\pi^{D(D-1)/2}}{\prod_{d=1}^{D-1} d!}. \quad (157)$$

Similarly, the volume of $U(D)$ is reduced by a factor of $(\sqrt{2})^{D^2}$, giving

$$\left(\text{volume of } U(D) \right)' = \frac{2^{D/2} \pi^{D(D+1)/2}}{\prod_{d=1}^{D-1} d!}, \quad (158)$$

and the volume of $SU(D)$ is reduced by a factor of $(\sqrt{2})^{D^2-1}$, giving

$$\left(\text{volume of } SU(D) \right)' = \frac{\sqrt{D} 2^{(D-1)/2} \pi^{(D+2)(D-1)/2}}{\prod_{d=1}^{D-1} d!}. \quad (159)$$

This result agrees with Eq. (A10) of C. Bernard, *Phys. Rev. A* **19**, 3013–3019 (1979) and also with Eq. (31) of M. S. Marinov, *J. Phys. A* **14**, 543–544 (1981), which corrects the corresponding equation in M. S. Marinov, *J. Phys. A* **13**, 3357–3366 (1980).

B. Metrics and volume elements on density-operator space

1. General formulation

There is no way to pick out a universally preferred line element on density operators, but we can restrict the possibilities by imposing the following natural restrictions: (i) displacements on the eigenvalue simplex are orthogonal to displacements describing basis changes, (ii) there are no preferred directions on the eigenvalue simplex, and (iii) the line element for basis changes is the same as the Haar metric except that we allow for the possibility of eigenvalue-dependent length scalings. The resulting line element has the form

$$\begin{aligned} ds^2 &= \sum_j \frac{\langle e_j | d\rho | e_j \rangle^2}{f(\lambda_j)} + \sum_{j \neq k} g(\lambda_j, \lambda_k) |\langle e_k | d\rho | e_j \rangle|^2 \\ &= \sum_j \frac{d\lambda_j^2}{f(\lambda_j)} + 2 \sum_{k < j} g(\lambda_j, \lambda_k) (\lambda_j - \lambda_k)^2 |\langle e_k | de_j \rangle|^2, \end{aligned} \quad (160)$$

where $f(\lambda_j)$ is a positive function and $g(\lambda_j, \lambda_k)$ is a symmetric, positive function.

To get the corresponding volume element, we focus first on the volume element on the eigenvalue simplex. At a point on the simplex specified by eigenvalues $\lambda_j^{(0)}$ ($\sum_j \lambda_j^{(0)} = 1$), consider a curve that runs orthogonal to the simplex into the region of unnormalized eigenvalues. Near the simplex such a curve is given by

$$\lambda_j - \lambda_j^{(0)} = \frac{f(\lambda_j^{(0)})}{\left(\sum_k f(\lambda_k^{(0)}) \right)^{1/2}} \ell, \quad (161)$$

where ℓ measures distance along the curve according to the simplex part of the line element (160). This allows us to write

$$\ell = \frac{\sum_j \lambda_j - 1}{\left(\sum_k f(\lambda_k^{(0)})\right)^{1/2}}. \quad (162)$$

At the point in question, the line element on the space of eigenvalues has the form

$$\sum_j \frac{d\lambda_j^2}{f(\lambda_j)} = d\ell^2 + d\nu_{D-1}^2, \quad (163)$$

where $d\nu_{D-1}^2$ is the line element on the simplex.

The volume element on the eigenvalue space thus has the form

$$\frac{d\lambda_1 \cdots d\lambda_D}{\sqrt{f(\lambda_1) \cdots f(\lambda_D)}} = d\ell d\mathcal{B}_{D-1}, \quad (164)$$

where $d\mathcal{B}_{D-1}$ is the volume element on the simplex. Thus we have

$$d\mathcal{B}_{D-1} = \delta(\ell) \frac{d\lambda_1 \cdots d\lambda_D}{\sqrt{f(\lambda_1) \cdots f(\lambda_D)}}. \quad (165)$$

Since

$$\delta(\ell) = \delta\left(\frac{1 - \sum_j \lambda_j}{\left(\sum_k f(\lambda_k)\right)^{1/2}}\right) = \left(\sum_j f(\lambda_j)\right)^{1/2} \delta\left(1 - \sum_j \lambda_j\right), \quad (166)$$

we can put the volume element on the eigenvalue simplex in the more convenient forms

$$\begin{aligned} d\mathcal{B}_{D-1} &= \delta\left(1 - \sum_j \lambda_j\right) \left(\sum_j f(\lambda_j)\right)^{1/2} \frac{d\lambda_1 \cdots d\lambda_D}{\sqrt{f(\lambda_1) \cdots f(\lambda_D)}} \\ &= \left(\frac{1}{D} \sum_j f(\lambda_j)\right)^{1/2} \frac{d\mathcal{A}_{D-1}}{\sqrt{f(\lambda_1) \cdots f(\lambda_D)}} \\ &= 2^{D-1} \left(\sum_j f(\lambda_j)\right)^{1/2} \sqrt{\frac{\lambda_1 \cdots \lambda_D}{f(\lambda_1) \cdots f(\lambda_D)}} d\mathcal{S}_{D-1}. \end{aligned} \quad (167)$$

Now the volume element on density-operator space becomes

$$\begin{aligned} d\mathcal{V}_D &= d\mathcal{B}_{D-1} \left(\prod_{k<j} 2g(\lambda_j, \lambda_k)(\lambda_j - \lambda_k)^2 \right) d\Gamma_D \cdots d\Gamma_2 \\ &= \left(\prod_{k<j} g(\lambda_j, \lambda_k)(\lambda_j - \lambda_k)^2 \right) d\mathcal{B}_{D-1} d\Upsilon_D . \end{aligned} \quad (168)$$

As discussed above, for integrating over all density operators, one should integrate over all of projective $U(D)$, but only over unordered sets of eigenvalues, i.e., over one of the $D!$ equivalent subsets of the eigenvalue simplex that are equivalent under permutations. When the integrand depends only on the eigenvalues, however, we can integrate over the entire simplex and over the entirety of projective $U(D)$, dividing by $D!$ to remove the overcounting. Thus we have for the volume of density-operator space

$$\mathcal{V}_D = \frac{\Upsilon_D}{D!} \int d\mathcal{B}_{D-1} \left(\prod_{k<j} g(\lambda_j, \lambda_k)(\lambda_j - \lambda_k)^2 \right) . \quad (169)$$

2. Examples

a. Flat metric

The simplest metric on density operators is the flat metric

$$ds^2 = \text{tr}(d\rho^2) = \sum_{j,k} |\langle e_j | d\rho | e_k \rangle|^2 = \sum_j d\lambda_j^2 + \sum_{k \neq j} (\lambda_j - \lambda_k)^2 |\langle e_k | de_j \rangle|^2 . \quad (170)$$

This metric is flat on the eigenvalue simplex, and its overall flatness requires a scaling factor $(\lambda_j - \lambda_k)^2$ relative to the Haar metric on projective $U(D)$. These factors reduce the distance corresponding to a change in basis vector relative to the distance corresponding to the same change for a pure state on projective Hilbert space. Thus this factor means that a smaller volume is assigned to basis-vector changes for highly mixed states than for nearly pure ones. Notice that the flat metric has $f(\lambda_j) = 1$ and $g(\lambda_j, \lambda_k) = 1$; the general scaling functions $f(\lambda_j)$ and $g(\lambda_j, \lambda_k)$ appearing in other line elements thus describe further scalings relative to the flat metric.

The volume element for the flat metric,

$$d\mathcal{V}_D = \left(\prod_{k<j} (\lambda_j - \lambda_k)^2 \right) d\mathcal{A}_{D-1} d\Upsilon_D , \quad (171)$$

leads to a total volume

$$\mathcal{V}_D = \frac{\Upsilon_D}{D!} \int d\mathcal{A}_{D-1} \left(\prod_{k<j} (\lambda_j - \lambda_k)^2 \right) = \frac{(2\pi)^{D(D-1)/2}}{\prod_{d=1}^D d!} \int d\mathcal{A}_{D-1} \left(\prod_{k<j} (\lambda_j - \lambda_k)^2 \right) . \quad (172)$$

For $D = 2$, this becomes

$$\mathcal{V}_2 = \pi \int d\mathcal{A}_1 (\lambda_2 - \lambda_1)^2 = \pi\sqrt{2} \int_0^1 d\lambda_1 (2\lambda_1 - 1)^2 = \frac{\pi\sqrt{2}}{3}. \quad (173)$$

b. Round metric

Another simple and natural choice is the round metric

$$ds^2 = \text{tr}((d\sqrt{\rho})^2) = \sum_{j,k} |\langle e_j | d\sqrt{\rho} | e_k \rangle|^2. \quad (174)$$

Writing

$$\sqrt{\rho} = \sum_j \sqrt{\lambda_j} |e_j\rangle\langle e_j|, \quad (175)$$

we find that a small displacement of $\sqrt{\rho}$ becomes

$$d\sqrt{\rho} = \sum_j \frac{d\lambda_j}{2\sqrt{\lambda_j}} + \sum_j \sqrt{\lambda_j} (|e_j\rangle\langle de_j| + |de_j\rangle\langle e_j|), \quad (176)$$

which gives

$$\langle e_j | d\sqrt{\rho} | e_k \rangle = \frac{d\lambda_j}{2\sqrt{\lambda_j}} \delta_{jk} + (\sqrt{\lambda_k} - \sqrt{\lambda_j}) \langle e_j | de_k \rangle = \begin{cases} d\lambda_j/2\sqrt{\lambda_j}, & j = k, \\ (\sqrt{\lambda_k} - \sqrt{\lambda_j}) \langle e_j | de_k \rangle, & j \neq k. \end{cases} \quad (177)$$

The resulting line element is

$$ds^2 = \sum_j \frac{d\lambda_j^2}{4\lambda_j} + \sum_{k \neq j} (\sqrt{\lambda_j} - \sqrt{\lambda_k})^2 |\langle e_k | de_j \rangle|^2. \quad (178)$$

This metric is the Wootters metric on the eigenvalue simplex, and its overall roundness requires a scaling factor $(\sqrt{\lambda_j} - \sqrt{\lambda_k})^2$ relative to the Haar metric on projective $U(D)$. Notice that the round metric has

$$f(\lambda_j) = 4\lambda_j \quad \text{and} \quad g(\lambda_j, \lambda_k) = \left(\frac{\sqrt{\lambda_j} - \sqrt{\lambda_k}}{\lambda_j - \lambda_k} \right)^2. \quad (179)$$

The volume element for the round metric,

$$d\mathcal{V}_D = \left(\prod_{k < j} (\sqrt{\lambda_j} - \sqrt{\lambda_k})^2 \right) d\mathcal{S}_{D-1} d\Upsilon_D, \quad (180)$$

leads to a total volume

$$\mathcal{V}_D = \frac{\Upsilon_D}{D!} \int d\mathcal{S}_{D-1} \left(\prod_{k < j} (\sqrt{\lambda_j} - \sqrt{\lambda_k})^2 \right) = \frac{(2\pi)^{D(D-1)/2}}{\prod_{d=1}^D d!} \int d\mathcal{S}_{D-1} \left(\prod_{k < j} (r_j - r_k)^2 \right). \quad (181)$$

For $D = 2$, this becomes

$$\mathcal{V}_2 = \pi \int d\mathcal{S}_1 (r_2 - r_1)^2 = \pi \int_0^{\pi/2} d\phi (\sin \phi - \cos \phi)^2 = \pi \int_0^{\pi/2} d\phi (1 - \sin 2\phi) = \pi \left(\frac{\pi}{2} - 1 \right). \quad (182)$$

c. Bures-Uhlmann metric

Statistical distance for density operators leads to the Bures-Uhlmann metric

$$ds^2 = \frac{1}{2} \text{tr}(d\rho \mathcal{L}_\rho(d\rho)) , \quad (183)$$

where \mathcal{L}_ρ is the lowering superoperator defined by

$$\mathcal{L}_\rho(B) = A \quad \text{if} \quad B = \rho A + A\rho = \mathcal{R}_\rho . \quad (184)$$

Thus we have that

$$\langle e_j | B | e_k \rangle = (\lambda_j + \lambda_k) \langle e_j | A | e_k \rangle , \quad (185)$$

which gives

$$\langle e_j | \mathcal{L}_\rho(B) | e_k \rangle = \langle e_j | A | e_k \rangle = \frac{\langle e_j | B | e_k \rangle}{\lambda_j + \lambda_k} . \quad (186)$$

The resulting line element is

$$\begin{aligned} ds^2 &= \frac{1}{2} \sum_{j,k} \langle e_k | d\rho | e_j \rangle \langle e_j | \mathcal{L}_\rho(d\rho) | e_k \rangle \\ &= \frac{1}{2} \sum_{j,k} \frac{|\langle e_j | d\rho | e_k \rangle|^2}{\lambda_j + \lambda_k} \\ &= \frac{d\lambda_j^2}{4\lambda_j} + \sum_{k \neq j} \frac{(\lambda_j - \lambda_k)^2}{2(\lambda_j + \lambda_k)} |\langle e_k | de_j \rangle|^2 . \end{aligned} \quad (187)$$

The Bures-Uhlmann metric is the Wootters metric on the eigenvalue simplex, with a “statistical distinguishability” scaling factor for basis changes. Notice that the Bures-Uhlmann metric has

$$f(\lambda_j) = 4\lambda_j = \frac{1}{g(\lambda_j, \lambda_j)} \quad \text{and} \quad g(\lambda_j, \lambda_k) = \frac{1}{2(\lambda_j + \lambda_k)} . \quad (188)$$

The volume element for the Bures-Uhlmann metric,

$$d\mathcal{V}_D = \frac{1}{2^{D(D-1)/2}} \left(\prod_{k < j} \frac{(\lambda_j - \lambda_k)^2}{\lambda_j + \lambda_k} \right) d\mathcal{S}_{D-1} d\Upsilon_D , \quad (189)$$

leads to a total volume

$$\begin{aligned} \mathcal{V}_D &= \frac{\Upsilon_D}{2^{D(D-1)/2} D!} \int d\mathcal{S}_{D-1} \left(\prod_{k < j} \frac{(\lambda_j - \lambda_k)^2}{\lambda_j + \lambda_k} \right) \\ &= \frac{\pi^{D(D-1)/2}}{\prod_{d=1}^D d!} \int d\mathcal{S}_{D-1} \left(\prod_{k < j} \frac{(r_j^2 - r_k^2)^2}{r_j^2 + r_k^2} \right) . \end{aligned} \quad (190)$$

For $D = 2$, this becomes

$$\mathcal{V}_2 = \frac{\pi}{2} \int d\mathcal{S}_1 (r_2^2 - r_1^2)^2 = \frac{\pi}{2} \int_0^{\pi/2} d\phi (\sin^2\phi - \cos^2\phi)^2 = \frac{\pi}{2} \int_0^{\pi/2} d\phi \cos^2 2\phi = \frac{\pi^2}{8}. \quad (191)$$

d. Another metric based on statistical distinguishability

Another way to introduce a metric based on statistical distinguishability is to use the isotropic, informationally complete POVM

$$dE(|\psi\rangle) \equiv \frac{D}{\Gamma_D} d\Gamma_D |\psi\rangle\langle\psi|, \quad (192)$$

where

$$\int dE(|\psi\rangle) = \frac{D}{\Gamma_D} \int d\Gamma_D |\psi\rangle\langle\psi| = 1. \quad (193)$$

This POVM generates probabilities

$$p(|\psi\rangle) d\Gamma_D = \text{tr}(\rho dE(|\psi\rangle)) = \frac{D}{\Gamma_D} \langle\psi|\rho|\psi\rangle d\Gamma_D, \quad (194)$$

whose Wootters metric induces a metric on density operators,

$$ds^2 = \frac{1}{4} \int d\Gamma_D \frac{dp^2(|\psi\rangle)}{p(|\psi\rangle)} = \frac{D}{4\Gamma_D} \int d\Gamma_D \frac{\langle\psi|d\rho|\psi\rangle^2}{\langle\psi|\rho|\psi\rangle}. \quad (195)$$

At the time of writing, I don't know how to evaluate this integral to put the line element in the standard form (160), so I confine myself to working out the $D = 2$ case below.

3. $D = 2$

For $D = 2$ the density operator can be written as

$$\rho = \frac{1}{2}(1 + r\mathbf{n} \cdot \sigma) = \underbrace{\frac{1+r}{2}}_{=\lambda_1} \frac{1}{2}(1 + \mathbf{n} \cdot \sigma) + \underbrace{\frac{1-r}{2}}_{=\lambda_2} \frac{1}{2}(1 - \mathbf{n} \cdot \sigma). \quad (196)$$

a. Flat metric

A small displacement of the density operator takes the form

$$d\rho = \frac{1}{2}(dr \mathbf{n} + r d\mathbf{n}) \cdot \sigma. \quad (197)$$

The resulting flat line element,

$$ds^2 = \text{tr}(d\rho^2) = \frac{1}{2}|dr \mathbf{n} + r d\mathbf{n}|^2 = \frac{1}{2}(dr^2 + r^2 d\mathbf{n} \cdot d\mathbf{n}), \quad (198)$$

is indeed the standard flat metric on the Bloch sphere, except that lengths are contracted by a factor of $1/\sqrt{2}$. The corresponding volume is thus

$$\mathcal{V}_2 = \frac{1}{2\sqrt{2}} \frac{4\pi}{3} = \frac{\pi\sqrt{2}}{3} . \quad (199)$$

b. Round metric

The square root of the density operator can be written as

$$\sqrt{\rho} = \sqrt{\frac{1+r}{2}} \frac{1}{2} (1 + \mathbf{n} \cdot \boldsymbol{\sigma}) + \sqrt{\frac{1-r}{2}} \frac{1}{2} (1 - \mathbf{n} \cdot \boldsymbol{\sigma}) . \quad (200)$$

Defining a new coordinate χ by $r = \sin 2\chi$, where $0 \leq \chi \leq \pi/4$, we have

$$\sqrt{\frac{1 \pm r}{2}} = \sqrt{\frac{1 \pm \sin 2\chi}{2}} = \sqrt{\frac{\sin^2 \chi + \cos^2 \chi \pm 2 \sin \chi \cos \chi}{2}} = \frac{1}{\sqrt{2}} (\cos \chi \pm \sin \chi) . \quad (201)$$

In terms of χ , the square root of the density operator becomes

$$\sqrt{\rho} = \frac{1}{\sqrt{2}} (\cos \chi + \sin \chi) \frac{1}{2} (1 + \mathbf{n} \cdot \boldsymbol{\sigma}) + \frac{1}{\sqrt{2}} (\cos \chi - \sin \chi) \frac{1}{2} (1 - \mathbf{n} \cdot \boldsymbol{\sigma}) = \frac{1}{\sqrt{2}} (\cos \chi 1 + \sin \chi \mathbf{n} \cdot \boldsymbol{\sigma}) , \quad (202)$$

and a small displacement in $\sqrt{\rho}$ takes the form

$$d\sqrt{\rho} = \frac{1}{\sqrt{2}} [-\sin \chi d\chi 1 + (\cos \chi d\chi \mathbf{n} + \sin \chi d\mathbf{n}) \cdot \boldsymbol{\sigma}] . \quad (203)$$

The resulting line element is

$$\begin{aligned} ds^2 &= \text{tr}((d\sqrt{\rho})^2) \\ &= \sin^2 \chi d\chi^2 + |\cos \chi d\chi \mathbf{n} + \sin \chi d\mathbf{n}|^2 \\ &= d\chi^2 + \sin^2 \chi d\mathbf{n} \cdot d\mathbf{n} \\ &= \frac{dr^2}{4(1-r^2)} + \frac{1}{2} (1 - \sqrt{1-r^2}) d\mathbf{n} \cdot d\mathbf{n} . \end{aligned} \quad (204)$$

Under the round metric the Bloch sphere has the geometry of the part of the unit 3-sphere that lies within $\pi/4$ of the north pole. The corresponding volume is

$$\mathcal{V}_2 = \int_0^{\pi/4} d\chi 4\pi \sin^2 \chi = 2\pi \int_0^{\pi/4} d\chi (1 - \cos 2\chi) = \pi \left(\frac{\pi}{2} - 1 \right) . \quad (205)$$

The quantity $\sqrt{r^2 g_{rr}/g_{\theta\theta}}$ measures the ratio of radial to angular distances relative to a unity ratio for the flat metric. For the round metric we have

$$\sqrt{\frac{r^2 g_{rr}}{g_{\theta\theta}}} = \frac{r}{\sqrt{2(1-r^2)(1-\sqrt{1-r^2})}} \rightarrow \begin{cases} 1, & r \ll 1, \\ 1/2\sqrt{1-r}, & r \simeq 1. \end{cases} \quad (206)$$

c. Bures-Uhlmann metric

Writing an arbitrary operator as

$$A = a_\alpha \sigma_\alpha = a_0 1 + \mathbf{a} \cdot \boldsymbol{\sigma}, \quad (207)$$

we find that

$$B = \rho A + A \rho = (a_0 + r \mathbf{a} \cdot \mathbf{n}) 1 + (\mathbf{a} + r a_0 \mathbf{n}) \cdot \boldsymbol{\sigma} = b_\alpha \sigma_\alpha, \quad (208)$$

which gives

$$b_0 = a_0 + r \mathbf{a} \cdot \mathbf{n} \quad \text{and} \quad \mathbf{b} = \mathbf{a} + r a_0 \mathbf{n}. \quad (209)$$

The vector relation gives immediately that

$$\mathbf{a} - \mathbf{n}(\mathbf{a} \cdot \mathbf{n}) = \mathbf{a}_\perp = \mathbf{b}_\perp = \mathbf{b} - \mathbf{n}(\mathbf{b} \cdot \mathbf{n}) \quad (210)$$

and

$$\mathbf{b} \cdot \mathbf{n} = \mathbf{a} \cdot \mathbf{n} + r a_0. \quad (211)$$

Inverting the equations for b_0 and $\mathbf{b} \cdot \mathbf{n}$, we find

$$a_0 = \frac{b_0 - r \mathbf{b} \cdot \mathbf{n}}{1 - r^2} \quad \text{and} \quad \mathbf{a} \cdot \mathbf{n} = \frac{\mathbf{b} \cdot \mathbf{n} - r b_0}{1 - r^2}. \quad (212)$$

Combining these relations with Eq. (210) yields

$$\mathbf{a} = \mathbf{b} - \mathbf{n} \underbrace{(\mathbf{b} \cdot \mathbf{n} - \mathbf{a} \cdot \mathbf{n})}_{= r a_0} = \mathbf{b} - \mathbf{n} \frac{r b_0 - r^2 \mathbf{b} \cdot \mathbf{n}}{1 - r^2}. \quad (213)$$

The result is an explicit form for the action of the lowering operator:

$$\mathcal{L}_\rho(B) = A = \frac{b_0 - r \mathbf{b} \cdot \mathbf{n}}{1 - r^2} 1 + \boldsymbol{\sigma} \cdot \left(\mathbf{b} - \mathbf{n} \frac{r b_0 - r^2 \mathbf{b} \cdot \mathbf{n}}{1 - r^2} \right). \quad (214)$$

We apply this result to the $d\rho$ of Eq. (197), for which $b_0 = 0$ and $\mathbf{b} = (dr \mathbf{n} + r d\mathbf{n})/2$:

$$\mathcal{L}_\rho(d\rho) = -\frac{1}{2} \frac{r dr}{1 - r^2} 1 + \frac{1}{2} \boldsymbol{\sigma} \cdot \left(\frac{dr}{1 - r^2} \mathbf{n} + r d\mathbf{n} \right). \quad (215)$$

The resulting Bures-Uhlmann line element is

$$ds^2 = \frac{1}{2} \text{tr}(d\rho \mathcal{L}_\rho(d\rho)) = \frac{1}{4} (dr \mathbf{n} + r d\mathbf{n}) \cdot \left(\frac{dr}{1-r^2} \mathbf{n} + r d\mathbf{n} \right) = \frac{1}{4} \left(\frac{dr^2}{1-r^2} + r^2 d\mathbf{n} \cdot d\mathbf{n} \right). \quad (216)$$

Introducing a new coördinate χ defined by $r = \sin \chi$, with $0 \leq \chi \leq \pi/2$, we find that the line element assumes the form

$$ds^2 = \frac{1}{4} (d\chi^2 + \sin^2 \chi d\mathbf{n} \cdot d\mathbf{n}). \quad (217)$$

which means that the Bloch sphere has the geometry of the northern hemisphere of a 3-sphere of radius $1/2$. The corresponding volume is

$$\mathcal{V}_2 = \frac{1}{2} \frac{\mathcal{S}_3}{8} = \frac{\pi^2}{8}. \quad (218)$$

For the Bures-Uhlmann metric, the quantity $\sqrt{r^2 g_{rr}/g_{\theta\theta}}$ takes the form

$$\sqrt{\frac{r^2 g_{rr}}{g_{\theta\theta}}} = \frac{1}{\sqrt{1-r^2}} \rightarrow \begin{cases} 1, & r \ll 1, \\ 1/\sqrt{2(1-r)}, & r \simeq 1. \end{cases} \quad (219)$$

Relative to the flat metric, the Bures-Uhlmann metric assigns a consistently greater distance to radial displacements than to angular displacements, reflecting the ease of distinguishing mixed states with the same eigenvectors relative to the distance assigned by the flat metric.

d. Another metric based on statistical distinguishability

Letting $|\psi\rangle\langle\psi| = \frac{1}{2}(1 + \mathbf{m} \cdot \sigma)$ and using $\langle\psi|\rho|\psi\rangle = \frac{1}{2}(1 + r\mathbf{n} \cdot \mathbf{m})$ and $\langle\psi|d\rho|\psi\rangle = \frac{1}{2}(dr \mathbf{n} + r d\mathbf{n}) \cdot \mathbf{m}$, the line element (195) becomes

$$ds^2 = \frac{1}{2} \int \frac{d\Omega_{\mathbf{m}}}{4\pi} \frac{\langle\psi|d\rho|\psi\rangle^2}{\langle\psi|\rho|\psi\rangle} = \frac{1}{16\pi} \int d\Omega_{\mathbf{m}} \frac{[(dr \mathbf{n} + r d\mathbf{n}) \cdot \mathbf{m}]^2}{1 + r\mathbf{n} \cdot \mathbf{m}}, \quad (220)$$

where $d\Gamma_D/\Gamma_D = d\Omega_{\mathbf{m}}/4\pi$. We can evaluate the integral by orienting the coördinates so that $\mathbf{n} = \mathbf{e}_z$ and thus $d\mathbf{n} = dn_x \mathbf{e}_x + dn_y \mathbf{e}_y$. With this choice we have

$$\begin{aligned} ds^2 &= \frac{1}{16\pi} \int d\Omega_{\mathbf{m}} \frac{(dr \cos \theta + r d\mathbf{n} \cdot \mathbf{m})^2}{1 + r \cos \theta} \\ &= \frac{1}{16\pi} \int d\Omega_{\mathbf{m}} \frac{dr^2 \cos^2 \theta + 2r dr \cos \theta d\mathbf{n} \cdot \mathbf{m} + r^2 (d\mathbf{n} \cdot \mathbf{m})^2}{1 + r \cos \theta} \\ &= \frac{1}{16\pi} \left(dr^2 \int d\Omega_{\mathbf{m}} \frac{\cos^2 \theta}{1 + r \cos \theta} + 2r dr dn_j \int d\Omega_{\mathbf{m}} \frac{m_j \cos \theta}{1 + r \cos \theta} \right. \\ &\quad \left. + r^2 dn_j dn_k \int d\Omega_{\mathbf{m}} \frac{m_j m_k}{1 + r \cos \theta} \right). \end{aligned} \quad (221)$$

In the two sums over dn_j , remember that j can only take on two values, x and y .

The integrals in the final line of Eq. (221) are easy to evaluate. The first integral is

$$\begin{aligned} \int d\Omega_{\mathbf{m}} \frac{\cos^2\theta}{1+r\cos\theta} &= 2\pi \int_0^\pi d\theta \frac{\sin\theta \cos^2\theta}{1+r\cos\theta} \\ &= \frac{2\pi}{r^3} \int_{1-r}^{1+r} du \frac{(u-1)^2}{u} \quad (u = 1+r\cos\theta, du = -r\sin\theta d\theta) \quad (222) \\ &= \frac{2\pi}{r^3} \left[\ln\left(\frac{1+r}{1-r}\right) - 2r \right]. \end{aligned}$$

The second integral vanishes due to reflection symmetry. The third integral vanishes for $j \neq k$ and has the same value for $j = k = x$ and $j = k = y$, which is given by

$$\begin{aligned} \int d\Omega_{\mathbf{m}} \frac{m_x^2}{1+r\cos\theta} &= \int_0^\pi d\theta \frac{\sin^3\theta}{1+r\cos\theta} \int_0^{2\pi} d\phi \cos^2\phi \\ &= \pi \left(\underbrace{\int_0^\pi d\theta \frac{\sin\theta}{1+r\cos\theta}}_{= \frac{1}{r} \ln\left(\frac{1+r}{1-r}\right)} - \underbrace{\int_0^\pi d\theta \frac{\sin\theta \cos^2\theta}{1+r\cos\theta}}_{= \frac{1}{r^3} \left[\ln\left(\frac{1+r}{1-r}\right) - 2r \right]} \right) \quad (223) \\ &= \frac{1}{r} \ln\left(\frac{1+r}{1-r}\right) - \frac{1}{r^3} \left[\ln\left(\frac{1+r}{1-r}\right) - 2r \right] \\ &= \frac{\pi}{r^3} \left[2r - (1-r^2) \ln\left(\frac{1+r}{1-r}\right) \right]. \end{aligned}$$

The resulting line element is

$$ds^2 = \frac{1}{12} \left(\frac{3}{2r^3} \left[\ln\left(\frac{1+r}{1-r}\right) - 2r \right] dr^2 + \frac{3}{4r} \left[2r - (1-r^2) \ln\left(\frac{1+r}{1-r}\right) \right] d\mathbf{n} \cdot d\mathbf{n} \right). \quad (224)$$

For small r , $\ln[(1+r)/(1-r)] = 2r + 2r^3/3$, so the line element takes on the flat form, $ds^2 = \frac{1}{12}(dr^2 + r^2 d\mathbf{n} \cdot d\mathbf{n})$, whereas for $r \simeq 1$, the line element goes to $ds^2 = \frac{1}{8}[-\ln(1-r)dr^2 + d\mathbf{n} \cdot d\mathbf{n}]$. The quantity $\sqrt{r^2 g_{rr}/g_{\theta\theta}}$ takes the form

$$\sqrt{\frac{r^2 g_{rr}}{g_{\theta\theta}}} = \sqrt{2 \frac{\ln\left(\frac{1+r}{1-r}\right) - 2r}{2r - (1-r^2) \ln\left(\frac{1+r}{1-r}\right)}} \rightarrow \begin{cases} 1, & r \ll 1, \\ \sqrt{-\ln(1-r)}, & r \simeq 1. \end{cases} \quad (225)$$

Relative to the flat metric, this line element assigns a consistently greater distance to radial displacements than to angular displacements, reflecting the ease of distinguishing mixed states with the same eigenvectors relative to the distance assigned by the flat metric. The distinguishability is nowhere near as good as for the Bures-Uhlmann metric, however, reflecting the fact that the Bures-Uhlmann metric uses the best measurement for distinguishing two neighboring density operators, whereas this line element refers to a particular metric that is optimal for distinguishing a density operator from all its neighbors in all directions.