

REPORT DOCUMENTATION PAGE

PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ORGANIZATION.

1. REPORT DATE MARCH 2023	2. REPORT TYPE JOURNAL ARTICLE (POST PRINT)	3. DATES COVERED	
		START DATE APRIL 2022	END DATE NOVEMBER 2022
4. TITLE AND SUBTITLE Distribution of density matrices at fixed purity for arbitrary dimensions			
5a. CONTRACT NUMBER NA	5b. GRANT NUMBER	5c. PROGRAM ELEMENT NUMBER	
5d. PROJECT NUMBER	5e. TASK NUMBER	5f. WORK UNIT NUMBER NA	
6. AUTHOR(S) Paul M. Alsing ,1,* Christopher C. Tison,1 James Schneeloch,1 Richard J. Birrittella,1,2 and Michael L. Fanto1			
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) 1Air Force Research Laboratory, Information Directorate, 525 Brooks Road, Rome, NY 13411 2National Research Council Postdoctoral Fellow, National Academy of Sciences, 500 Fifth St N.W. Washington, D.C. 20001			8.PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES) Air Force Research Laboratory/RITQ 525 Brooks Road Rome NY 13441-4505		10.SPONSOR/MONITOR'S ACRONYM(S) AFRL/RI	11.SPONSOR/MONITOR'SREPORT NUMBER(S) AFRL-RI-RS-TP-2023-015
12. DISTRIBUTION/AVAILABILITY STATEMENT Approved for Public Release; Distribution Unlimited. PA# AFRL-2022-1631 Date Cleared: 6 Apr 22			
13. SUPPLEMENTARY NOTES © Published by the American Physical Society under the terms of the Creative Commons Attribution 4.0 International license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.			
14. ABSTRACT Uniformly sampling quantum density matrices has been demonstrated for a long time [Mezzadri, Notices AMS 54, 592 (2007), Zyczkowski, J. Math. Phys. 52, 062201 (2011)] and is a valuable tool in the analysis and testing of quantum relations (e.g., the tightness of an uncertainty relation); in ranking the performance of various tools to witness entanglement, nonlocality, discord, etc.; and in probing the geometry of fundamental quantum properties (e.g, the boundary between separable and entangled states).			
15. SUBJECT TERMS Quantum states, density matrices, uniform distributions, purity			
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT SAR
a. REPORT U	b. ABSTRACT U	c. THIS PAGE U	
			18. NUMBER OF PAGES 29
19a. NAME OF RESPONSIBLE PERSON PAUL M. ALSING			19b. PHONE NUMBER (Include area code) N/A

STANDARD FORM 298 (REV. 5/2020)

Distribution of density matrices at fixed purity for arbitrary dimensions

Paul M. Alsing^{1,*}, Christopher C. Tison,¹ James Schneeloch,¹ Richard J. Birrittella,^{1,2} and Michael L. Fanto¹

¹*Air Force Research Laboratory, Information Directorate, 525 Brooks Road, Rome, New York 13411, USA*

²*National Research Council Postdoctoral Fellow, National Academy of Sciences, 500 Fifth Street, N.W. Washington, D.C. 20001, USA*



(Received 22 April 2022; accepted 20 October 2022; published 17 November 2022)

Uniformly sampling quantum density matrices has been demonstrated for a long time [Mezzadri, *Notices AMS* 54, 592 (2007), Życzkowski, *J. Math. Phys.* 52, 062201 (2011)] and is a valuable tool in the analysis and testing of quantum relations (e.g., the tightness of an uncertainty relation); in ranking the performance of various tools to witness entanglement, nonlocality, discord, etc.; and in probing the geometry of fundamental quantum properties (e.g, the boundary between separable and entangled states). While uniformly sampling quantum states has been shown to be quite valuable, there is to our knowledge no such method to sample these states uniformly at a constant amount of mixedness. This challenge becomes increasingly acute as post-selecting a subensemble of states within a narrow range of, say, purities from this fully uniform sampling becomes overwhelmingly inefficient at high dimension. In this work, we demonstrate how to analytically construct the distribution of density matrices at constant purity (the trace of the square of a density matrix) as our mixedness measure. With this technique at our disposal: we provide analytic formulas for the cumulative radial distribution functions for the uniform distribution of density matrices at constant purity for arbitrary total dimension N , with closed form expressions up to $N = 4$, and perform numerical integration to analyze the statistics of these uniform-purity distributions at higher dimensions (up to $N = 100$). Moreover, we use our new capabilities to: compare different measures of entanglement and nonclassicality, including Wootters' concurrence, the logarithmic negativity and quantum discord, as a function of purity at dimension $N = 4$ (two qubits); to find the probability distribution of purities of marginal density matrices from a uniform distribution of joint pure states (and thus the entanglement statistics of this uniform ensemble); and to numerically test a conjectured uncertainty relation between quantum mutual information and the sum of classical mutual informations in complementary bases.

DOI: 10.1103/PhysRevResearch.4.043114

I. INTRODUCTION

The random generation of density matrices uniformly distributed according to the Haar measure is well known [1,2], and constitutes an extremely powerful tool in quantum information science from the exploration of measures of entanglement [3] to quantum data locking protocols [4,5]. While the numerical algorithm to generate uniformly random density matrices ρ_N of arbitrary dimension N (denoted as UE for uniform ensemble) is straightforward, the samples are biased toward the lower values of purity $\mu_N(\rho) = \text{Tr}[\rho^2] \in [\frac{1}{N}, 1]$ (nearer the maximally mixed state (MMS) $\rho_{\text{MMS}} = I_{N \times N}/N$ with $\mu(\rho_{\text{MMS}}) = \frac{1}{N}$), with ever increasing rarity to sample pure state ρ_N [$\mu_N(\rho) \rightarrow 1$]. The implication is that one has to generate an extremely large set random density matrices to obtain a statistically relevant number of samples as the purity nears unity. This problem is only exacerbated as the dimension N of the quantum state increases.

In this work, we derive the cumulative distribution functions (CDFs) of density matrices ρ_N for fixed purity, that will allow us to uniformly generate random density matrices, but now at a user-chosen fixed purity (denoted as UP for uniform purity ensemble), across the complete range $\mu_N(\rho) \in [\frac{1}{N}, 1]$. These formulas will reveal the distribution of the eigenvalues of ρ_N on the sphere $S^{(N-2)}$ of radius $r_N \equiv \sqrt{\mu_N - 1/N} \in [0, 1 - \frac{1}{N}]$ centered on the MMS, as a function of the purity μ_N .

While most witnesses or measures of entanglement are based on quantities derived from properties the reduced density matrix of a higher-dimensional composite quantum state (pure or mixed), having the ability to sample the later at fixed purity provides a surgical tool to numerically explore the entanglement relationship between the subsystems derived from the composite state. As an example, for the $N = d^2$ -dimensional Werner state, given by the convex combination of the d -dimensional maximally entangled bipartite Bell state $|\Psi\rangle_{ab} = \frac{1}{\sqrt{d}} \sum_0^{d-1} |n, n\rangle_{ab}$ with the MMS, written as $\rho^{(W,N)} = p|\Psi\rangle_{ab}\langle\Psi| + (1-p)I_{N \times N}/N$ with $p \in [0, 1]$, one can compute logarithmic negativity (LN) analytically (see Appendix A) as $\text{LN} = \log_2(1 + 2\mathcal{N})$, where the negativity [sum of the absolute values of the negative eigenvalues of the partial transpose (PT) of the composite state], is given by $\mathcal{N} = \frac{1}{2} \frac{d-1}{d} [(d+1)p - 1]$. Further, one can then show that

*paul.alsing@us.af.mil

Published by the American Physical Society under the terms of the Creative Commons Attribution 4.0 International license. Further distribution of this work must maintain attribution to the author(s) and the published article's title, journal citation, and DOI.

the probability p and the purity $\mu_{(W,d^2)} \in [\frac{1}{d^2}, 1]$ are related by $p = (\frac{d^2 \mu_{(W,d^2)} - 1}{d^2 - 1})^{1/2}$. Thus, the LN entanglement measure is directly seen as an analytic function of the purity of the composite state. The CDFs derived in this work allow the exploration, for example, of the LN to the purity of the composite random state ρ_N for arbitrary dimension N . For the case of $N = 4$, i.e., two-qubits, we will numerically compare the relationship of the LN to the purity of the composite state with the Wootters' concurrence [6], the only entanglement measure valid for both pure and mixed states (applicable as well to $N = 6$, a qubit-qutrit system).

This paper is outlined as follows: In Sec. II we review the UE generation of random unitary matrices $U_N \in U(N)$, which can then be used generate random density matrices via the prescription $\rho_N = U_N \rho_N^{(\text{diag})} U_N^\dagger$, where $\rho_N^{(\text{diag})}$ is a random diagonal density matrix of dimension N , whose eigenvalues are unchanged by the similarity transformation generating ρ_N . We review several easily implementable methods for the uniform generation of $\rho_N^{(\text{diag})}$. In Sec. III we provide a parametrization of $\rho_N^{(\text{diag})}$ as a vector $\vec{p}_E^{(N)} \in \mathbb{R}^N$ in the Weyl chamber (WC) (see Chapter 8.5 of Ref. [3]) whose components are the probability eigenvalues of $\rho_N^{(\text{diag})}$. Where the convex hull (i.e., set of all convex combinations) of all probability vectors $\vec{p}_E^{(N)} \in \mathbb{R}^N$ defines an $N - 1$ -dimensional simplex in \mathbb{R}^N (denoted as Δ_{N-1}), the Weyl chamber can be defined as the convex hull of all truncated maximally mixed states (i.e., maximally mixed, but truncated to a fixed number of nonzero entries; see Eq. (4), for example), and this convex hull is also an $N - 1$ -dimension simplex (here denote as $\tilde{\Delta}_{N-1}$). We then transform $\vec{p}_E^{(N)}$ to a vector $\vec{p}_e^{(N)}$ centered about the MMS (and whose first component is always given by $\sqrt{\mu_N} = \sqrt{1/N}$), and associate the remaining $N - 1$ components with a vector lying on a sphere $S^{(N-2)}$ of radius $r_N = \sqrt{\mu_N - 1/N}$, for fixed value of the purity μ_N . We then analytically solve for the boundary ranges of the $N - 3$ spherical polar angles. We provide a formulation of these bounds for arbitrary dimension N . In Sec. IV we illustrate the previous formulas for the analytically tractable cases of $N = 2$ (which is trivial), $N = 3$ (a qutrit), and $N = 4$ (a pair of qubits). We provide closed form analytic solutions for the cumulative distribution functions (CDF) of both the (spherical polar) angles and the purity radius vector r_N for $N = \{3, 4\}$. The CDFs for the radial purity vector allows us to examine the probability of obtaining a density matrix of a given purity [7] if one were to generate density matrices by the standard method employing the uniform distribution of ρ_N according to the Haar measure (UE). We compare our results to that of previous numerical simulations employing the uniform Haar measure generation method. In Sec. V we explore applications of the above formulas for $N = 4$. For the case of two-qubits $N = 4$, we compare the logarithmic negativity to the Wootters' concurrence as a function of the composite state purity μ_4 . In addition, we compare these measures to a "baseline" entanglement witness based on the difference of the purities of the composite bipartite state with its reduced single qubit state, extending the concept the linear entropy for pure states, to mixed states. We also investigate the distribution of eigenvalues of a reduced N -dimensional density matrix obtained by tracing out the reservoir of its higher-dimensional purification. Last, we

numerically investigate a recently proposed complementary-quantum correlation conjecture [8] which lower bounds the quantum mutual information of a bipartite system by the sum of classical mutual informations obtained from two pairs of mutually unbiased measurements. In Sec. VI we discuss the case of $N = 5$ which serves as an instructive example for how these formulas are applied for all higher dimensions $N > 4$. The formulation ceases to be purely analytically tractable due the presence of powers of the sine of the angles in the integration measure. At this point one must turn to numerical simulation employing the nontrivial analytically specified boundary regions for each polar angle. We further numerically explore the case of $N = 6$, a qubit-qutrit system, and provide a simple, implementable few-line numerical code (which easily generalizes to higher dimension) to generate its radial CDF. For very high dimensions $N \gg 6$, we provide numerically generated radial CDFs for the case of $N \in \{10, 25, 50, 100\}$. The numerical UP generation of density matrices for these higher dimensions (using a more sophisticated numerical integration scheme) were recently used in a complementary paper by the authors [9] exploring the logarithmic negativity versus purity and entropy as witnesses for entanglement. The objective of the work presented here is primarily focused on the analytic formulation of the UP generated density matrices, and their application to the familiar realm of $N = 4$ (2 qubits). In Sec. VII we summarize our results and discuss avenues for future research directions.

II. GENERATION UNITARY AND DENSITY MATRICES DISTRIBUTED WITH RESPECT TO THE HAAR MEASURE

There are many well-known schemes for uniformly generating density matrices according to the Haar measure (UE). One of the oldest constructive approaches dating back to Hurwitz in 1887 (see Ref. [10] and references therein) relies on the N^2 angle parametrization of $U(N) = SU(N) \times U(1)$ by all possible products of 2×2 $SU(2)$ rotation matrices

$$E^{(i,j)} = \begin{pmatrix} \cos \phi_{ij} e^{i\psi_{ij}} & \sin \phi_{ij} e^{i\chi_{ij}} \\ -\sin \phi_{ij} e^{-i\chi_{ij}} & \cos \phi_{ij} e^{-i\psi_{ij}} \end{pmatrix} \quad (1)$$

embedded within $N \times N$ matrices, with the cos terms at position (i, i) and (j, j) with $1 \leq i < j \leq N$, and the $\pm \sin$ terms at positions (i, j) and (j, i) , respectively, with the remaining elements unity on the diagonal $k \neq (i, j)$, and zeros on the off diagonals (see Ref. [10] and Appendix B). There is an overall $U(1)$ phase $e^{i\alpha}$. The angles are taken from the intervals $0 \leq \phi_{rs} \leq \pi/2$, $0 \leq \psi_{rs}, \chi_{rs} \leq \pi/2$ and $0 \leq \alpha \leq 2\pi$ uniformly with respect to the Haar measure with probability measure $P_U(dU) = \sqrt{N!2^{N(N-1)}} \prod_{1 \leq r < s \leq N} (\frac{1}{2r}) d[(\sin \phi_{rs})^{2r}] \prod_{1 \leq s \leq N} d\chi_{1s}$. One then samples $\alpha, \phi_{rs}, \chi_{1s}$ uniformly on the interval $[0, 2\pi)$. Additionally, one takes $\phi_{rs} = \sin^{-1}(\xi^{1/2r})$ with ξ drawn uniformly in $[0, 1)$, for $r \in \{1, 2, \dots, N-1\}$.

With today's fast and accurate computer linear algebra subroutines, a simple (requiring only a few lines of code) routine centers around the QR decomposition [11] of an invertible $N \times N$ complex matrix Z with entries z_{jk} (the Ginibre ensemble) (see Mezzadri [1] and Appendix B). Such matrices have matrix elements that are independent and identically distributed (i.i.d.) standard

normal complex random variables with probability distribution $p(z_{jk}) = \frac{1}{\pi} e^{-|z_{jk}|^2}$. The joint probability distribution for the matrix elements (also statistically independent) is given by $P(Z) = \frac{1}{\pi^{N^2}} \prod_{j,k=1}^N e^{-|z_{jk}|^2} = \frac{1}{\pi^{N^2}} \exp[\sum_{j,k=1}^N e^{-|z_{jk}|^2}] = \frac{1}{\pi^{N^2}} \exp(-\text{Tr}[Z^\dagger Z])$. $P(Z)$ is normalized to unity via $\int_{\mathbb{C}^{N^2}} P(Z) dZ = 1$ where $dZ = \prod_{j,k=1}^N dx_{jk} dy_{jk}$ and $z_{jk} = x_{jk} + iy_{jk}$. The integration measure on the Ginibre ensemble $\mathbb{C}^{N \times N} \cong \mathbb{C}^{N^2}$ is $d\mu_G(Z) = P(Z) dZ$ which can be thought of as an infinitesimal volume in \mathbb{C}^{N^2} . The crucial point is that $d\mu_G(Z)$ is invariant under left and right multiplications of Z by arbitrary unitary matrices, i.e., $d\mu_G(UZ) = d\mu_G(ZV) = d\mu_G(Z)$ for $U, V \in U(N)$. The proof follows trivially from the property of the trace in the definition of $P(Z)$ since $\text{Tr}[(UZ)^\dagger (UZ)] = \text{Tr}[(ZV)^\dagger (ZV)] = \text{Tr}[Z^\dagger Z]$, and hence $P(UZ) = P(ZV) = P(Z)$. This Haar measure is the matrix analog of a uniform probability distribution in one dimension $p(\theta) = \frac{1}{2\pi}$.

The above algorithm to generate random unitary matrices distributed with the Haar measure uses the QR decomposition of Z (versus the less stable, at higher dimensions, Gram-Schmidt orthonormalization routine). Here Q is a unitary matrix and R is an upper-triangular matrix. One caveat exists though. The QR decomposition is not unique, since if $Z = QR$ then so is $Z = Q'R' \equiv (Q\Lambda)(\Lambda^{-1}R)$, with Λ a diagonal matrix so that Q' and R' are again unitary and upper-triangular matrices. To make the decomposition unique, the solution (see Mezzadri [1] for details) is to choose $\Lambda_{ii} = R_{ii}/|R_{ii}|$ where R_{ii} are the diagonal elements of R . Thus, the diagonal matrix elements of $R' = (\Lambda^{-1}R)$ are real and strictly positive, which renders the matrix $Q' = Q\Lambda$ unique and uniformly distributed with the Haar measure. This is the procedure implemented in the Appendix B Mathematica codes.

Given a code to generate random unitary matrices U , one can subsequently uniformly generate density matrices ρ (positive semidefinite Hermitian matrices of unit trace) by the simple decomposition $\rho = U \rho_N^{(\text{diag})} U^\dagger > 0$. To generate the diagonal density matrix $\rho_N^{(\text{diag})}$, an element of the Weyl chamber (see Sec. 8.5 of Ref. [3]) such that $\sum_{i=1}^N (\rho_N^{(\text{diag})})_{ii} = 1$, one simply generates another random unitary U' and takes the absolute square of a random row (or column) as the diagonal entries. The above is the method (UE) used in this work to generate uniformly random unitary matrices. These codes are easily implementable in commonly used coding languages, such as Python, or Mathematica (see Appendix B).

Last, another insightful method to generate an element $\rho_N^{(\text{diag})} = \text{diagonal}\{\lambda_1, \lambda_2, \dots, \lambda_{N-1}\}$ of the WC (the subset of the $N - 1$ simplex $\Delta_{(N-1)}$ defined by the eigenvalues arranged in decreasing order $\{\lambda_1 \geq \lambda_2 \dots \geq \lambda_{N-1}\}$ with $\lambda_N \equiv 1 - \sum_k^{N-1} \lambda_k$) is to choose the eigenvalues according to the formula (see Appendix A of Zyczkowski *et al.* [12], and Appendix B):

$$\lambda_k = [1 - \xi_1^{1/(N-k)}] \left(1 - \sum_{i=1}^{k-1} \lambda_i \right), \quad \lambda_1 = 1 - \xi_1^{1/(N-1)}, \quad (2a)$$

$$\lambda_2 = [1 - \xi_2^{1/(N-2)}] (1 - \lambda_1), \quad \lambda_N \equiv 1 - \sum_{k=1}^{N-1} \lambda_k, \quad (2b)$$

where the $\{\xi_k\}$ for $k \in \{1, 2, \dots, N - 1\}$ are uniform deviates in $[0,1]$. For $N = 2$ we have trivially $\lambda_1 = 1 - \xi_1$, so that λ_1 is uniform in $[0,1]$. Since $\rho_{(N=2)} = \frac{1}{2}(\mathbb{I} + \vec{r} \cdot \vec{\sigma})$ with eigenvalues $\lambda_{\pm} = \frac{1}{2}(1 \pm r)$ with $r = \sqrt{2} r_2 = \sqrt{2} \mu_2 - 1$, we see that $\lambda_1 = \lambda_+$ and hence r_2 (μ_2) is distributed uniformly (quadratically) in $[0, \frac{1}{\sqrt{2}}]$ ($[\frac{1}{2}, 1]$). For $N = 3$ we have $\lambda_1 = 1 - \sqrt{\xi_1}$, $\lambda_2 = (1 - \xi_2)\sqrt{\xi_1}$ with $\lambda_3 = \xi_2 \sqrt{\xi_1}$. Note the term $\sqrt{\xi_1}$ appears with alternating signs in λ_1 and λ_2 , while the same is true for the term $\xi_2 \sqrt{\xi_1}$ in λ_2 and λ_3 . These terms cancel in successive sums of eigenvalues (in decreasing order) to ensure the unit trace condition $\text{Tr}[\rho_{\text{diagonal}}] = \sum_{k=1}^N \lambda_k = 1$.

The formulas in Eqs. (2a) and (2b) are derived by assuming a generic form of $\lambda_1 = 1 - z_1$ and $\lambda_k = (1 - z_k) \prod_{i=1}^{k-1} z_i$ for $k = \{2, \dots, N - 1\}$ and $\lambda_N = 1 - \sum_{k=1}^{N-1} \lambda_k$ which by construction, trivially enforces the unit trace condition. Then, by assuming $z_k = (\xi_k)^{\alpha_k}$, and requiring that the Jacobian $\det[\frac{\partial \lambda_i(\xi_j)}{\partial \xi_j}]$ of the transformation between the λ and ξ variables is a constant (so that the ξ variables are uniformly distributed [11]), the powers $\alpha_k = \frac{1}{N-k}$ appearing in Eqs. (2) and (2b) are obtained.

III. SPHERICAL POLAR REPRESENTATION OF DIAGONAL DENSITY MATRICES IN THE WEYL CHAMBER

The previous section discussed the uniform generation of density matrices (UE) satisfying the unit trace (linear eigenvalue) constraint $\text{Tr}[\rho_N] = 1$. In this section we turn our attention to the main focus of this work, namely, the uniform generation of density matrices with the additional implementation of the quadratic constraint of fixed (chosen) purity $\mu_N = \text{Tr}[\rho_N^2]$ (UP). Before we begin we first introduce several different coordinate systems that will be useful in our derivation. We will illustrate this with examples for $N = 4$.

A. Bases

1. E-basis in \mathbb{R}^N

Let us call the orthogonal ‘‘E-basis’’ the canonical basis in \mathbb{R}^N with basis vectors $E_i = \{0, \dots, 1, \dots, 0\}^T = \delta_{i,j}$ for $i, j \in \{1, \dots, N\}$. In this basis we define the $N = 4$ diagonal density matrix (ddm) ρ_d as the $N = 4$ vector $\vec{\lambda}_E^{(4)}$

$$\vec{\lambda}_E^{(4)} = \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \end{pmatrix}, \quad \sum_{i=1}^4 \lambda_i = 1, \quad \sum_{i=1}^4 \lambda_i^2 \equiv \mu_4. \quad (3)$$

2. The (nonorthogonal) P-basis: Vertices of the Weyl chamber (N - 1)-simplex in dimension N

We now define the vertices of the $(N - 1)$ -simplex of the Weyl chamber (denoted) $\tilde{\Delta}_{N-1}$ in dimension N Fig. 1(c) (right) as the vectors $\vec{P}_E^{(k,N)}$ as (here illustrated for $N = 4$)

$$\vec{P}_E^{(1,4)} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \vec{P}_E^{(2,4)} = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix},$$

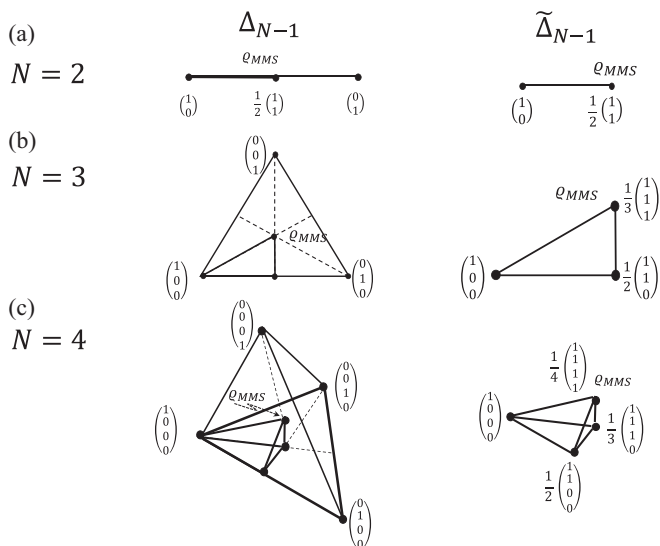


FIG. 1. (left) Eigenvalue simplex Δ_{N-1} and (right) Weyl chamber (WC) $\tilde{\Delta}_{N-1}$ for (a) $N = 2$, (b) $N = 3$, and (c) $N = 4$.

$$\vec{P}_E^{(3,4)} = \frac{1}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \quad \vec{P}_E^{(4,4)} = \frac{1}{4} \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \quad (4)$$

which should be read as *the MMS of dimension k embedded in dimension $N = 4$* . That is, for $N = 1$ we can regard the 0-Simplex as the 1D “vector” $\vec{P}_E^{(1,1)} \equiv (1)$. For $N = 2$ we embed $\vec{P}_E^{(1,1)} \equiv (1) \mapsto \vec{P}_E^{(1,2)} \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix} \in \mathbb{R}^2$, and then “add” the MMS in dimension $N = 2$ as $\vec{P}_E^{(2,2)} = \frac{1}{2} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, which are the vertices of the (one dimensional) 1-Simplex Δ_1 . For $N = 3$ we continue this process by embedding $\vec{P}_E^{(1,2)} \mapsto \vec{P}_E^{(1,3)}$ and $\vec{P}_E^{(2,2)} \mapsto \vec{P}_E^{(2,3)}$ in \mathbb{R}^3 , and then “adding” the MMS in dimension $N = 3$ as $\vec{P}_E^{(3,3)} = \frac{1}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$. Continuing this process for $N = 4$ produces Eq. (4), which can be trivially extended iteratively to arbitrary dimension N . Note that in dimension N , the vector $\vec{P}_E^{(1,N)}$ is a *pure state*, while $\vec{P}_E^{(N,N)}$ is the MMS for that dimension.

In dimension N , there are $N!$ ways to order the eigenvalues $\{\lambda_k\}$, $k \in \{1, \dots, N\}$ of the ddm ρ_d (in the E-basis). We define the *Weyl chamber* (WC) as the particular *descending order* $\{\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_N\}$, which is denoted as the $(N - 1)$ -simplex $\tilde{\Delta}_{N-1}$.

3. The (orthogonal) e -basis: The “in-WC” basis

We now form the e -basis, or the *in-WC* basis formed from normalized successive differences of the $\tilde{\Delta}_{N-1}$ vertex vectors $\vec{P}_E^{(k,N)}$ for $k \in \{0, \dots, N - 2\}$,

$$\hat{e}_1 = \frac{\vec{P}_E^{(N,N)}}{|\vec{P}_E^{(N,N)}|}, \quad \hat{e}_{k+2} = \frac{\vec{P}_E^{(N-(k+1),N)} - \vec{P}_E^{(N-k,N)}}{|\vec{P}_E^{(N-(k+1),N)} - \vec{P}_E^{(N-k,N)}|}. \quad (5)$$

For $N = 4$ these are the the normalized vectors $\{\vec{P}_E^{(4,4)}, \vec{P}_E^{(3,4)} - \vec{P}_E^{(4,4)}, \vec{P}_E^{(2,4)} - \vec{P}_E^{(3,4)}, \vec{P}_E^{(1,4)} - \vec{P}_E^{(2,4)}\} \mapsto \{\hat{e}_1, \hat{e}_2, \hat{e}_3, \hat{e}_4\}$. Here, \hat{e}_1 is a unit vector pointing from the origin to the MMS $\vec{P}_E^{(N,N)}$, and lies “outside” the WC. The vectors \hat{e}_{k+2} , $(k \in \{0, N - 2\})$ are then unit vectors that lie within

the WC and point from the embedded $(N - k)$ -dimensional MMS to the embedded $[N - (k + 1)]$ -dimensional MMS. We will designate the *orthogonal* matrix whose rows are the unit vectors \hat{e}_k as \mathbf{e} , and its transpose as \mathbf{e}^T . For $N = \{3, 4\}$ we explicitly have

$$\mathbf{e}_{N=3} = \begin{pmatrix} \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\sqrt{\frac{2}{3}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \end{pmatrix},$$

$$\mathbf{e}_{N=4} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{3}} & \frac{1}{2\sqrt{3}} & -\frac{\sqrt{3}}{2} \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{6}} & -\sqrt{\frac{2}{3}} & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \end{pmatrix}, \quad (6)$$

where $\mathbf{e}_N \cdot \mathbf{e}_N^T = \mathbf{1}$. These matrices will be useful for transforming (column) vectors \vec{p} between the E-basis $\in \mathbb{R}^N$ and the MMS-centered e -basis:

$$\vec{p}_{E\text{-basis}}^{(N)} = \mathbf{e} \cdot \vec{p}_{e\text{-basis}}^{(N)}, \quad \vec{p}_{e\text{-basis}}^{(N)} = \mathbf{e}^T \cdot \vec{p}_{E\text{-basis}}^{(N)}. \quad (7)$$

The utility of the particular formulation will be the simplicity (regularity) of the vector $\vec{\lambda}_e^{(N)}$ when transformed to the e -basis. For $N = 4$ we have $\vec{\lambda}_e^{(N)} = \mathbf{e} \cdot \vec{\lambda}_E^{(N)}$,

$$\vec{\lambda}_e^{(N)} = \begin{pmatrix} \frac{1}{2\sqrt{3}} [(\lambda_1 - \lambda_4) + (\lambda_2 - \lambda_4) + (\lambda_3 - \lambda_4)] \\ \frac{1}{\sqrt{2}\sqrt{3}} [(\lambda_1 - \lambda_3) + (\lambda_2 - \lambda_3)] \\ \frac{1}{\sqrt{2}} (\lambda_1 - \lambda_2) \end{pmatrix},$$

$$\equiv \begin{pmatrix} \frac{1}{2} \\ r_{\mu_4} \sin \varphi_3 \cos \varphi_2 \\ r_{\mu_4} \sin \varphi_3 \sin \varphi_2 \\ r_{\mu_4} \cos \varphi_3 \end{pmatrix}, \quad (8)$$

where we have defined the spherical coordinates $(r_{\mu_4}, \varphi_2, \varphi_3)$ on S^2 , which maps the WC tetrahedron to the ball with purity $\mu_4 \in [\frac{1}{4}, 1]$ for $N = 4$. (Note: the reason for the ordering of the components and the numbering of the angles starting from φ_2 will be made clear shortly). In fact, the first component of $\vec{\lambda}_e^{(4)}$ is actually $\sqrt{(\mu_{4,\min} = 1/4)} = 1/2$. For arbitrary N this generalizes to the first component being $\sqrt{(\mu_{N,\min} = 1/N)} = 1/\sqrt{N}$.

Note that the first matrix in Eq. (8) is written in such a way that in the WC each term in parenthesis is positive (greater or equal to zero). This implies that the tetrahedron for $N = 4$ has been mapped to the positive octant of S^2 (this is generalized for arbitrary N). Given a randomly generated $\vec{\lambda}_E^{(4)} \mapsto \vec{\lambda}_e^{(4)}$ we can back out the spherical coordinates as follows. Since $\mu_4 = \vec{\lambda}_E^{(4)} \cdot \vec{\lambda}_E^{(4)} = \vec{\lambda}_e^{(4)} \cdot \vec{\lambda}_e^{(4)} = \frac{1}{4} + r_{\mu_4}^2$ we have that $r_{\mu_4} = \sqrt{\mu_4 - 1/4}$. Comparing the terms in Eq. (8) yields for $N = 4$,

$$r_{\mu_4} = \sqrt{\mu_4 - 1/4}, \quad (9a)$$

$$\cos \varphi_3 = \frac{(\lambda_1 - \lambda_2)}{\sqrt{2} r}, \quad (9b)$$

$$\tan \varphi_2 = \sqrt{2} \frac{(\lambda_1 - \lambda_3) + (\lambda_2 - \lambda_3)}{(\lambda_1 - \lambda_4) + (\lambda_2 - \lambda_4) + (\lambda_3 - \lambda_4)}, \quad (9c)$$

showing that the spherical polar angles (φ_2, φ_3) on S^2 depend on the values of the eigenvalues selected.

In the next section we present a different parametrization of the WC, leading again to a mapping on the sphere S^{N-2} (via a transformation of an WC eigenvalue vector in the E-basis, to the e-basis, via \mathbf{e}) analogous to Eq. (8), but with a “nicer” (more amenable) structure.

**B. Parameterization of the WC in terms of its vertices $\vec{P}_E^{(k,N)}$:
Purity coordinates**

In this section we present a systematic parametrization of the WC in terms of its vertices $\vec{P}_E^{(k,N)}$. We will build this up recursively from $N = 2$ to a general N .

1. Derivation of the purity coordinates μ_k

For $N = 2$ the WC $\tilde{\Delta}_1$ is a one-dimensional line with a single coordinate interpolating between the pure state $\vec{P}_E^{(1,2)}$ and the MMS of dimension $N = 2$, $\vec{P}_E^{(2,2)}$ (i.e., a convex combination of the 2D vertices of the 1D line). Let us write a point $\vec{p}^{(N=2)_E}$ on this line in the E-basis as

$$\vec{p}_E^{(2)}(x_2) = x_2 \vec{P}_E^{(1,2)} + (1 - x_2) \vec{P}_E^{(2,2)}, \quad \text{Tr}[\vec{p}_E^{(2)}] = 1, \tag{10a}$$

$$1/2 \leq \mu_2 = \vec{p}_E^{(2)} \cdot \vec{p}_E^{(2)} \leq 1, \quad \vec{p}_E^{(2)}(x_2) = \vec{p}_E^{(2)}(\mu_2). \tag{10b}$$

Note that $\text{Tr}[\vec{p}_E^{(2)}] = 1$ follows since (i) $\text{Tr}[\vec{P}_E^{(k,N)}] = 1$ holds for every k -dimensional MMS embedded in dimension N , and (ii) by construction of Eq. (10a) we have made a convex combination of the vertices. Note that we have also defined the $N = 2$ purity μ_2 as $1/2 \leq \mu_2 = \vec{p}_E^{(2)} \cdot \vec{p}_E^{(2)} \leq 1$.

To extend this from the 1D line to the 2D triangle we need to add a new “polar angle” which we accomplish as follows:

$$\vec{p}_E^{(3)}(x_3, x_2) = x_3 \vec{p}_E^{(2)}(x_2) + (1 - x_3) \vec{P}_E^{(3,3)}, \tag{11a}$$

$$\text{Tr}[\vec{p}_E^{(3)}] = 1, \tag{11a}$$

$$= x_3(x_2 \vec{P}_E^{(1,3)} + (1 - x_2) \vec{P}_E^{(2,3)}) + (1 - x_3) \vec{P}_E^{(3,3)}, \tag{11b}$$

$$1/3 \leq \mu_3 = \vec{p}_E^{(3)} \cdot \vec{p}_E^{(3)} \leq 1,$$

$$\vec{p}_E^{(3)}(x_3, x_2) = \vec{p}_E^{(3)}(\mu_3, \mu_2). \tag{11c}$$

Equation (11a) states that we now have a convex combination of points $\vec{p}_E^{(2)}(x_2)$ on the 1D WC line, parameterized by the x_2 , or equivalent the $N = 2$ purity μ_2 , and the MMS in dimension $N = 3$, $\vec{P}_E^{(3,3)}$. The new coordinate that governs this convex combination from points on the 1D line $\tilde{\Delta}_1$ for $N = 2$ to points into the 2D triangle $\tilde{\Delta}_2$ for $N = 3$ is x_3 , or equivalently the $N = 3$ purity μ_3 . [Note: we will find it convenient to use both the x_k and μ_k coordinates, and later demonstrate that $x_k = x_k(\mu_k, \mu_{k-1})$ for each k . That is, for a fixed $k \geq 2$, x_k only depends on μ_k and μ_{k-1} , where we define $\mu_1 \equiv 1$.]

We now derive an important relationship between the x_k and the μ_k coordinates for $N = 3$, which readily generalizes

readily to arbitrary N . Consider the following calculation:

$$\begin{aligned} \mu_3 &= \vec{p}_E^{(3)} \cdot \vec{p}_E^{(3)}, \tag{12a} \\ &= [x_3 \vec{p}_E^{(2)} + (1 - x_3) \vec{P}_E^{(3,3)}]^2, \\ &= x_3^2 (\vec{p}_E^{(2)} \cdot \vec{p}_E^{(2)}) + 2x_3(1 - x_3) (\vec{p}_E^{(2)} \cdot \vec{P}_E^{(3,3)}) \\ &\quad + (1 - x_3)^2 (\vec{P}_E^{(3,3)} \cdot \vec{P}_E^{(3,3)}), \\ &= x_3^2 \mu_2 + 2x_3(1 - x_3) \mu_3^{(\min)} + (1 - x_3)^2 \mu_3^{(\min)}, \\ &= x_3^2 \mu_2 + (1 - x_3^2) \mu_3^{(\min)}, \end{aligned}$$

$$\Rightarrow x_3 = \sqrt{\frac{\mu_3 - \mu_3^{(\min)}}{\mu_2 - \mu_3^{(\min)}}}, \quad \mu_3^{(\min)} = 1/3, \quad \mu_1 \equiv 1, \tag{12b}$$

$$\Rightarrow x_k = \sqrt{\frac{\mu_k - \mu_k^{(\min)}}{\mu_{k-1} - \mu_k^{(\min)}}} = \sqrt{\frac{k \mu_k - 1}{k \mu_{k-1} - 1}}, \quad \mu_k^{(\min)} = 1/k. \tag{12c}$$

In the above we have used that for the MMS in dimension N , we have $\vec{P}_E^{(N,N)} = \frac{1}{N} (1, \dots, 1)$ so that $\vec{p}_E^{(k)} \cdot \vec{P}_E^{(N,N)} = \frac{1}{N} \text{Tr}[\vec{p}_E^{(k)}] = \frac{1}{N} = \mu_N^{(\min)}$. In addition, we also have $\vec{P}_E^{(N,N)} \cdot \vec{P}_E^{(N,N)} = \frac{1}{N} = \mu_N^{(\min)}$.

Equation (12c) is the central result of this approach, which then characterizes the ddm in dimension N in terms of all the purities $\{\mu_N, \mu_{N-1}, \dots, \mu_3, \mu_2\}$ of dimensions $k \in [2, N]$ [13].

For completeness, for the case of $N = 4$, we have

$$\begin{aligned} \vec{p}_E^{(4)}(x_4, x_3, x_2) &= x_4 \vec{p}_E^{(3)}(x_3, x_2) + (1 - x_4) \vec{P}_E^{(4,4)}, \\ \text{Tr}[\vec{p}_E^{(4)}] &= 1, \tag{13a} \\ &= x_4 \{x_3 [x_2 \vec{P}_E^{(1,3)} + (1 - x_2) \vec{P}_E^{(2,3)}] \\ &\quad + (1 - x_3) \vec{P}_E^{(3,3)}\} + (1 - x_4) \vec{P}_E^{(4,4)}, \tag{13b} \end{aligned}$$

$$1/4 \leq \mu_4 = \vec{p}_E^{(4)} \cdot \vec{p}_E^{(4)} \leq 1,$$

$$\vec{p}_E^{(4)}(x_4, x_3, x_2) = \vec{p}_E^{(4)}(\mu_4, \mu_3, \mu_2). \tag{13c}$$

2. $\vec{p}_E^{(4)}(x_4, x_3, x_2) \mapsto \vec{p}_e^{(4)}(x_4, x_3, x_2)$ and derivation of the angle constraints

Upon computing $\vec{p}_e^{(4)}(x_4, x_3, x_2) = \mathbf{e} \cdot \vec{p}_E^{(4)}(x_4, x_3, x_2)$ we obtain the very “nice” (regular) form

$$\begin{aligned} \vec{p}_e^{(4)}(x_4, x_3, x_2) &= \begin{pmatrix} \frac{1}{2} \\ \frac{1}{\sqrt{4 \cdot 3}} x_4 \\ \frac{1}{\sqrt{3 \cdot 2}} x_4 x_3 \\ \frac{1}{\sqrt{2 \cdot 1}} x_4 x_3 x_2 \end{pmatrix} \\ &\equiv \begin{pmatrix} \frac{1}{2} \\ r_{\mu_4} \cos \varphi_3 \\ r_{\mu_4} \sin \varphi_3 \cos \varphi_2 \\ r_{\mu_4} \sin \varphi_3 \sin \varphi_2 \end{pmatrix}, \tag{14} \end{aligned}$$

where we have introduced the polar and azimuthal angles φ_3 and φ_2 , respectively, and the radius $r_{\mu_4} = \sqrt{\mu_4 - 1/4}$ as before. Note that we have also permuted the order of the spherical coordinates to make an easier identification with the

x_k coordinates. By taking ratios of the coordinates we can easily determine that

$$x_4 = 2\sqrt{3}r_{\mu_4} \cos \varphi_3, \tag{15}$$

$$x_3 = \frac{1}{\sqrt{2}} \tan \varphi_3 \cos \varphi_2, \tag{16}$$

$$x_2 = \frac{1}{\sqrt{3}} \tan \varphi_2. \tag{17}$$

Note that since a ddm in the WC is a valid convex combinations of WC vertices, we must require *in general* that for each

$k, 0 \leq x_k \leq 1$. If we now employ Eq. (12c), a little algebra reveals that

$$\tan \varphi_2 = \sqrt{3}x_2 = \sqrt{3} \sqrt{\frac{2\mu_2 - 1}{2\mu_1 - 1}} = \sqrt{3} \sqrt{2\mu_2 - 1}, \tag{18a}$$

$$\begin{aligned} \tan \varphi_3 &= \frac{\sqrt{2}}{\cos \varphi_2} x_3 = \sqrt{2} (\sqrt{2} \sqrt{3\mu_2 - 1}) \sqrt{\frac{3\mu_3 - 1}{3\mu_2 - 1}} \\ &= \sqrt{4} \sqrt{3\mu_3 - 1}. \end{aligned} \tag{18b}$$

We can easily prove by induction that for arbitrary k the above pattern generalizes to

$$\tan \varphi_k = \sqrt{k+1} \sqrt{k\mu_k - 1}, \Rightarrow 0 \leq \tan \varphi_k \leq \sqrt{k^2 - 1}, \tag{19a}$$

$$\Rightarrow \sin \varphi_k = \sqrt{\frac{k+1}{k}} \sqrt{\frac{k\mu_k - 1}{(k+1)\mu_k - 1}}, \Rightarrow 0 \leq \sin \varphi_k \leq \frac{\sqrt{k^2 - 1}}{k}, \tag{19b}$$

$$\Rightarrow \cos \varphi_k = \frac{1}{\sqrt{k}} \frac{1}{\sqrt{(k+1)\mu_k - 1}}, \Rightarrow \frac{1}{k} \leq \cos \varphi_k \leq 1, \tag{19c}$$

where we obtained the bounds on the above angles by examining the expressions on the left at $\mu_k \rightarrow \mu_k^{(\min)} = 1/k$ and $\mu_k \rightarrow \mu_k^{(\max)} = 1$.

Finally, let us examine the condition $0 \leq x_k \leq 1$ (for creating convex combinations of vertices) and the restrictions on the angles as given above to obtain

$$\begin{aligned} 0 \leq x_4 = \sqrt{2}\sqrt{3}r_{\mu_4} \cos \varphi_3 \leq 1 &\Rightarrow \left(0 \leq \cos \varphi_3 \leq \frac{1}{\sqrt{2}\sqrt{3}r_{\mu_4}}\right) \cap \left(\frac{1}{3} \leq \cos \varphi_3 \leq 1\right), \\ &\Rightarrow \frac{1}{3} \leq X_3 \equiv \cos \varphi_3 \leq \text{Min}\left[\frac{1}{\sqrt{2}\sqrt{3}r_{\mu_4}}, 1\right], \end{aligned} \tag{20a}$$

and

$$\begin{aligned} 0 \leq x_3 = \frac{1}{\sqrt{2}} \tan \varphi_3 \cos \varphi_2 \leq 1 &\Rightarrow \left(0 \leq \cos \varphi_2 \leq \frac{\sqrt{2}}{\tan \varphi_3}\right) \cap \left(\frac{1}{2} \leq \cos \varphi_2 \leq 1\right), \\ &\Rightarrow \frac{1}{2} \leq \cos \varphi_2 \leq \text{Min}\left[\frac{\sqrt{2}}{\tan \varphi_3}, 1\right], \end{aligned} \tag{20b}$$

$$\Rightarrow \cos^{-1}\left(\text{Min}\left[\frac{\sqrt{2}}{\tan \varphi_3}, 1\right]\right) \leq X_2 = \varphi_2 \leq \cos^{-1}(1/2) = \frac{\pi}{3}. \tag{20c}$$

In the above we have defined the uniform deviates $X_3 = \cos \varphi_3$ and $X'_2 = \varphi_2$, since the volume element on $\mathbb{R}^3 = \mathbb{R} \times S^2$ is given by

$$\begin{aligned} dV &= dr (r d\varphi_3) (r \sin \varphi_3 d\varphi_2) = dr r^2 \sin \varphi_3 d\varphi_3 d\varphi_2, \\ &= d(r^3/3) d(\cos \varphi_3) d(\varphi_2), \end{aligned} \tag{21a}$$

$$\equiv dX_4 dX_3 dX'_2, \Rightarrow \text{(flat)}, \tag{21b}$$

$$\text{with } X_4 = r^3/3, \quad X_3 = \cos \varphi_3, \quad X'_2 = \varphi_2, \tag{21c}$$

[modulo an insignificant minus sign on $d(\cos \varphi_3)$ which simply changes the order of the upper and lower bounds; the volume comes from a Jacobian which involves an absolute value so that this sign drops out, i.e., $|-1| = 1$]. The implication of the above is that the variables that constitute the

uniform deviates are $X_3 = \cos \varphi_3$ and $X'_2 = \varphi_2$ [i.e., not the angles (φ_3, φ_2) directly]. The variables X_3 and X'_2 should be chosen *uniformly* over the range of their upper and lower limits. Determining those limits is the whole issue at hand here.

C. Angle ranges for arbitrary N

To generalize the above formulas for arbitrary N , it is instructive to write out the x_k for $N = \{2, 3, 4, 5, 6\}$ to discern the general pattern by induction:

$$N = 2 : x_2 = \sqrt{2} \cdot 1 r_2 \cos \varphi_1 = \sqrt{2} r_2, \quad (\varphi_1 \equiv \pi/2), \tag{22a}$$

$$N = 3 : x_2 = \frac{\tan \varphi_2}{\sqrt{3}}, \quad x_3 = \sqrt{3} \cdot 2 r_3 \cos \varphi_2, \tag{22b}$$

$$N = 4 : x_2 = \frac{\tan \varphi_2}{\sqrt{3}}, \quad x_3 = \frac{\cos \varphi_2 \tan \varphi_3}{\sqrt{2}},$$

$$x_4 = \sqrt{4 \cdot 3} r_4 \cos \varphi_3, \tag{22c}$$

$$x_5 = \sqrt{\frac{2}{3}} \cos \varphi_4 \tan \varphi_5,$$

$$x_6 = \sqrt{6 \cdot 5} r_6 \cos \varphi_5, \tag{22e}$$

$$N = 5 : x_2 = \frac{\tan \varphi_2}{\sqrt{3}}, \quad x_3 = \frac{\cos \varphi_2 \tan \varphi_3}{\sqrt{2}},$$

$$x_4 = \sqrt{\frac{3}{5}} r_4 \cos \varphi_3 \tan \varphi_4,$$

$$x_5 = \sqrt{5 \cdot 4} r_5 \cos \varphi_5, \tag{22d}$$

$$N = 6 : x_2 = \frac{\tan \varphi_2}{\sqrt{3}}, \quad x_3 = \frac{\cos \varphi_2 \tan \varphi_3}{\sqrt{2}},$$

$$x_4 = \sqrt{\frac{3}{5}} \cos \varphi_3 \tan \varphi_4,$$

with $r_k = \sqrt{\mu_k - 1/k}$. From inspection of the above equations a general pattern is deduced. For a given N , we have the $N - 2$ angles ($\varphi_2; \varphi_{k \in \{3, \dots, N-2\}}; \varphi_{N-1}$) which we denote as lowest angle: φ_2 , middle angles: $\varphi_{k \in \{3, \dots, N-2\}}$, and highest angle: φ_{N-1} , which form the angles of an $(N - 2)$ -sphere $S^{(N-2)}$ for a fixed radius r_k . Further, the condition (range) on the variables $0 \leq \{x_k\} \leq 1$ for $k \in \{1, 2, \dots, N\}$ used to construct the convex combinations of vertices in the WC are given for arbitrary N by

$$\text{radius: } 0 \leq r_{\mu_N} \equiv \sqrt{\mu_N - 1/N} \leq \sqrt{1 - 1/N}, \quad 1/N \leq \mu_N \equiv \text{Tr}[\rho_N^2] \leq 1, \tag{23a}$$

$$\text{highest indexed angle: } 0 \leq x_N = \frac{\cos \varphi_{N-1}}{\left(\frac{1}{\sqrt{N(N-1)}} r_{\mu_N}\right)} \equiv \frac{X_{N-1}}{\bar{X}_{N-1}} \leq 1, \tag{23b}$$

$$\text{middle indexed angles: } 0 \leq x_k = \cos \varphi_{k-1} \frac{\tan \varphi_k}{\sqrt{\frac{k+1}{k-1}}} \leq 1, \quad k \in \{3, \dots, N - 1\}, \tag{23c}$$

$$\text{smallest indexed angle: } 0 \leq x_2 = \frac{\tan \varphi_2}{\sqrt{3}} \leq 1, \tag{23d}$$

where we have defined the variable (capital) $X_k \equiv \cos \varphi_k$ which satisfies

$$\frac{1}{k} \leq X_k \equiv \cos \varphi_k \equiv \frac{1}{\sqrt{k}} \frac{1}{\sqrt{(k+1)\mu_k - 1}} \leq 1,$$

$$\frac{1}{k} \leq \mu_k \leq 1, \tag{24}$$

where the left and right bounds in Eq. (24) arise from evaluating the $\cos \varphi_k$ at $\mu_k = 1$ and $\mu_k = 1/k$, respectively.

In addition to the bounds imposed by the definition of $X_k \equiv \cos \varphi_k$, we must also impose the range restrictions Eqs. (23a)–(23d) imposed by the coefficients $\{x_k\}$ (little “x”) of the convex combinations of WC vertices. For this, we note the following:

$$0 \leq \tan \varphi_k \equiv \sqrt{k+1} \sqrt{k \mu_k - 1},$$

$$= \frac{\sqrt{1 - X_k^2}}{X_k} \leq \sqrt{k^2 - 1}, \quad \frac{1}{k} \leq \mu_k \leq 1. \tag{25}$$

Therefore, the constraint Eq. (23d) becomes (shifting $k \rightarrow k + 1$)

$$\frac{1}{k} \leq X_k \equiv \cos \varphi_k \leq \text{Min} \left[\frac{\sqrt{\frac{k+2}{k}} X_{k+1}}{\sqrt{1 - X_{k+1}^2}}, 1 \right],$$

$$k \in \{2, \dots, N - 2\}, \tag{26a}$$

$$\Rightarrow \cos^{-1} \left(\text{Min} \left[\frac{\sqrt{\frac{k+2}{k}} X_{k+1}}{\sqrt{1 - X_{k+1}^2}}, 1 \right] \right) \leq \varphi_k \leq \cos^{-1}(1/k), \tag{26b}$$

where we have used the fact that since $\cos(\varphi)$ is monotonically decreasing for our range of interest, then $a \leq \cos(\varphi) \leq b \Rightarrow \cos^{-1}(b) \leq \varphi \leq \cos^{-1}(a)$. For the lowest indexed angle φ_2 , we additionally have the constraint Eq. (23d), $0 \leq \tan \varphi_2 \leq \sqrt{3} \Rightarrow 0 \leq \tan^{-1}(\sqrt{3}) = \cos^{-1}(1/2) = \pi/3$, which is self-consistent with Eq. (26b) for $k = 2$. The constraint for the highest indexed angle X_{N-1} for the variable $0 \leq x_N \leq 1$ can be written from Eq. (26b) as

$$\frac{1}{N - 1} \leq X_{N-1} = \cos \varphi_{N-1}$$

$$\leq \bar{X}_{N-1} \equiv \text{Min} \left\{ \frac{1}{[r_{\mu_N} \sqrt{N(N-1)}]}, 1 \right\}, \tag{27a}$$

$$\Rightarrow \cos^{-1} \left(\text{Min} \left\{ \frac{1}{[r_{\mu_N} \sqrt{N(N-1)}]}, 1 \right\} \right)$$

$$\leq \varphi_{N-1} \leq \cos^{-1} \left(\frac{1}{N - 1} \right), \tag{27b}$$

where the limits on $0 \leq r_{\mu_N} \equiv \sqrt{\mu_N - 1/N} \leq \sqrt{1 - 1/N}$, are given by Eq. (23a).

The important point to note here is that $X_k^{(\text{min})} = 1/k$, while $X_k^{(\text{max})} = X_k^{(\text{max})}(X_{k+1})$, namely, the upper limit of X_k is a function of the value of X_{k+1} . This means that in terms of nested integrals, we can give the values of the highest indexed X_k , which will determine the range of integration over the lower indexed $X_{k' < k}$. In terms of computing the CDFs, we should start from X_2 (or φ_2) and integrate “upwards” successively in the angle variables $X_2 \rightarrow X_3 \rightarrow \dots \rightarrow X_{N-1}$. After integration over these angle variables, we can then integrate over the

radius variable r_{μ_N} to find the CDF for the distribution of density matrices as a function of their purity.

In applying these formulas for generating density matrices of fixed purity, we actually work “downwards,” i.e., given an r_N , we then uniformly sample X_{N-1} whose upper bound is determined by the former. The sampled value of X_{N-1} then determines the upper bound of X_{N-2} , the next lower angle moving downwards. The sampled value of X_{N-2} then determines the upper bound of X_{N-3} , and so on, until we reach X_2 (although for this lowest angle we will work with φ_2 directly).

In the following section we will illustrate these analytic formulas for the case of $N = 2$ (which is trivial), and $N = 3$ (qutrit) and $N = 4$ (two qubits). We then indicate the minor changes that occur for $N = 5$, which is the first dimension with proper lowest, middle and highest angles, from which the case of arbitrary $N > 5$ is readily inferred.

D. Volume element for arbitrary N

For a given value of N , we have defined above coordinates on an $(N - 2)$ -sphere S^{N-2} with volume element given by

$$dV = r_{\mu_N}^{N-2} dr_{\mu_N} d\varphi_2 d\varphi_3 \dots d\varphi_{N-1} \sin \varphi_3 \sin \varphi_4^2 \dots \sin \varphi_{N-1}^{N-3}, \quad (28a)$$

$$= r_{\mu_N}^{N-2} dr_{\mu_N} \prod_{k=2}^{N-1} \sin^{k-2} \varphi_k d\varphi_k. \quad (28b)$$

In particular, we have

$$N = 2 : dV_2 = dr_2, \quad (29a)$$

$$N = 3 : dV_3 = dr_3 d\varphi_2, \quad (29b)$$

$$N = 4 : dV_4 = r_{\mu_4}^2 dr_{\mu_4} (\sin \varphi_3 d\varphi_3) (d\varphi_2) \equiv r_{\mu_4}^2 dr_{\mu_4} dX_3 d\varphi_2, \quad (29c)$$

$$N = 5 : dV_5 = r_{\mu_5}^3 dr_{\mu_5} (\sin^2 \varphi_4 d\varphi_4) (\sin \varphi_3 d\varphi_3) (d\varphi_2) \equiv r_{\mu_5}^3 dr_{\mu_5} (1 - X_4^2)^{1/2} dX_4 dX_3 d\varphi_2, \quad (29d)$$

$$N : \Rightarrow dV_N = r_{\mu_N}^{N-2} dr_{\mu_N} \left(\prod_{k=3}^{N-1} (1 - X_k^2)^{(k-3)/2} dX_k \right) d\varphi_2, \quad (29e)$$

$$X_k = \cos \varphi_k, \quad k \in \{2, \dots, N - 1\}. \quad (29f)$$

Note that while in general $X_k \leftrightarrow \cos \varphi_k$, the variable φ_2 is already a uniform deviate, so we have separated it out. That is, the definition of $\cos \varphi_k = \{k[(k + 1)\mu_k - 1]\}^{-1/2}$ holds for all $k \in \{2, \dots, N - 1\}$, while the assignment $X_k \rightarrow \cos \varphi_k$ holds for $k \in \{3, \dots, N - 1\}$.

Integrating out successive sets of variables, starting from the lowest angle ($k = 2$), to the highest angle ($k = N - 1$), and then over the radius variable ($k = N$), will produced the desire cumulative distribution functions from which we can uniformly sample the variables.

IV. ANALYTIC CDFs FOR $N = \{2, 3, 4\}$

For $N = \{2, 3, 4\}$ the above formulas can be computed analytically. They are then very informative explicit examples

of the type of features exhibited in the CDF for larger values of N .

A. $N = 2$: A single qubit

In this section we give more details on the derivation of the cumulative distribution functions for $N = 2$. This is in fact a trivial case, but it serves to illustrate the previous applicability of the general formulas at the “boundary condition” of the smallest density matrix dimension, $N = 2$. For $N = 2$ we have $\bar{p}_e^{(2)}(x_2)$ given by

$$N = 2 : \bar{p}_e^{(2)}(x_2) = \left(\frac{1}{\sqrt{2}} \right)_{\frac{1}{\sqrt{2.1}} x_2} \equiv \left(\frac{1}{\sqrt{2}} \right)_{r_2 \cos \varphi_1}, \quad (30)$$

$$r_2 = \sqrt{\mu_2 - 1/2}.$$

This implies $0 \leq x_2 = \sqrt{2} r_2 \cos \varphi_1 \leq 1$. However, from the general formula $\frac{1}{k} |_{\mu_k=1} \leq X_k = \cos \varphi_k = \frac{1}{\sqrt{k} \sqrt{(k+1)\mu_k - 1}} \leq 1 |_{\mu_k=\frac{1}{k}}$, we have for $k = 1$ and $\mu_1 \stackrel{\text{def}}{=} 1$ that $1 \leq X_1 = \cos \varphi_1 \leq 1 \Rightarrow \cos \varphi_1 = \frac{\pi}{2}$. This implies that $0 \leq x_2 = \sqrt{2} r_2 = \sqrt{2 \mu_2 - 1} \leq 1$, which is consistent with $\mu_4^{(1)} \in [\frac{1}{2}, 1]$. Since x_2 is uniformly distributed in $x_2 \in [0, 1]$, then so is r_2 in $r_2^{(1)} \in [0, \frac{1}{\sqrt{2}}]$. Both of these variables act as the coordinate along the 1D simplex in Fig. 1(a). We therefore have

$$F_2^{(N=2)}(r_2) = \frac{\int_0^{r_2 \leq r_2^{\max}=1/\sqrt{2}} dr'_2}{\int_0^{r_2^{\max}=1/\sqrt{2}} dr'_2} = \frac{r_2}{1/\sqrt{2}} = \sqrt{2 \mu_2 - 1}, \quad (31a)$$

$$\equiv \frac{F_2^{(N=2)\text{Num}}(r_2)}{F_2^{(N=2)\text{Denom}}} \quad (31b)$$

where we have employed the notation (to be used henceforth) $F_k^{(N)}$ to indicate the CDF for the variable X_k for a given dimension N . Note that in this “boundary condition” case of $N = 2$ there are no angles φ_k ; only the radius vector r_2 . In Eq. (31b) we have introduced the notation $F_2^{(N=2)\text{Num}}(r_2)$ and $F_2^{(N=2)\text{Denom}}$ where the latter is the CDF normalizing denominator. The difference in the two expressions is that the denominator $F_2^{(N=2)\text{Denom}}$ is integrated over the full range of the variable $r'_2 \in [0, r_2^{\max} = \frac{1}{\sqrt{2}}]$ while the numerator $F_2^{(N=2)\text{Num}}$ is integrated over $r'_2 \in [0, r_2 \leq r_2^{\max}]$. We will see that the denominator expressions are then reused in iterated integrals for the computation of CDFs for larger N . For larger dimensions, and for the middle angles we will have that $F_k^{(N)\text{Num}}(X_k; X_{k+1})$ represents the numerator of the CDF for X_k , whose upper limits depends on the choice of the next higher up “angle” X_{k+1} , while $F_k^{(N)\text{Denom}}(X_{k+1})$ represents the normalizing denominator. This notation will be used throughout the rest of this work.

B. $N = 3$: A single qutrit

For $N = 3$, the eigenvalue simplex is an equilateral triangle Fig. 1(b) (left) with coordinates (φ_2, r_3) . Here, the new polar angle φ_2 is measured relative to the $N = 3$ MMS Fig. 1(b) (right). Since the volume element is $dV_2 = dr_3 d\varphi_2$ we shall always use the angle φ_2 directly (versus our use of $X_k \equiv \cos \varphi_k$ for $k \geq 3$).

For $N = 3$ we have $\vec{p}_e^{(3)}(x_2, x_3)$ given by

$$\vec{p}_e^{(3)}(x_2, x_3) = \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3.2}} x_2 \\ \frac{1}{\sqrt{2.1}} x_3 x_2 \end{pmatrix} \equiv \begin{pmatrix} \frac{1}{\sqrt{3}} \\ r_3 \cos \varphi_2 \\ r_3 \sin \varphi_2 \end{pmatrix},$$

$$r_3 = \sqrt{\mu_3 - 1/3}. \tag{32}$$

This implies $0 \leq x_2 = \sqrt{6} r_3 \cos \varphi_2 \leq 1$. However, from the general formula $\frac{1}{k} |_{\mu_k=1} \leq X_k = \cos \varphi_k = \frac{1}{\sqrt{k}} \frac{1}{\sqrt{(k+1)\mu_k-1}} \leq 1 |_{\mu_k=\frac{1}{k}}$, we have for $k = 2$ that $\frac{1}{2} \leq X_2 = \cos \varphi_2 \leq 1$. This implies that $0 \leq x_2 = \sqrt{6} r_3 \cos \varphi_2 \leq 1$, or that

$$\frac{1}{2} \leq X_2 \equiv \cos \varphi_2 \leq 1, \tag{33a}$$

$$\Rightarrow \bar{\varphi}_2^{\min}(r_3) \equiv \cos^{-1} \left(\text{Min} \left[\frac{1}{\sqrt{3.2} r_3}, 1 \right] \right) \leq \varphi_2 \leq \cos^{-1} \left(\frac{1}{2} \right) = \frac{\pi}{3} \equiv \bar{\varphi}_2^{\max}, \tag{33b}$$

$$\text{where } \bar{\varphi}_2^{\min} = \begin{cases} 0, & r_3^{(1)} \in [0, \frac{1}{\sqrt{3.2}}] \leftrightarrow \mu_3^{(1)} \in [\frac{1}{3}, \frac{1}{2}], \\ \cos^{-1} \left(\frac{1}{\sqrt{3.2} r_3} \right) \equiv \tilde{\varphi}_2(r_3), & r_3^{(2)} \in [\frac{1}{\sqrt{3.2}}, \sqrt{\frac{2}{3}}] \leftrightarrow \mu_3^{(2)} \in [\frac{1}{2}, 1], \end{cases} \tag{33c}$$

where for notational convenience we have defined $\bar{\varphi}_2(r_3) \stackrel{\text{def}}{=} \cos^{-1} \left(\frac{1}{\sqrt{3.2} r_3} \right)$. In Eq. (33b) we see that the upper limit of the angle φ_2 is always $\bar{\varphi}_2^{\max} = \frac{\pi}{3}$, while the lower limit $\bar{\varphi}_2^{\min}(r_3)$ depends on the selection of the radius $r_3 = \sqrt{\mu_3 - 1/3}$. Since $X_2 = \cos \varphi_2 \leq \frac{1}{\sqrt{6} r_3}$, $\bar{\varphi}_2^{\min}(r_3)$ naturally breaks up into two regions depending on the magnitude of $\frac{1}{\sqrt{6} r_3}$ being greater or less than unity. The dividing (or ‘‘breakpoint’’) occurs when $\frac{1}{\sqrt{6} r_3} = 1$ corresponding to $\mu_3 = \frac{1}{3}$.

We will see that this last result is a general feature, namely, for the highest angle φ_{N-1} (φ_2 in this case), its range of values will always be divided into two regions $[\frac{1}{N}, \frac{1}{N-1}] \cup [\frac{1}{N-1}, 1]$. It will be seen that the first purity region $\mu_N^{(1)} \equiv [\frac{1}{N}, \frac{1}{N-1}]$ (where in general we define the μ_N -regions $\mu_N^{(i)} \stackrel{\text{def}}{=} [\frac{1}{N-(i-1)}, \frac{1}{N-i}]$ for $i \in \{1, \dots, N-1\}$), is where the diagonal density matrices in the simplex are uniformly distributed. The purity value $\mu_N = \frac{1}{N-1}$ is the largest ‘‘ μ -radius’’ for which the sphere $S^{(N-2)}$ can be inscribed within the $N-1$ simplex $\Delta^{(N-1)}$ (the ‘‘in-sphere,’’ see Ref. [3]). For the regions $\mu_N^{(i>1)}$ the sphere of fixed μ -radius extends beyond the simplex $\Delta^{(N-1)}$, and intersects it in disjoint regions, which this work

details for the WC. The other $N! - 1$ regions of $\Delta^{(N-1)}$ are easily obtained by first randomly permuting the values of the diagonal density $\rho_{N,d}$ matrices before applying the unitary similarity transformation to obtain the density matrix $\rho_N = U \rho_{N,d} U^\dagger$.

We now compute the angle φ_2 , and radius r_3 , CDFs for $N = 3$ illustrating the complex dependency of their limits upon each other. This will be needed for subsequent calculations of CDFs for $N \geq 4$.

1. CDF $F_2^{(N=3)}(\varphi_2; r_3)$

Using the above expressions for $\bar{\varphi}_2^{\min}(r_3)$, we then have

$$F_2^{(N=3)}(\varphi_2; r_3) = \frac{\int_{\bar{\varphi}_2^{\min}(r_3)}^{\varphi_2 \leq \bar{\varphi}_2^{\max} = \pi/3} d\varphi'_2}{\int_{\bar{\varphi}_2^{\min}(r_3)}^{\bar{\varphi}_2^{\max} = \pi/3} d\varphi'_2} = \frac{\varphi_2 - \bar{\varphi}_2^{\min}(r_3)}{\pi/3 - \bar{\varphi}_2^{\min}(r_3)}$$

$$\equiv \frac{F_2^{(N=3)\text{Num}}(\varphi_2; r_3)}{F_2^{(N=3)\text{Denom}}(r_3)}. \tag{34}$$

We compute the r_3 -dependent denominator $F_2^{(N=3)\text{Denom}}(r_3)$ as follows:

$$F_2^{(N=3)\text{Denom}}(r_3) = \begin{cases} \int_{\bar{\varphi}_2^{\min}(r_3)=0}^{\bar{\varphi}_2^{\max}=\pi/3} d\varphi'_2 = \frac{\pi}{3}, & r_3^{(1)} \in [0, \frac{1}{\sqrt{3.2}}], \\ \int_{\bar{\varphi}_2^{\min}(r_3)=\tilde{\varphi}_2(r_3)}^{\bar{\varphi}_2^{\max}=\pi/3} d\varphi'_2 = \frac{\pi}{3} - \cos^{-1} \left(\frac{1}{\sqrt{3.2} r_3} \right), & r_3^{(2)} \in [\frac{1}{\sqrt{3.2}}, \sqrt{\frac{2}{3}}]. \end{cases} \tag{35}$$

We therefore have

$$F_2^{(N=3)}(\varphi_2; r_3) = \begin{cases} \frac{\varphi_2}{\frac{\pi}{3}}, & r_3^{(1)} \in [0, \frac{1}{\sqrt{3.2}}], \\ \frac{\varphi_2 - \cos^{-1} \left(\frac{1}{\sqrt{3.2} r_3} \right)}{\frac{\pi}{3} - \cos^{-1} \left(\frac{1}{\sqrt{3.2} r_3} \right)}, & r_3^{(2)} \in [\frac{1}{\sqrt{3.2}}, \sqrt{\frac{2}{3}}]. \end{cases} \tag{36}$$

2. $F_3^{(N=3)}(r_3)$

To compute the radial CDF $F_3^{(N=3)}(r_3)$ we use the expression above for $F_2^{(N=3)\text{Denom}}(r_3)$ in Eq. (35)

$$F_3^{(N=3)}(r_3) = \frac{\int_0^{r_3 \leq r_3^{\max} = \sqrt{2/3}} dr'_3 r'_3 F_2^{(N=3)\text{Denom}}(r'_3)}{\int_0^{r_3^{\max} = \sqrt{2/3}} dr'_3 r'_3 F_2^{(N=3)\text{Denom}}(r'_3)}, \quad (37a)$$

$$\equiv \frac{F_3^{(N=3)\text{Num}}(r_3)}{F_3^{(N=3)\text{Denom}}}. \quad (37b)$$

Here, $F_3^{(N=3)\text{Denom}}$ is integrated over the whole range of $r_3 \in r_3^{(1)} \cup r_3^{(2)} = [0, \frac{1}{\sqrt{3.2}}] \cup [\frac{1}{\sqrt{3.2}}, \sqrt{\frac{2}{3}}]$, and hence is a

constant. Using Eq. (35) we have

$$F_3^{(N=3)\text{Denom}} = \int_0^{\frac{1}{\sqrt{6}}} dr'_3 r'_3 \frac{\pi}{3} + \int_{\frac{1}{\sqrt{6}}}^{r_3^{\max} = \sqrt{2/3}} dr'_3 r'_3 \times \left[\frac{\pi}{3} - \cos^{-1} \left(\frac{1}{\sqrt{3 \cdot 2} r_3} \right) \right] = \frac{1}{4\sqrt{3}}. \quad (38)$$

We then have for $r_3^{(1)} \in [0, \frac{1}{\sqrt{3.2}}] \leftrightarrow \mu_3^{(1)} \in [\frac{1}{3}, \frac{1}{2}]$, and $r_3^{(2)} \in [\frac{1}{\sqrt{3.2}}, \sqrt{\frac{2}{3}}] \leftrightarrow \mu_3^{(2)} \in [\frac{1}{2}, 1]$,

$$F_3^{(N=3)}(r_3) = \frac{\int_0^{r_3 \leq \frac{1}{\sqrt{6}}} dr'_3 r'_3 \frac{\pi}{3}}{F_3^{(N=3)\text{Denom}}} = \frac{\frac{\pi r_3^2}{6}}{\frac{1}{4\sqrt{3}}} = \frac{2\pi r_3^2}{\sqrt{3}}, \quad (39a)$$

$$= \frac{\int_0^{\frac{1}{\sqrt{6}}} dr'_3 r'_3 \frac{\pi}{3} + \int_{\frac{1}{\sqrt{6}}}^{r_3 \leq \sqrt{\frac{2}{3}}} dr'_3 r'_3 \left[\frac{\pi}{3} - \cos^{-1} \left(\frac{1}{\sqrt{3 \cdot 2} r'_3} \right) \right]}{F_3^{(N=3)\text{Denom}}}, \quad (39b)$$

$$\equiv \frac{g_3^{(N=3)}(r_3)}{\frac{1}{4\sqrt{3}}}, \quad (39c)$$

$$g_3^{(N=3)}(r_3) = \frac{1}{12} \left[2\pi r_3^2 + \sqrt{6r_3^2 - 1} - 6r_3^2 \cos^{-1} \left(\frac{1}{\sqrt{6}r_3} \right) \right]. \quad (39c)$$

Note that as a function of purity μ_3 we simply substitute for these expressions $r_3 \rightarrow \sqrt{\mu_3 - 1/3}$, i.e., $F_3^{(N=3)}(\mu_3) = F_3^{(N=3)}(r_3 = \sqrt{\mu_3 - 1/3})$. We will hold off plotting these CDFs until after the next section where we compute the CDFs for $N = 4$.

C. $N = 4$: A pair of qubits

For the case of $N = 4$, representing a pair of qubits, we have the variables $(\varphi_2, X_3 = \cos \varphi_3, r_4)$, with volume element $dV_4 = r_4^2 dr_4 dX_3 d\varphi_2$. In this section we analytically compute the CDFs $F_2^{(N=4)}(\varphi_2; X_3)$, $F_3^{(N=4)}(X_3; r_4)$, and $F_4^{(N=4)}(r_4)$ where the $F_k^{(N=4)}$ are functions of the first argument, for fixed selected value of the second argument. For $N = 4$ the lower angle is φ_2 , there are no middle angles, and the highest angle is X_3 . As such we now have the limiting values of φ_2 and X_3 given by

$$\bar{\varphi}_2^{\min}(X_3) = \cos^{-1} \left(\text{Min} \left[\bar{X}_2(X_3) \equiv \frac{\sqrt{2}X_3}{\sqrt{1-X_3^2}}, 1 \right] \right), \quad (40a)$$

$$= \begin{cases} \cos^{-1}(\bar{X}_2(X_3)), & X_3 \in [\frac{1}{3}, \frac{1}{\sqrt{3}}] \equiv X_3^{(I)}, \\ 0, & X_3 \in [\frac{1}{\sqrt{3}}, 1] \equiv X_3^{(II)}, \end{cases} \quad (40b)$$

$$X_3^{\max}(r_4) = \text{Min} \left[\bar{X}_3(r_4) \equiv \frac{1}{\sqrt{4 \cdot 3} r_4}, 1 \right], \quad (40c)$$

$$= \begin{cases} 1, & r_4 \in [0, \frac{1}{2\sqrt{3}}] \leftrightarrow \mu_4 \in [\frac{1}{4}, \frac{1}{3}], \\ \frac{1}{2\sqrt{3} r_4}, & r_4 \in [\frac{1}{2\sqrt{3}}, 1] \leftrightarrow \mu_4 \in [\frac{1}{3}, 1], \end{cases} \quad (40d)$$

with $\bar{\varphi}_2^{\max} \equiv \frac{\pi}{3}$, and $X_k^{(\min)} = \frac{1}{k}$ for all N .

1. CDF: $F_2^{(N=4)}(\varphi_2; X_3)$

For the CDF of φ_2 , given a value of X_3 , which we denote as $F_2^{(N=4)}(\varphi_2; X_3)$, we have

$$F_2^{(N=4)}(\varphi_2; X_3) = \frac{\int_{\bar{\varphi}_2^{\min}(X_3)}^{\varphi_2 \leq \pi/3} d\varphi'_2}{\int_{\bar{\varphi}_2^{\min}(X_3)}^{\pi/3} d\varphi'_2}, \quad (41a)$$

$$\equiv \frac{F_2^{(N=4)\text{Num}}(\varphi_2; X_3)}{F_2^{(N=4)\text{Denom}}(X_3)}, \quad (41b)$$

$$= \begin{cases} \frac{\varphi_2 - \cos^{-1} \left(\frac{\sqrt{2}X_3}{\sqrt{1-X_3^2}} \right)}{\pi/3 - \cos^{-1} \left(\frac{\sqrt{2}X_3}{\sqrt{1-X_3^2}} \right)}, & X_3 \in X_3^{(I)}, \end{cases} \quad (41c)$$

$$= \begin{cases} \frac{\varphi_2}{\pi/3}, & X_3 \in X_3^{(II)}, \end{cases} \quad (41d)$$

where in the last line we have used that in $X_3 \in [\frac{1}{\sqrt{3}}, 1] \equiv X_3^{(II)}$ we have $\cos^{-1}(\text{Min}[\frac{\sqrt{2}X_3}{\sqrt{1-X_3^2}}, 1]) = \cos^{-1}(1) = 0$. The

normalizing denominator $F_2^{(N=4)\text{Denom}}(X_3)$ is given by

$$F_2^{(N=4)\text{Denom}}(X_3) = \begin{cases} \pi/3 - \cos^{-1}\left(\frac{\sqrt{2}X_3}{\sqrt{1-X_3^2}}\right), & X_3 \in X_3^{(I)}, \\ \pi/3, & X_3 \in X_3^{(II)}. \end{cases} \tag{42}$$

2. CDF: $F_3^{(N=4)}(X_3; r_4)$

For the CDF of X_3 , given a value of $r_4 \leftrightarrow \mu_4$, we have

$$F_3^{(N=4)}(X_3; r_4) = \frac{\int_{1/3}^{X_3 \leq \bar{X}_3^{\max}(r_4)} dX'_3 F_2^{(N=4)\text{Denom}}(X'_3)}{\int_{1/3}^{\bar{X}_3^{\max}(r_4)} dX'_3 F_2^{(N=4)\text{Denom}}(X'_3)} = \frac{\int_{1/3}^{X_3 \leq \bar{X}_3^{\max}(r_4)} dX'_3 \int_{\bar{\varphi}_{2,c}^{\min}(X'_3)}^{\pi/3} d\varphi'_2}{\int_{1/3}^{\bar{X}_3^{\max}(r_4)} dX'_3 \int_{\bar{\varphi}_{2,c}^{\min}(X'_3)}^{\pi/3} d\varphi'_2}, \tag{43a}$$

$$\equiv \frac{F_3^{(N=4)(i)\text{Num}}(X_3; r_4)}{F_3^{(N=4)(i)\text{Denom}}(r_4)}, \text{ for } \mu_4 \in \mu_4^{(i)}. \tag{43b}$$

Defining (for notational convenience) $\bar{\varphi}_{2,c}^{(\min)}(X_3) \equiv \cos^{-1}\left(\frac{\sqrt{2}X_3}{\sqrt{1-X_3^2}}\right)$ we have $F_3^{(N=4)\text{Num}}(X_3; r_4)$ by μ_4 -region given by

Num:

Region 1: $1/4 \leq \mu_4 \leq 1/3, \Leftrightarrow 1_{(\mu_4=1/3)} \leq \frac{1}{2\sqrt{3}r_{\mu_4}} \leq \infty_{(\mu_4=1/4)},$

$$F_3^{(N=4)(1)\text{Num}}(r_4) = \begin{cases} \int_{1/3}^{X_3 \leq 1/\sqrt{3}} dX_3 \int_{\bar{\varphi}_{2,c}^{(\min)}(X_3)}^{\pi/3} d\varphi_2, \\ = f_{\text{NL}}(X_3), & X_3 \in X_3^{(I)}, \end{cases} \tag{44a}$$

$$= \begin{cases} \int_{1/3}^{1/\sqrt{3}} dX_3 \int_{\bar{\varphi}_{2,c}^{(\min)}(X_3)}^{\pi/3} d\varphi_2 + \int_{1/\sqrt{3}}^{X_3 \leq \bar{X}_3 = \frac{1}{2\sqrt{3}r_{\mu_4}} = 1} dX_3 \int_0^{\pi/3} d\varphi_2, \\ \frac{\pi}{6} (2X_3 - 1), & X_3 \in X_3^{(II)}, \end{cases} \tag{44b}$$

Region 2: $1/3 \leq \mu_4 \leq 1/2, \Leftrightarrow 1/\sqrt{3}_{(\mu_4=1/2)} \leq \frac{1}{2\sqrt{3}r_{\mu_4}} \leq 1_{(\mu_4=1/3)},$

$$F_3^{(N=4)(2)\text{Num}}(r_4) = \begin{cases} \int_{1/3}^{X_3 \leq \bar{X}_3(r_4) \leq 1/\sqrt{3}} dX_3 \int_{\bar{\varphi}_{2,c}^{(\min)}(X_3)}^{\pi/3} d\varphi_2, \\ = f_{\text{NL}}(X_3), & X_3 \in X_3^{(I)}, \end{cases} \tag{44c}$$

$$= \begin{cases} \int_{1/3}^{1/\sqrt{3}} dX_3 \int_{\bar{\varphi}_{2,c}^{(\min)}(X_3)}^{\pi/3} d\varphi_2 + \int_{1/\sqrt{3}}^{X_3 \leq \bar{X}_3 = \frac{1}{2\sqrt{3}r_{\mu_4}} < 1} dX_3 \int_0^{\pi/3} d\varphi_2, \\ = \frac{\pi}{6} (2X_3 - 1), & X_3 \in [1/\sqrt{3}, \bar{X}_3(r_4)], \end{cases} \tag{44d}$$

Region 3: $1/2 \leq \mu_4 \leq 1, \Leftrightarrow 1/3_{(\mu_4=1)} \leq \frac{1}{2\sqrt{3}r_{\mu_4}} \leq 1/\sqrt{3}_{(\mu_4=1/2)},$

$$F_3^{(N=4)(3)\text{Num}}(r_4) = \int_{1/3}^{X_3 \leq \bar{X}_3 = \frac{1}{2\sqrt{3}r_{\mu_4}} \leq \frac{1}{\sqrt{3}}} dX_3 \int_{\bar{\varphi}_{2,c}^{(\min)}(X_3)}^{\pi/3} d\varphi_2, \\ \equiv f_{\text{NL}}(X_3) = X_3 \left(\frac{\pi}{3} - y(X_3)\right) + \sin^{-1}\left(\frac{\sin y(X_3)}{\sqrt{3}}\right) - \frac{\pi}{6}, \quad X_3 \in \left[\frac{1}{3}, \bar{X}_3(r_4)\right],$$

$$\text{with } y(X_3) = \cos^{-1}\left(\frac{\sqrt{2}X_3}{\sqrt{1-X_3^2}}\right) \equiv \bar{\varphi}_{2,c}^{(\min)}(X_3),$$

$$\bar{X}_3(r_4) = \frac{1}{2\sqrt{3}r_4}, \tag{44e}$$

where we have defined the functions $f_{\text{NL}}(X_3)$, $y(X_3)$, and $\bar{X}_3(r_4)$ in Eq. (44e).

Repeating the same calculations as above, but now with $X_3 \rightarrow X_3^{\max}(r_4)$, we have for the normalizing denominator $F_3^{(N=4)\text{Denom}}(r_4)$ by μ_4 -region.

Denom:

Region 1: $1/4 \leq \mu_4 \leq 1/3, \Leftrightarrow 1_{(\mu_4=1/3)} \leq \frac{1}{2\sqrt{3}r_{\mu_4}} \leq \infty_{(\mu_4=1/4)},$

$$F_3^{(N=4)(1)\text{Denom}}(r_4) = \int_{1/3}^{1/\sqrt{3}} dX_3 \int_{\bar{\varphi}_{2,c}^{(\min)}(X_3)}^{\pi/3} d\varphi_2 + \int_{1/\sqrt{3}}^1 dX_3 \int_0^{\pi/3} d\varphi_2 = \frac{\pi}{6} \equiv \frac{4\pi}{4!}, \tag{45a}$$

Region 2: $1/3 \leq \mu_4 \leq 1/2, \Leftrightarrow 1/\sqrt{3}_{(\mu_4=1/2)} \leq \frac{1}{2\sqrt{3}r_{\mu_4}} \leq 1_{(\mu_4=1/3)},$

$$F_3^{(N=4)(2)\text{Denom}}(r_4) = \int_{1/3}^{1/\sqrt{3}} dX_3 \int_{\varphi_{2,c}^{(\min)}(X_3)}^{\pi/3} d\varphi_2 + \int_{1/\sqrt{3}}^{\frac{1}{2\sqrt{3}r_{\mu_4}} \leq 1} dX_3 \int_0^{\pi/3} d\varphi_2,$$

$$= \frac{\pi}{6} (2\bar{X}_3 - 1), \tag{45b}$$

Region 3: $1/2 \leq \mu_4 \leq 1, \Leftrightarrow 1/3_{(\mu_4=1)} \leq \frac{1}{2\sqrt{3}r_{\mu_4}} \leq 1/\sqrt{3}_{(\mu_4=1/2)},$

$$F_3^{(N=4)(3)\text{Denom}}(r_4) = \int_{1/3}^{\frac{1}{2\sqrt{3}r_{\mu_4}} \leq \frac{1}{\sqrt{3}}} dX_3 \int_{\varphi_{2,c}^{(\min)}(X_3)}^{\pi/3} d\varphi_2$$

$$= f_{\text{NL}}(\bar{X}_3), \quad \bar{X}_3(r_4) = \frac{1}{2\sqrt{3}r_4}. \tag{45c}$$

Putting this altogether we finally obtain the CDF for $F_3^{(N=4)}(X_3; r_4)$ by μ_4 -region

Region 1: $1/4 \leq \mu_4 \leq 1/3, \Leftrightarrow 1_{(\mu_4=1/3)} \leq \frac{1}{2\sqrt{3}r_{\mu_4}} \leq \infty_{(\mu_4=1/4)},$

$$F_3^{(N=4)(1)}(X_3; r_4) = \begin{cases} \frac{f_{\text{NL}}(X_3)}{\pi/6}, & X_3 \in X_3^{(I)}, \\ 2X_3 - 1, & X_3 \in X_3^{(II)}, \end{cases} \tag{46a}$$

Region 2: $1/3 \leq \mu_4 \leq 1/2, \Leftrightarrow 1/\sqrt{3}_{(\mu_4=1/2)} \leq \frac{1}{2\sqrt{3}r_{\mu_4}} \leq 1_{(\mu_4=1/3)}$

$$F_3^{(N=4)(2)}(X_3; r_4) = \begin{cases} \frac{f_{\text{NL}}(X_3)}{\frac{\pi}{6}(2\bar{X}_3-1)}, & X_3 \in X_3^{(I)}, \\ \frac{2X_3-1}{2\bar{X}_3-1}, & \frac{1}{\sqrt{3}} \leq X_3 \leq \bar{X}_3 = \frac{1}{2\sqrt{3}r_{\mu_4}}, \end{cases} \tag{46b}$$

Region 3: $1/2 \leq \mu_4 \leq 1, \Leftrightarrow 1/3_{(\mu_4=1)} \leq \frac{1}{2\sqrt{3}r_{\mu_4}} \leq 1/\sqrt{3}_{(\mu_4=1/2)},$

$$F_3^{(N=4)(3)}(X_3; r_4) = \frac{f_{\text{NL}}(X_3)}{f_{\text{NL}}(\bar{X}_3)}, \quad \frac{1}{3} \leq X_3 \leq \bar{X}_3 = \frac{1}{2\sqrt{3}r_{\mu_4}}, \tag{46c}$$

$$\text{where } f_{\text{NL}}(X_3) = X_3 \left(\frac{\pi}{3} - y(X_3) \right) + \sin^{-1} \left(\frac{\sin y(X_3)}{\sqrt{3}} \right) - \frac{\pi}{6}, \tag{46d}$$

$$y(X_3) = \cos^{-1} \left(\frac{\sqrt{2}X_3}{\sqrt{1-X_3^2}} \right). \tag{46e}$$

From the above we see that for all regions $\mu_4 \in [\frac{1}{4}, 1]$ we have $F_3^{(N=4)(1,2,3)\text{Num}}(r_4) = f_{\text{NL}}(X_3)$ if $X_3 \in [\frac{1}{3}, \frac{1}{\sqrt{3}}] \equiv X_3^{(I)}$, and $F_3^{(N=4)(1,2)\text{Num}}(r_4) = \frac{\pi}{6} (2X_3 - 1)$ if $X_3 \in [\frac{1}{\sqrt{3}}, 1] \equiv X_3^{(II)}$ [since for $F_3^{(N=4)(3)\text{Num}}(r_4)$ there simply is no region $X_3^{(II)}$]. While the numerator $F_3^{(N=4)(1,2,3)\text{Num}}(r_4)$ is essentially the same in each $\mu_4^{(1,2,3)}$ region, what makes the CDF different in each region is the different normalizing denominators $F_3^{(N=4)(1,2,3)\text{Denom}}(r_4)$ in each of the three $\mu_4^{(1,2,3)}$ regions, i.e., $F_3^{(N=4)(1,2,3)}(r_4) = F_3^{(N=4)(1,2,3)\text{Num}}(r_4)/F_3^{(N=4)(1,2,3)\text{Denom}}(r_4)$.

It is also interesting to note that in region $\mu_4^{(1)} F_3^{(N=4)(1)\text{Denom}}(r_4) = \frac{\pi}{6} \equiv \frac{4\pi}{4!}$. This just indicates that region $\mu_4^{(1)}$ describes the ‘‘in-sphere’’ which can be completely inscribed inside the tetrahedron simplex Δ_3 , for which the WC represents a fractional area of $1/(N = 4)!$.

3. CDF for $r_4 : F_4^{(N=4)}(r_4)$

We now compute the radial CDF for $r_{\mu_4} : F_4^{(N=4)}(r_{\mu_4})$ via ($r_4 \equiv r_{\mu_4}$)

$$F_4^{(N=4)}(r_4) = \frac{\int_0^{r_4 \leq \bar{r}^{\max} = \frac{1}{2\sqrt{3}}} dr'_4 r_4'^2 F^{(N=4)\text{Denom}}(\bar{X}_3)}{\int_0^{\bar{r}^{\max} = \frac{1}{2\sqrt{3}}} dr'_4 r_4'^2 F^{(N=4)\text{Denom}}(\bar{X}_3)}, \tag{47a}$$

$$\equiv \frac{F_4^{(N=4)\text{Num}}(r_4)}{F_4^{(N=4)\text{Denom}}} \tag{47b}$$

in each of the three purity regions (Region 1, Region 2, Region 3) given, respectively, by $\mu_4^{(1)} \in [\frac{1}{4}, \frac{1}{3}] \Leftrightarrow r_4^{(1)} \in [0, \frac{1}{2\sqrt{3}}]$, $\mu_4^{(2)} \in [\frac{1}{3}, \frac{1}{2}] \Leftrightarrow r_4^{(2)} \in [2\sqrt{3}, \frac{1}{2}]$, $\mu_4^{(3)} \in [\frac{1}{2}, 1] \Leftrightarrow r_4^{(3)} \in [\frac{1}{2}, \frac{\sqrt{3}}{2}]$, using the $F_3^{(N=4)(i=(1,2,3))\text{Denom}}(r_4)$ from

Eqs. (45a)–(45c). Note that the normalizing denominator $F_4^{(N=4)\text{Denom}}$ in Eq. (47a) is a constant, while the numerator $F_4^{(N=4)\text{Num}}(r_4)$ is r_4 -dependent.

We proceed by first computing the indefinite integrals $F_4^{(N=4)(I,II,III)\text{Num}}(r_4)$ required for $F_4^{(N=4)(i)\text{Num}}(r_4)$ for each Region i :

Region 1: $\mu_4^{(1)} \in [\frac{1}{4}, \frac{1}{3}] \leftrightarrow r_4^{(1)} \in [0, \frac{1}{2\sqrt{3}}]$,

$$F_4^{(N=4)(I)\text{Num}}(r_4) = \int^{r_4} dr_4 r_4^2 \frac{\pi}{6} = \frac{\pi}{6} \frac{r_4^3}{3}, \quad (48a)$$

Region 2: $\mu_4^{(2)} \in [\frac{1}{3}, \frac{1}{2}] \leftrightarrow r_4^{(2)} \in [\frac{1}{2\sqrt{3}}, \frac{1}{2}]$,

$$\begin{aligned} F_4^{(N=4)(II)\text{Num}}(r_4) &= \int^{r_4} dr_4 r_4^2 \frac{\pi}{6} (2\bar{X}_3 - 1), \\ &= \frac{\pi}{36} (\sqrt{3} - 2r_4) r_4^2, \end{aligned} \quad (48b)$$

Region 3: $\mu_4^{(3)} \in [\frac{1}{2}, 1] \leftrightarrow r_4^{(3)} \in [\frac{1}{2}, \frac{\sqrt{3}}{2}]$,

$$\begin{aligned} F_4^{(N=4)(III)\text{Num}}(r_4) &= \int^{r_4} dr_4 r_4^2 f_{\text{NL}}(\bar{X}_3(r_4)), \\ &\equiv g_{\text{NL}}(r_4), \end{aligned} \quad (48c)$$

where

$$\begin{aligned} g_{\text{NL}}(r_4) &= \frac{1}{432} \left[3\sqrt{8r_4^2 - 2} + \sqrt{3}\pi(12r_4^4 + 8\sqrt{3}r_4^3 - 1) \right. \\ &\quad \left. - \sqrt{3}(36r_4^2) \sec^{-1} \left(\sqrt{6r_4^2 - \frac{1}{2}} \right) \right. \\ &\quad \left. + 144r_4^3 \sin^{-1} \left(\sqrt{\frac{4r_4^2 - 1}{12r_4^2 - 1}} \right) \right], \end{aligned} \quad (49)$$

with $f_{\text{NL}}(\bar{X}_3(r_4))$ defined in Eq. (45c) with $\bar{X}_3(r_4) = \frac{1}{2\sqrt{3}r_4}$. Note: It is surprising that these integrals can be computed analytically in closed form.

With the above integrals we can now compute the normalizing constant denominator $F_4^{(N=4)\text{Denom}}$:

$$\begin{aligned} F_4^{(N=4)\text{Denom}} &= \left[F_4^{(N=4)(I)\text{Num}} \left(\frac{1}{2\sqrt{3}} \right) - F_4^{(N=4)(I)\text{Num}}(0) \right], \\ &\quad + \left[F_4^{(N=4)(II)\text{Num}} \left(\frac{1}{2} \right) - F_4^{(N=4)(II)\text{Num}} \left(\frac{1}{2\sqrt{3}} \right) \right] \\ &\quad + \left[F_4^{(N=4)(III)\text{Num}} \left(\frac{\sqrt{3}}{2} \right) - F_4^{(N=4)(III)\text{Num}} \left(\frac{1}{2} \right) \right], \end{aligned} \quad (50a)$$

$$= \frac{1}{72}. \quad (50b)$$

Using the above results we then have

Region 1: $\mu_4^{(1)} \in [\frac{1}{4}, \frac{1}{3}] \leftrightarrow r_4^{(1)} \in [0, \frac{1}{2\sqrt{3}}]$,

$$\begin{aligned} F_4^{(N=4)(1)}(r_4) &= \frac{[F_4^{(N=4)(I)\text{Num}}(r_4 \leq \frac{1}{2\sqrt{3}}) - F_4^{(N=4)(I)\text{Num}}(0)]}{F_4^{(N=4)\text{Denom}}}, \\ &= 4\pi r_4^3, \end{aligned} \quad (51a)$$

Region 2: $\mu_4^{(2)} \in [\frac{1}{3}, \frac{1}{2}] \leftrightarrow r_4^{(2)} \in [\frac{1}{2\sqrt{3}}, \frac{1}{2}]$,

$$\begin{aligned} F_4^{(N=4)(2)}(r_4) &= \frac{F_4^{(N=4)(1)}(\frac{1}{2\sqrt{3}})}{F_4^{(N=4)\text{Denom}}} + \frac{[F_4^{(N=4)(II)\text{Num}}(r_4 \leq \frac{1}{2}) - F_4^{(N=4)(II)\text{Num}}(\frac{1}{2\sqrt{3}})]}{F_4^{(N=4)\text{Denom}}}, \\ &= 2\sqrt{3}\pi r_4^2 - 4\pi r_4^3 - \frac{\pi}{6\sqrt{3}}, \end{aligned} \quad (51b)$$

Region 3: $\mu_4^{(3)} \in [\frac{1}{2}, 1] \leftrightarrow r_4^{(3)} \in [\frac{1}{2}, \frac{\sqrt{3}}{2}]$,

$$\begin{aligned} F_4^{(N=4)(3)}(r_4) &= \frac{F_4^{(N=4)(2)}(\frac{1}{2})}{F_4^{(N=4)\text{Denom}}}, \\ &\quad + \frac{[F_4^{(N=4)(III)\text{Num}}(r_4 \leq \frac{\sqrt{3}}{2}) - F_4^{(N=4)(III)\text{Num}}(\frac{1}{2})]}{F_4^{(N=4)\text{Denom}}}, \end{aligned} \quad (51c)$$

$$\begin{aligned} F_4^{(N=4)(3)}(r_4) &= 2\sqrt{3}\pi r_4^2 + 4\pi r_4^3 - \frac{\pi}{6\sqrt{3}} + \sqrt{2r_4^2 - \frac{1}{2}} \\ &\quad + \frac{(36r_4^2 - 1)}{2\sqrt{3}} \sec \left(\sqrt{6r_4^2 - \frac{1}{2}} \right) + 24r_4^3 \sin^{-1} \left(\sqrt{\frac{4r_4^2 - 1}{12r_4^2 - 1}} \right). \end{aligned} \quad (51d)$$

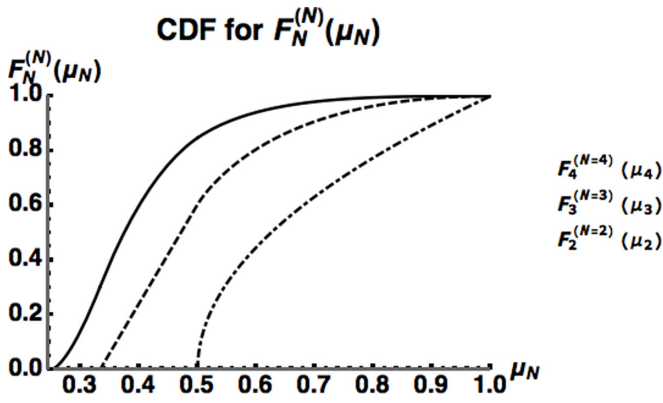


FIG. 2. Radial CDFs $F_N^{(N)}(\mu_N)$ for $N \in \{2, 3, 4\}$ from analytic expressions Eqs. (31a), (39a)–(39c), and (51a)–(51d) respectively.

D. Plots of radial CDFs from analytic formulas

In this section we show plots of the radial CDFs for $N = \{2, 3, 4\}$ from the analytic formulas derived in the previous section, and scatter plots of the distribution of the diagonal density matrices on $S^{(1)}$ and $S^{(2)}$ for $N = 3$ and $N = 4$, respectively.

1. Composite plot of the radial CDF for $N \in \{2, 3, 4\}$

In Fig. 2 we show the radial CDFs for $N = \{2, 3, 4\}$ in a single composite plot. Note that as N increases, the curves become increasingly flat for higher purities, i.e. $F_N^{(N)}(\mu_N) \sim 1 - \epsilon$ for $\mu_N \rightarrow \mu_N^{(N)} \in [\frac{1}{2}, 1]$. At $N > 4$ this increase becomes more severe, and as discussed earlier, in the case of $N = 4$, poses numerical challenges for the interpolation of the CDFs and for the numerical inversion of the inverse CDFs (and not just for r_N , but also for higher angles $\varphi_k \sim N$, i.e., k near N). This is exacerbated by the fact that the integration measure for a given N contains a factor of $\sin^{(N-3)} \varphi_N$ (and $\sin^{(N-3-k)} \varphi_k$ for lower angles) which become increasingly peaked at $\varphi_k \sim \pi/2$ or $X_k = \cos \varphi_k \sim 1$. We discuss an approximation scheme for larger N based on this fact in a later section.

In Table I we show the percentage of purity by region obtained from the analytically generated radial CDFs. The last two columns, illustrates the increasing flatness of $F_N^{(N)}(\mu_N)$ with increasing $N \in \{2, 3, 4\}$, which shows the increasing rarity of obtaining near maximal purity states by random sampling. As an example, for $N = 4$ one would expect $\sim 5(660)$ samples in the region $\mu_4 \in [0.99, 1]$ ($[0.95, 1]$) per every 10^7 trials of density matrices generated from conventional uniform sampling (via the Haar measure) of random unitary

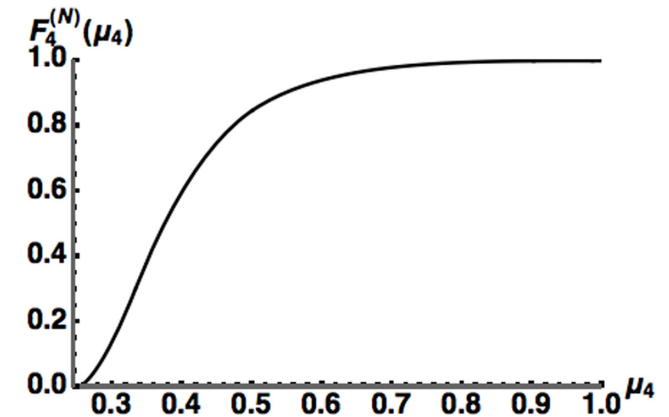
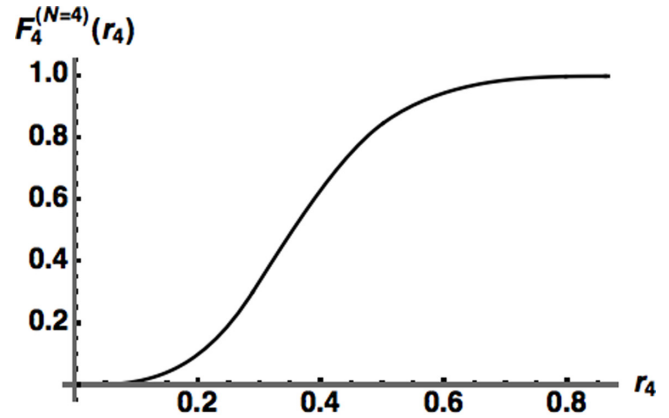


FIG. 3. Analytical (top) radial CDF vs $r_{\mu_4} : F_4^{(N=4)}(r_4)$, (bottom) vs purity CDF for $\mu_4 : F_4^{(N=4)}(r_4(\mu_4))$ where $r_{\mu_4} = \sqrt{\mu_4 - 1/4}$, from Eqs. (51a)–(51d).

matrices (UE). In comparison, in the plots generated in the next section, 10^3 density matrices with exactly $\mu_4 \equiv 0.99$ were generated in approximately 2 s (in *Mathematica*, with no optimization).

In Fig. 3 we plot the analytic radial CDF for (top) $F_4^{(N=4)}(r_4)$ and (bottom) $F_4^{(N=4)}(r_4(\mu_4))$ where the later is obtained from the former by the variable substitution $r_{\mu_4} = \sqrt{\mu_4 - 1/4}$. The three regions $r_4^{(i=\{1,2,3\})}$ and $\mu_4^{(i=\{1,2,3\})}$ are indicated on the abscissa.

In Fig. 4 we plot the inverse CDF for μ_4 , which simply switches the abscissa and ordinate in the bottom plot of Fig. 3. However, this figure illustrates two things. First, to uniformly sample a value of μ_4 according to the CDF $F_4^{(N=4)}(\mu_4)$ we treat $p = F_4^{(N=4)}(\mu_4) \in [0, 1]$ as a uniform deviate (abscissa in Fig. 4) which then determines a value of $\mu_4(p)$ (ordinate

TABLE I. Percentage of Purity by Region for (columns 2–4) $N \in \{2, 3, 4\}$, and (columns 5 and 6) $\mu \in [0.95, 1]$ and $\mu \in [0.99, 1]$, respectively, illustrating the increasing rarity of obtaining near maximal purity states from uniform random sampling via the Haar measure.

% of states by Purity μ and dimension N					
N	$\mu \in [\frac{1}{4}, \frac{1}{3}]$	$\mu \in [\frac{1}{3}, \frac{1}{2}]$	$\mu \in [\frac{1}{2}, 1]$	$\mu \in [0.95, 1]$	$\mu \in [0.99, 1]$
2	–	–	100	5.13	1.01
3	–	60.46	39.54	0.20	7.5×10^{-3}
4	30.23	54.54	15.23	6.6×10^{-3}	5.1×10^{-5}

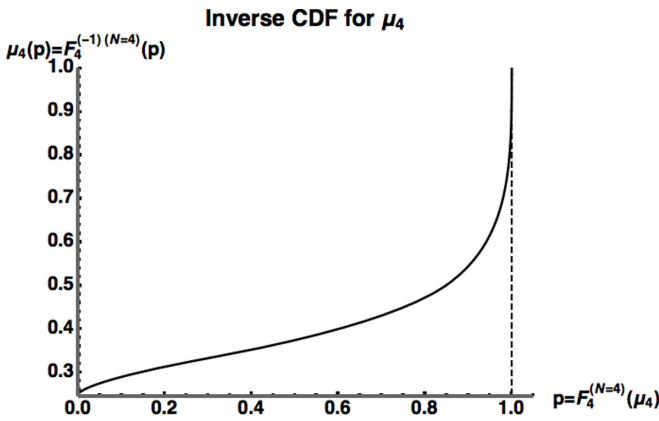


FIG. 4. Inverse radial CDF for $\mu_4 : F^{(N=4)}(r_4(\mu_4))$.

in Fig. 4). Second, we see that for $p \sim 1 - \epsilon$, the slope of $\mu_4(p)$ is nearly vertical (infinite), and interpolation of the values $\{p, \mu_4(p)\}$ becomes increasingly inaccurate. This is equivalent to the statement that in Fig. 3, $F_4^{(N=4)}(\mu_4) \sim 1 - \epsilon$ for $\mu_4 \sim 1 - \delta$, i.e., values of $F_4^{(N=4)}(\mu_4)$ are infinitesimally close to 1 as $\mu_4 \rightarrow 1$, and thus becomes computationally hard to represent and distinguish since the addition (subtraction) of a large number 1 with an infinitesimal number ϵ becomes increasingly inaccurate in floating point arithmetic on a computer. Care must be taken in the interpolation of pairs of values $\{\mu_4, p(\mu_4)\}$ and its numerical inversion $\{p, \mu_4(p)\}$. Both the former and latter become significant numerical issues as we numerically compute the CDF integrals for $\{X_k, F_k^{(N)}(X_k; X_{k+1})\}$ for $N > 4$, and then perform the numerical interpolation (or root finding procedure) of its inverse CDF of pairs $\{p = F_k^{(N)}(X_k; X_{k+1}), X_k(p)\}$.

2. $N = 3$: 1-spheres $S^{(1)}$ in simplex Δ_2 for fixed μ_3

In Fig. 5 we plot the inverse CDF for $F_2^{(N=3)}(\varphi_2; r_3)$ from Eq. (36). That is given a uniform deviate $p = F_2^{(N=3)}(\varphi_2; r_3) \in [0, 1]$ for a fixed value of the purity-radius $r_3 = \sqrt{\mu_3 - 1/3}$, we compute $\varphi_2(p; r_3)$, which then uniformly samples φ_2 over $F_2^{(N=3)}$. Since $F_2^{(N=3)}$ is linear in φ_2 , this can be analytically performed (trivially). We then compute $\vec{p}_e^{(N=3)} = (\frac{1}{\sqrt{3}}, \vec{r}^{(N=3)}(r_3, \varphi_2))$, which is the diagonal eigenvalue vector $\vec{\lambda}_E^{(N=3)} = (\lambda_1, \lambda_2, \lambda_3)$ transformed to the e -basis (where the first component is always $\frac{1}{\sqrt{3}}$), and plot the two-vector $\vec{r}^{(N=3)} \equiv (r_3 \cos \varphi_2, r_3 \sin \varphi_2)$. The latter is a 2D vector in plane of the equilateral triangle that is the $N = 3$ eigenvalue simplex Δ_2 , and is centered on the MMS ($r_3 = 0 \leftrightarrow \mu_3 = \frac{1}{3}$) at the triangle's center. The direction $\varphi_2 = 0$ points to the $N = 2$ MMS $\frac{1}{2}(1, 1, 0)$ embedded in $N = 3$ WC $\tilde{\Delta}_2$ (white triangle in lower left corner of Fig. 5), while $\varphi_2 = \frac{\pi}{3}$ points to the WC pure state $(1, 0, 0)$.

Each (blue) concentric circle represents diagonal density matrices of fixed radius $r_3 = \sqrt{\mu_3 - 1/3}$. The center of the triangle $r_3 = 0$ is the MMS of purity $\mu_3 = \frac{1}{3}$. The largest inscribed circle is at the “in-radius” $r_3 = \frac{1}{\sqrt{6}} = r_3^*$ at $\mu_3 = \frac{1}{2}$. For $r_3 > r_3^*$ the concentric circles lie outside the equilateral triangle and therefore only intersect the triangle in three segments near the vertices. The minimum angle is no longer

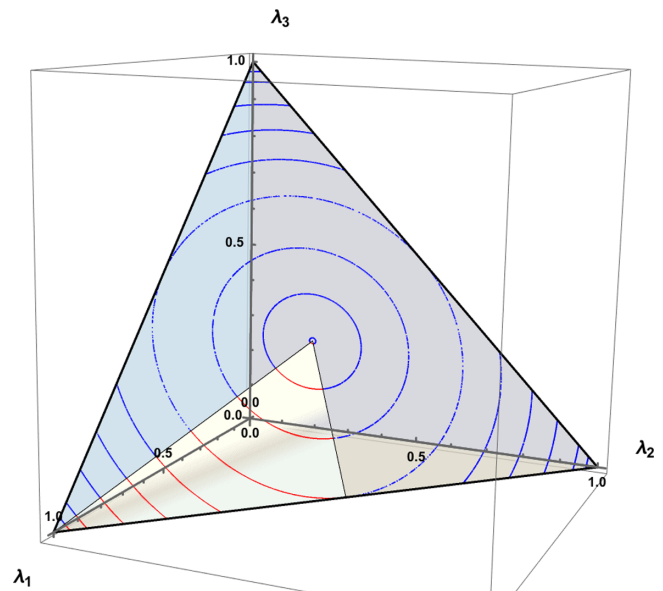


FIG. 5. Uniform sample of 1-spheres $S^{(1)}$ (blue) of fixed $\mu_3 = \{0.3334, 0.35, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90, 0.95, 0.99\}$ outward from the center ($\mu_3 = 1/3$) of 2-simplex Δ_2 to the vertices ($\mu_3 = 1$). The white triangle in the lower left corner is the WC ($1/3!$ of Δ_2) with partial circular arcs (red) uniformly sampled from $F_2^{N=3}(\mu_3)$ in Eq. (36).

0, and is given by $\cos^{-1}(\frac{1}{\sqrt{3} \cdot 2r_3})$ as in Eq. (33c), while the maximum angle in the WC is still $\pi/3$.

The above is a generic feature for higher dimensions. Namely, for a dimension N the eigenvalue simplex Δ_{N-1} is an equilateral simplex (hypertriangle) of dimension $N - 1$. The “in-radius” for the largest inscribed sphere $S^{(N-1)}$ occurs at $r_N^* = \sqrt{\frac{1}{N-1} - \frac{1}{N}} \leftrightarrow \mu_N = \frac{1}{N-1}$. For $r_N > r_N^*$ the spheres $S^{(N-1)}$ lie outside the simplex Δ_{N-1} , and therefore intersect it near its pure state vertices $\vec{e}_i = (0, \dots, 1_i, \dots, 0)$. This is the origin of the complicated, nested angle bound on φ_k for general N . We’ll see this explicitly for the 2-spheres $S^{(2)}$ in the tetrahedron eigenvalue simplex for $N = 4$ in the next section.

3. $N = 4$: 2-spheres $S^{(2)}$ in simplex Δ_3 for fixed μ_4

In Fig. 6 (top left) we plot $\vec{p}_e^{(N=4)} = (\frac{1}{\sqrt{4}}, \vec{r}^{(N=4)}(r_4, \varphi_3, \varphi_2))$, which is the diagonal eigenvalue vector $\vec{\lambda}_E^{(N=4)} = (\lambda_1, \lambda_2, \lambda_3, \lambda_4)$ transformed to the e -basis (where the first component is always $\frac{1}{\sqrt{4}}$), and plot the three-vector $\vec{r}^{(N=4)} \equiv (r_4 \cos \varphi_3, r_4 \sin \varphi_3 \cos \varphi_2, r_4 \sin \varphi_3 \sin \varphi_2)$ for $\mu_4 = 0.3334 \approx \frac{1}{3}$. This is the “in-sphere,” i.e., the largest S^2 that can be inscribed within the tetrahedron Δ_3 . In Fig. 6 (top right) the “clipping” of the sphere S^2 is due its intersection with the triangular face of the eigenvalue simplex tetrahedron Δ_3 , since $\mu_4 = 0.40 > \mu_4^* = \frac{1}{N-1} = \frac{1}{3}$. This clipping is even more pronounced in Fig. 6 (bottom left) and occurs more closely to the vertices of Δ_3 . Finally, in Fig. 6 (bottom right) shows the spheres and clipped-spheres for $\mu_4 = \{0.3334, 0.40, 0.55, 0.75\}$. To create these images

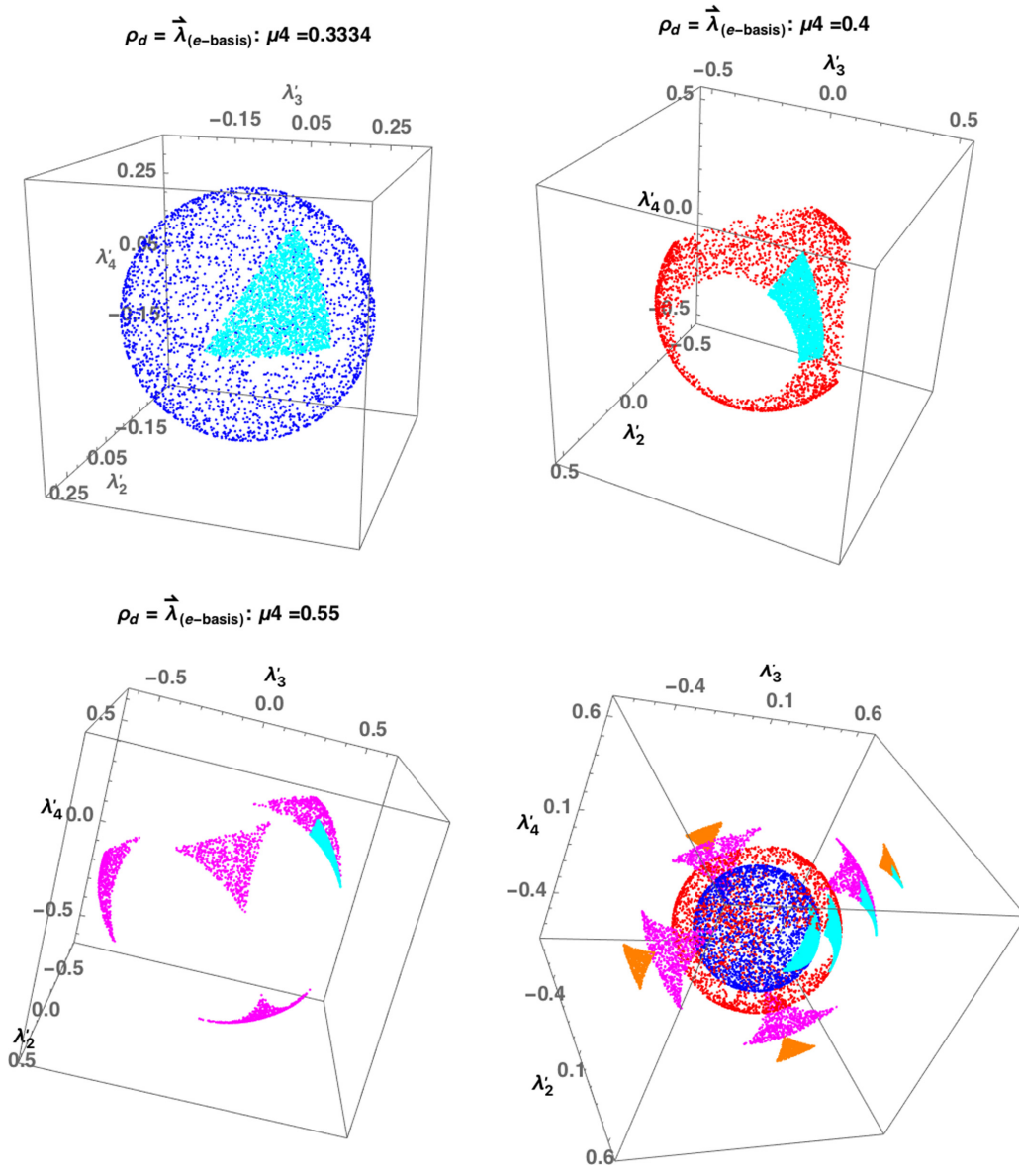


FIG. 6. Diagonal density matrices $\vec{r}^{(N=4)}(r_4 \varphi_3, \varphi_2)$ in the tetrahedral eigenvalue simplex Δ_3 for $N = 4$ for (top left, blue) $\mu_4 = 0.3334$, (top right, red) $\mu_4 = 0.40$, (bottom left, magenta) $\mu_4 = 0.55$, and (bottom right, blue, red, magenta, orange) $\mu_4 = \{0.3334, 0.40, 0.55, 0.75\}$. The cyan patches are the WC $\tilde{\Delta}_3$ where the eigenvalues are arranged in decreasing order.

by uniformly sampling from the marginal CDFs, we work “top-down” in the following sense.

- Procedure for uniformly sample CDFs at fixed $\mu_{N=4}$:
- (a) Given a chosen purity $\frac{1}{4} \leq \mu_4 \leq 1 \Leftrightarrow 0 \leq r_4 \leq \sqrt{1-1/4} = \frac{\sqrt{3}}{2}$,
 - (b) Given an r_4 , pick an $X_3 = \cos \varphi_3$ such that $\frac{1}{3} \leq X_3 \leq \bar{X}_3^{\max}(r_4) = \text{Min}[\bar{X}_3 \equiv \frac{1}{2\sqrt{3}r_4}, 1]$, where $\bar{X}_3 = 1$ at $r_4 = \frac{1}{\sqrt{43}} = \frac{1}{2\sqrt{3}} \Leftrightarrow \mu_4 = \frac{1}{3}$,
 - (c) Given an X_3 , pick an $X_2 = \cos \varphi_2$ such that $\frac{1}{2} \leq X_2 \leq \bar{X}_2^{\max}(X_3) = \text{Min}[\bar{X}_2 \equiv \frac{\sqrt{2}X_3}{\sqrt{1-X_3^2}}, 1]$ where $\bar{X}_2 = 1$ at $X_2 = \frac{1}{\sqrt{3}} \equiv X_2^*$, or $\text{Min}[\bar{\varphi}_2 \equiv \cos^{-1}(\bar{X}_2 \equiv \frac{\sqrt{2}X_3}{\sqrt{1-X_3^2}}), 1] \leq \bar{\varphi}_2^{\min} \leq \cos^{-1}(\frac{1}{2}) = \frac{\pi}{3}$.

Note that the value of the chosen r_4 determines the “break points” for $\bar{X}_3^{\max}(r_4)$ given by the value at $\bar{X}_3 \equiv \frac{1}{2\sqrt{3}r_4} = \{\frac{1}{3}, \frac{1}{\sqrt{3}}, 1, \infty\}$ at $r_4 = \{\frac{\sqrt{3}}{2}, \frac{1}{2}, \frac{1}{2\sqrt{3}}, 0\} \Leftrightarrow \mu_4 = \{1, \frac{1}{2}, \frac{1}{3}, \frac{1}{4}\}$. We will see that later on, that for a given N the previous determined break points for $N' < N$ still apply (i.e., hold).

In Fig. 7 we plot a histogram of the purity for $N = 4$ generated by two methods: (i) our uniform sampling (UP) of diagonal density matrices ρ_{diag} at fixed purity μ_4 , and (ii) the conventional method of uniformly sampling unitary matrices according to the Haar measure (UE). In (ii) ρ_{diag} is the absolute square of a random row of U' , and $\rho = U \rho_{\text{diag}} U^\dagger$ with $\mu_4 = \text{Tr}[\rho^2]$. In (i) we compute 10^3 samples per fixed value of the purity μ_4 , and obtained 10^3 identical purity values per chosen μ_4 (see thin vertical bars). In (ii) we computed a total of 10^5 uniformly sampled unitary matrices, and used a bin

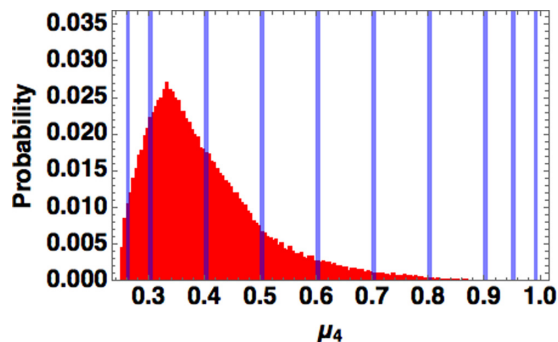


FIG. 7. Histogram of purity values for $N = 4$ generated by (blue vertical bars, extending to unity) uniform sampling (UP) of diagonal density matrices of fixed purity (2500 for each μ_4 value) for $\mu_4 = \{0.26, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90, 0.95, 0.99\}$, (red) uniform sampling (10^5 total samples, bin width 0.005) of random (UE) unitary matrices U' , U such that ρ_{diag} is the absolute square of a random row of U' , and $\rho = U \rho_{\text{diag}} U^\dagger$ with $\mu_4 = \text{Tr}[\rho^2]$.

width of 0.005 for the histogram of purity values (red). We note that while the unitary matrices are sampled uniformly in (ii), the purity is sampled nonuniformly, being weighted toward lower values of the purity, especially in Regions 1 and 2, $\mu_4 \in [\frac{1}{4}, \frac{1}{2}]$. As indicated in Table I, we expect on the order of 7 samples per 10^5 to be in the purity range $\mu_4 \in [0.95, 1]$, which is borne out in the histogram in Fig. 7.

For general N with variables $(X_2, X_3, \dots, X_{N-1}, r_N)$, the bounds for the angles $X_k = \cos \varphi_k$ ($X_2 = \varphi_2$) were outlined in Eqs. (23a)–(23c), (26a), (26b), (27a), and (27b). The procedure for uniformly sampling diagonal density matrices for fixed μ_N follows similarly to the case of $N = 4$ above. Given a fixed value of the purity μ_N , one uniformly samples $F_{N-1}^{(N)}(X_{N-1}; r_N)$ for the highest angle X_{N-1} whose r_N -dependent bound is given by Eq. (27a). For the lowest and middle angles X_k for $k \in \{N-2, \dots, 2\}$ one then successively uniformly samples, in descending k -order, $F_k^{(N)}(X_k; X_{k+1})$ whose X_{k+1} -dependent bound is given in Eq. (26b). Once the diagonal density matrix $\rho_N^{(\text{diag})}$ of fixed purity μ_N is uniformly sampled by the above procedure, the general density ρ_N can be obtained, as usual, from a uniformly (Haar) sampled unitary matrix U via $\rho_N = U \rho_N^{(\text{diag})} U^\dagger$, with identical eigenvalue spectrum and purity.

V. APPLICATIONS

A. Entanglement in $N = 4$

In this section we apply the $N = 4$ analytic expressions for the CDFs $F_{k=\{2,3\}}^{(N=4)}$ to investigate well-known measures of entanglement of 2-qubit systems, but now as functions of fixed values of the purity $\mu_4(\rho_{ab})$ of the composite systems, as well of the purity $\mu_2(\rho_a)$ of a subsystem. As the canonical entanglement measure for 2-qubits we use the concurrence, \mathcal{C} [6,14] as well as the (more generalizable) logarithmic negativity (LN) [15–17], and the quantum discord (QD) [18–20]. We will also explore the classical correlations \mathcal{J} , defined in relation to the quantum discord, as the alternative definition of the mutual information between subsystems A and B conditioned on measurements on subsystem B [19,21–23], as well as a “baseline” entanglement witness (ΔLE) based on the

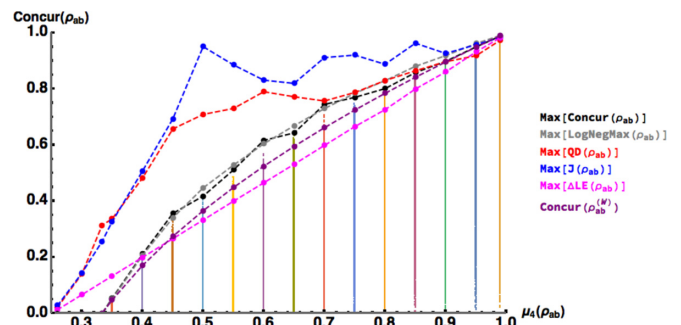


FIG. 8. Plot of various entanglement measures (points with dashed curves) for 2-qubits ($N = 4$) vs μ_4 : (black) $\text{Max}[\mathcal{C}(\rho_{ab})]$ (concurrence), (gray) $\text{Max}[\text{LN}(\rho_{ab})]$ (logarithmic negativity), (red) $\text{Max}[\mathcal{Q}(\rho_{ab})]$ (quantum discord), (blue) $\text{Max}[\mathcal{J}(\rho_{ab})]$ (classical correlations), (magenta) $\text{Max}[\Delta\text{LE}(\rho_{ab})]$ (Δ Linear Entropy), and (purple) $\mathcal{C}(\rho_{ab}^{(\text{Werner})})$ (concurrence for 2-qubit Werner state). The vertical points at fixed $\mu_4 = \{0.26, 0.30, 0.3334, 0.35, 0.40, 0.45, 0.50, 0.55, 0.60, 0.65, 0.70, 0.75, 0.80, 0.85, 0.90, 0.95, 0.99\}$ are the concurrences of 2500 randomly sampled 2-qubit density matrices at fixed purity.

difference in purity between the composite system ab and its subsystem a , attempting to generalize the LE.

In Fig. 8 we plot the functions of the density matrix discussed above for fixed discrete values of the purity $\mu_4 = \{0.26, 0.30, 0.3334, 0.35, 0.40, 0.45, 0.50, 0.55, 0.60, 0.65, 0.70, 0.75, 0.80, 0.85, 0.90, 0.95, 0.99\}$ (colored vertical “lines” of points). As is well-known [3,12], we see that separability occurs in the region $\mu_4^{(1)} \in [\frac{1}{4}, \frac{1}{3}]$ where the concurrence \mathcal{C} goes to zero. At each fixed values of μ_4 , 2500 composite density matrices ρ_{ab} were generated and their concurrences computed, and values plotted vertically. The black-dashed curved represents $\text{max}_{\{\rho_{ab}\}}[\mathcal{C}(\rho_{ab}|\mu_4)]$, that is, the maximum concurrence over the 2500 ρ_{ab} sampled at the same fixed value of the composite purity μ_4 . The dashed-gray curve in Fig. 8 represents $\text{max}_{\{\rho_{ab}\}}[\text{LN}(\rho_{ab}|\mu_4)]$, the corresponding maximum, now using the logarithmic negativity LN [24] and is essentially the same as that for the concurrence, although the latter appears statistically slightly larger than the former at purities above $\mu_4 \gtrsim 0.75$.

The dashed-purple curve in Fig. 8 represents the concurrence for the 2-qubit Werner state $\rho_{ab}^{(W)} = p|\Phi^{(+)}\rangle\langle\Phi^{(+)}| + \frac{(1-p)}{4}\mathbb{I}$, where $|\Phi^{(+)}\rangle = \frac{1}{\sqrt{2}}(|00\rangle_{ab} + |11\rangle_{ab})$ is the maximally entangled (symmetric) Bell state, and $\frac{1}{4}\mathbb{I}$ is the 2-qubit MMS. A straightforward calculation of $\mu_N = \text{Tr}[(\rho_{ab}^{(W,N)})^2]$ for a Werner state with a d -dimensional Bell state $|\Phi_N^{(+)}\rangle = \frac{1}{\sqrt{d}} \sum_{n=0}^{d-1} |n, n\rangle_{ab}$ (see Appendix A) reveals that $p(\mu_N) = \sqrt{\frac{d^2 \mu_N - 1}{d^2 - 1}}$ with a sudden death of entanglement (as measured by the LN) at a critical value of $p_N^* = \frac{1}{d+1}$ corresponding to $\mu_N^* = \frac{2}{d(d+1)}$, as is borne out in Fig. 8 for the case of $d = 2$. Note that while $\mathcal{C}(\rho_{ab}^{(W)})$ qualitatively follows the same curve as $\text{max}_{\{\rho_{ab}\}}[\mathcal{C}(\rho_{ab}|\mu_4)]$, the former is strictly less than the latter, except at the endpoints $\mu_4 = 1/4$ and $\mu_4 = 1$.

The red-dashed and blue-dashed curves in Fig. 8 plot $\text{max}_{\{\rho_{ab}\}}[\mathcal{Q}(\rho_{ab}|\mu_4)]$ and $\text{max}_{\{\rho_{ab}\}}[\mathcal{J}(\rho_{ab}|\mu_4)]$, respectively, for 1.5×10^4 UP samples at fixed μ_4 . (This time intensive

calculation involves the numerical calculation of the supremum of \mathcal{Q} and \mathcal{J} over all possible measurements [23]). The curves do show instances where $\mathcal{Q} > \mathcal{J}$, as noted by Luo [19] in the special case of the 2-qubit Werner state, but now for random ρ_{ab} . As is well known, $\mathcal{Q} > 0$ (and $\mathcal{J} > 0$) for all $\mu_4 \in (\frac{1}{4}, 1]$ and therefore is nonzero in the no-entanglement region $\mu_4 \in [\frac{1}{4}, \frac{1}{3}]$. Instead, $\mathcal{Q} > 0$ measures the quantum information-disturbance such that a classical state is defined by the fact that any projective measurement on ρ_{ab} leaves it in the state before the measurement. The behavior of \mathcal{Q} and \mathcal{J} exhibits a nearly linear growth with respect to μ_4 in the region $\mu_4 \in [\frac{1}{4}, \frac{1}{2}]$, with a crescent-like behavior in the region $\mu_4 \in [\frac{1}{2}, 1]$ (analogous to Fig. 16).

Finally, the dashed-magenta curve is a plot of a “baseline” entanglement witness $\max_{\{\rho_{ab}\}}[\Delta\text{LE}(\rho_{ab}|\mu_4)]$ for $N = 4$, where we have defined for arbitrary dimension N ,

$$\Delta\text{LE} \stackrel{\text{def}}{=} \frac{(\mu(\rho_{ab}^{(N)}) - \frac{1}{N}) - (\mu(\rho_a^{(N_a)}) - \frac{1}{N_a})}{(1 - \frac{1}{N})},$$

$$\text{where } N_a = \dim(\rho_a), \quad \rho_a = \text{Tr}_b[\rho_{ab}]. \quad (52)$$

The reasoning behind Eq. (52) is that if the purity of the subsystem ρ_a is less than that of the composite state ρ_{ab} , i.e., $\mu(\rho_a^{(N_a)}) < \mu(\rho_{ab}^{(N)})$, then the system is more mixed, and hence must contain entanglement [9]. However, since $\mu(\rho_{ab}^{(N)}) \in [\frac{1}{N}, 1]$ and $\mu(\rho_a^{(N_a)}) \in [\frac{1}{N_a}, 1]$ we should measure these purities relative to their respective MMS. The denominator in Eq. (52) simply normalizes ΔLE to unity for a maximally entangled state with $\mu(\rho_{ab}^{(N)}) = 1$ and correspondingly $\mu(\rho_a^{(N_a)}) = \frac{1}{N_a}$. We also have $\Delta\text{LE}(\rho_{ab}) = 0$ when $\rho_{ab} = \mathbb{I}/N$ is the N -dimensional MMS. The dashed-magenta curve for $\max_{\{\rho_{ab}\}}[\Delta\text{LE}(\rho_{ab}|\mu_4)]$ in Fig. 8 is a linear interpolation [25] of the purity μ_4 in the range $[\frac{1}{4}, 1]$ and acts as a lower bound to $\max_{\{\rho_{ab}\}}[\mathcal{C}(\rho_{ab}|\mu_4)]$ in the approximate region $\mu_4 \approx [0.37, 1]$, where the intersection of the two curves occurs at $\mu_4 \approx 0.37 > \frac{1}{3}$. $\max_{\{\rho_{ab}\}}[\Delta\text{LE}(\rho_{ab}|\mu_4)]$ is nonzero in the complement region $\mu_4 \approx [\frac{1}{4}, 0.37]$, and in a sense behaves more like the quantum discord $\max_{\{\rho_{ab}\}}[\mathcal{Q}(\rho_{ab}|\mu_4)]$ in this region (although the two measure different things). Another way to view $\max_{\{\rho_{ab}\}}[\Delta\text{LE}(\rho_{ab}|\mu_4)]$ is that for all $\mu_4 \in [\frac{1}{4}, 1]$, it acts as a witness (proper lower bound) to both $\max_{\{\rho_{ab}\}}[\mathcal{Q}(\rho_{ab}|\mu_4)]$ and $\max_{\{\rho_{ab}\}}[\mathcal{J}(\rho_{ab}|\mu_4)]$.

Of course, the results of Fig. 8 could have also been obtained from the conventional method of density matrix generation via sampling random unitaries with respect to the Haar measure. However, considering the distribution of purities μ_4 given in the histogram in Fig. 7, it would have been much more difficult and time consuming to obtain the corresponding results for higher purity values in Fig. 8.

Another informative approach to examining the above data is to plot the concurrence $\mathcal{C}(\rho_{ab})$ versus $\mu_2(\rho_a)$ the purity of the reduced density matrix of (say) subsystem a . In Fig. 9 we plot 2500 generated density matrices for each fixed value $\mu_4(\rho_{ab})$ (different colored points) of the composite system ρ_{ab} versus the purity $\mu_2(\rho_a)$ of the reduced density matrix ρ_a . We see that as the subsystem purity $\mu_2(\rho_a)$ increases the concurrence approaches zero, indicating a separable composite system, while at low values of $\mu_2(\rho_a)$ the concurrence approaches its maximum $\mu_4(\rho_{ab})$ -dependent value. As the pu-

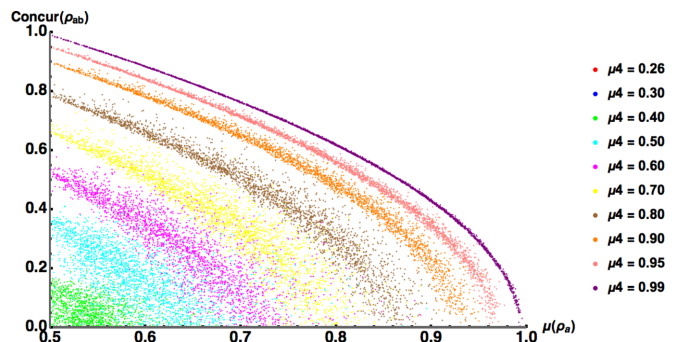


FIG. 9. Concurrence $\mathcal{C}(\rho_{ab})$ vs purity $\mu_2(\rho_a)$ of the subsystem a for fixed composite purity values (colored points) $\mu_4(\rho_{ab}) = \{0.26, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90, 0.95, 0.99\}$. For each fixed value of the purity $\mu_4(\rho_{ab})$, 2500 density matrices (same colored points) were (UP) generated.

urity $\mu_4(\rho_{ab})$ of the composite system increases toward unity, the (colored) bands of the 2500 density matrices becomes narrower, and more pronounced.

In Fig. 10 (top) we plot (top) the logarithmic negativity $\text{LN}(\rho_{ab})$ and (bottom) $\Delta\text{LE}(\rho_{ab})$ Eq. (52) versus the concurrence $\mathcal{C}(\rho_{ab})$ for the same composite purity values $\mu_4(\rho_{ab})$ as in Fig. 9 [again, 2500 density matrices per fixed $\mu_4(\rho_{ab})$ (color) value]. The tight clustering of all points in Fig. 10 (top) for all values of $\mu_4(\rho_{ab})$ indicates that the logarithmic negativity is a very close approximation to a one-to-one function

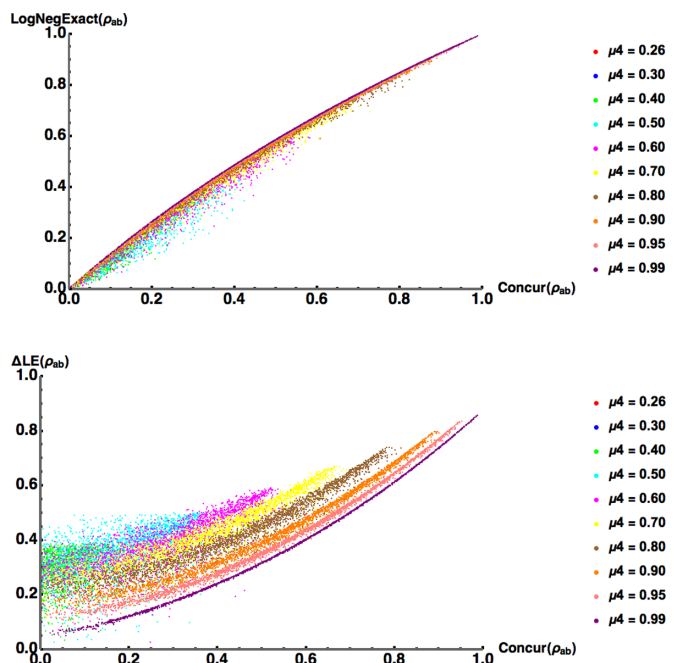


FIG. 10. (top) Logarithmic negativity $\text{LN}(\rho_{ab})$ and (bottom) $\Delta\text{LE}(\rho_{ab})$ vs the concurrence $\mathcal{C}(\rho_{ab})$. For each fixed value of the composite purity $\mu_4(\rho_{ab}) = \{0.26, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90, 0.95, 0.99\}$, 2500 density matrices (same colored points) were (UP) generated.

the concurrence (though it is well known that the former does not detect bound entanglement). The much broader widths in Fig. 10 (bottom) indicates that the $\Delta\text{LE}(\rho_{ab})$ from Eq. (52) is much less accurate approximation of the concurrence than $\text{LN}(\rho_{ab})$ (top), though still exhibiting some structural dependence on the purities.

B. Induced measures

With the formulas developed above, we now have a geometric representation (in the WC) of the eigenvalues $\{\lambda_i\}$ in

dimension N . Transforming back to the E -basis we have the following forms $\vec{\lambda}_N$ for the eigenvalues for $N = 2$ and $N = 3$:

$$\begin{aligned} \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix}_{N=2} &= \frac{1}{2} \begin{pmatrix} 1 + \sqrt{2} r_2 \\ 1 - \sqrt{2} r_2 \end{pmatrix}, \\ \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{pmatrix}_{N=3} &= \frac{1}{6} \begin{pmatrix} 2 + r_3 \cos \varphi_2 + \sqrt{3} r_3 \sin \varphi_2 \\ 2 + r_3 \cos \varphi_2 + \sqrt{3} r_3 \sin \varphi_2 \\ 2(1 - r_3 \cos \varphi_2) \end{pmatrix}, \end{aligned} \quad (53a)$$

and for $N = 4$

$$\begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \end{pmatrix}_{N=4} = \frac{1}{12} \begin{pmatrix} 3 + 2\sqrt{3} r_4 \cos \varphi_3 + 2\sqrt{6} r_4 \sin \varphi_3 \cos \varphi_2 + 6\sqrt{2} r_4 \sin \varphi_3 \sin \varphi_2 \\ 3 + 2\sqrt{3} r_4 \cos \varphi_3 + 2\sqrt{6} r_4 \sin \varphi_3 \cos \varphi_2 - 6\sqrt{2} r_4 \sin \varphi_3 \sin \varphi_2 \\ 3 + 2\sqrt{3} r_4 \cos \varphi_3 - 4\sqrt{6} r_4 \sin \varphi_3 \cos \varphi_2 \\ 3(1 - 2\sqrt{3} r_4 \cos \varphi_3) \end{pmatrix}, \quad (53b)$$

each with unit trace. These formulas can be easily generated for arbitrary N .

1. The probability distribution of the eigenvalues of ρ_N

With the above formulas, one can then explore metrics and measures on the space of density matrices $\mathcal{M}^{(N)}$ of dimension N . For example (see Secs. 15.3 and 15.4, pp. 410–414, of Ref. [3] for further details), $P_{\text{HS}}(\lambda_1, \dots, \lambda_N)$ is the Hilbert-Schmidt (HS) probability distribution of eigenvalues of $\rho = U \rho_d U^\dagger$ when averaged over all unitaries $U \in \text{SU}(N)$ with respect to the Haar measure (uniform measure on sphere S^{N^2-1}), where $\rho_d \equiv \Lambda = \text{diagonal}(\lambda_1, \dots, \lambda_N) \leftrightarrow \vec{\lambda}_N$. This probability distribution of eigenvalues is given by

$$P_{\text{HS}}(\lambda_1, \dots, \lambda_N) = C_N^{\text{HS}} \delta\left(1 - \sum_{j=1}^N \lambda_j\right) \prod_{j < k}^N (\lambda_j - \lambda_k)^2, \quad (54a)$$

$$C_N^{\text{HS}} = \frac{\Gamma(NK)}{\prod_{k=1}^N \Gamma(k) \Gamma(k+1)}, \quad (54b)$$

$$\int_0^1 d\lambda_N \cdots \int_0^1 d\lambda_1 P_{\text{HS}}(\lambda_1, \dots, \lambda_N) = 1. \quad (54c)$$

Here, the δ function $\delta(1 - \sum_{j=1}^N \lambda_j)$ enforces the unit trace condition on the ddm. The second term $\prod_{j < k}^N (\lambda_j - \lambda_k)^2$ arises from the introduction of the unitary U in $\rho = U \rho_d U^\dagger$, providing the eigenvectors for ρ . The HS metric is then defined by $ds_{\text{HS}}^2 = \frac{1}{2} \text{Tr}[(d\rho)^2]$, where the factor of $\frac{1}{2}$ is used to make closed geodesics on $\mathbb{C}P^N \sim S^{2N+1}$ have length π . Writing $d\rho = U[d\Lambda + U^\dagger dU \Lambda - \Lambda U^\dagger dU]U^\dagger$ [employing $d(U dU^\dagger) = 0$], one has that in the spectral representation $d\rho_{ij} = d\lambda_i \delta_{ij} + (\lambda_j - \lambda_i)(U^\dagger dU)_{ij}$. The first (diagonal) term is the classical-like Fisher-Rao metric (of the eigenvalue probability vector), while the second term introduces the off-diagonal differences of eigenvalues $(\lambda_j - \lambda_i)$. [Note: writing $U = e^{-iH}$, one then has $(U^\dagger dU)_{ij} = -i H_{ij}$]. Thus, the HS metric becomes (taking “one” factor from each squared term of $d\rho$) $ds_{\text{HS}}^2 = \frac{1}{2} \sum_{i=1}^N (d\lambda_i)^2 + \sum_{i < j}^N (\lambda_i - \lambda_j)^2 |(U^\dagger dU)_{ij}|^2$.

This leads to the HS volume element (taking into account a normalization factor respecting the δ function, i.e., that $\lambda_N \stackrel{\text{def}}{=} 1 - \sum_{i=1}^{N-1} \lambda_i$) given by

$$dV_{\text{HS}} = \sqrt{\frac{N}{2^{N-1}}} \prod_{j=1}^{N-1} d\lambda_j \prod_{j < k}^{1 \dots N} (\lambda_i - \lambda_j)^2 \times \left| \prod_{j < k}^{1 \dots N} \text{Re}(U^\dagger dU)_{jk} \text{Im}(U^\dagger dU)_{jk} \right|, \quad (55a)$$

$$\equiv P_{\text{HS}}(\vec{\lambda}) \times Q(\mathbf{F}^N). \quad (55b)$$

The above shows that $P(\rho) = P_{\text{HS}}(\vec{\lambda}) \times Q(\mathbf{F}^N)$ is a *product metric* with $P_{\text{HS}}(\vec{\lambda})$ depending on the eigenvalues of ρ acting as the *radial* portion, and $Q(\mathbf{F}^N)$ depending on the eigenvectors of ρ (i.e., the column vectors of U) acting as the *angular* portion, which one can roughly think of as $d\Omega_{\mathbb{C}P^N = S^{2N+1}}$. (Technically, \mathbf{F}^N is *Flag Manifold* [3,26].) Thus, $P_{\text{HS}}(\vec{\lambda})$ in Eq. (54a) is just the radial portion of dV_{HS} in Eq. (55a), depending only on the eigenvalues of ρ . In many cases one is *not* interested in the “angular” distribution of the eigenvalues $\vec{\lambda}$ and so one integrates over this angular portion. This is what $P_{\text{HS}}(\vec{\lambda})$ in Eq. (54a) represents, i.e., a random $\rho_N = U \rho_d U^\dagger$ averaged over all unitaries U with respect to the Haar measure.

2. ρ_N considered as the reduced density matrix of a randomly chosen pure state of composite dimension NK

From a fiber-bundle perspective, one can also think of $\mathcal{M}^{(N)}$ as the base space in which the ρ_N live. Above each ρ_N (labeled by their eigenvalues $\vec{\lambda}_N$) is a fiber containing all the purifications of the density matrix, each of which maps down from bundle space to ρ_N in the base space. These pure states $|\Psi\rangle_{N,K}$ lie in a composite Hilbert space $\mathcal{H}_{N,K} = \mathcal{H}_N \otimes \mathcal{H}_K$, where \mathcal{H}_N is the *system* subspace of dimension N , and \mathcal{H}_K is the *ancilla (reservoir)* subspace of dimension K , which we will take as $K \geq N$. We can conveniently write $|\Psi\rangle_{N,K} = \sum_{n,k} A_{nk} |n\rangle_N \otimes |k\rangle_K$ for an $N \times K$ rectangular complex matrix A with matrix elements

$A_{nk} = {}_{N,K}\langle n, k | \Psi_{N,K} \rangle$, with orthogonal bases $|n\rangle_N \in \mathcal{H}_N$ and $|k\rangle_K \in \mathcal{H}_K$, respectively. The only restriction placed upon A is that $|\Psi_{N,K}\rangle|^2 = \text{Tr}[AA^\dagger] = 1$. The corresponding density matrix $\rho_{NK} = |\Psi_{N,K}\rangle\langle\Psi_{N,K}|$ is represented by a 4-indexed object $(\rho_{NK})_{nk,n'k'}$ which upon partial tracing over \mathcal{H}_K yields the $N \times N$ reduced density matrix $\rho_N = \text{Tr}_K[AA^\dagger]$. One can then define a family of measures in the space of mixed states $\mathcal{M}^{(N)}$ labeled by the size K of the reservoir.

Here we will consider the measures $P_{N,K}^{\text{trace}}(\lambda_1, \dots, \lambda_N)$ induced by the above partial tracing over the reservoir. Since we consider pure states $|\Psi\rangle_{N,K}$ that are drawn randomly (with respect to the Fubini-Study metric), the induced measure $P_{N,K}^{\text{trace}}$ also has the product form of Eq. (55b). Hence, the distribution of eigenvectors is determined by the Haar measure on $U(N)$. The radial distribution of eigenvalues can be derived and is given by (see Eq. (15.59), p. 417 in Ref. [3])

$$P_{N,K \geq N}^{\text{trace}}(\lambda_1, \dots, \lambda_N) = C_N^{\text{HS}} \delta\left(1 - \sum_{j=1}^N \lambda_j\right) \times \prod_{j < k}^N (\lambda_j - \lambda_k)^2 \prod_i^N (\lambda_i)^{K-N}, \quad (56a)$$

$$C_{N,K} = \frac{\Gamma(NK)}{\prod_{j=0}^{N-1} \Gamma(K-j)\Gamma(K-j+1)}, \quad (56b)$$

$$\int_0^1 d\lambda_N \cdots \int_0^1 d\lambda_1 P_{N,K}^{\text{trace}}(\lambda_1, \dots, \lambda_N) = 1. \quad (56c)$$

The net effect of tracing over the reservoir system of dimension K is to modify the previous metric P_{HS} Eq. (54a) with the extra product terms $\prod_i^N (\lambda_i)^{K-N}$ (here written for $K \geq N$) in Eq. (56a). Note that for $K \rightarrow N \Rightarrow P_{N,N}^{\text{trace}} = P_{\text{HS}}$. In other words, for a composite bipartite system composed of two subsystems of equal dimension N , tracing out over one of the systems produces the distribution of eigenvalues given by P_{HS} .

While in the past many authors have been interested in $P_{N,K}^{\text{trace}}(\lambda_1, \dots, \lambda_N)$ and have used it to derive the average purity, entropy, etc. (see Chapter 15 of Ref. [3] and references therein) of systems, a new feature of this present work is that we are able to produce *exact analytic expressions* for the

joint probability distribution $P_{N,K}^{\text{trace}}$ in terms of the geometric coordinates $(\varphi_2, \varphi_3, \dots, \varphi_N, r_N)$ for an arbitrary dimension N by using the expressions $\vec{\lambda}_N$ as in Eqs. (53a) and (53b), and their (easy to produce) generalizations. By integrating over the angular variables, given their boundary regions of the previous sections, we are able to produce marginal probability and cumulative distribution functions in terms of the radius r_N or purity μ_N . In some cases, as we shall show below, we can actually perform the integrations analytically and obtain closed-form expressions. In general, these analytic equations quickly become unwieldy for general N, K , and one must resort to numerical integration.

Thus, in the following we will show analytic formulas and plots for the case of $N = 2, K = 2^{k \in \{1,2,3,4\}}$, though we generate a formula for arbitrary K . This system is a qubit in a reservoir of (1,2,3,4) qubits. The case $N = 2$ is not surprising, since the independent eigenvalue λ_1 (with $\lambda_2 \equiv 1 - \lambda_1$) of a qubit ($N = 2$) is completely characterized by its purity μ_2 , i.e. $\lambda_1 = \frac{1}{2}(1 + \sqrt{\mu_2 - 1/2})$. The first nontrivial case occurs for $N = 3$ which depends on the coordinates (r_3, φ_2) and thus we investigate the explicit case $N = 3, K = \{3, 6, 9\}$ analytically. Here the system is a qutrit, and the reservoir consists of 1-qutrit, a qubit-qutrit, and 2-qutrits, respectively. Last, we investigate the case of $N = 4, K = 4$ in which the system is a ‘‘ququad’’ (\mathbb{C}^4 , of which a system of 2 qubits is a subset), and the reservoir is of the same size, $K = 4$. This system does not yield a closed form analytic expression. Hence, we integrate (the nontrivial task) out $(X_3 = \cos \varphi_3, \varphi_2)$ and produce probability distributions and cumulative probability distributions as a function of μ_4 (r_4) alone.

3. $N = 2$

The case of $N = 2$ is straightforward since any 2×2 matrix is completely determined by two invariants, its trace and determinant. Comparing $\vec{p}_E^{(2)}(x_2)$ from Eq. (10a) with $\vec{\lambda}^{(N=2)} = (\lambda_1, \lambda_2 = 1 - \lambda_1)^T$ in either the E-basis or e-basis, one finds that $\lambda_1 = (1 + x_2)/2 = (1 + \sqrt{2\mu_2 - 1})/2$. Using Eq. (56a) for the case of $N = 2$ and carrying out the Jacobian transformations $J_{\lambda,x} J_{x,\mu} = \det(\frac{d\lambda_1}{dx_2}) \det(\frac{dx_2}{d\mu_2})$ to convert $d\lambda_1 = J_{\lambda,x} dx_2 = J_{\lambda,x} J_{x,\mu} d\mu_2$ one derives for arbitrary $K \geq N$

$$P_{N=2,K}^{\text{trace}}(\mu_2) = \frac{(1 - \mu_2)^{K-2} (2\mu_2 - 1)^{1/2} \Gamma(2K)}{2^{K-1} \Gamma(K) \Gamma(K - 1)}, \quad (57a)$$

$$F_{N=2,K}^{\text{trace}}(\mu_2) = \int_{1/2}^{\mu_2} d\mu'_2 P_{N=2,K}^{\text{trace}}(\mu'_2), \\ = \frac{(2\mu_2 - 1)^{3/2} {}_2F_1\left(\frac{3}{2}, 2 - K, \frac{5}{2}, 2\mu_2 - 1\right) \Gamma(2K)}{3 \cdot 2^{2K-3} \Gamma(K) \Gamma(K - 1)}, \quad (57b)$$

where ${}_2F_1(a, b; c; z) = \sum_{k=0}^{\infty} \frac{(a)_k (b)_k}{(c)_k} \frac{z^k}{k!}$ is the hypergeometric function, with Pochhammer symbol $(a)_k \equiv a(a + 1) \dots (a + k - 1) = \frac{\Gamma(a+k)}{\Gamma(a)}$. These are plotted in Fig. 11 for $K = 2^{k \in \{1,2,3,4\}}$. The general trend of these plots is that as the dimension K of the reservoir system increases, the probability

distribution $P_{N=2,K}^{\text{trace}}(\mu_2)$ peaks further and further to the left, approaching $\mu_2 \rightarrow 1/2$, i.e., the MMS (where it approaches an almost δ function-like behavior). This is also reflected in the cumulative probability distribution $F_{N=2,K}^{\text{trace}}(\mu_2)$ which saturates to unity for smaller values of μ_2 as K increases.

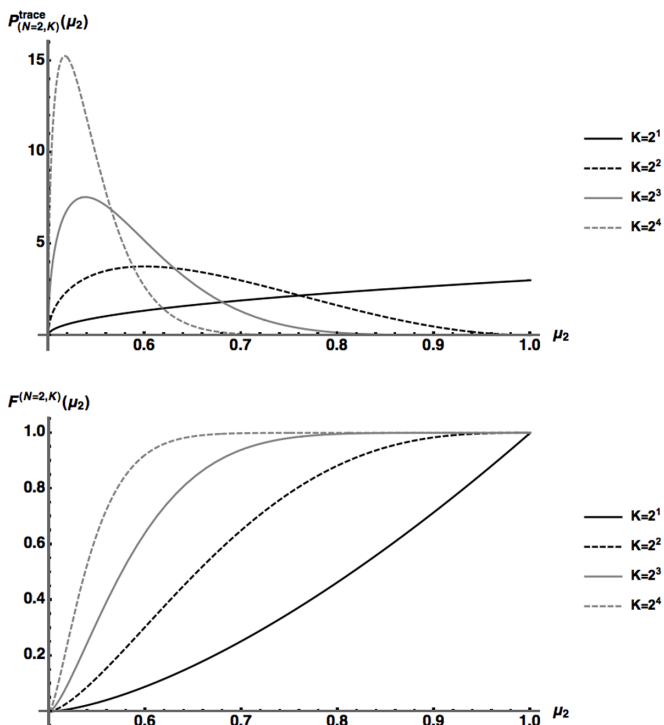


FIG. 11. Analytic (top) probability $P_{N=2,K}^{\text{trace}}(\mu_2)$, (bottom) cumulative probability distribution function $F_{N=2,K}^{\text{trace}}(\mu_2)$ for $N = 2$, and $K = 2^{k \in \{1,2,3,4\}}$, from Eqs. (57a) and (57b).

We can use $P_{N=2,K}^{\text{trace}}(\mu_2)$ to obtain the probability distribution as a function of the Rényi entropy $S_2^{(N)} = S_2(\rho_N) = -\ln(\sum_{i=1}^N \lambda_i^2) \in \{0, \ln(N)\} \leftrightarrow \{\text{pure, MMS}\}$ which takes its minimum value 0 on pure states and its maximum value $\ln(N)$ ($\ln(2) \approx 0.693$) on the MMS. Here we use the fact that $P(S_2) dS_2 = P(\mu_2) d\mu_2 \Rightarrow P(S_2) = P(\mu_2 \rightarrow e^{-S_2}) | \frac{d\mu_2}{dS_2} |$ to obtain

$$P_{N=2,K}^{\text{trace}}(S_2) = \frac{(1 - e^{-S_2})^{K-2} (2e^{-S_2} - 1)^{1/2} \Gamma(2K)}{2^{K-1} \Gamma(K) \Gamma(K-1)} e^{-S_2}. \tag{58}$$

This is plotted in Fig. 12 (top) for $K = 2^{k \in \{1,2,3,4\}}$ and also $K = 2^{k \in \{1,2,3,4,5,6\}}$ on the (bottom), to exhibit the spikey behavior near the MMS for very large K .

4. N = 3

For the case of $N = 3$, we substitute Eq. (53a) (right) into the unnormalized portion $\tilde{P}_{N,K \geq N}^{\text{trace}}(\lambda_1, \dots, \lambda_N) \stackrel{\text{def}}{=} \prod_{j < k}^N (\lambda_j - \lambda_k)^2 \prod_i^N (\lambda_i)^{K-N}$ of the probability distribution in Eq. (56c) (and also include the Jacobian $J_{\lambda, \varphi} \stackrel{\text{def}}{=} \text{Det}[\frac{\partial(\lambda_1, \lambda_2)}{\partial(r_3, \varphi_2)}]$) of the transformation between the (λ_1, λ_2) and (r_3, φ_2) coordinates) to obtain

$$\tilde{P}_{N=3,K=3}^{\text{trace}} = \frac{r_3^6}{2^4 3^3} \sin^2(3\varphi_2), \tag{59a}$$

$$\tilde{P}_{N=3,K \geq 4}^{\text{trace}} = \frac{r_3^6}{2^{2(K-1)} 3^{3(K-2)}} \sin^2(3\varphi_2) \times [4 - 3r_3^2 - r_3^3 \cos(3\varphi_2)]^{K-3}. \tag{59b}$$

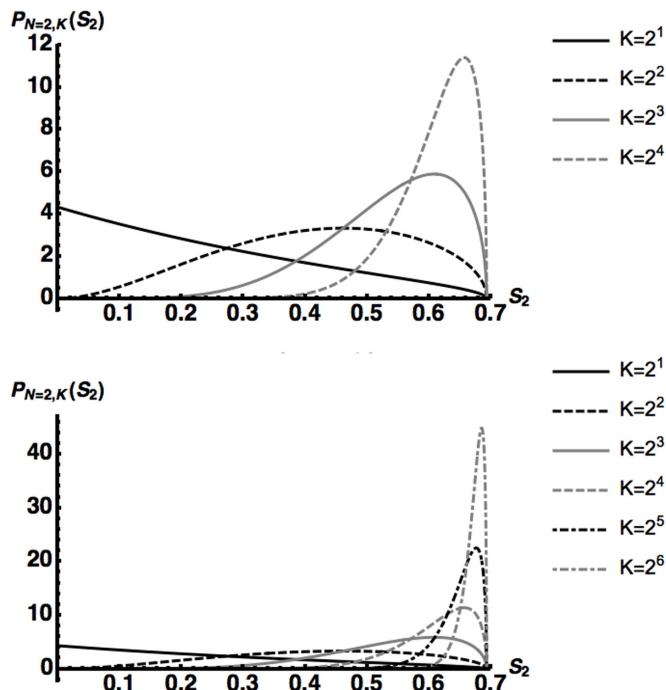


FIG. 12. Analytic probability $P_{N=2,K}^{\text{trace}}(S_2^{(N)})$, as a function of the Rényi entropy $S_2^{(N)} = -\ln(\mu_N)$ for $N = 2$, and (top) $K = 2^{k \in \{1,2,3,4\}}$, and (bottom) $K = 2^{k \in \{1,2,3,4,5,6\}}$. Note: $S_2^{(N)} = S_2(\rho_N) = -\ln(\sum_{i=1}^N \lambda_i^2) \in \{0, \ln(N)\} \leftrightarrow \{\text{pure, MMS}\}$, from Eq. (58).

We then compute

$$P_{N=3,K}^{\text{trace}}(r_3) = \frac{\int_{\varphi_2^{\min}(r_3)}^{\pi/3} d\varphi_2 \tilde{P}_{N=3,K}^{\text{trace}}(r_3, \varphi_2)}{\int_0^{r_3^{\max}=\sqrt{2/3}} dr_3' \int_{\varphi_2^{\min}(r_3')}^{\pi/3} \tilde{P}_{N=3,K}^{\text{trace}}(r_3', \varphi_2)}, \tag{60a}$$

$$\varphi_2^{\min}(r_3) = \cos^{-1} \left(\text{Min} \left[\frac{1}{\sqrt{3} \times 2r_3}, 1 \right] \right), \tag{60b}$$

$$P_{N=3,K}^{\text{trace}}(\mu_3) = P_{N=3,K}^{\text{trace}}(r_3(\mu_3)) \frac{1}{2\sqrt{\mu_3 - 1/3}}, \tag{60c}$$

where in the last line we have used the fundamental law of probability that $P(\mu_3) d\mu_3 = P(r_3) dr_3 \Rightarrow P(\mu_3) J_{r_3, \mu_3}$ where here the Jacobian of the transformation is simply $J_{r_3, \mu_3} = \frac{dr_3}{d\mu_3} = \frac{1}{2\sqrt{\mu_3 - 1/3}}$, using $r_3 = \sqrt{\mu_3 - 1/3}$. In the r_3 variable, we can then compute the CDF $F_{N=3,K}^{\text{trace}}(r_3)$ as

$$F_{N=3,K}^{\text{trace}}(r_3) = \int_0^{r_3 \leq r_3^{\max}} dr_3' P_{N=3,K}^{\text{trace}}(r_3', \varphi_2). \tag{61}$$

To plot $F_{N=3,K}^{\text{trace}}(r_3)$ as a function of μ_3 we can simply substitute in $r_3 = \sqrt{\mu_3 - 1/3}$. Remarkably, all the above integrals can be performed analytically in closed form, though they are somewhat unwieldy to write down. In Fig. 13 we plot $P_{N=3,K}^{\text{trace}}(r_3)$ and $F_{N=3,K}^{\text{trace}}(r_3)$ for $K = \{3, 6, 9\}$. The general trend is the same as for $N = 2$ case, namely, that as K increases, $P_{N=3,K}^{\text{trace}}(r_3)$ moves leftward, centered on lower values of μ_3 , and at the same time narrows, and increases in height (eventually δ -function spiking at the MMS at $\mu_3 = 1/3$ as $K \rightarrow \infty$). This feature is reflected in the CDF $F_{N=3,K}^{\text{trace}}(r_3)$ which also moves leftward, and saturates earlier near unity value at ever smaller values of μ_3 as K increases [27].

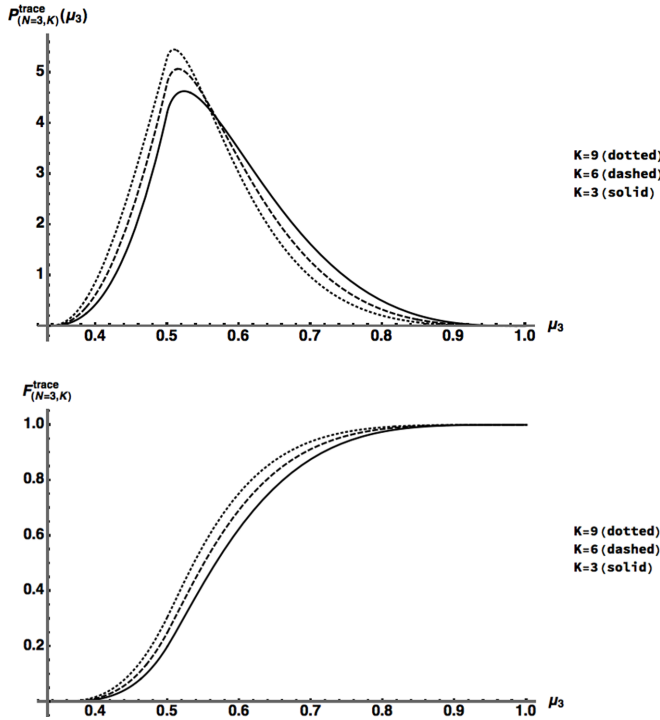


FIG. 13. Analytically derived plots of (top) $P_{N=3,K}^{\text{trace}}(\mu_3)$ and (bottom) $F_{N=3,K}^{\text{trace}}(\mu_3)$ for $K = \{3, 6, 9\}$, from Eqs. (60a)–(60c).

5. $N = 4$

The case of $N = 4$ follows analogously to the case of $N = 3$ above, with some minor modification of the limits. For $N = 4$ the variables are now $(r_4, X_3 = \cos \varphi_3, \varphi_2)$. The expression for $\tilde{P}_{N=4,K=4}^{\text{trace}}(r_4)$ [including the Jacobian of the transformation between the $(\lambda_1, \lambda_2, \lambda_3)$ and the $(r_4, X_3 = \cos \varphi_3, \varphi_2)$ coordinates] is given by

$$\begin{aligned} \tilde{P}_{N=4,K=4}^{\text{trace}}(r_4) = & \frac{r_4^{14}}{2^6 3^3} \sin^2(\varphi_2) \sin^7(\varphi_3) [1 + 2 \cos^2(2\varphi_2)]^2 \\ & \times [21 \cos(\varphi_3) + 11 \cos(3\varphi_3) \\ & - \sqrt{8} \cos(3\varphi_2) \sin^2(\varphi_3)]^2. \end{aligned} \quad (62)$$

As we integrate out both X_3 and φ_2 to obtain the marginal distributions for $P_{N=4,K}^{\text{trace}}(r_4)$ and $F_{N=4,K}^{\text{trace}}(r_4)$ we must remember to now use $\tilde{\varphi}_2^{\min}(X_3) = \cos^{-1}(\text{Min}[\frac{\sqrt{2}X_3}{\sqrt{1-X_3^2}}, 1])$, $\tilde{X}_3^{\max} = \text{Min}[\frac{1}{\sqrt{4-3r_4}}, 1]$ and $X_3^{(\min)} = 1/3$. These integrals cannot be performed in closed form analytically and so must be computed numerically. In Fig. 14 we illustrate the $N = 4$ case for $K = 4$. As in the $N = 3$ case, we see that $P_{N=4,K=4}^{\text{trace}}(\mu_4)$ is already becoming narrower and left-shifted, and $F_{N=4,K=4}^{\text{trace}}(\mu_4)$ is plateauing to unity at much lower values of the purity μ_4 than for the corresponding case for $N = 3$ in Fig. 13.

C. Complementary-quantum correlation (CQC) relation: $N = 4$

As a final application we re-examine the complementary-quantum correlation (CQC) relation conjectured by Schneeloch *et al.* [8] which lower bounds the quantum mutual information (QMI) of a bipartite system AB of dimension $M \otimes N$ by the sum of the classical mutual informations (CMI)

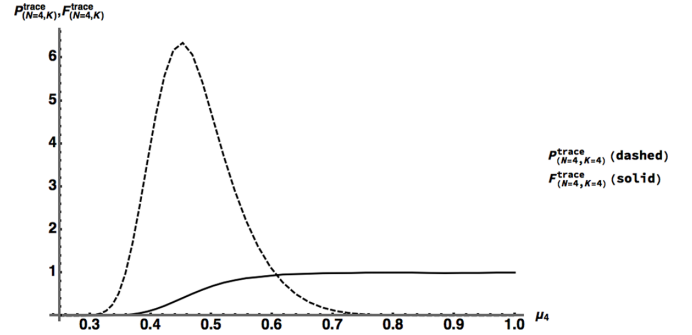


FIG. 14. Composite plot of numerically integrated $P_{N=4,K=4}^{\text{trace}}(\mu_4)$ and $F_{N=4,K=4}^{\text{trace}}(\mu_4)$, from Eq. (62).

obtained from pairs of mutually unbiased measurements on the subsystems. As usual, the QMI is given by $I(A : B) = S(A) + S(B) - S(AB)$ where S is the von Neumann entropy $S(\rho) = -\text{Tr}[\rho \log \rho]$. For the CMI, the authors considered the post-measurement-QMI obtained by local projective measurements of observables \hat{Q}^A and \hat{Q}^B on A and B , respectively. The post-measurement-QMI is equal to the CMI obtained from the joint probability distribution of measurement outcomes $P(q_i^A, q_j^B)$, where i and j run over all measurement outcomes. The CMI for the measurements $\{\hat{Q}^A, \hat{Q}^B\}$ is then given by $H(\hat{Q}^A : \hat{Q}^B) = H(\hat{Q}^A) + H(\hat{Q}^B) - H(\hat{Q}^A, \hat{Q}^B)$, where $H(\vec{p}) = -\sum_i p_i \log p_i$ is the classical Shannon entropy.

The CQC relation conjectured in Ref. [8] was given by

$$I(A : B) \geq H(\hat{Q}^A : \hat{Q}^B) + H(\hat{R}^A : \hat{R}^B), \quad (63)$$

where $\{\hat{R}^A, \hat{R}^B\}$ is another set of arbitrary measurement observables subject only to the constraint that they are mutually unbiased to the observables $\{\hat{Q}^A, \hat{Q}^B\}$ for each subsystem, respectively. Numerical evidence on $k \otimes k$ systems for $k \in \{2, 3, 4\}$ showed that for (10^7) density matrices generated randomly from unitary matrices distributed according to the Haar measure, that pairs of points (CMI $_{Z+X}$, QMI) always lay within and filled the triangle with vertices $\{(0, 0), (0, k), (k, k)\}$. Here, we have denoted CMI $_{Z+X}$ as the right-hand side of Eq. (63) for $\hat{Q} \rightarrow \hat{Z}$ and $\hat{R} \rightarrow \hat{X}$, where $\{\hat{X}, \hat{Y}, \hat{Z}\}$ are the usual single qubit Pauli spin operators. In the following we examine the case of $k = 2$ ($N = 4$, two-qubits), but now from the perspective of sampling density matrices at fixed purity values $\mu_4 \equiv \text{Tr}[\rho_{AB}^2]$.

Plotting pairs of points (not shown) (CMI $_{Z+X}$, QMI) for 2500 density matrices, each at a fixed value of purity $\mu_4 \equiv \text{Tr}[\rho_{AB}^2]$, for $\mu_4 \in \{0.26, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90, 0.95, 0.99\}$ reveals that each fixed value of μ_4 produces a scaled down version of the (gray) triangle shown in Fig. 15 (left), similar to the full triangle for $N = 4$, with vertices $\{(0, 0), (0, 2), (2, 2)\}$. Such triangles exhibit a constant maximum value of QMI for all values of CMI $_{Z+X}$ that increases with larger values of the purity μ_4 , and further include a curved edge concave-down facing the diagonal line QMI = CMI $_{Z+X}$. In Fig. 15 the gray points in the (left) plot represents 10^6 (UP) random density matrices all at fixed purity $\mu_4 = 0.999$ (note: for density matrices UE-generated from

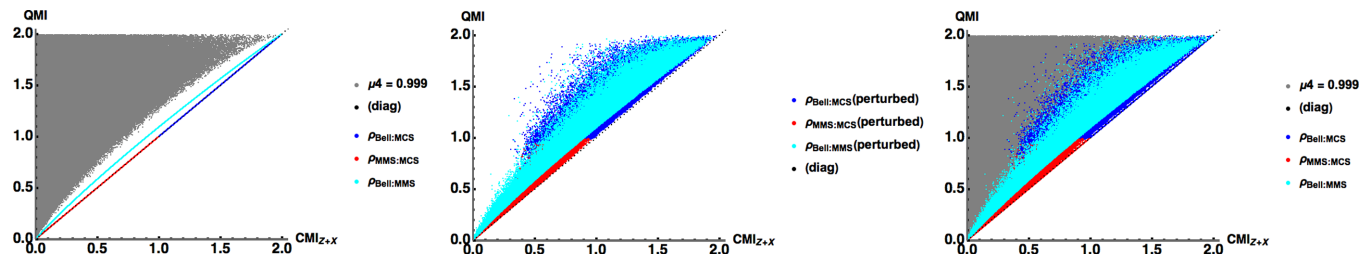


FIG. 15. Pairs of points (CMI_{Z+X}, QMI) for (left, gray) 10^6 density matrices at $\mu_4 = 0.999$, and 10^4 convex combinations of density matrices: (left, blue) Bell and maximally correlated states (MCS) $\rho_{Bell:MCS}$, (left, red) maximally mixed state and MCS $\rho_{MMS:MCS}$, and (left, cyan) Bell and MMS $\rho_{Bell:MMS}$. (center) 2.5×10^4 perturbations $U \rho U^\dagger$ of each (left) convex combinations ρ , with U near the identity matrix. (right) Composite plot of left and middle plots.

unitary matrices uniformly sampled from the Haar measure, this would have required $\sim \mathcal{O}(10^{13})$ samples to obtain the same number of states with $\mu_4 = 0.999$. We observe that the $N = 4$ triangle with vertices $\{(0, 0), (0, 2), (2, 2)\}$ is almost, though not fully populated by states with $\mu_4 = 0.999$, missing a (white) crescent shaped region near the diagonal [28]. Thus, in the (left) figure, we also plot various convex combinations of the maximally entangled Bell state $|\text{Bell}\rangle\langle\text{Bell}|$ (with $|\text{Bell}\rangle = \frac{1}{\sqrt{N}} \sum_i |ii\rangle_{ab}$), with the maximally correlated state (MCS, left, blue) given by $\rho_{MCS} = \sum_i |i, i\rangle_{ab}\langle i, i|$, and with the maximally mixed state (MMS, left cyan) given by $\rho_{MMS} = \sum_{i,j} |i, j\rangle_{ab}\langle i, j|$. The (left red) are convex combinations of the MMS with the MCS. We see that (blue) $\rho_{Bell:MCS} = p|\text{Bell}\rangle\langle\text{Bell}| + (1-p)\rho_{MCS}$ and (red) $\rho_{MMS:MCS} = p\rho_{MMS} + (1-p)\rho_{MCS}$ fill the upper and lower ends of the diagonal of the triangle, while (cyan) $\rho_{MMS:MCS} = p|\text{MMS}\rangle\langle\text{Bell}| + (1-p)\rho_{MCS}$ is a curved upper bound to the diagonal, lying outside the gray sampled points.

Thus, to fill in the white crescent shaped region, we perturb the previous mixed states by $\rho \rightarrow U \rho U^\dagger$ with U a unitary near the identity [29], as shown in Fig. 15 (middle) (using the same color coding as in the left plot). In Fig. 15 (right) we show the composite of the (left) and (middle) figures, which now almost completely fills the full $N = 4$ triangle with vertices $\{(0, 0), (0, 2), (2, 2)\}$ using only the additional randomly sampled states with fixed purity (gray) $\mu_4 = 0.999$ (note: states of purity with $\mu_4 = 1 - \epsilon$ with $\epsilon \rightarrow 0$ would completely fill the triangle).

The apparent constant maximum value of QMI (for all CMI) as a function of purity μ_4 suggests there exists a well defined purity dependent upper bound to the QMI. In Fig. 16 the red points are the values of QMI corresponding to $\text{Max}[CMI_{Z+X}]$ (blue points) now sampled with 2.5×10^4 density matrices for each fixed value of the purity (additionally including $\mu_4 = \{0.35, 0.45, 0.55, 0.65, 0.75, 0.85\}$). These $QMI = \text{Max}[QMI]$ values (a numerical approximation to the supremum of the QMI over all ρ of each fixed μ_4) clearly outline three crescent shaped curves for each of the three purity regions $\mu_4^{(1)} = [\frac{1}{4}, \frac{1}{3}]$, $\mu_4^{(2)} = [\frac{1}{3}, \frac{1}{2}]$, and $\mu_4^{(3)} = [\frac{1}{2}, 1]$. The (black, solid) curve represents the upper bound based on the using the minimum entropy in each $\mu_4^{(i)}$ region, to be described shortly. In fact, the black solid curve is actually the maximum value to the QMI given the joint purity μ_4 , since there are states saturating this bound [30]. Note that in

regions $\mu_4^{(1)}$ and $\mu_4^{(2)}$ the red points nearly coincide with the black curve, but deviate from it in region $\mu_4^{(3)}$. We conjecture that red points of $\text{Max}[QMI]$ should actually lie on the upper bound black curve, and the deviation arises solely from finite sampling size. The (black, dashed) curve is simply a linear trend line (for visual guidance) between the points $(1/4, 0)$ and $(1, 2)$. The difference $\text{Max}[QMI] - \text{Max}[CMI]$ then gives the minimum “gap” between the quantum and classical mutual information at each fixed purity value μ_4 .

The (black, solid) curve is derived as follows. For a given purity, there is an exact lower limit to the von Neumann entropy because there is a minimum entropy probability distribution for constant purity [31]. In Ref. [9], we express those distributions in terms of the purity. In particular, our lower bound to the joint entropy has the form:

$$S(AB) \geq \frac{-(1-g) \log\left(\frac{1-g}{1+\kappa}\right) - (\kappa+g) \log\left[\frac{\kappa+g}{\kappa(1+\kappa)}\right]}{1+\kappa}, \quad (64)$$

where $g = \sqrt{\kappa[\mu_4(\kappa+1) - 1]}$ and $\kappa = \text{Floor}[\frac{1}{\mu_4}]$, i.e., the value of $\frac{1}{\mu_4}$ rounded down to the nearest integer. We obtain Eq. (64) by considering diagonal density matrices of the following form $\rho_d \rightarrow \vec{p}_{\min} = (p_0, \dots, p_0, 1 - \kappa p_0, 0, 0, \dots, 0)$, where κ dictates the number of p_0 entries. Note that $p_0 = 1 \Rightarrow \kappa = 1$, a pure state, which has the minimum (zero) value of the von Neumann entropy. Therefore, \vec{p}_{\min} represents diagonal density matrices that

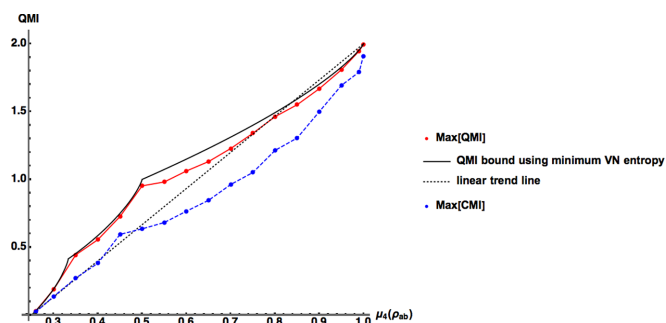


FIG. 16. (red) $QMI (\equiv \text{Max}[QMI])$ value corresponding to (blue) $\text{Max}[CMI_{Z+X}]$ from 25 000 density matrices, each at a fixed value of purity $\mu_4 \equiv \text{Tr}[\rho_{AB}^2]$, for $\mu_4 \in \{0.26, 0.30, 0.40, 0.50, 0.60, 0.70, 0.80, 0.90, 0.95, 0.99\}$. (black, solid) QMI bound using minimum von Neumann entropy (as described in text); (black, dashed) linear trend line.

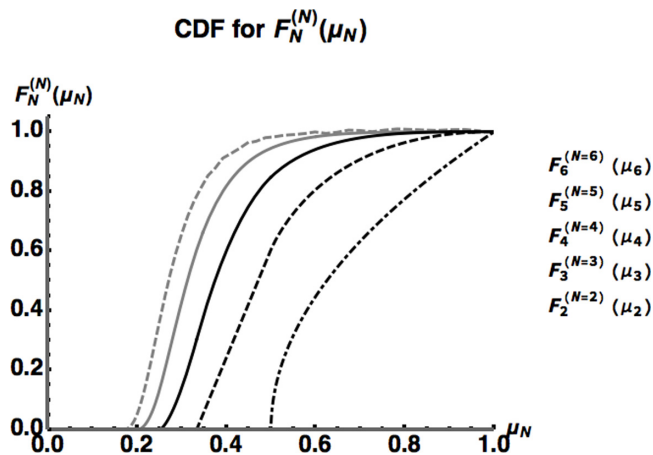


FIG. 17. Radial CDFs $F_N^{(N)}(\mu_N)$ same as (analytical) Fig. 2 but now additionally including (mostly analytic) $N = 5$ (gray-solid) and (numerical) $N = 6$ (gray-dashed).

deviate from the pure state as p_0 decreases from unity. We now fix p_0 by setting $\bar{p}_{\min}^2 = \mu_4$ and solving for $p_0 = p_0(\mu_4)$ (choosing the root that gives $p_0 = \mu_4$ if $\kappa \equiv \frac{1}{\mu_4}$). We then simply compute $S_{\min} = -p_0(\mu_4) \log_2 p_0(\mu_4) - [1 - p_0(\mu_4)] \log_2 [1 - p_0(\mu_4)]$ with $\kappa \rightarrow \text{Floor}[\frac{1}{\mu_4}]$ to obtain the (black) upper bound.

It is interesting to note that the (black) serrated curve yields a much tighter bound than a simple upper bound estimate obtained [9] by considering the maximum of the von Neumann entropy S_{\max} derived from considering $\bar{p}_{\max} = [p_0, \dots, p_0, 1 - (N-1)p_0]$, where all but one entry is given by p_0 . Again we fix p_0 by setting $\bar{p}_{\max}^2 = \mu_4$, and solve for $p_0 = p_0(\mu_4)$ (choosing the root such that $p_0 \leq 1 - (N-1)p_0$). One then notes that the collision entropy defined by $S_2(\mu_4) = -\log_2(\mu_4)$ [27] is always less than or equal to the joint von Neumann entropy $S(A, B)$, so that $S_{\max} \equiv S(A) + S(B) - S_2(\mu_4) \geq I(A : B)$. The curve for S_{\max} would be a smooth concave arc in Fig. 16 (not shown) with endpoints at points $(\frac{1}{4}, 0)$ and $(1, 2)$ which also just touches the Max[QMI] values at the cusp values at $\mu_4 = \frac{1}{3}$ and $\mu_4 = \frac{1}{2}$, i.e., at all the four boundary points of the three $\mu_4^{(i)}$ regions. As observed in Fig. 16, the bound using the minimum entropy S_{\min} produces a much tighter bound (in fact, the maximum value of the QMI) than that using S_{\min} .

VI. $N = 5, 6$ AND HIGHER DIMENSIONS, PLUS NUMERICAL CONSIDERATIONS

In Fig. 17 we plot the same radial CDFs $F_N^{(N)}(\mu_N)$ versus μ_N but now additionally including $N = 5$ (gray-solid) and $N = 6$ (gray-dashed). As N increases we observe a steeper transition from low to high CDF values occurring at much lower purity values. The more extended flat region of $F_N^{(N)}(\mu_N) \sim 1$ as N increases presents challenges for both numerical accuracy in this region, as well as for numerically computing the inverse of the CDF for the purposes of sampling.

The curve for $F_5^{(N=5)}(\mu_5)$ in Fig. 17 was computed as in terms of $r_5 = \sqrt{\mu_5 - \frac{1}{5}}$ as

$$F_5^{(N=5)}(r_5) = \frac{\int_0^{r_5 \leq r_5^{(\max)}} dr'_5 r_5'^3 F_4^{(N=5)\text{Denom}}(r'_5)}{\int_0^{r_5^{(\max)} = \sqrt{4/5}} dr'_5 r_5'^3 F_4^{(N=5)\text{Denom}}(r'_5)}, \quad (65a)$$

$$\equiv \frac{F_5^{(N=5)\text{Num}}(r_5)}{F_5^{(N=5)\text{Denom}}}. \quad (65b)$$

Here $F_5^{(N=5)\text{Denom}}$ is the r_5 -independent normalization constant given by the denominator of Eq. (65a), which is just the numerator of Eq. (65a) evaluated at the maximum purity value $\mu_5 = 1 \leftrightarrow r_5 = \sqrt{4/5}$. In turn, the descending $F_{k=4,3,2}^{(N=5)\text{Denom}}$ terms are given by

$$F_4^{(N=5)\text{Denom}}(r_5) = \int_{1/4}^{\bar{X}_4^{\max}(r_5) = \text{Min}[\frac{1}{5.4r_5}, 1]} dX_4 \times \sqrt{1 - X_4^2} F_3^{(N=5)\text{Denom}}(X_4), \quad (66a)$$

$$F_3^{(N=5)\text{Denom}}(X_4) = \int_{1/3}^{\bar{X}_3^{\max}(X_4) = \text{Min}[\frac{\sqrt{5/3}X_4}{\sqrt{1-X_4^2}}, 1]} dX_3 \times F_2^{(N=5)\text{Denom}}(X_3), \quad (66b)$$

$$F_2^{(N=5)\text{Denom}}(X_3) = \int_{\bar{\varphi}_2^{\max}(X_3) = \cos^{-1}(\text{Min}[\frac{\sqrt{2}X_3}{\sqrt{1-X_3^2}}, 1])}^{\pi/3} d\varphi_2. \quad (66c)$$

Now, for all N , $F_2^{(N)\text{Denom}}(X_3)$ is the expression given in Eq. (42) for $F_2^{(N=4)\text{Denom}}(X_3)$, since it is the lowest angle. For $N \geq 5$, $F_3^{(N=5)\text{Denom}}(X_4)$ is given by the expressions in Eqs. (45a)–(45c) for $F_3^{(N=4)\text{Denom}}(r_4)$ with the substitution of $\bar{X}_3^{\max}(r_4) = \text{Min}[\frac{1}{\sqrt{4.3}r_4}, 1] \rightarrow \bar{X}_3^{\max}(X_4) = \text{Min}[\frac{\sqrt{5/3}X_4}{\sqrt{1-X_4^2}}, 1]$. This occurs since for $N = 4$, $X_{3=N-1}$ is the highest angle. However, for $N \geq 5$, X_3 is now a bona fide middle angle. The highest angle for $N = 5$ is now $X_{4=N-1}$ with $\bar{X}_4^{\max}(r_5) = \text{Min}[\frac{1}{\sqrt{5.4}r_5}, 1]$. In addition, each $F_{k>2}^{(N)\text{Denom}}(X_{k+1})$ is integrated over $(1 - X_k^2)^{(k-3)/2} dX_k$ coming from the $\sin^{(k-2)}(\varphi_k) d\varphi_k$ in the volume measure dV_N . The procedure in Eq. (65a) through Eq. (66c) generalizes to arbitrary N .

Surprisingly, for all but one of the subintegrations over r_5 in $F_5^{(N=5)\text{Denom}}(r_5)$, the numerator of Eq. (65a) can be carried out in closed form. The “holdout” term arises from the subexpression $\tan^{-1}[\sqrt{\frac{1-6X_4^2}{2(1-X_4^2)}}]$ that occurs in $F_3^{(N=5)\text{Denom}}(X_4)$ in the region $X_4 \in [\frac{1}{4}, \frac{1}{\sqrt{6}}]$, which when integrated over $\sqrt{1 - X_4^2}$ to contribute to $F_4^{(N=5)\text{Denom}}(r_5)$, cannot be done in closed form. This latter integration must be performed numerically, and once again when integrated over r_5^3 to contribute to the final result $F_5^{(N=5)\text{Denom}}(r_5)$.

The gray-solid line in Fig. 17 for the CDF $F_5^{(N=5)}(r_5)$ was computed using as many analytic formulas as possible, with numerical integration reserved for the “holdout” term just discussed.

This reduction to mostly analytic expressions quickly fails at the $N \geq 6$ level, primarily due to the volume integration factors of $(1 - X_k^2)^{(k-3)/2}$. Thus, in contrast to the involved analytical integration over various regions of $\{\varphi_2, X_3, \dots, X_{N-1}, r_N\}$ as was carried out for $F_5^{(N=5)}(r_5)$, the gray-dashed curve in Fig. 17 for $F_6^{(N=6)}(r_6)$ was carried out by a straightforward nested integration over $\{\varphi_2, X_3, X_4, X_5, r_6\}$ for $N = 6$, which is trivially coded up in just a few lines as shown in Listing 1. This was the *Mathematica* code used to produce the gray-dashed curve for $N = 6$ in Fig. 17.

Listing 1. Nested integral Mathematica example: $N = 6$.

```

F6N6r6Num[r6value_] :=
Block[{$MaxExtraPrecision = 1000},
  NIntegrate[r6^4 (1 - X5^2) sqrt[1 - X4^2],
    {r6, 0, r6value},
    {X5, 1/5, Min[1/sqrt[6x5 r6], 1]},
    {X4, 1/4, Min[sqrt[6/4 X5], sqrt[1 - X5^2], 1]},
    {X3, 1/3, Min[sqrt[5/3 X4], sqrt[1 - X4^2], 1]},
    {phi2, Min[sqrt[4/2 X3], sqrt[1 - X3^2], 1], pi/3},
  Method -> "Trapezoidal,"
  WorkingPrecision -> 20]
]
(*given mu6, r6value = sqrt[mu6 - 1]/6; call as*)
F6N6Denom = F6N6r6Num[sqrt[4/5]]; (* once *)
F6N6 = F6N6r6Num[r6value]/F6N6Denom

```

While in the straightforward Listing 1 a modest attempt has been made to increase the precision of the nested numerical integrations, more attention must be made to this issue as revealed by the undulations at higher purity values (flat regions of the CDF) in the gray-dashed curve in Fig. 17 for $N = 6$. This issue arises since in the region where $F_N^{(N)}(\mu_N) \sim 1 - \epsilon$, differences in values of the CDF are exponentially small, which compound the inaccuracies when a small number $\epsilon_2 \ll 1$ is added in the integration procedure to a prior large number $1 - \epsilon_1 \sim \mathcal{O}(1)$ to obtain the next $\mathcal{O}(1)$ value $1 + (\epsilon_2 - \epsilon_1)$. For $N = 6$ it was found that a globally adaptive integration strategy produced a much smoother curve of $F_6^{(N=6)}(\mu_6)$ (not shown), especially for higher purity values, over that using a locally adaptive integration strategy (at least in *Mathematica*).

To create a uniform sampling procedure for a fixed purity μ_N (or r_N), all CDFs $F_k^{(N)}(X_k; X_{k+1})$ for $k \in \{2, \dots, N - 1\}$ must be computed, which can be performed numerically analogous to Listing 1 by truncating the nested integrals at level k , and appropriately adjusting the limits of the highest angle $k = N - 1$. One then forms $F_k^{(N)Num}(X_k; X_{k+1})$, from which $F_k^{(N)Denom}(X_{k+1})$ is evaluated at $X_k \rightarrow \bar{X}_k^{max}$ and the CDF is formed by $F_k^{(N)}(X_k; X_{k+1}) = F_k^{(N)Num}(X_k; X_{k+1})/F_k^{(N)Denom}(X_{k+1})$. The UP sampling procedure above was performed using a more involved numerical integration scheme than that of the straightforward (yet easily coded) procedure in Listing 1 to compute the radial

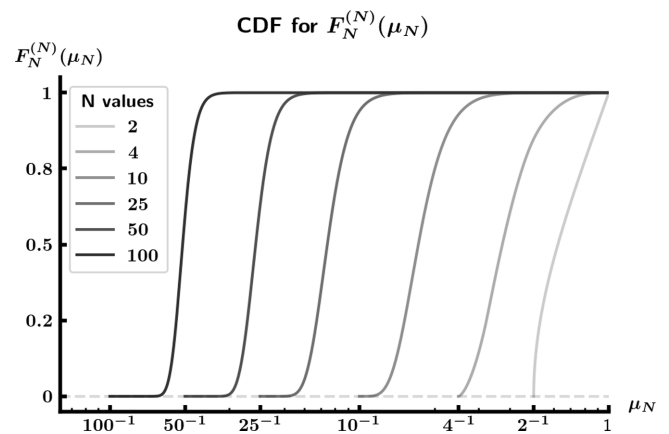


FIG. 18. Numerically integrated radial CDFs $F_N^{(N)}(\mu_N)$ for high dimensions $N \in \{2, 4, 10, 25, 50, 100\}$ using a more sophisticated integration scheme than Listing 1.

CDFs for very high dimensions as shown in Fig. 18 for $N \in \{2, 4, 10, 25, 50, 100\}$. (Note: the code also produced reliable results for dimensions as high as $N = 15^2 = 225$, before errors due to precision limits dominated). The results in Fig. 18 were numerically calculated through successive integration of the cumulative distribution function (CDF) evaluated at a fixed number of points ($\sim 10^4$) for all parameters involved in the integrations. The integration scheme included the points where it is known that discontinuities due to the minimum integration bound of the CDF occur, leading to a nonuniform parameter space. Additionally, we stored only relative changes in the CDF, and reconstruct it using decreasing values of its argument which avoids decimation in the region where the CDF is close to unity. The samples generated from this more sophisticated code were recently used in a complementary paper by the authors [9] to explore measure of entanglement at high dimensions up to $N = 100$.

Last, for extremely high dimensions it is noteworthy that the factors of $(\sin \varphi_k)^{k-2} \leftrightarrow (1 - X_k^2)^{(k-3)/2}$ arising from the volume integration measure become sharply peaked around $\varphi_k \sim \pi/2 \leftrightarrow X_k \sim 1$, a well known fact for the volumes of N -spheres [3]. This implies that for large N , $(1 - X_k^2)^{(k-3)/2} \sim 1 - \frac{(k-3)}{2} X_k^2 \approx e^{-\frac{(k-3)}{2} X_k^2}$ is an ever increasingly accurate approximation such that one can additionally add the constraint to the limits of integration of X_k that it be sampled from

$$X_{k \gg 3} \in 7 \left[\sqrt{\frac{2}{k-3}}, \text{Max} \left[\sqrt{\frac{2}{k-3}}, \text{Min} \left[\sqrt{\frac{k+2}{k}} \frac{X_{k+1}}{\sqrt{1 - X_{k+1}^2}}, 1 \right] \right] \right], \quad (67)$$

which implies that sampling of X_k ceases when $\bar{X}_k^{max}(X_{k+1}) \equiv \sqrt{\frac{k+2}{k}} \frac{X_{k+1}}{\sqrt{1 - X_{k+1}^2}} < \sqrt{\frac{2}{k-3}}$. This approximation could aid in sampling from the relevant nonnegligible contributions to the integration over X_k for very large values of N .

VII. SUMMARY AND CONCLUSION

In this work we have presented a formulation to uniformly sample density matrices ρ of fixed purity for arbitrary dimensions N based on generating fixed purity random diagonal density matrices ρ_{diag} , where $\rho = U \rho_{\text{diag}} U^\dagger$, with U a unitary matrix uniformly sampled from the Haar measure. We have provided analytic formulas for the case of generating ρ_{diag} in dimensions $N \in \{2, 3, 4\}$, and analytical/numerical formulation for $N = 5$, and provided simple implementable nested-integration numerical code for any dimension (particularly for $N \geq 6$). We have further has shown results (up to $N = 100$) for numerical sampling at fixed purity using a more sophisticated (and involved) numerical procedure allowing us to generate radial CDFs at very high dimensions. We used the analytic formulation for $N = 4$, the case of two-qubits, to explore the relation of well known entanglement measures, and a “baseline” entanglement witness, on the purity $\mu_4(\rho_{ab})$ of the two-qubit composite state, as well as on the purity of $\mu_2(\rho_a)$ of the reduced single qubit system. In addition, we have used our method to sample density matrices at arbitrary constant purity to explore the complementary-quantum correlation (CQC) conjecture. While the investigations for $N = 4$ could in principle be carried out purely by uniformly sampling U from the Haar measure (where ρ_{diag} can be obtained as the absolute square of another randomly generated U'), we have shown that this latter sampling is heavily weighted toward lower values of the purity $\mu_4(\rho_{ab})$. This rarity of generating high purity states by the latter method is only exacerbated as the dimension increases, as we have shown by computing the radial cumulative probability distribution function (CDF) for $N \in \{2, 3, 4, 5, 6, 10, 25, 50, 100\}$.

Many entanglement measures (or witnesses) rely on constructions utilizing a reduced density matrix of the composite system (such as entropy-based methods), or on the manipulations of the composite density matrix itself (such as the eigenvalues of the partial transpose of the composite density matrix in the case of the logarithmic negativity). While clearly the eigenvalues $\{\lambda_i\}$ of the composite system ρ are the same as its diagonal (spectral representation) ρ_{diag} , the reduced density matrices $\rho_a = \text{Tr}[\rho_{ab}]$ (where here, both a and b each now represent a possible collection of subsystems) depend on both the eigenvalues $\{\lambda_i\}$ as well as the reduced matrix elements of the random U , since $d\rho = U[d\rho_{\text{diag}} + U^{-1}dU\rho_{\text{diag}} - \rho_{\text{diag}}U^{-1}dU]U^{-1} \Rightarrow (d\rho)_{ij} = d\lambda_i\delta_{ij} + (\lambda_j - \lambda_i)(U^{-1}dU)_{ij}$ [3]. Thus, it is in general impossible to construct a uniform distribution of reduced density matrices of fixed purity $\mu(\rho_a)$ starting from a higher dimensional mixed composite system ρ_{ab} . However, what we have shown is the opposite, namely that we can construct composite mixed density matrices of fixed purity $\mu(\rho_{ab})$ and study the dependence of the entanglement measures (or witnesses) constructed from the subsequent further randomized sets of purities $\mu(\rho_a)$ of the lower dimensional reduced density matrices. This is especially important as we study effects of entanglement measures resulting from composite systems of high purity, where our method can act as an efficient means to generate a statistically relevant sample of random states to more accurately explore this purity regime [9].

Further, as in Sec. VB, we can alternatively consider ρ_N to be the reduced density matrix (averaged over all unitary equivalents) derived from a higher-dimensional purification with arbitrary reservoir dimension K . The formalism presented in this work then allows for a spherical polar description of the eigenvalues $(\lambda_1, \lambda_2, \dots, \lambda_N)$ in terms of the variables $(\varphi_2, \varphi_3, \dots, \varphi_{N-1}, r_N)$ describing these eigenvalues in the Weyl-Chamber. For the joint probability distribution of the eigenvalues we can obtain closed formed analytic expressions in terms of the spherical polar variables for arbitrary N and K . By integrating out the angular variables $\{\varphi_k\}$ we can construct probability and cumulative probability distribution functions of the reduced state ρ_N in terms of its purity μ_N , which for certain lower dimensional cases can be expressed analytically.

Even at the lower purity regime, favored by the uniform (w.r.t. to the Haar measure) U approach, our method act can act as a surgical tool to more efficiently and precisely explore certain questions. It is well known that for the case of $N = 4$ (two-qubits) and $N = 6$ (qubit-qutrit) the boundary between separable and entangled states occurs at composite purity $\mu_N = \frac{1}{N-1}$. For all other dimensions, separable states lie somewhere just outside the regime $\mu_N^{(1)} \in \{\frac{1}{N}, \frac{1}{N-1}\}$ (for a proof, see Ref. [12]). Our method of generating composite density matrices of fixed purity can be used in a numerical search routine to more precisely pinpoint this transition boundary between separable and entangled states (say using the logarithmic negativity as the entanglement measure) than would be obtained by uniform (Haar) random UE approach (see also the work of Zyczkowski [32]). This, and other aspects of high dimensional entanglement as a function of purity, will be explored in future work.

ACKNOWLEDGMENTS

P.M.A. and J.S. acknowledge support of this work from the Air Force Office of Scientific Research. Any opinions, findings, conclusions, or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of Air Force Research Laboratory. The appearance of external hyperlinks does not constitute endorsement by the United States Department of Defense (DoD) of the linked websites, or the information, products, or services contained therein. The DoD does not exercise any editorial, security, or other control over the information you may find at these locations.

APPENDIX A: WERNER STATES: LOGARITHMIC NEGATIVITY LN AND VARIANT OF LINEAR ENTROPY ΔE

Because they are analytically tractable, it is informative to examine bipartite Werner states of dimension d^2 [where $d = (M + 1)$], i.e., $\rho_{ab}^{(W, d^2)} = p|\Psi_{\text{Bell}}\rangle_{ab}\langle\Psi_{\text{Bell}}| + \frac{(1-p)}{d^2}I_{d^2 \times d^2}$ with $|\Psi_{\text{Bell}}\rangle_{ab} = \frac{1}{\sqrt{d}}\sum_{n=0}^{d-1}|nn\rangle_{ab}$. (Note: $|\Psi_{\text{Bell}}\rangle$ is a $d^2 \times 1$ vector, so $\rho_{ab}^{(W, d^2)}$ is a $d^2 \times d^2$ matrix.) In Fig. 19 we show the logarithmic negativity $\text{LN}(\rho_{ab})$, for Werner states with (top) $M = 1$ (two qubits) and $M = \{3, 8, 18\}$.

It is straightforward to compute that for the Werner state the negative eigenvalues of the partial transpose are given

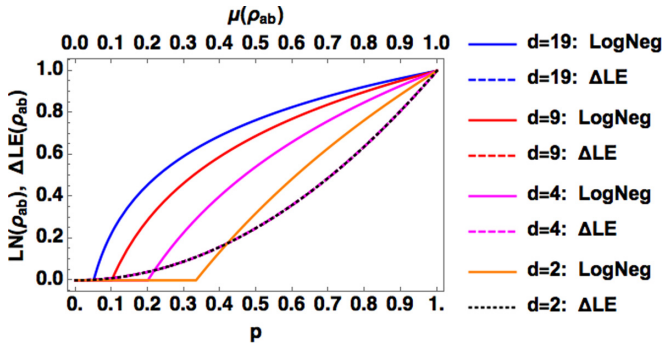


FIG. 19. Scaled $\text{LN}(\rho_{ab}^{(W, d^2)})$ [by $\log_2(d)$]: for $d^2 = (M + 1)^2$ dimensional Werner states with probability (to be in the pure state) $0 \leq p \leq 1$, for dimensions (left to right) $d = \{19, 9, 4, 2\} \leftrightarrow \{\text{blue, red, magenta, orange}\}$ for (solid) $\text{LN}(\rho_{ab})$, and (dashed) $\Delta\text{LE}(\rho_{ab})$. Note: All $\Delta\text{LE}(\rho_{ab})$ (dashed) curves are identical, and fall on the black-dashed curve associated with $d = 2$.

by $\lambda_- = \frac{1}{d^2} [1 - (d + 1)p]$ for $\frac{1}{d+1} \leq p \leq 1$ with multiplicity $\binom{d}{2} = \frac{d(d-1)}{2}$. Therefore, the negativity in this region is given by $\mathcal{N} = \frac{1}{2} \frac{d-1}{d} [(d + 1)p - 1]$ with $\text{LN} = \log_2(1 + 2\mathcal{N})$, yielding $\text{LN}(p = \frac{1}{d+1}) = 0$ and $\text{LN}(p = 1) = \log_2(d)$. Thus, $\rho_{ab}^{(W, d^2)}$ is entangled ($\text{LN} > 0$) for $\frac{1}{(d+1)} < p \leq 1$ and separable ($\text{LN} \leq 0$) for $0 \leq p \leq \frac{1}{(d+1)}$. The dimensions $d = (M + 1) = \{2, 4, 9, 19\}$ where chosen so that the sudden death of entanglement occurred at easily recognizable points $p = \{\frac{1}{3}, \frac{1}{5}, \frac{1}{10}, \frac{1}{20}\}$ on the abscissa in Fig. 19.

Finally, one can also show that the purity $\mu(\rho) = \text{Tr}[\rho^2]$ for the Werner states is given by $\mu_{(W, d^2)} = \frac{1+(d^2-1)p}{d^2}$ corresponding to a critical value $\mu_{(W, d^2)}^* = \frac{2}{d(d+1)}$ at the sudden death of entanglement at $p = \frac{1}{d+1}$. This is plotted as the top abscissa in Fig. 19.

In Fig. 19 we also plot $\Delta\text{LE}(\rho_{ab})$ as given by

$$\Delta\text{LE}(\rho_{ab}) = \text{Max} \left[0, \frac{(\mu(\rho_{ab}) - \frac{1}{d^2}) - (\mu(\rho_a) - \frac{1}{d})}{1 - \frac{1}{d^2}} \right]. \tag{A1}$$

Note that the $\Delta\text{LE}(\rho_{ab})$ curves all fall on the same (multi-colored dashed) curve. This occurs because the d -dimensional Bell state has reduced density matrix ρ_a equal to the MMS for all dimensions d . $\Delta\text{LE}(\rho_{ab})$ acts a better lower bound to $\text{LN}(\rho_{ab})$ the more d increases.

APPENDIX B: UNIFORM GENERATION OF RANDOM UNITARY AND DIAGONAL DENSITY MATRICES

The following *Mathematica* codes follow the procedure outlined in Mezzadri [1] to generate a uniform random $n \times n$ unitary U matrix (with respect to the Haar measure), and then subsequently generate a uniform random density matrix of dimension n .

Listing 2. Mathematica code to generate random unitary U .

```
URandom[n_] :=
Module[{Z, Q, R, diagR, Λ},
  RG:=RandomVariate[NormalDistribution[]];
  Z = Table[ $\frac{1}{\sqrt{2}}$ (RG + I RG), {n}, {n}];
  {Q,R}=QRDecomposition[Z];
  (* Note: Z=Q.R=(Q Λ).(Λ-1R).*)
  (*Make R (hence Q) unique by forcing R*)
  (*to have positive diagonal entries*)
  diagR=Diagonal[R];
  (* diagonal matrix  $\frac{R_{ii}}{|R_{ii}|}$  *)
  (* Note: Λ-1R makes diagonal entries *)
  (* of R to be |Rii| *)
  Λ=DiagonalMatrix[diagR/Abs[diagR]]//Chop;
  (* return unique unitary matrix *)
  Q = Q.Λ // Chop
]
```

Listing 3. Mathematica code to generate random ρ .

```
ρRandom[n_] :=
Module[{U, ρd},
  RI:=RandomInteger[{1,n}];
  (* ρd = ρdiagonal: take a random row of U*)
  U=URandom[n];
  ρd = Abs[U[[RI]]]^2 // Chop;
  (*form ρ = U.ρd.U†*)
  U=URandom[n];
  (*return random density matrix ρ*)
  ρ = U.ρd.U† // Chop
]
```

[1] F. Mezzadri, How to generate random matrices from the classical compact groups, *Notices AMS* **54**, 592 (2007).
 [2] K. Życzkowski, K. Penson, I. Nechita, and B. Collins, Generating random density matrices, *J. Math. Phys.* **52**, 062201 (2011).

[3] I. Bengtsson and K. Życzkowski, *The Geometry of Quantum States*, 2nd ed. (Cambridge University Press, Cambridge, UK, 2020).
 [4] S. Lloyd, Quantum enigma machines, [arXiv:1307.0380](https://arxiv.org/abs/1307.0380).

- [5] D. Lum, J. C. Howell, M. S. Allman, T. Gerrits, V. B. Verma, S. W. Nam, C. Lupo, and S. Lloyd, Quantum enigma machine: Experimentally demonstrating quantum data locking, *Phys. Rev. A* **94**, 022315 (2016).
- [6] W. K. Wootters, Entanglement of Formation of an Arbitrary State of Two Qubits, *Phys. Rev. Lett.* **80**, 2245 (1998).
- [7] For a general probability density function (PDF) $p(x)$, the cumulative distribution function (CDF) is given by $F(x) = \int_{x_0}^x p(x') dx'$ such that $\text{Prob}(a \leq x \leq b) = \int_a^b p(x') dx' = \int_{x_0}^b p(x') dx' - \int_{x_0}^a p(x') dx' = F(b) - F(a)$.
- [8] J. Schneeloch, C. J. Broadbent, and J. C. Howell, Uncertainty relation for mutual information, *Phys. Rev. A* **90**, 062119 (2014).
- [9] J. Schneeloch, H. S. Jacinto, C. C. Tison, and P. M. Alsing, Negativity vs. purity and entropy for witnessing entanglement, [arXiv:2009.06765v2](https://arxiv.org/abs/2009.06765v2).
- [10] K. Życzkowski and M. Kus, Random unitary matrices, *J. Phys. A: Math. Gen.* **27**, 4235 (1994).
- [11] W. Press, S. Teuklosky, W. Vetterling, and B. Flannery, *Numerical Recipes in C* (Cambridge University Press, Cambridge, UK, 1992), Chap. 2.10, pp. 98–102.
- [12] K. Życzkowski, P. Horodecki, A. Sanpera, and M. Lewenstein, Volume of the set of separable states, *Phys. Rev. A* **58**, 883 (1998).
- [13] Unfortunately, this fortuitous dependence of x_k only on the two purities (μ_k, μ_{k-1}) does not occur for other traces of higher powers of ρ , i.e., $\text{Tr}[\rho^q]$ for $q > 2$, and so the enumeration of the range of the coordinates is intractable analytically, except for case of $q = 2$.
- [14] W. Wootters, Entanglement of formation and concurrence, *Q. Inf. Comput.* **1**, 27 (2001).
- [15] A. Peres, Separability Criterion for Density Matrices, *Phys. Rev. Lett.* **77**, 1413 (1996).
- [16] P. Horodecki, Separability criterion and inseparable mixed states with positive partial transposition, *Phys. Lett. A* **232**, 333 (1997).
- [17] G. S. Agarwal, *Quantum Optics* (Cambridge University Press, Cambridge, UK, 2013).
- [18] H. Ollivier and W. H. Zurek, Quantum Discord: A Measure of the Quantumness of Correlations, *Phys. Rev. Lett.* **88**, 017901 (2001).
- [19] S. Luo, Quantum discord for two-qubit systems, *Phys. Rev. A* **77**, 042303 (2008).
- [20] C. C. Rulli and M. S. Sarandy, Global quantum discord in multipartite systems, *Phys. Rev. A* **84**, 042109 (2011).
- [21] L. Henderson and V. Vedral, Global quantum discord in multipartite systems, *J. Phys. A* **34**, 6899 (2001).
- [22] V. Vedral, Classical Correlations and Entanglement in Quantum Measurements, *Phys. Rev. Lett.* **90**, 050401 (2003).
- [23] Recall that the quantum discord \mathcal{Q} for a bipartite system ρ_{ab} is defined as the difference between two expressions for the quantum mutual information: (i) $\mathcal{I}(\rho_{ab}) = S(\rho_a) + S(\rho_b) - S(\rho_{ab})$ and (ii) $\mathcal{J}(\rho_{ab}|\{\Pi_b^k\}) = S(\rho_a) - S(\rho_{ab}|\{\Pi_b^k\})$ where $\{\Pi_b^k\}$ are a complete set of projective measurements on subsystem b . Here $S(\rho_{ab}|\{\Pi_b^k\}) \stackrel{\text{def}}{=} \sum_k p_k S(\rho_a^{(k)})$ with $\rho_a^{(k)} = \frac{1}{p_k} (I_a \otimes \Pi_b^k) \rho_{ab} (I_a \otimes \Pi_b^k)$ and $p_k = \text{Tr}[(I \otimes \Pi_b^k) \rho_{ab} (I \otimes \Pi_b^k)]$. The classical correlations are defined as $\mathcal{J}(\rho_{ab}) = \sup_{\{\Pi_b^k\}} \mathcal{J}(\rho_{ab}|\{\Pi_b^k\})$, and the quantum discord is defined as the difference $\mathcal{Q}(\rho_{ab}) = \mathcal{I}(\rho_{ab}) - \mathcal{J}(\rho_{ab})$.
- [24] The logarithmic negativity LN is given by $\text{LN}(\rho_{ab}) = \log_2[1 + 2\mathcal{N}(\rho_{ab})]$, where the negativity $\mathcal{N}(\rho_{ab})$ is defined as the sum of the absolute values of the negative eigenvalues of the partial transpose (on either subsystem a or b) of the composite state ρ_{ab} .
- [25] For the case of the Werner state used here with the d -dimensional Bell state, whose reduced density matrix is maximally mixed, the second term $\mu(\rho_a^{(N_a)}) - \frac{1}{N_a}$ in Eq. (52) is exactly zero, and ΔLE is strictly a linear function of $\mu(\rho_{ab}^{(N)})$. For other choices of the pure state component of the Werner state, this second term would not be zero, and would come into play.
- [26] Technically, \mathbf{F}^N is *Flag Manifold*, i.e., a Cartesian product of spheres [see Ref. [3] Eq. (15.23)] $\mathbf{F}^N = \frac{U(N)}{[U(1)]^N} \approx \frac{U(N)}{U(N-1) \times U(1)} \frac{U(N-1)}{U(N-2) \times U(1)} \cdots \frac{U(2)}{U(1) \times U(1)} \approx \mathbb{C}P^{N-1} \times \mathbb{C}P^{N-2} \times \cdots \times \mathbb{C}P^1$. Here $\mathbb{C}^k = S^{2k-1}$ (complex projective space of dimension k) are the complex k -tuples (Z_1, \dots, Z_k) such that $\sum_{i=1}^k |Z_i|^2 = 1$, i.e., k complex numbers (i.e., $2k$ real numbers) whose squares sum to unity, i.e., the sphere S^{2k-1} . The flag manifolds \mathbf{F}^N informs one of the symmetry group (see Table 8.1 in Ref. [3], p. 234) of ρ_d , whose symmetry depends on how many of the eigenvalues are equal (i.e., none equal—the interior of the WC, to all equal—the MMS $\lambda_i = 1/N$ for all $i \in \{1, \dots, N\}$).
- [27] If desired, we could also use the probability distribution $P_{N=3,K}^{\text{trace}}(\mu_3)$ to write $P_{N=3,K}^{\text{trace}}(S_3)$ in terms of the Rényi entropy $S_3^{(N)} = S_3(\rho_N) = -\ln(\sum_{i=1}^N \lambda_i^3)$ as in Fig. 12. The family of Rényi entropies $S_\alpha(AB) = S_\alpha(\hat{\rho}_{AB}) \equiv \frac{1}{1-\alpha} \log(\text{Tr}[\hat{\rho}_{AB}^\alpha])$ include the von Neuman entropy $\lim_{\alpha \rightarrow 1} S_\alpha(AB) = -\text{Tr}[\hat{\rho}_{AB} \log(\hat{\rho}_{AB})]$, and the collision entropy $\lim_{\alpha \rightarrow 2} S_\alpha(AB) = -\log(\text{Tr}[\hat{\rho}_{AB}^2]) = -\log(\mu(\rho_{ab}))$.
- [28] It is worth noting that one can prove that the entire triangle can be filled out (not counting possible violations). The hypotenuse represents mixtures of the maximally entangled state, maximally correlated mixed state, and the maximally mixed state. By changing the local basis upon which classical correlations are measured, one can trace out a flat horizontal line from each point on the diagonal to a point on the left side of the triangle, filling it entirely.
- [29] We generate the unitary U near the identity as follows. We create an $N \times N$ matrix with entries drawn from a normal distribution with unit variance, and scale the entries by a fixed chosen $\epsilon < 1$ which sets the scale of the deviation of U from the $N \times N$ identity matrix (in the plot we chose $\epsilon = 0.15$). Next, we replace the diagonal entries by unity, and Gram-Schmidt orthonormalize the matrix (`Orthogonalize` in *Mathematica*) to produce the unitary U .
- [30] In particular, consider a mixture of four orthogonal Bell states with a total purity of μ_4 but whose eigenvalues form a minimum entropy distribution at constant purity. For this set of mixed states, the marginal states are maximally mixed, and the quantum mutual information will be what is given by the black solid curve.
- [31] D. W. Berry and B. C. Sanders, Bounds on general entropy measures, *J. Phys. A: Math. Gen.* **36**, 12255 (2003).
- [32] K. Życzkowski, Volume of separable states II, *Phys. Rev. A* **60**, 3496 (1999).