Halving the length of approximate classical representations of pure quantum states with probabilistic encoding

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Pure quantum states are often approximately encoded as classical bit strings such as those representing probability amplitudes and those describing circuits that generate the quantum states. The crucial quantity is the minimum length of classical bit strings from which the original pure states are approximately reconstructible. We derive asymptotically tight bounds on the minimum bit length required for probabilistic encodings with which one can approximately reconstruct the original pure state as an ensemble of the quantum states encoded in classical strings. Our results imply that such a probabilistic encoding asymptotically halves the bit length required for “deterministic” ones.

I. INTRODUCTION

In classical physics, the state of a physical system, called a classical state, is either one of deterministic states or a probabilistic mixture of them, where the latter merely represents our lack of knowledge about the state. A unique feature of classical states is that any deterministic state can be cloned, which is distinct from other probabilistic models, including the one corresponding to quantum physics [1]. This also ensures the consistency of information encoded in classical states, in contrast to the inconsistency of inferences drawn from outcomes obtained by measuring quantum states [2]. Due to these remarkable features, quantum states are often approximately encoded in classical states, such as bit strings representing density matrices and circuit descriptions that generate the quantum states. Additionally, various classical encodings are used in quantum information processing tasks, such as predicting expectation values of observables from limited measurement outcomes within a certain precision and with a high probability [3–5]; classically transmitting a quantum state so as to approximately sample outcomes of an arbitrary quantum measurement [6]; and reconstructing a quantum state from measurement outcomes within a certain precision in state tomography or state estimation.

The key issue is the minimum encoding. Here, we investigate it in terms of the minimum length of classical bit strings, with which one can approximately achieve any information processing task achievable with the original pure state on a d-dimensional system. That is, from the classical strings, one can construct a quantum state \( \hat{\rho} \) that is indistinguishable from the original state \( \phi \) within a certain precision. In addition to deterministic encodings, which deterministically associate \( \phi \) with a classical bit string, we consider probabilistic encodings, which associate \( \phi \) with one of multiple classical strings according to some distribution. That is, in probabilistic encodings, \( \phi \) is associated with an ensemble of classical strings from which \( \hat{\rho} \) is constructed as an ensemble of the quantum states encoded in the classical strings. Note that a lower bound for a particular task called distributed quantum sampling [2] immediately implies \( n = \Omega(d) \).

In deterministic encodings, classical strings do nothing but encode elements in an \( \epsilon \)-covering (sometimes called an \( \epsilon \)-net) of the set of pure states. Thus, the minimum bit length \( n \) is the logarithm of the minimum size of \( \epsilon \)-coverings (called the covering number). Due to its prominent role in high-dimensional analyses based on probability theory, the covering number has been well studied [7–9], and it is known that \( n = O(d) \) bits are enough to encode an \( \epsilon \)-covering. Taking lower bound \( n = \Omega(d) \) into account, it seems that the most compact probabilistic encoding can be realized by a deterministic one.

Contrary to this intuition, we show that the bit rate realized by the most compact probabilistic encoding is exactly half of the one realized by the most compact deterministic encoding within the asymptotic limits of the dimension or precision. Thus, the most compact encoding must associate some pure states with ensembles of classical strings describing distinct quantum states, which may be counter-intuitive, considering that pure states themselves are not probabilistic mixtures of distinct quantum states. The excessive bits required for deterministic encodings can be interpreted as a consequence of their excessive predictive capability such that they can not only reconstruct quantum states within a certain precision but also deterministically compute the probability distribution of any measurements within the same precision. Such a deterministic computation is impossible by using either the most compact (probabilistic) encoding or the original quantum states. Technically, our proof includes a refined estimation of the covering number and a minimax relationship between the fidelity and the trace distance.
II. PRELIMINARIES

In this section, we summarize basic notations used throughout the paper. Note that we consider only finite-dimensional Hilbert spaces. In particular, two-dimensional Hilbert space \( \mathbb{C}^2 \) is called a qubit. \( \mathbf{L}(\mathcal{H}) \) and \( \mathbf{Pos}(\mathcal{H}) \) represent the set of linear operators and positive semidefinite operators on Hilbert space \( \mathcal{H} \), respectively. \( \mathbf{S}(\mathcal{H}) := \{ \rho \in \mathbf{Pos}(\mathcal{H}) : \text{tr} [\rho] = 1 \} \) and \( \mathbf{P}(\mathcal{H}) := \{ \rho \in \mathbf{S}(\mathcal{H}) : \text{tr} [\rho^2] = 1 \} \) represent the set of quantum states and that of pure states, respectively. Pure state \( \phi \in \mathbf{P}(\mathcal{H}) \) is sometimes alternatively represented by complex unit vector \( |\phi\rangle \in \mathcal{H} \) satisfying \( \phi = |\phi\rangle \langle \phi| \). Any physical transformation of the quantum state can be represented by a completely positive and trace preserving (CPTP) linear mapping \( \Gamma : \mathbf{L}(\mathcal{H}) \to \mathbf{L}(\mathcal{H}) \).

The trace distance \( \| \rho - \sigma \|_{\text{tr}} \) of two quantum states \( \rho, \sigma \in \mathbf{S}(\mathcal{H}) \) is defined by using the Schatten 1-norm as \( \| M \|_{1} := \frac{1}{2} \text{tr} \sqrt{M^* M} \) for \( M \in \mathbf{L}(\mathcal{H}) \). It represents the maximum total variation distance between probability distributions obtained by measurements performed on two quantum states. A similar notion measuring the distinguishability of \( \rho \) and \( \sigma \) is the fidelity function, defined by \( F(\rho, \sigma) := \max \{ \text{tr} [\Phi^p \Phi^s] \} \), where \( \Phi^p \in \mathbf{P}(\mathcal{H} \otimes \mathcal{H}) \) is a purification of \( \rho, \sigma = \text{tr}_{\mathcal{H}'} [\Phi^p] \), and the maximization is taken over all the purifications.

Fuchs-van de Graaf inequalities \[1\] provide relationships between the two measures with respect to the distinguishability as follows:

\[
1 - \sqrt{F(\rho, \sigma)} \leq \| \rho - \sigma \|_{\text{tr}} \leq \sqrt{1 - F(\rho, \sigma)} \tag{1}
\]

holds for any states \( \rho, \sigma \in \mathbf{S}(\mathcal{H}) \), where the equality of the right inequality holds when \( \rho \) and \( \sigma \) are pure.

III. CLASSICAL ENCODING OF PURE STATES

![FIG. 1. Probabilistic encoding of pure state \( \phi \) on a d-dimensional system using \( n \) bit strings and physical transformation \( \Gamma \) corresponding to a decoder of the bit strings to quantum states. State \( \phi \) is randomly encoded in label \( x \) in finite set \( X \) according to probability distribution \( p_{\phi} : X \to [0, 1] \), where \( n = \lceil \log_2 |X| \rceil \).](image)

The existence of a probabilistic encoding is equivalent to the existence of physical transformation \( \Gamma \) that can approximately reconstruct arbitrary pure state \( \phi \) from probabilistic classical state \( \{ p_{\phi}(x), x \}_{x \in X} \) as shown in Fig. 1. Physical transformation \( \Gamma \) can be regarded as a decoder of the classical states to quantum states and represented by a classical-quantum channel \[1\], which is defined as \( \Gamma(\sigma) = \sum_{x \in X} x |\sigma| x \rho_x \), where \( \{ |x\rangle \in \mathbb{C}^{|X|} \} \) is an orthonormal basis and \( \rho_x \in \mathbf{S}(\mathbb{C}^d) \). We require that with the output state \( \hat{\rho} := \sum_x p_{\phi}(x) \rho_x \) of \( \Gamma \), one can approximately sample any measurement outcomes performed on \( \phi \) within total variation distance \( \epsilon \), i.e., \( \| \phi - \hat{\rho} \|_{\text{tr}} < \epsilon \) for \( \epsilon \in (0, 1] \). Thus, we say that a probabilistic encoding exists if and only if there exists classical-quantum channel \( \Gamma \) satisfying

\[
\max_{\phi \in \mathbf{P}(\mathbb{C}^d)} \min_{\sigma \in \mathbf{S}(\mathbb{C}^{|X|})} \| \phi - \Gamma(\sigma) \|_{\text{tr}} < \epsilon. \tag{2}
\]

Note that, in the above equation, the input state \( \sigma \) is allowed to be a quantum state since it is equally transformed as probabilistic classical state \( \{(x |\sigma| x), x \}_{x \in X} \) by \( \Gamma \). Since any mixed state is a probabilistic mixture of pure states and trace distance is convex, Eq. (2) also guarantees that an arbitrary mixed state is also approximately reconstructible within the same precision as pure states.

A. Most compact deterministic encoding

First, we consider deterministic encodings, which can be defined as particular probabilistic encodings. Concretely, the domain of input state \( \sigma \) in Eq. (2) is replaced by the set of deterministic classical states, i.e., \( \{ |x\rangle \langle x| \}_{x \in X} \). Thus, we say that a deterministic encoding exists if and only if there exists set of quantum states \( \{ \rho_x \in \mathbf{S}(\mathbb{C}^d) \}_{x \in X} \) satisfying

\[
\max_{\phi \in \mathbf{P}(\mathbb{C}^d)} \min_{x \in X} \| \phi - \rho_x \|_{\text{tr}} < \epsilon, \tag{3}
\]

which is called an external \( \epsilon \)-covering of \( \mathbf{P}(\mathbb{C}^d) \). A set of pure states \( \{ \rho_x \in \mathbf{P}(\mathbb{C}^d) \}_{x \in X} \) satisfying Eq. (3) is called an internal \( \epsilon \)-covering of \( \mathbf{P}(\mathbb{C}^d) \), which corresponds to particular deterministic encodings such as one storing probability amplitudes approximately representing \( \phi \). The minimum size of internal (or external) \( \epsilon \)-coverings is called the internal (or external) covering number and denoted by \( I_{\text{in}} \) (or \( I_{\text{ex}} \)). Note that \( I_{\text{ex}} \leq I_{\text{in}} \) by definition and the minimum bit length \( n \) required for deterministic encodings equals to \( \lceil \log_2 I_{\text{ex}} \rceil \).

Since the condition of the \( \epsilon \)-coverings in Eq. (3) is equivalent to that for the set of \( \epsilon \)-balls \( \{ B_{\epsilon}(\rho_x) := \{ \psi \in \mathbf{P}(\mathbb{C}^d) : \| \psi - \rho_x \|_{\text{tr}} < \epsilon \} \}_{x \in X} \) to cover \( \mathbf{P}(\mathbb{C}^d) \), a detailed analysis of the volume of the \( \epsilon \)-ball provides a good estimation of the covering numbers. As shown in Appendix A, the volume can be calculated as \( \mu(B_{\epsilon}(\phi)) = \epsilon^{2(d-1)} \) with respect to the unitarily invariant probability measure \( \mu \) for any \( \phi \in \mathbf{P}(\mathbb{C}^d) \). This directly provides a lower bound on \( I_{\text{in}} \) and also its upper bound by applying the method of constructing an internal \( \epsilon \)-covering developed in \[1\]. We obtain the following estimation of \( I_{\text{in}} \), which is tighter than previous estimations \[1\] in large dimensions. For completeness, we provide a construction of an internal \( \epsilon \)-covering and an estimation of the parameters appearing in the construction in Appendix A.
Lemma 1. The internal covering number $I_{in}$ of $P\left(C^d\right)$ is bounded as follows: For any $r > 2$, there exists $d_0 \in \mathbb{N}$ such that

$$\left(\frac{1}{\epsilon}\right)^{2(d-1)} \leq I_{in} \leq rd \ln d \left(\frac{1}{\epsilon}\right)^{2(d-1)},$$

where the left inequality holds for any $\epsilon \in (0, 1]$ and $d \in \mathbb{N}$, and the right inequality holds for any $\epsilon \in (0, 1]$ and $d \geq d_0$. For example, if $r = 5$, we can set $d_0 = 2$.

To obtain a lower bound on $I_{ex}$, we use the following upper bounds on the volume of the $\epsilon$-ball as shown in Appendix [C]

$$\forall \epsilon \in \left(0, \frac{1}{2}\right], \mu(B_\epsilon(\varnothing)) \leq \left\{\begin{array}{ll} 2^d & \text{for } d \geq 1 \\
(2^d - 1) & \text{for } d \geq 4. \end{array}\right.$$  

(5)

This bound and $\mu(B_\epsilon(\varnothing)) = \epsilon^{2(d-1)}$ imply that the volume of the $\epsilon$-ball can be maximized by setting its center as a pure state if $d \geq 4$, which is contrary to what happens in a qubit ($d = 2$), where $B_\epsilon(\varnothing)$ corresponds to the intersection of the Bloch sphere and a ball centered at $\varnothing$ and the intersection is maximized not by a ball centered at a point on the Bloch sphere but by a ball centered at a point inside the Bloch ball. The qubit case also implies that the condition $d \geq 4$ for the second inequality cannot be fully relaxed. $\mu(B_\epsilon(\varnothing)) = 1$ if $\epsilon > 1 - \frac{1}{2}$ with the maximally mixed state $\sigma = \frac{1}{d}I$ implies another condition $\epsilon \in (0, \frac{1}{2}]$ is also not fully removable. By using Eq. (5), we easily obtain the following lower bound on $I_{ex}$.

Lemma 2. The external covering number $I_{ex}$ of $P\left(C^d\right)$ is bounded as follows: For any $\epsilon \in \left(0, \frac{1}{2}\right]$, $I_{ex} \geq \left\{\begin{array}{ll} \left(\frac{1}{\epsilon}\right)^{2(d-1)} & \text{for } d \geq 1 \\
\frac{1}{\epsilon^{2(d-1)}} & \text{for } d \geq 4. \end{array}\right.$  

(6)

Using the two lemmas by setting $r = 5$, we obtain the following theorem straightforwardly.

Theorem 1. The size of label set $X$ used in the most compact deterministic encoding is bounded by

$$2r(d, 2\epsilon) \leq \log_2 |X| \leq 2r(d, \epsilon) + \log_2(5d \ln d).$$

(7)

for any $\epsilon \in (0, \frac{1}{2}]$ and $d \geq 2$, where $r(d, \epsilon) := (d - 1)\log_2 \left(\frac{1}{\epsilon}\right)$. Moreover, if $d \geq 4$, the lower bound can be strengthened as $2r(d, \epsilon) \leq \log_2 |X|$. $I_{ex}$.

Using Theorem 1 and $n = [\log_2 |X|]$, we obtain the asymptotic bit rate per dimension $\lim_{d \to \infty} \frac{n}{d} = 2 \log_2 \left(\frac{1}{\epsilon}\right)$ of the most compact deterministic encoding if $\epsilon \in (0, \frac{1}{2}]$. We can also obtain the asymptotic bit rate per precision $\lim_{\epsilon \to 0} \frac{n}{\log_2 \epsilon} = 2(d - 1)$ of the most compact deterministic encoding if $d \geq 2$.

B. Most compact probabilistic encoding

We prove the existence of a probabilistic encoding that achieves exactly half the asymptotic bit rate of the most compact deterministic encoding, and its optimality. The main tool for the proof is the following minimax relationship between the fidelity and the trace distance.

Lemma 3. For any $d, D \in \mathbb{N}$ and any physical transformation $\Lambda$, it holds that

$$\max_{\phi \in P(C^d)} \min_{\sigma \in S(C^d)} \|\phi - \Lambda(\sigma)\|_{tr} = 1 - \min_{\sigma \in P(C^d)} \max_{\phi \in P(C^d)} F(\Lambda(\psi), \phi).$$

(8)

Proof. We use the minimax theorem as follows:

$$\text{L.H.S.} = \max_{\phi \in P(C^d)} \min_{\sigma \in S(C^d)} \max_{0 \leq M \leq 1} \text{tr}[M(\phi - \Lambda(\sigma))]$$

(9)

$$= \max_{\phi \in P(C^d)} \min_{\sigma \in S(C^d)} \max_{0 \leq M \leq 1} \text{tr}[M(\phi - \Lambda(\sigma))]$$

(10)

$$= \max_{\phi \in P(C^d)} \min_{\sigma \in S(C^d)} \max_{0 \leq M \leq 1} \left(\max_{\psi \in P(C^d)} \text{tr}[M\Lambda(\psi)] - \max_{\psi \in P(C^d)} \text{tr}[M\Lambda(\psi)]\right)$$

(11)

$$= \text{R.H.S.}$$

(12)

Note that the minimax theorem, used in the second equation, is applicable since $f(\sigma, M) := \text{tr}[M(\phi - \Lambda(\sigma))]$ is affine with respect to each variable and the domain of $M$ and $\sigma$ are compact and convex. The last equality holds since the maximum is achieved if $\text{rank}M = 1$.

Using Lemma 3, the condition for the existence of a classical encoding, Eq. (2), is equivalent to

$$\min_{\phi \in P(C^d)} \max_{x \in X} F(\rho_x, \phi) > 1 - \epsilon.$$  

(13)

For $F(\Gamma(\psi), \phi) = \sum_x |\langle x | \psi \rangle|^2 \text{tr}[\rho_x |\phi_x\rangle \rangle$ is maximized only if $\psi = |x\rangle |\langle x|\rangle$ for some $x \in X$. If $\rho_x$ is pure, Eq. (13) is also equivalent to the condition for $\{\rho_x \in P\left(C^d\right)\}_{x \in X}$ to be an internal $\sqrt{\epsilon}$-covering of $P\left(C^d\right)$ due to the equality in Eq. (11) holding when $\rho$ and $\sigma$ are pure.

The translation from the trace distance to the fidelity enables us to show the following main theorem concerning the most compact classical encoding.

Theorem 2. The size of label set $X$ used in the most compact probabilistic encoding is bounded by

$$r(d, \epsilon) - \log_2 d \leq \log_2 |X| \leq r(d, \epsilon) + \log_2(5d \ln d).$$

(14)

for any $\epsilon \in (0, 1]$ and $d \geq 2$, where $r(d, \epsilon) := (d - 1)\log_2 \left(\frac{1}{\epsilon}\right)$. Moreover, if $d \geq 4$, the lower bound can be strengthened as $2r(d, \epsilon) \leq \log_2 |X|$. $I_{ex}$.

Proof. Since setting $\{\rho_x\}_{x \in X}$ as an internal $\sqrt{\epsilon}$-covering of $P\left(C^d\right)$ is sufficient to satisfy Eq. (13), the upper bound can be obtained by applying Lemma 1 by setting $r = 5$.

Next, we show the lower bound. Assume Eq. (13) is satisfied, and let $\rho_x = \sum_i |i\rangle \langle i| \phi_{i|x}$. Then, Eq. (13) implies that $\{|i\rangle \langle i|\}_{i \in X}$ is an internal $\sqrt{\epsilon}$-covering of $P\left(C^d\right)$. Thus, the lower bound can be obtained by applying Lemma 1 as $|X|d \geq \left(\frac{1}{\epsilon}\right)^{d-1}$.  

$\square$
Using Theorem 2 and $n = \lceil \log_2 |X| \rceil$, we obtain the asymptotic bit rate per dimension $\lim_{d \to \infty} \frac{d}{2} = \log_2 \left( \frac{1}{2} \right)$ of the most compact probabilistic encoding for any $\epsilon \in (0, 1)$, and one per precision $\lim_{\epsilon \to 0} \frac{n}{\log_2 \epsilon} = d - 1$ of the most compact probabilistic encoding for any $d \geq 2$, which are exactly half of those of the most compact deterministic encoding.

The reason a $\sqrt{\epsilon}$-covering is sufficient to approximate arbitrary pure state within precision $\epsilon$ by using its probabilistic mixture can be intuitively understood by the curvature of the sphere as illustrated in Fig. 2. Indeed, Lemma 3 and the Bloch representation imply that for any compact and convex set $K$ whose extreme points $\text{ext}(K)$ reside on sphere $S$ with radius $\frac{1}{\sqrt{2}}$, the distance $\epsilon$ between $K$ and the farthest point on $S$ from $K$ and the distance $\delta$ between $\text{ext}(K)$ and the farthest point on $S$ from $\text{ext}(K)$ satisfy $\delta = \sqrt{\epsilon}$, which can be also derived by elementary geometric observations.

FIG. 2. For any pure qubit state $\phi$, we can find probability mixture $\hat{\rho}$ of six pure states, which are the eigenstates of the Pauli operators and represented by the extreme points of the octahedron in the Bloch ball, such that $\|\phi - \hat{\rho}\|_1 \leq \epsilon = \frac{1}{\sqrt{2}} (\sqrt{3} - 1)$. A farthest pure state from the octahedron and its best approximation are illustrated by a red point and a green point, respectively. Note that the trace distance between two quantum states is equal to the Euclidean distance between the corresponding points in the Bloch ball if we represent the Bloch sphere by a sphere with radius $\frac{1}{\sqrt{2}}$. On the other hand, the distance $\delta$ between the red point and the closest extreme point of the octahedron, illustrated by a blue point, satisfies $\delta = \sqrt{\epsilon}$.

IV. CONCLUSION

In this paper, we have considered the most compact probabilistic encoding so as to approximately reconstruct an arbitrary pure state $\phi \in \mathbb{P} (\mathbb{C}^d)$ from an $n$-bit string within precision $\epsilon$ with respect to the trace distance. We then demonstrated that it cannot be realized by simply storing an element of the minimum $\epsilon$-covering. More precisely, we proved that the bit rate required for probabilistic encodings is exactly half of that of the minimum length of bits necessary to store elements of an $\epsilon$-covering of $\mathbb{P} (\mathbb{C}^d)$ in asymptotic limit $\epsilon \to 0$ or in limit $d \to \infty$ when $\epsilon \in (0, \frac{1}{2})$. In limit $d \to \infty$ when $\epsilon \in (\frac{1}{2}, 1]$, the same result holds if we consider only internal $\epsilon$-coverings; however, in general, whether the same result holds or not is an open problem. Several numerical calculations suggest the positive answer. Our result could provide a new quantitative guiding principle to explore further capabilities and limitations of manipulating a quantum system as well as the foundations of quantum theory, including the following two related topics:

1. The results demonstrate an information theoretical separation of the memory size to store a pure quantum state between strong simulations and weak ones, which are two types of classical simulation of a quantum computer [12–14] (the former approximately computes the probability distribution over the outcomes, whereas the latter only approximately samples the outcomes.)

2. The complex projective space representation of pure states can be regarded as a classical encoding of pure states in deterministic classical states describing operators in $\mathbb{P} (\mathcal{H})$. The fact that any distinct pure states are encoded in indistinguishable classical states inclines us to think that the indistinguishability of non-orthogonal pure states results from our limited ability to measure them. To interpret the indistinguishability as an intrinsic feature of pure states, classical encodings of pure states in probabilistic classical states have been constructed in $\psi$-epistemic models [15–17], in which the encodings use indistinguishable and probabilistic classical states to encode some distinct pure states. Our results show that indistinguishable classical states encoding distinct elements in an $\epsilon$-covering are not only helpful for such an interpretation but also necessary for the minimum probabilistic encoding.

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Appendix A: Volume of $\epsilon$-ball in $\mathbf{P}(\mathbb{C}^d)$

To construct an $\epsilon$-covering, we first derive the volume of $\epsilon$-ball $B_\epsilon(\phi) := \{ \psi \in \mathbf{P}(\mathbb{C}^d) : \|\psi - \phi\|_\text{tr} < \epsilon \}$ in $\mathbf{P}(\mathbb{C}^d)$ as follows:

$$\forall d \in \mathbb{N}, \forall \epsilon \in (0, 1], \forall \phi \in \mathbf{P}(\mathbb{C}^d), \mu(B_\epsilon(\phi)) = \epsilon^{2(d-1)},$$

(A1)

where $\mu$ is the unitarily invariant probability measure on the Borel sets of $\mathbf{P}(\mathbb{C}^d)$.

When $d = 1$, Eq. (A1) holds. By assuming $d \geq 2$, we proceed as follows:

$$\mu(B_\epsilon(\phi)) = \mu(\{ \psi \in \mathbf{P}(\mathbb{C}^d) : \|0\rangle \langle 0\| - \psi\|_\text{tr} < \epsilon \})$$

(A2)

$$= \mu(\{ \psi \in \mathbf{P}(\mathbb{C}^d) : |\langle 0\|\psi\rangle|^2 > 1 - \epsilon^2 \})$$

(A3)

$$= \xi(\{ x \in \mathbb{R}^{2d} : \|x\|_2 = 1 \land x_1^2 + x_2^2 > 1 - \epsilon^2 \}),$$

(A4)

where the first equality uses fixed pure state $|0\rangle$ and the trace distance, the second equality uses Eq. (A1), and the third equality uses the relationship between $\mu$ and the uniform spherical probability measure $\xi$. Using a spherical coordinate system, we can proceed as follows:

$$\mu(B_\epsilon(\phi)) = \frac{V(\epsilon)}{V(1)},$$

(A5)

where $V(\epsilon) := \int_{D_\epsilon} \sin^{2d-2}\theta \sin^{2d-3}\phi d\theta d\phi$

(A6)

$$= 4 \int_{D_\epsilon} \sin^{2d-2}\theta \sin^{2d-3}\phi d\theta d\phi$$

(A7)

and the domain of the integration $D_\epsilon$ is given by $\{ (\theta, \phi) : \theta, \phi \in (0, \pi), \sin \theta \sin \phi < \epsilon \}$. Since the domain and that of the integrand have reflection symmetries about two lines $\theta = \frac{\pi}{2}$ and $\phi = \frac{\pi}{2}$, it is sufficient to perform the integration in domain $\hat{D}_\epsilon := \{ (\theta, \phi) : \theta, \phi \in (0, \frac{\pi}{2}) \}, \sin \theta \sin \phi < \epsilon \}$. By changing the variables as

$$\begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} \sin \theta \sin \phi \\ \sin \theta \end{pmatrix},$$

we obtain

$$V(\epsilon) = 4 \int_{0}^{1} dx x^{2d-3} \int_{0}^{1} dy \frac{y}{\sqrt{1 - x^2} \sqrt{1 - y^2 - x^2}}$$

(A8)

$$= 4 \int_{0}^{1} dx x^{2d-3} \left[ \arcsin \left( \frac{\sqrt{1 - y^2}}{1 - x^2} \right) \right]_{0}^{y}$$

(A9)

$$= \frac{\pi}{d-1} \epsilon^{2(d-1)},$$

(A10)

for $\epsilon \in [0, 1]$. This completes the calculation.

Appendix B: Upper bound for internal covering number $I_{\text{in}}$

We construct an internal $\epsilon$-covering ($\epsilon \in (0, 1]$) following the proof in [9, Corollary 5.5]. The construction is basically based on the fact that sufficiently many pure states randomly sampled form an $\epsilon$-covering. However, since the probability of a new random pure state residing in the uncovered region decreases when many random $\epsilon$-balls are sampled, it is better to stop sampling a pure state and change the strategy of the construction.

In the proof, we represent some parameters explicitly, which are tailored to the $\epsilon$-covering with respect to the trace distance. Assume $d \geq 2$ and let $D = 2(d-1)(\geq 2)$. Let $\{ \phi_j \in \mathbf{P}(\mathbb{C}^d) \}_{j=1}^{J_\epsilon}$ be a set of finite randomly sampled pure states with respect to product measure $\mu^{J_\epsilon}$. The expected volume of the region not covered by $A := \bigcup_{j=1}^{J_\epsilon} B_{\epsilon}(\phi_j)$
(0 < \epsilon_R \leq 1) can be calculated as follows:

\[ \int d\mu^J \mu(A^c) \]

\[ = \int d\mu^J \int d\mu(\psi) \prod_{j=1}^{J_R} I [||\psi - \phi_j||_{tr} \geq \epsilon_R] \]

\[ = \int d\mu(\psi) \prod_{j=1}^{J_R} I [||\psi - \phi_j||_{tr} \geq \epsilon_R] \]

\[ = (1 - \epsilon_R^{D})^{J_R} \leq \exp (-J_R \epsilon_R^{D}), \]

where we use Fubini’s theorem and Eq. \ref{eq:A1} in the second equation and the third equation, respectively. Note that \( I[X] \in \{0, 1\} \) is the indicator function, i.e., \( I[X] = 1 \) iff \( X \) is true.

Thus, there exists \( \{\phi_j\}_{j=1}^{J_R} \) such that \( \mu(A^c) \leq \exp (-J_R \epsilon_R^{D}) \). Pick \( \{\psi_j\}_{j=1}^{J_F} \) as much as possible such that \( B_{\epsilon^F}(\psi_j) \) are disjoint and contained in \( A^c \). When \( 0 < \epsilon_F \leq \epsilon_R \leq 1 \), we can verify that \( \{\phi_j\}_{j=1}^{J_R} \cup \{\psi_j\}_{j=1}^{J_F} \) is an \( (\epsilon_R + \epsilon_F) \)-covering and its size \( J := J_R + J_F \) is upper bounded as

\[ J \leq J_R + \frac{\exp (-J_R \epsilon_R^{D})}{\epsilon_F}. \]

By setting \( J_R = \left[ \frac{D \ln x}{\epsilon_F} \right] \), \( \epsilon_F = \frac{D \ln x}{x} \) and \( \epsilon_R = \frac{D}{x + 1} \epsilon \) with \( x \geq 1 \), we obtain the following upper bound:

\[ J \leq \left[ \frac{D \ln x}{\epsilon_F} \right] + 1 \leq \frac{1}{\epsilon_R^{D}} \left( (1 + 1/x)^D (D \ln x + 1) + 1 \right) = \frac{2\epsilon^{D}}{\epsilon_R^{D}} \cdot \frac{\alpha(d, x)}{2 \ln d}, \]

where \( \alpha(d, x) = (1 + \frac{1}{x})^D (D \ln x + 1) + 1. \) Since \( \lim_{d \to \infty} \frac{\alpha(d, D \ln d)}{2 \ln d} = 1 \), we obtain that for any \( r > 2 \) there exists \( d_0 \in \mathbb{N} \) such that

\[ \forall d \geq d_0, \forall \epsilon \in (0, 1], J \leq rd \ln d \left( \frac{1}{\epsilon} \right)^{2(d-1)}. \]

For example, if \( r = 5 \), we can set \( d_0 = 2 \). This completes the proof.

Appendix C: Lower bound for external covering number \( l_{ex} \)

We can derive a lower bound for the external covering number as a direct consequence of the following upper bounds on the volume of the maximum intersection of \( \epsilon \)-ball in \( S(\mathbb{C}^d) \) and \( P(\mathbb{C}^d) \), which will be proven in this section: For any \( \rho \in S(\mathbb{C}^d) \) and any \( \epsilon \in (0, \frac{1}{2}] \),

\[ \forall d \geq 1, \mu(B_{\epsilon}(\rho)) \leq (2\epsilon)^{2(d-1)}, \quad (C1) \]

\[ \forall d \geq 4, \mu(B_{\epsilon}(\rho)) \leq \epsilon^{2(d-1)}. \quad (C2) \]

Combined with Eq. \ref{eq:A1}, Eq. \ref{eq:C2} implies that the maximum intersection is achieved when \( \rho \) is pure if two conditions \( d \geq 4 \) and \( \epsilon \in (0, \frac{1}{2}] \) are satisfied. These two conditions are not tight but cannot be fully relaxed since \( \mu(B_{\epsilon}(\sigma)) = 1 \) for any \( d \in \mathbb{N} \) and \( \epsilon > 1 - \frac{1}{d} \), where \( \sigma \) is the maximally mixed state \( \frac{1}{d} \mathbb{I} \).

1. Proof of Eq. \ref{eq:C4}

By defining \( \phi := \arg \min_{\phi \in P(\mathbb{C}^d)} ||\phi - \rho||_{tr} \), we obtain \( B_{\epsilon}(\rho) \subseteq B_{2\epsilon}(\phi) \). For \( ||\psi - \phi||_{tr} \leq ||\psi - \rho||_{tr} + ||\phi - \rho||_{tr} \leq 2 ||\psi - \rho||_{tr} < 2\epsilon \) for any pure state \( \psi \in B_{\epsilon}(\rho) \). This completes the proof since \( \mu(B_{\epsilon}(\rho)) \leq \mu(B_{2\epsilon}(\phi)) = (2\epsilon)^{2(d-1)} \) for any \( \epsilon \in (0, \frac{1}{2}] \).
2. Proof of Eq. (C2)

Let $\rho = \sum_{i=0}^{d-1} p_i |i\rangle\langle i|$, where \{|i\rangle\} is a set of eigenvectors of $\rho$ and eigenvalues are arranged in decreasing order, i.e., $p_0 \geq p_1 \geq \cdots$. Since $\mu(B_\epsilon(\rho))$ depends not on the eigenvectors but on the eigenvalues of $\rho$, it is sufficient to consider only diagonal $\rho$ with respect to a fixed basis. However, it is difficult to exactly calculate $\mu(B_\epsilon(\rho))$ due to a complicated relationship between $\psi$ and the largest eigenvalue of $\psi - \rho$, resulting from the condition $\epsilon > \|\psi - \rho\|_\text{tr} = \lambda_{\text{max}}(\psi - \rho)$.

We derive lower bound $f_\rho(\psi)$ of $\|\psi - \rho\|_\text{tr}$ and use the relationship $\mu(B_\epsilon(\rho)) \leq \mu\{\psi : f_\rho(\psi) < \epsilon\}$ to show Eq. (C2), where $f_\rho$ is a measurable function. Since simple bound $f_\rho(\psi) = 1 - F(\psi, \rho)$ is too loose to show Eq. (C2), we derive a tighter lower bound as follows: Let $\Pi$ and $\Pi^\perp$ be the Hermitian projectors on two-dimensional subspace $\mathcal{V} \supseteq \langle \{0\}, |\psi\rangle \rangle$ and its orthogonal complement, respectively. We then obtain

$$
\|\psi - \rho\|_\text{tr} \geq \|\Pi(\psi - \rho)\Pi + \Pi^\perp(\psi - \rho)\Pi^\perp\|_\text{tr}
$$

(C3)

$$
= \|\psi - \Pi \rho \Pi\|_\text{tr} + \|\Pi^\perp \rho \Pi^\perp\|_\text{tr},
$$

(C4)

where we use the monotonicity of the trace distance under a CPTP mapping in the first inequality. Define $f_\rho(\psi)$ as the value in Eq. (C4), which can be explicitly written as

$$
f_\rho(\psi) = \frac{1}{2}\sqrt{(1 + p_0 - q)^2 - 4(p_0 - q)|\langle 0|\psi \rangle|^2} + \frac{1}{2}(1 - p_0 - q),
$$

(C5)

where $q = \langle 0|\rho|0\rangle$ and $\{|0\}, |0\rangle\}$ is an orthonormal basis of $\mathcal{V}$. The explicit formula implies $f_\rho$ is uniquely defined (although neither $\mathcal{V}$ nor $q$ is uniquely defined if $\psi = |0\rangle\langle 0|$) and continuous, thus measurable. Since $\mu(B_\epsilon(\rho)) = 0$, satisfying Eq. (C2), if $p_0 \leq 1 - \epsilon$, we consider the case $p_0 > 1 - \epsilon$. By further assuming $\epsilon \in (0, \frac{1}{d}]$, we obtain

$$
f_\rho(\psi) < \epsilon \leftrightarrow |\langle 0|\psi \rangle|^2 > \frac{(\epsilon + p_0)(1 - q - \epsilon)}{p_0 - q},
$$

(C6)

where this condition is not trivial, i.e., $\frac{(\epsilon + p_0)(1 - q - \epsilon)}{p_0 - q} \in (0, 1)$. Assuming $d \geq 4$, we calculate an upper bound on $\mu(B_\epsilon(\rho))$ as follows: By defining $U(\mathcal{H})$ as the set of unitary operators on $\mathcal{H}$ and $C : U(C^{d-1}) \rightarrow U(C^d)$ as $C(U) := |0\rangle\langle 0| \oplus U$, we can show that for any unitary operator $U \in U(C^{d-1})$,

$$
\mu\{\psi \in D(C^d) : f_\rho(\psi) < \epsilon\}
$$

(C7)

$$
= \mu\{\psi : f_\rho(C(U)|\psi C(U)^{\dagger}) < \epsilon\}
$$

(C8)

$$
= \int_{\mathcal{P}(C^d)} d\mu(\psi) \mathbb{I} \left[ |\langle 0|\psi \rangle|^2 > \frac{(\epsilon + p_0)(1 - q - \epsilon)}{p_0 - q} \right]
$$

(C9)

where we use the unitarily invariance of $\mu$ in the first equality, $q_U = |0\rangle\langle 0| C(U)^{\dagger} \rho C(U) |0\rangle\langle 0|$, and $\mathbb{I}[X] \in \{0, 1\}$ is the indicator function, i.e., $\mathbb{I}[X] = 1$ iff $X$ is true. By integrating Eq. (C9) with respect to the Haar measure on $U(C^{d-1})$ and using Fubini’s theorem, we obtain

$$
\mu\{\psi \in D(C^d) : f_\rho(\psi) < \epsilon\} = \int_{\mathcal{P}(C^d)} d\mu(\psi) \int_{\mathcal{P}(C^{d-1})} d\mu(\phi) \mathbb{I} \left[ |\langle 0|\psi \rangle|^2 > \frac{(\epsilon + p_0)(1 - F(\rho, \phi) - \epsilon)}{p_0 - F(\rho, \phi)} \right],
$$

(C10)

where $\phi \in \mathcal{P}(C^{d-1})$ is identified with a pure state on $\mathcal{P}(C^d)$ acting on subspace $\langle \{1\}, \cdots, |d - 1\rangle \rangle$. Using Fubini’s theorem again and Eq. (A1), we can proceed with the calculation:

$$
= \int_{\mathcal{P}(C^{d-1})} d\mu(\phi) \delta(F(\rho, \phi))^{2(d-1)}
$$

(C11)

$$
= \int_{\mathcal{P}(C^{d-1})} d\mu(\phi) \delta \left( \sum_{i=1}^{d-1} p_i |\langle i|\phi \rangle|^2 \right)^{2(d-1)}
$$

(C12)

$$
\leq \int_{\mathcal{P}(C^{d-1})} d\mu(\phi) \delta \left( (1 - p_0) |\langle 1|\phi \rangle|^2 \right)^{2(d-1)}
$$

(C13)

$$
= (d - 2) \int_0^1 (1 - x)^{2(d-3)} \delta((1 - p_0) x)^{2(d-1)} dx =: g_{d, \epsilon}(p_0),
$$

(C14)
where $\delta(q) = \sqrt{\frac{(q+1)(p_0+q-1)}{p_0-q}}$, we use the convexity of $\delta^{2(d-1)}$ and the unitary invariance of $\mu$ in the last inequality, and we use the probability density of $x = |\langle 1|\phi \rangle|^2$ derived by Eq. (A1) in the last equality. To confirm the calculation, we plot a comparison between $\mu(B_4(\rho))$ and its upper bound $g_{d,\epsilon}(p_0)$ for a particular $\rho$ as shown in Fig. 3 where we use the following explicit expression of $g_{d,\epsilon}(p_0)$:

$$g_{d,\epsilon}(p_0) = 2(p_0 + \epsilon - 1)^3 \left\{ \frac{1 - 6b - ab^2}{2b^2} + \frac{3(a + 1)}{a(b - a)} \left( 1 - \frac{a}{b} - \log \frac{b}{a} \right) \right\}, \quad (C15)$$

where $a = \frac{2p_0 - 1}{\epsilon + p_0}$ and $b = \frac{p_0}{\epsilon + p_0}$ and $p_0 \in (1 - \epsilon, 1)$. Note that $g_{4,\epsilon}(1) = e^6 = \lim_{p_0 \to 1} g_{4,\epsilon}(p_0)$.

![FIG. 3. Plots of estimated values of $\mu(B_4(\rho))$ (dots) and $g_{4,\epsilon}(p_0)$ (curve) for $\rho = p_0|0\rangle\langle 0| + (1 - p_0)|1\rangle\langle 1| \in S(\mathbb{C}^4)$. $\mu(B_4(\rho))$ is estimated by uniformly sampling $10^7$ pure states. The plots indicate $\mu(B_4(\rho))$ is well upper bounded by $g_{4,\epsilon}(p_0)$.](image)

It is sufficient to show that under the two conditions $\epsilon \in (0, \frac{1}{2}]$ and $d \geq 4$,

$$\forall p_0 \in (1 - \epsilon, 1), \frac{dg_{d,\epsilon}}{dp_0} \geq 0 \quad (C16)$$

since $g_{d,\epsilon}(1) = e^{2(d-1)}$. Since the integrand of $g_{d,\epsilon}$ and its partial derivative with respect to $p_0$ are continuous, we can interchange the partial differential and integral operators:

$$\frac{dg_{d,\epsilon}}{dp_0} = (d - 2) \int_0^1 (1 - x)^{d-3} \frac{\partial}{\partial p_0} \delta((1 - p_0)x)^{2(d-1)} dx = \alpha_{d,\epsilon}(p_0) \int_0^1 \beta_\epsilon(p_0, x) \gamma_{d,\epsilon}(p_0, x) dx, \quad (C17)$$

where $\alpha_{d,\epsilon}(p_0) = (d - 2)(d - 1)(p_0 + \epsilon - 1)^{d-2}, \beta_\epsilon(p_0, x) = -(1 - p_0)^2 x^2 + (1 - \epsilon - \epsilon^2 - p_0^2) x + (1 - \epsilon)\epsilon$ and $\gamma_{d,\epsilon}(p_0, x) = \frac{(1-x)^{d-3}(\epsilon + (1-p_0)x)^{d-2}}{(p_0 - (1-p_0)x)^d}$. Since $\alpha_{d,\epsilon}$ and $\gamma_{d,\epsilon}$ are non-negative in the entire considered region $R := \{(p_0, x) : p_0 \in (1 - \epsilon, 1) \land x \in [0, 1]\}$, $\frac{dg_{d,\epsilon}}{dp_0} \geq 0$ if $\beta_\epsilon$ is non-negative for all $x \in [0, 1]$. However, $\beta_\epsilon$ can be negative for some $x \in [0, 1]$ if and only if $\beta_\epsilon(p_0, 1) < 0$. Taking account of considered region $R$, it is sufficient to show $\frac{dg_{d,\epsilon}}{dp_0} \geq 0$ for all $p_0 \in \left( \frac{1}{2}, 1 \right) \subseteq (1 - \epsilon, 1)$, where $\beta_\epsilon$ can be negative.

For fixed $p^* \in \left( \frac{1}{2}, 1 \right)$, let $x^* \in (0, 1)$ satisfy $\beta_\epsilon(p^*, x) = 0$. Since $\beta_\epsilon(p^*, x)$ is monotonically decreasing in $x \geq 0$, $x^*$ is uniquely defined, $\beta_\epsilon(p^*, x) > 0$ if $x \in [0, x^*)$ and $\beta_\epsilon(p^*, x) < 0$ if $x \in (x^*, 1]$. Thus, showing

$$\forall d \geq 4, \exists c > 0, \begin{cases} \gamma_{d+1,\epsilon}(p^*, x) \geq c \gamma_{d,\epsilon}(p^*, x) & \text{for } x \in [0, x^*) \\ \gamma_{d+1,\epsilon}(p^*, x) \leq c \gamma_{d,\epsilon}(p^*, x) & \text{for } x \in (x^*, 1] \end{cases} \quad (C18)$$

and

$$\frac{dg_{d,\epsilon}}{dp_0} \bigg|_{p_0=p^*} \geq 0, \quad (C19)$$
is sufficient for $\forall d \geq 4, \left. \frac{dgd_{d,e}}{dp_0} \right|_{p_0=p^*} \geq 0$. For

$$\alpha_{d+1,e}(p^*)^{-1} \left. \frac{dg_{d+1,e}}{dp_0} \right|_{p_0=p^*}$$

(C20)

$$= \int_0^{x^*} \beta_e(p^*, x) \gamma_{d+1,e}(p^*, x) dx + \int_{x^*}^1 \beta_e(p^*, x) \gamma_{d+1,e}(p^*, x) dx$$

(C21)

$$\geq c \left\{ \int_0^{x^*} \beta_e(p^*, x) \gamma_{d,e}(p^*, x) dx + \int_{x^*}^1 \beta_e(p^*, x) \gamma_{d,e}(p^*, x) dx \right\}$$

(C22)

$$= c \alpha_{d,e}(p^*)^{-1} \left. \frac{dg_{d,e}}{dp_0} \right|_{p_0=p^*}$$

(C23)

holds for any $d \geq 4$.

First, we show Eq. (C18). By observing that for any $d \geq 4$,

$$\gamma_{d+1,e}(p^*, x) - c \gamma_{d,e}(p^*, x) = \gamma_{d,e}(p^*, x) \left( \frac{(1-x)(\epsilon + (1-p^*)x)}{p^* - (1-p^*)x} - c \right),$$

(C24)

$h_{\epsilon,p^*}(x) := \frac{(1-x)(\epsilon + (1-p^*)x)}{p^* - (1-p^*)x}$ is monotonically decreasing in $x \in [\hat{x}, 1]$ and $h_{\epsilon,p^*}(x) \geq h_{\epsilon,p^*}(\hat{x})$ for $x \in [0, \hat{x}]$ with

$$\hat{x} := \max \left\{ 0, 1 - \frac{2p^* - 1}{p^*(1-p^*)} \right\} \leq x^*,$$

setting $c = h_{\epsilon,p^*}(x^*)(>0)$ implies Eq. (C18).

Next, Eq. (C19) can be verified by using the explicit expression Eq. (C15).