Quantum Measurements in the Light of Quantum State Estimation

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Starting from a simple estimation problem, here we propose a general approach for decoding quantum measurements from the perspective of information extraction. By virtue of the estimation fidelity only, we provide surprisingly simple characterizations of rank-1 projective measurements, mutually unbiased measurements, and symmetric informationally complete measurements. Notably, our conclusions do not rely on any assumption on the rank, purity, or the number of measurement outcomes, and we do not need bases to start with. Our work demonstrates that all these elementary quantum measurements are uniquely determined by their information-extraction capabilities, which are not even anticipated before. In addition, we offer a new perspective for understanding noncommutativity and incompatibility from tomographic performances, which also leads to a universal criterion for detecting quantum incompatibility. Furthermore, we show that the estimation fidelity can be used to distinguish inequivalent mutually unbiased bases and symmetric informationally complete measurements. In the course of study, we introduce the concept of (weighted complex projective) 1/2-designs and show that all 1/2-designs are tied to symmetric informationally complete measurements, and vice versa.

I. INTRODUCTION

Quantum measurements are a basic tool for extracting information from quantum systems and a bridge for connecting the quantum world with the classical world [1–3]. They also play indispensable roles in almost all quantum information processing tasks, such as quantum computation, quantum communication, quantum metrology, quantum sensing, quantum simulation, and quantum characterization, verification, and validation. Although there are numerous works on quantum measurements, the mysteries about quantum measurements have never been fully explored, even for the simplest quantum measurements.

Prominent examples of quantum measurements include *rank*-1 *projective measurements*, *mutually unbiased measurements* (MUMs) based on *mutually unbiased bases* (MUB) [4–8], and *symmetric informationally complete measurements* (SICs for short) [8–12]. These quantum measurements stand out because of their crucial roles in foundational studies and practical quantum information

processing. Notably, rank-1 projective measurements are the canonical quantum measurements discussed in most elementary textbooks on quantum mechanics. MUMs are tied to the complementarity principle [13], uncertainty relations [14–18], and are useful in quantum state estimation [5–7,19–21] and quantum cryptography [7,18,22]. SICs play a crucial role in connecting the Born rule with the law of total probability and in the Bayesian interpretation of quantum theory [23,24]; SICs are also useful in constructing quasiprobability representations with minimal negativity [25] and in quantum state estimation [26–29]. In addition, the rich mathematical structures underlying MUB and SICs are a source of inspiration and have attracted the attention of numerous researchers; see Refs. [7,8,12,30] for reviews.

All the quantum measurements mentioned above have very simple algebraic descriptions in the language of positive operator-valued measures (POVMs) [2,3]. However, such algebraic descriptions lack clear operational meanings beyond the Born rule. Notably, the information theoretical significance of these measurements is far from being clear despite the efforts of many researchers. This awkward situation is in sharp contrast with the rapid development of quantum information science. Now, it is natural to ask if these measurements can be characterized by simple tasks in quantum information processing. What is so special about rank-1 projective measurements from the

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perspective of information extraction? How about other elementary quantum measurements, such as MUMs and SICs?

In this work, we propose a general approach for decoding quantum measurements from a simple and well-studied estimation problem: estimation of Haar random pure states [31–41]. Here Haar random pure states can also be replaced by certain discrete sets, which are amenable to experiments. By virtue of tomographic performances as quantified by the estimation fidelity, we provide surprisingly simple operational characterizations of various typical and important quantum measurements, including rank-1 projective measurements, MUMs, and SICs. Remarkably, our characterizations do not need any assumption on the rank, purity, or the number of measurement outcomes, and we do not need bases to start with. Our work demonstrates that all these elementary quantum measurements are uniquely determined by their information-extraction capabilities and can therefore be defined in purely information theoretic terms, in sharp contrast with traditional algebraic definitions, which lack clear operational meanings.

In addition, we offer a new perspective for understanding noncommuting and incompatible measurements [3,42–44] from tomographic performances. Notably, we show that incompatibility is a resource rather than a limitation to enhance the estimation fidelity. Moreover, we prove a tight upper bound for the two-copy estimation fidelity based on compatible measurements, which reveals an intriguing connection between quantum incompatibility and SICs and also provides a universal criterion for detecting quantum incompatibility. The connection with entropic uncertainty relations [17,18,45] is also discussed briefly. Furthermore, our work leads to a simple operational approach for distinguishing inequivalent MUB and SICs, which cannot be distinguished by inspecting pairwise overlaps alone. The approach we introduce is also very useful to studying other discrete symmetric structures tied to the quantum state space. Moreover, all these results are amenable to experimental demonstration with current technologies.

In the course of study, we derive a number of results on quantum measurements and (weighted complex projective) t-designs [9,10,26,46], which are of interest beyond the main focus of this work. Notably, we introduce the concept of 1/2-designs and show that SICs are essentially the only 1/2-designs. This result may shed some light on the search for general "fractional designs", although this is not the focus of this work. In addition, we introduce the concept of cross frame potential, which is surprisingly useful to studying typical quantum measurements and discrete symmetric structures tied to the quantum state space. Furthermore, we establish a simple connection between the estimation fidelity and the tth frame potential with $t = 1/2$, thereby clarifying the operational significance of this frame potential. Our work may have implications

for a number of active research areas, including quantum measurements, quantum estimation theory, geometry of quantum states, t-designs, and foundational studies on quantum incompatibility and steering.

The rest of this paper is organized as follows. In Sec. II we first introduce basic concepts on quantum measurements and an order relation under data processing; then we derive several results on rank-1 projective measurements and MUMs. In Sec. III we discuss the connections between t-designs and quantum measurements and explore the applications of a special frame potential. In Sec. IV we propose a general approach for decoding quantum measurements based on a simple estimation problem. In Sec. V by virtue of the estimation fidelity we offer surprisingly simple characterizations of various typical quantum measurements. In Sec. VI we explore the connections between the estimation fidelity and quantum incompatibility. In Sec. VII we provide an operational approach for distinguishing inequivalent MUB and SICs. Section VIII summarizes this paper. To streamline the presentation of the main results, technical proofs are relegated to the appendices.

II. QUANTUM MEASUREMENTS

A. Basic concepts

Let $\mathcal{H}$ be a d-dimensional Hilbert space associated with the quantum system under consideration. Quantum states on $\mathcal{H}$ are usually represented by density operators, which are positive (semidefinite) operators of trace 1. Quantum measurements on $\mathcal{H}$ are basic tools for extracting information from the quantum system as encoded in the quantum state. In this work we are interested in the information-extraction capabilities of quantum measurements, but not the postmeasurement quantum states. In this context, a quantum measurement on $\mathcal{H}$ can be described by a POVM, which is composed of a set (or collection) of positive operators on $\mathcal{H}$, usually called POVM elements, that sum up to the identity operator [2,3]. Here we use the same notation for the identity operator as the number 1 to simplify the notation; in addition, numbers in operator equations are implicitly multiplied by the identity operator.

Let ρ be a quantum state on $\mathcal{H}$, and let $\mathscr{A} = \{A_j\}_j$ be a POVM on $\mathcal{H}$. If we perform the POVM $\mathscr{A}$ on ρ, then the probability p_j of obtaining outcome j reads $p_j = \mathrm{tr}(\rho A_j)$ according to the Born rule. The POVM $\mathscr{A}$ is informationally complete if its POVM elements span the whole operator space on $\mathcal{H}$ [26,27,47]. This condition guarantees that any quantum state on $\mathcal{H}$ can be reconstructed accurately from frequencies of measurement outcomes as long as the POVM can be performed sufficiently many times. For comparison, the POVM $\mathscr{A}$ is trivial if all POVM elements are proportional to the identity operator, in which case no information can be extracted by performing the POVM. The POVM $\mathscr{A}$ is rank 1 if each POVM element is

proportional to a rank-1 projector. The POVM $\mathscr{A}$ is unbiased if all POVM elements have the same trace, in which case the completely mixed state will yield a flat probability distribution when the POVM is performed. Suppose that $\mathscr{A}$ is an unbiased rank-1 POVM; then $\mathscr{A}$ is equiangular if all the pairwise overlaps $\mathrm{tr}(A_j A_k)$ for $j \neq k$ are equal.

B. An order relation and simple POVMs

The idea of data (information) processing leads to a natural order relation on POVMs. Let $\mathscr{A} = \{A_j\}_j$ and $\{B_k\}_k$ be two POVMs on $\mathcal{H}$. The POVM $\mathscr{A}$ is a *coarse graining* of $\mathscr{B}$, denoted by $\mathscr{A} \preceq \mathscr{B}$ or $\mathscr{B} \succeq \mathscr{A}$, if $\mathscr{A}$ can be constructed from $\mathscr{B}$ by data processing [48–50]. More specifically, $\mathscr{A} \preceq \mathscr{B}$ if the POVM elements of $\mathscr{A}$ can be expressed as

$$A_j = \sum_k \Lambda_{jk} B_k \quad \text{for all } j, \tag{1}$$

where Λ is a stochastic matrix, which satisfies the normalization condition $\sum_j \Lambda_{jk} = 1$. In this case the measurement statistics of $\mathscr{A}$ can be simulated by performing $\mathscr{B}$ and then applying suitable data processing. Alternatively, we also say $\mathscr{B}$ *refines* $\mathscr{A}$ or $\mathscr{B}$ is a *refinement* of $\mathscr{A}$. Intuitively, coarse graining can never lead to information gain, while refinement can never lead to information loss.

Two POVMs are *equivalent* if they are coarse graining of each other (note the distinction from unitary equivalence); such POVMs are essentially the same from the perspective of information extraction. A coarse graining or refinement of a POVM $\mathscr{A}$ is trivial (nontrivial) if it is (not) equivalent to $\mathscr{A}$. To clarify when a coarse graining is nontrivial, we need to introduce a special function on POVMs. The *purity* of a POVM $\mathscr{A} = \{A_j\}_j$ [51] is defined as

$$\wp(\mathscr{A}) = \sum_j \frac{1}{d} \frac{\mathrm{tr}(A_j^2)}{\mathrm{tr} A_j} = \sum_j \frac{\mathrm{tr} A_j}{d} \frac{\mathrm{tr}(A_j^2)}{(\mathrm{tr} A_j)^2}, \tag{2}$$

where d is the dimension of the underlying Hilbert space, and the summation runs over nonzero POVM elements in $\mathscr{A}$. From this definition, it is easy to verify that

$$\frac{1}{d} \leq \wp(\mathscr{A}) \leq 1; \tag{3}$$

the lower bound is saturated iff all POVM elements are proportional to the identity operator, so that the POVM is trivial, while the upper bound is saturated iff all nonzero POVM elements are rank 1, so that the POVM is rank 1.

Lemma 1. *Suppose that $\mathscr{A} = \{A_j\}_j$ is a coarse graining of $\mathscr{B} = \{B_k\}_k$ as defined in Eq. (1). Then $\wp(\mathscr{A}) \leq \wp(\mathscr{B})$ and the following three statements are equivalent:*

1. *$\mathscr{A}$ is equivalent to $\mathscr{B}$;*
2. *$\wp(\mathscr{A}) = \wp(\mathscr{B})$;*
3. *$\Lambda_{jk}\Lambda_{jl} = 0$ whenever B_k, B_l are linearly independent.*

Lemma 1 is proved in Appendix A. It shows that a coarse graining is trivial iff it only mixes POVM elements that are proportional to each other in addition to the zero POVM element. Lemma 1 also shows that the purity is a strict order-monotonic function [50]. Such functions are useful not only for studying quantum incompatibility, but also for studying quantum steering [49,50,52].

A POVM is *simple* if no POVM element is proportional to another POVM element, that is, all POVM elements are pairwise linearly independent. By definition, a simple POVM has no POVM element that is equal to the zero operator. The following result was originally proved in Ref. [48] (see also Ref. [53]); it is also a simple corollary of Lemma 1, as shown in Appendix A.

Lemma 2. *Two simple POVMs are equivalent iff they are identical up to relabeling. Every POVM is equivalent to a unique simple POVM up to relabeling.*

Restriction to simple POVMs is quite helpful to avoiding unnecessary complications, but usually does not cause any loss of generality. For example, all results on simple POVMs derived in this work can be easily extended to general POVMs with minor modifications. Nevertheless, nonsimple POVMs are occasionally useful in technical analysis, so we do not assume that all POVMs are simple. In the rest of this paper we instead take the weaker assumption that no POVM element is equal to the zero operator unless stated otherwise.

A POVM is *maximal* if any refinement is equivalent to itself. Suppose that $\mathscr{A}$ and $\mathscr{B}$ are equivalent POVMs; then $\mathscr{A}$ is maximal iff $\mathscr{B}$ is maximal. The following proposition is a variant of a result proved in Ref. [48], which characterizes the set of rank-1 POVMs via the order relation based on data processing. It is also a simple corollary of Lemma 1.

Proposition 1. *A POVM is maximal iff it is rank* 1.

Lemma 1 and Proposition 1 show that every refinement of a rank-1 POVM is equivalent to the POVM; in other words, any rank-1 POVM has no nontrivial refinement. In addition, a rank-1 POVM cannot be equivalent to any POVM that is not rank 1. These observations lead to the following proposition.

Proposition 2. *Suppose that $\mathscr{A}$ is a coarse graining of a rank-1 POVM $\mathscr{B}$. Then $\mathscr{A}$ is equivalent to (is a trivial coarse graining of) $\mathscr{B}$ iff $\mathscr{A}$ is rank* 1.

C. Quantum incompatibility

Let $\mathscr{A}$ and $\mathscr{B}$ be two arbitrary POVMs on $\mathcal{H}$. Then $\mathscr{A}$ and $\mathscr{B}$ commute if all POVM elements in $\mathscr{A}$ commute with all POVM elements in $\mathscr{B}$. This definition also applies to two sets of positive operators. By contrast, $\mathscr{A}$ and $\mathscr{B}$ are *compatible* or jointly measurable if they admit a common refinement [42–44,49,54,55]. In that case, the measurement statistics of both $\mathscr{A}$ and $\mathscr{B}$ can be simulated by performing the common refinement. Otherwise, $\mathscr{A}$ and $\mathscr{B}$ are *incompatible*. Generalizations to three or more POVMs are immediate. Note that commuting POVMs are automatically compatible, but not vice versa in general. By definition, the compatibility relation is closely tied to the order relation discussed in Sec. II B. This connection is very useful to detecting quantum incompatibility [43,49,50,52] (cf. Sec. VI).

Proposition 3. *Suppose that $\mathscr{A}$ and $\mathscr{B}$ are two POVMs on $\mathcal{H}$ with $\mathscr{B}$ being rank 1. Then $\mathscr{A}$ and $\mathscr{B}$ are compatible iff $\mathscr{A}$ is a coarse graining of $\mathscr{B}$.*

Proposition 4. *Two rank-1 POVMs are compatible iff they are equivalent. Two simple rank-1 POVMs are compatible iff they are identical up to relabeling.*

Proposition 3 is a simple corollary of Proposition 1. Proposition 4 is a simple corollary of Proposition 3 and Lemma 2.

D. Projective measurements and mutually unbiased measurements

A POVM is *reducible* if its POVM elements can be divided into two groups such that each group contains at least one nonzero POVM element and all POVM elements in one group are orthogonal to all POVM elements in the other group (cf. Ref. [56]). In this case, the POVM is a direct sum of two POVMs. Notably, any POVM containing a projector that is not equal to the identity or the zero operator is reducible; note that such a projector is necessarily orthogonal to all other POVM elements. A POVM is *irreducible* if it is not reducible; such a POVM cannot be expressed as a direct sum of two POVMs.

A projective measurement (also known as a von Neumann measurement) is a special POVM in which all the POVM elements are mutually orthogonal projectors and is thus reducible except for the trivial projective measurement. It is usually characterized by a Hermitian operator via spectral decomposition. Rank-1 projective measurements are special projective measurements in which all POVM elements are mutually orthogonal rank-1 projectors. They are associated with nondegenerate Hermitian operators and are the canonical example of quantum measurements, as discussed in most textbooks [1]. In addition, they are in one-to-one correspondence with orthonormal

bases if we identify bases that differ only by overall phase factors. In view of the crucial roles played by rank-1 projective measurements, here we summarize their main characteristics that are useful in the current study. The detailed proofs are relegated to Appendix B.

Lemma 3. *Any simple rank-1 POVM $\mathscr{A}$ on $\mathcal{H}$ has at least d POVM elements and satisfies the inequality $\dim(\mathrm{span}(\mathscr{A})) \geq d$. Each bound is saturated iff $\mathscr{A}$ is a rank-1 projective measurement.*

Lemma 4. *Suppose that $\mathscr{A}$ is a simple rank-1 POVM on $\mathcal{H}$ and that $\mathscr{B}$ is a set of distinct rank-1 projectors on $\mathcal{H}$. Then $\mathscr{A}$ and $\mathscr{B}$ commute iff $\mathscr{B} \subseteq \mathscr{A}$ and the projectors in $\mathscr{B}$ are mutually orthogonal.*

Note that every rank-1 positive operator on $\mathcal{H}$ is proportional to a rank-1 projector. As an implication of Lemma 4 and this observation, if a simple rank-1 POVM $\mathscr{A}$ commutes with a nonempty set of pairwise linearly independent rank-1 positive operators (say some POVM elements in another simple rank-1 POVM), then these positive operators must be mutually orthogonal, and $\mathscr{A}$ contains a set of rank-1 projectors that are proportional to these rank-1 positive operators, respectively. In this case, the POVM $\mathscr{A}$ is a direct sum of a rank-1 projective measurement and another POVM and is thus reducible.

Lemma 5. *Two simple rank-1 POVMs commute iff they are identical rank-1 projective measurements up to relabeling.*

Lemma 5 is a simple corollary of Lemma 4; a direct proof is presented in Appendix B. As an implication of Lemma 5, any simple rank-1 POVM that commutes with itself is a rank-1 projective measurement.

Two orthonormal bases $\{|\psi_j\rangle\}_{j=1}^d$ and $\{|\varphi_k\rangle\}_{k=1}^d$ for $\mathcal{H}$ are *mutually unbiased* (MU) or complementary if all the transition probabilities $|\langle\psi_j|\varphi_k\rangle|^2$ are equal to $1/d$. In this case, the corresponding measurements are also referred to as MU and are often regarded as maximally incompatible [4–8,57]. Such measurements are quite useful in many tasks in quantum information processing, including quantum state estimation [5–7,19–21] and quantum cryptography [7,18,22] in particular. It is known that the number of bases in any MUB cannot surpass $d + 1$; when the upper bound is saturated, the MUB is called a complete set of MUB (CMUB), and the corresponding measurements are called a complete set of MUMs (CMUMs).

As a generalization, two positive operators A and B on $\mathcal{H}$ are MU if $\mathrm{tr}(AB) = \mathrm{tr}(A)\,\mathrm{tr}(B)/d$. Two POVMs $\{A_j\}_j$ and $\{B_k\}_k$ on $\mathcal{H}$ are MU if each POVM element in $\mathscr{A}$ and each POVM element in $\mathscr{B}$ are MU, that is, $\mathrm{tr}(A_j B_k) = \mathrm{tr}(A_j)\,\mathrm{tr}(B_k)/d$. The following theorem sets an upper bound for the number of rank-1 POVMs that are

MU, which is reminiscent of the upper bound for MUB [5–7].

Theorem 1. *Any set of MU simple rank-1 POVMs on $\mathcal{H}$ contains at most $d + 1$ POVMs. If the upper bound is saturated, then all the POVMs in the set are rank-1 projective measurements, which form a CMUMs.*

At this point, it is worth pointing out that the assumption of simplicity of POVMs in Lemmas 3–5 and Theorem 1 is convenient, but not essential, as pointed out in Sec. II B. Without this assumption, these results still hold after minor modifications, as presented below, given that every POVM is equivalent to a simple POVM according to Lemma 2. Similar remarks apply to other results presented in this manuscript.

Lemma 3*. *Any rank-1 POVM $\mathscr{A}$ on $\mathcal{H}$ has at least d POVM elements, and the lower bound is saturated iff $\mathscr{A}$ is a rank-1 projective measurement. Meanwhile, $\dim(\mathrm{span}(\mathscr{A})) \geq d$, and the bound is saturated iff $\mathscr{A}$ is equivalent to a rank-1 projective measurement.*

Lemma 4*. *Suppose that $\mathscr{A}$ is a rank-1 POVM on $\mathcal{H}$ and that $\mathscr{B}$ is a set of rank-1 positive operators on $\mathcal{H}$. Then $\mathscr{A}$ and $\mathscr{B}$ commute iff*

$$\sum_{A \in \mathscr{A} \,|\, A \propto B} = \frac{B}{\mathrm{tr}\, B} \quad \text{for all } B \in \mathscr{B}, \tag{4}$$

and any two operators in $\mathscr{B}$ are either mutually orthogonal or proportional to each other.

Lemma 5*. *Two rank-1 POVMs commute iff they are equivalent to the same rank-1 projective measurement.*

Theorem 1*. *Any set of MU rank-1 POVMs on $\mathcal{H}$ contains at most $d + 1$ POVMs. If the upper bound is saturated, then all the POVMs in the set are equivalent to rank-1 projective measurements, and the corresponding bases form a CMUB.*

III. QUANTUM MEASUREMENTS AND *t*-DESIGNS

A. *t*-designs

Let $\mathcal{S} = \{|\psi_j\rangle, w_j\}_{j=1}^m$ be a weighted set (or collection) of states in $\mathcal{H}$, where $w_j > 0$ and $\sum_j w_j = d$ (to avoid unnecessary complications, in this paper we assume that all weights are strictly positive unless stated otherwise; Lemma 7 in Sec. III C is an exception). As in the discussion of orthonormal bases, here we identify weighted sets that differ only by overall phase factors. Then a weighted set is also regarded as a distribution on the set of all pure states, which forms the complex projective space CP^{d-1}.

When the weights are not mentioned explicitly, we take the convention that all states have the same weight.

Given a positive integer t, the set $\mathcal{S}$ is a (weighted complex projective) t-design if $\sum_j w_j (|\psi_j\rangle\langle\psi_j|)^{\otimes t}$ is proportional to the projector P_t onto the symmetric subspace in $\mathcal{H}^{\otimes t}$ [9,10,26,46] (see Ref. [58] for mixed-state designs). In view of the normalization condition $\sum_j w_j = d$, the set $\mathcal{S}$ is a t-design iff

$$\sum_j w_j (|\psi_j\rangle\langle\psi_j|)^{\otimes t} = \frac{dP_t}{D_t}, \tag{5}$$

where $D_t = \mathrm{tr}(P_t)$ is the dimension of the t-partite symmetric subspace and its explicit expression reads

$$D_t = \binom{d + t - 1}{t}. \tag{6}$$

By definition, it is easy to verify that a t-design is also a t'-design for any positive integer t' that is smaller than or equal to t, that is, $t' \leq t$.

Given any pair of positive integers d and t, one can construct a t-design in dimension d with a finite number of elements [59]. To achieve this goal, nevertheless, the number of elements is at least [26,46]

$$\binom{d + \lceil t/2 \rceil - 1}{\lceil t/2 \rceil}\binom{d + \lfloor t/2 \rfloor - 1}{\lfloor t/2 \rfloor}, \tag{7}$$

which is equal to $d, d^2, d^2(d + 1)/2, d^2(d + 1)^2/4$ for $t = 1, 2, 3, 4$, respectively. An orthonormal basis (with uniform weights) is the simplest 1-design. Prominent examples of 2-designs include CMUB and SICs. In particular, a SIC stands out as a minimal 2-design, which saturates the lower bound in Eq. (7) with $t = 2$. Recall that a SIC in dimension d is composed of d^2 quantum states $|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_{d^2}\rangle$ with an equal pairwise fidelity of $1/(d + 1)$ [8–12], that is,

$$|\langle\psi_j|\psi_k\rangle|^2 = \frac{d\delta_{jk} + 1}{d + 1}, \quad j, k = 1, 2, \ldots, d^2. \tag{8}$$

Here each state has weight $1/d$ according to the current normalization convention, but we shall not mention this weight explicitly for simplicity when there is no danger of confusion. In addition, the set characterized by Eq. (8) and the corresponding POVM are both referred to as a SIC (cf. Sec. III B). When the dimension d is a power of 2, any orbit of the Clifford group is a 3-design; in particular, the set of stabilizer states forms a 3-design [60–62]. In addition, special orbits of the Clifford group can form 4-designs [63,64].

The tth *frame potential* is an important tool for studying t-designs; given the weighted set $\mathcal{S} = \{|\psi_j\rangle, w_j\}_{j=1}^m$, it is

defined as [9,10,26]

$$\Phi_t(\mathcal{S}) := \sum_{j,k} w_j w_k |\langle \psi_j | \psi_k \rangle|^{2t}. \qquad (9)$$

It is well known that this frame potential satisfies the inequality

$$\Phi_t(\mathcal{S}) \geq \frac{d^2}{D_t}, \qquad (10)$$

which is saturated iff $\mathcal{S}$ is a t-design. This inequality provides a simple criterion for determining whether a weighted set is a t-design.

To generalize the concept of frame potential mentioned above, let $\mathcal{S} = \{|\psi_j\rangle, w_j\}_{j=1}^m$ and $\mathcal{T} = \{|\varphi_k\rangle, w'_k\}_{k=1}^n$ be two weighted sets of states in $\mathcal{H}$, which satisfy $w_j, w'_k > 0$ and $\sum_j w_j = \sum_k w'_k = d$. The tth *cross frame potential* between $\mathcal{S}$ and $\mathcal{T}$ is defined as

$$\Phi_t(\mathcal{S}, \mathcal{T}) = \Phi_t(\mathcal{T}, \mathcal{S}) := \sum_{j,k} w_j w'_k |\langle \psi_j | \varphi_k \rangle|^{2t}. \qquad (11)$$

Note that the definitions in Eqs. (9) and (11) are applicable even if some weights w_j, w'_k are equal to zero. In addition, $\Phi_t(\mathcal{S}, \mathcal{S}) = \Phi_t(\mathcal{S})$, so the frame potential $\Phi_t(\mathcal{S})$ can be regarded as the cross frame potential between $\mathcal{S}$ and itself. We highlight the significance of the cross frame potential in Secs. III C and IV B.

Although the frame potential Φ_t was originally introduced when t is a positive integer, the definition in Eq. (9) applies to any positive real number t. Similar generalization applies to the cross frame potential defined in Eq. (11). However, it is not so easy to generalize the concept of t-designs in this way (the special case $t = 1/2$ will be discussed in Sec. III C). For example, the tth frame potentials of an orthonormal basis, SIC, and CMUB are respectively given by

$$\Phi_t(\text{basis}) = d, \qquad (12)$$

$$\Phi_t(\text{SIC}) = 1 + \frac{d^2 - 1}{(d+1)^t}, \qquad (13)$$

$$\Phi_t(\text{CMUB}) = \frac{d + d^{3-t}}{d+1}. \qquad (14)$$

In addition, the tth frame potential of Haar random pure states can be computed as

$$\begin{aligned}
\Phi_t(\text{Haar}) &= d^2 \int_{\text{CP}^{d-1}} |\langle 0 | \psi \rangle|^{2t} d\mu(\psi) \\
&= \frac{d^2 \int_{\theta=0}^{\pi/2} (\cos\theta)^{2t+1} (\sin\theta)^{2d-3} d\theta}{\int_{\theta=0}^{\pi/2} \cos\theta (\sin\theta)^{2d-3} d\theta} \\
&= \frac{d^2 \Gamma(d) \Gamma(t+1)}{\Gamma(d+t)}, \qquad (15)
\end{aligned}$$

where $d\mu(\psi)$ denotes the normalized measure on the complex projective space CP^{d-1} that is induced by the Haar measure on the unitary group. If t is an integer, then the above equation yields

$$\Phi_t(\text{Haar}) = \frac{d^2 t!}{d(d+1)\cdots(d+t-1)} = \frac{d^2}{D_t}, \qquad (16)$$

which saturates the lower bound in Eq. (10). So the ensemble of Haar random pure states forms a t-design for any positive integer t, as expected. In view of this fact, the ensemble of Haar random pure states is regarded as an ∞-design.

B. Connection between t-designs and quantum measurements

Given any t-design $\{|\psi_j\rangle, w_j\}_{j=1}^m$ with $t \geq 1$, we can construct a rank-1 POVM of the form $\{w_j |\psi_j\rangle\langle\psi_j|\}_{j=1}^m$. Conversely, any rank-1 POVM determines a t-design up to irrelevant overall phase factors. Quantum measurements based on t-designs have numerous applications in quantum information processing. Notably, collective measurements based on t-designs are optimal for pure-state estimation [28,29,41]. Measurements constructed from 2-designs are optimal for linear quantum state tomography [19,26–28] and quantum state verification [65–67]. Measurements constructed from 3-designs are useful in shadow estimation and entanglement detection [68–70]. In addition, the quantum measurement constructed from Haar random pure states, referred to as the *isotropic measurement* henceforth, is of special interest in quantum state estimation [20,28] and discrimination [71].

Thanks to the connection mentioned above, some concepts defined for t-designs can be generalized to rank-1 POVMs, and vice versa. Notably, the definitions of the tth frame potential and cross frame potential can be extended to rank-1 POVMs. To be concrete, let $\mathscr{A} = \{A_j\}_j$ and $\mathscr{B} = \{B_k\}_k$ be two rank-1 POVMs. Then the tth frame potential of $\mathscr{A} = \{A_j\}$ reads

$$\Phi_t(\mathscr{A}) = \sum_{j,k} \frac{[\text{tr}(A_j A_k)]^t}{[\text{tr}(A_j)\,\text{tr}(A_k)]^{t-1}}, \qquad (17)$$

which is applicable for any positive number t. Similarly, the tth cross frame potential between $\mathscr{A}$ and $\mathscr{B}$ reads

$$\Phi_t(\mathscr{A}, \mathscr{B}) = \sum_{j,k} \frac{[\text{tr}(A_j B_k)]^t}{[\text{tr}(A_j)\,\text{tr}(B_k)]^{t-1}}. \qquad (18)$$

The definitions of frame potential and cross frame potential in Eqs. (17) and (18) can be further generalized to POVMs that are not necessarily rank 1, although they are more useful if the POVMs are rank 1. In addition, these definitions are applicable even if some POVM elements are equal to

the zero operator as long as the summations are restricted to POVM elements that are not equal to the zero operator. Note that equivalent POVMs have the same frame potential; similarly, equivalent pairs of POVMs have the same cross frame potential.

On the other hand, a *t*-design is called simple if the corresponding POVM is simple. Two *t*-designs are MU if the corresponding POVMs are MU. This definition reduces to the usual definition of MUB when each weighted set is an orthonormal basis with uniform weights.

C. Applications of the frame potential $\Phi_{1/2}$

Here we are particularly interested in the (cross) frame potential Φ_t with $t = 1/2$, whose significance will become clear shortly. A weighted set of states in $\mathcal{H}$ is a 1/2-*design* if it is a 1-design and can attain the maximum frame potential $\Phi_{1/2}$ among all 1-designs. Here we choose the maximum frame potential because the square-root function is concave rather than convex. By definition, a 1/2-design is automatically a 1-design; this requirement is motivated by our study on quantum measurements: any rank-1 measurement corresponds to a 1-design, and vice versa. By contrast, a 1-design is not necessarily a 1/2-design, although a $(t + 1)$-design is automatically a *t*-design when t is a positive integer. The intuition about *t*-designs for an integer t cannot be taken for granted in the current study. Incidentally, the search for "fractional designs" has been a long-standing open problem. So far, it is still not clear how to define *t*-designs with arbitrary real parameter *t*. This problem deserves further study, but is not crucial to the current work.

According to Eqs. (12)–(15), the frame potentials $\Phi_{1/2}$ for an orthonormal basis, SIC, CMUB, and Haar random pure states are respectively given by

$$\Phi_{1/2}(\text{basis}) = d, \tag{19}$$

$$\Phi_{1/2}(\text{SIC}) = 1 + (d - 1)\sqrt{d + 1}, \tag{20}$$

$$\Phi_{1/2}(\text{CMUB}) = \frac{d + d^{5/2}}{d + 1}, \tag{21}$$

$$\Phi_{1/2}(\text{Haar}) = \frac{\sqrt{\pi} d^2 \Gamma(d)}{2 \Gamma(d + 1/2)}. \tag{22}$$

Quite unexpectedly, the frame potential attains its minimum at an orthonormal basis and its maximum at a SIC, as illustrated in Fig. 1. What is more surprising is that this conclusion holds even if we consider all possible 1-designs, as shown in Lemma 6 below.

Lemma 6. *Any* 1-*design $\mathcal{S}$ in $\mathcal{H}$ satisfies*

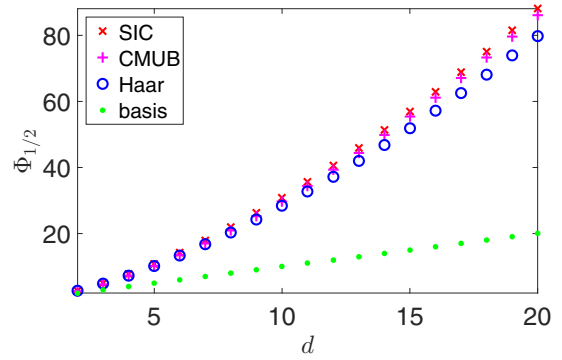$$d \leq \Phi_{1/2}(\mathcal{S}) \leq 1 + (d - 1)\sqrt{d + 1}. \tag{23}$$

FIG. 1. Frame potentials $\Phi_{1/2}$ of an orthonormal basis, SIC, CMUB, and Haar random pure states, respectively. Here d is the dimension of the underlying Hilbert space $\mathcal{H}$.

If $\mathcal{S}$ is simple, then the lower bound is saturated iff $\mathcal{S}$ is an orthonormal basis, while the upper bound is saturated iff $\mathcal{S}$ is a SIC.

Lemma 6 reveals intriguing connections between the frame potential $\Phi_{1/2}(\mathcal{S})$ and orthonormal bases as well as SICs. Notably, it shows that, among all 1-designs (including *t*-designs for any positive integer *t*), SICs are essentially the only 1/2-designs; in other words, all 1/2-designs are tied to SICs. Remarkably, SICs are uniquely characterized by the maximum frame potential, without any assumption even on the number of elements. These observations will have profound implications for understanding quantum measurements from the perspective of quantum state estimation, as we will see later. The detailed proof of Lemma 6 is presented in Appendix C. Here it is worth pointing out that the proof is tied to a surprising result on the 1/2-moment in statistics, as formulated and proved in Appendix C 2, which is of independent interest.

When the number of states is limited, the upper bound in Lemma 6 can be improved, and the maximum frame potential is tied to tight equiangular lines. Recall that a set $\{|\psi_j\rangle\}_{j=1}^m$ composed of *m* states is equiangular if all pairwise fidelities are equal [9,72]. The equiangular set is tight if $\sum_j |\psi_j\rangle\langle\psi_j|$ is proportional to the identity (automatically guaranteed for 1-designs), in which case the pairwise fidelities saturate the Welch bound [73]:

$$|\langle \psi_j | \psi_k \rangle|^2 = \begin{cases} 1, & j = k, \\ \dfrac{m - d}{d(m - 1)}, & j \neq k. \end{cases} \tag{24}$$

Any set of equiangular states in dimension *d* can contain at most d^2 states, and the upper bound is saturated iff the set is a SIC [9,72,74]. In Lemma 7 below we assume that all weights in $\mathcal{S}$ are nonnegative, but not necessarily strictly positive.

Lemma 7. *Any 1-design $\mathcal{S}$ composed of m states satisfies*

$$\Phi_{1/2}(\mathcal{S}) \leq \frac{d^2}{m} + \frac{d}{m}\sqrt{d(m-1)(m-d)}. \qquad (25)$$

When $m > d^2$, the upper bound cannot be saturated; when $d \leq m \leq d^2$, the bound is saturated iff $\mathcal{S}$ is composed of m equiangular states (with uniform weights).

Note that the upper bound in Eq. (25) is strictly monotonically increasing in m.

Next, we turn to the cross frame potential $\Phi_{1/2}(\mathcal{S}, \mathcal{T})$, which will play important roles in studying MUMs and SICs.

Lemma 8. *Any pair of 1-designs $\mathcal{S}$ and $\mathcal{T}$ in $\mathcal{H}$ satisfies*

$$d \leq \Phi_{1/2}(\mathcal{S}, \mathcal{T}) \leq d^{3/2}. \qquad (26)$$

The upper bound is saturated iff $\mathcal{S}$ and $\mathcal{T}$ are MU. If $\mathcal{S}$ and $\mathcal{T}$ are simple, then the lower bound is saturated iff $\mathcal{S}$ and $\mathcal{T}$ are identical orthonormal bases up to relabeling.

Lemma 9. *Suppose that $\mathcal{S}$ and $\mathcal{T}$ are 1-designs in $\mathcal{H}$, and that one of them is a 2-design; then*

$$\Phi_{1/2}(\mathcal{S}, \mathcal{T}) \leq 1 + (d-1)\sqrt{d+1}. \qquad (27)$$

If $\mathcal{S}$ and $\mathcal{T}$ are simple, then the upper bound is saturated iff $\mathcal{S}$ and $\mathcal{T}$ are identical SICs up to relabeling.

Here we identify weighted sets that differ only by overall phase factors as mentioned before. Thanks to the connections between 1-designs and POVMs, Lemmas 6–9 above can be generalized to rank-1 POVMs immediately as summarized in Lemmas 10–13 below.

Lemma 10. *Any rank-1 POVM $\mathscr{A}$ satisfies*

$$d \leq \Phi_{1/2}(\mathscr{A}) \leq 1 + (d-1)\sqrt{d+1}. \qquad (28)$$

If $\mathscr{A}$ is simple, then the lower bound is saturated iff $\mathscr{A}$ is a rank-1 projective measurement, while the upper bound is saturated iff $\mathscr{A}$ is a SIC.

Lemma 11. *Any rank-1 POVM $\mathscr{A}$ composed of m POVM elements satisfies*

$$\Phi_{1/2}(\mathscr{A}) \leq \frac{d^2}{m} + \frac{d}{m}\sqrt{d(m-1)(m-d)}. \qquad (29)$$

When $m > d^2$, the upper bound cannot be saturated; when $d \leq m \leq d^2$, the upper bound is saturated iff $\mathscr{A}$ is unbiased and equiangular.

Lemma 12. *Any pair of rank-1 POVMs $\mathscr{A}$ and $\mathscr{B}$ on $\mathcal{H}$ satisfies*

$$d \leq \Phi_{1/2}(\mathscr{A}, \mathscr{B}) \leq d^{3/2}. \qquad (30)$$

The upper bound is saturated iff $\mathscr{A}$ and $\mathscr{B}$ are MU. If $\mathscr{A}$ and $\mathscr{B}$ are simple, then the lower bound is saturated iff $\mathscr{A}$ and $\mathscr{B}$ are identical rank-1 projective measurements up to relabeling.

Lemma 13. *Suppose that $\mathscr{A}$ and $\mathscr{B}$ are rank-1 POVMs on $\mathcal{H}$, and that one of them is constructed from a 2-design; then*

$$\Phi_{1/2}(\mathscr{A}, \mathscr{B}) \leq 1 + (d-1)\sqrt{d+1}. \qquad (31)$$

If $\mathscr{A}$ and $\mathscr{B}$ are simple, then the upper bound is saturated iff $\mathscr{A}$ and $\mathscr{B}$ are identical SICs up to relabeling.

The above results demonstrate the significance of the (cross) frame potential $\Phi_{1/2}$ in characterizing typical quantum measurements. These results are the stepping stones for understanding quantum measurements from the perspective of quantum state estimation, as we will see shortly.

IV. DECODING QUANTUM MEASUREMENTS FROM A SIMPLE ESTIMATION PROBLEM

A. Reexamination of a simple estimation problem

Suppose that a quantum device can prepare a random pure quantum state ρ on $\mathcal{H}$ according to the normalized Haar measure and that we are asked to estimate the identity of ρ based on suitable quantum measurements. A natural figure of merit is the fidelity averaged over the measurement outcome and the random pure state. Given N copies of the pure state ρ, then what average fidelity can we achieve? This problem is well known in the quantum information community and has been studied by many eminent researchers [31–41], whose works have greatly improved our understanding about information extraction from quantum systems. However, the significance of this problem in decoding quantum measurements has not been fully appreciated.

If we perform the POVM $\mathscr{A} = \{A_j\}_j$ on $\rho^{\otimes N}$, then the probability of obtaining outcome A_j is $p_j = \text{tr}(\rho^{\otimes N} A_j)$. Let $\hat{\rho}_j$ be the estimator corresponding to outcome j. Then the

average fidelity reads

$$
\begin{aligned}
\bar{F} &= \sum_j \int_{\mathrm{CP}^{d-1}} \mathrm{d}\mu(\psi) p_j \, \mathrm{tr}(\rho \hat{\rho}_j) \\
&= \sum_j \int_{\mathrm{CP}^{d-1}} \mathrm{d}\mu(\psi) \, \mathrm{tr}[\rho^{\otimes N+1}(A_j \otimes \hat{\rho}_j)] \\
&= \frac{1}{D_{N+1}} \sum_j \mathrm{tr}[P_{N+1}(A_j \otimes \hat{\rho}_j)] \\
&= \frac{1}{D_{N+1}} \sum_j \mathrm{tr}[\tilde{\mathcal{Q}}(A_j)\hat{\rho}_j],
\end{aligned}
\tag{32}
$$

where $\mathrm{d}\mu(\psi)$ denotes the normalized measure on the complex projective space CP^{d-1} that is induced by the Haar measure on the unitary group, $\rho = |\psi\rangle\langle\psi|$, and

$$
\tilde{\mathcal{Q}}(A_j) := \mathrm{tr}_{1,\dots,N}[P_{N+1}(A_j \otimes 1)]. \tag{33}
$$

Note that

$$
\mathrm{tr}[\tilde{\mathcal{Q}}(A_j)\hat{\rho}_j] \leq \|\tilde{\mathcal{Q}}(A_j)\| = \max_\rho \mathrm{tr}[P_{N+1}(A_j \otimes \rho)], \tag{34}
$$

where $\|\tilde{\mathcal{Q}}(A_j)\|$ denotes the operator norm of $\tilde{\mathcal{Q}}(A_j)$ and the maximization is taken over all normalized pure states on $\mathcal{H}$. In addition, the upper bound is saturated if the estimator $\hat{\rho}_j$ is supported in the eigenspace of $\tilde{\mathcal{Q}}(A_j)$ corresponding to the largest eigenvalue and only then.

The *estimation fidelity* of $\mathscr{A}$ is defined as the maximum fidelity that can be achieved by the POVM $\mathscr{A}$ (with a judicial choice of each estimator $\hat{\rho}_j$) and is given by

$$
F(\mathscr{A}) = \sum_j \frac{\|\tilde{\mathcal{Q}}(A_j)\|}{D_{N+1}}. \tag{35}
$$

Define

$$
\mathcal{Q}(O) := (N+1)! \, \tilde{\mathcal{Q}}(O) \tag{36}
$$

for any linear operator O acting on $\mathcal{H}^{\otimes N}$. Then the estimation fidelity in Eq. (35) can be expressed as

$$
F(\mathscr{A}) = \sum_j \frac{\|\mathcal{Q}(A_j)\|}{(N+1)! \, D_{N+1}} = \sum_j \frac{\|\mathcal{Q}(A_j)\|}{d(d+1)\cdots(d+N)}. \tag{37}
$$

As we will see shortly, $F(\mathscr{A})$ encodes valuable information about the POVM $\mathscr{A}$. To facilitate the following discussions, here we summarize a number of simple but instructive facts. Let $\mathscr{I}$ be the trivial POVM that is composed of the identity on $\mathcal{H}$ as the only POVM element.

Lemma 14. *Suppose that $\mathscr{A}, \mathscr{B}$ are POVMs on $\mathcal{H}^{\otimes N}$, $\mathscr{C}$ is a POVM on $\mathcal{H}^{\otimes k}$, and that U is a unitary operator on $\mathcal{H}$. Then*

$$
F\left(U^{\otimes N} \mathscr{A} U^{\dagger \otimes N}\right) = F(\mathscr{A}), \tag{38}
$$

$$
F(\mathscr{A} \otimes \mathscr{I}^{\otimes k}) = F(\mathscr{A}), \tag{39}
$$

$$
F(\mathscr{A}) \leq F(\mathscr{B}) \quad \text{if } \mathscr{A} \preceq \mathscr{B}, \tag{40}
$$

$$
F(\mathscr{C} \otimes \mathscr{A}) = F(\mathscr{A} \otimes \mathscr{C}) \geq \max\{F(\mathscr{A}), F(\mathscr{C})\}. \tag{41}
$$

Here the notation $\mathscr{A} \preceq \mathscr{B}$ means $\mathscr{A}$ is a coarse graining of $\mathscr{B}$ as defined in Sec. II B. Lemma 14 in particular implies that equivalent POVMs can achieve the same estimation fidelity, as expected.

At this point, it is worth pointing out that the above results still apply if the ensemble of Haar random pure states involved in the estimation problem is replaced by any ensemble of pure states that forms a t-design with $t = N + 1$. This observation is quite helpful in devising experiments for demonstrating these results.

B. Calculation of the estimation fidelity

Next, we derive a number of basic results that are useful to computing the estimation fidelity in Eq. (37), especially for product measurements. Let A, B, C be linear operators on $\mathcal{H}$. Straightforward calculation shows that

$$
\mathcal{Q}(A) = \mathrm{tr}(A) + A, \tag{42}
$$

$$
\mathcal{Q}(A \otimes B) = \mathrm{tr}(A)\,\mathrm{tr}(B) + \mathrm{tr}(AB) + \mathrm{tr}(B)A + \mathrm{tr}(A)B + AB + BA, \tag{43}
$$

$$
\begin{aligned}
\mathcal{Q}(A \otimes B \otimes C) &= \mathrm{tr}(A)\,\mathrm{tr}(B)\,\mathrm{tr}(C) + \mathrm{tr}(AB)\,\mathrm{tr}(C) + \mathrm{tr}(BC)\,\mathrm{tr}(A) + \mathrm{tr}(CA)\,\mathrm{tr}(B) \\
&\quad + \mathrm{tr}(ABC) + \mathrm{tr}(ACB) + \mathrm{tr}(B)\,\mathrm{tr}(C)A + \mathrm{tr}(C)\,\mathrm{tr}(A)B + \mathrm{tr}(A)\,\mathrm{tr}(B)C \\
&\quad + \mathrm{tr}(BC)A + \mathrm{tr}(CA)B + \mathrm{tr}(AB)C + \mathrm{tr}(C)(AB + BA) + \mathrm{tr}(B)(AC + CA) \\
&\quad + \mathrm{tr}(A)(BC + CB) + ABC + ACB + BCA + BAC + CAB + CBA. \tag{44}
\end{aligned}
$$

Here numbers in operator equations, such as tr(A), are implicitly multiplied by the identity operator; a similar convention applies to other equations in this paper. When tr(A) = tr(B) = tr(C) = 1, Eqs. (42)–(44) simplify to

$$\mathcal{Q}(A) = 1 + A, \tag{45}$$

$$\mathcal{Q}(A \otimes B) = 1 + f + A + B + AB + BA, \tag{46}$$

$$\mathcal{Q}(A \otimes B \otimes C) = 1 + f_{12} + f_{23} + f_{31} + f_{123} + f_{132} + (1 + f_{23})A + (1 + f_{31})B + (1 + f_{12})C + AB + BA + AC + CA$$
$$+ BC + CB + ABC + ACB + BCA + BAC + CAB + CBA, \tag{47}$$

where $f = f_{12} = \mathrm{tr}(AB)$, $f_{23} = \mathrm{tr}(BC)$, $f_{31} = \mathrm{tr}(CA)$, $f_{123} = \mathrm{tr}(ABC)$, and $f_{132} = \mathrm{tr}(ACB)$. These equations indicate that the three-copy estimation fidelity may depend on the triple products of POVM elements in addition to pairwise overlaps (cf. Sec. VII).

Equation (42) implies that

$$\|\mathcal{Q}(A)\| = \mathrm{tr}(A) + \|A\|, \tag{48}$$

from which we can derive the following lemma.

Lemma 15. *The estimation fidelity $F(\mathscr{A})$ of any POVM $\mathscr{A} = \{A_j\}_j$ on $\mathcal{H}$ satisfies*

$$\frac{1}{d} \leq F(\mathscr{A}) = \frac{1}{d+1} + \frac{1}{d(d+1)} \sum_j \|A_j\| \leq \frac{2}{d+1}, \tag{49}$$

and the lower bound is saturated iff $\mathscr{A}$ is trivial, while the upper bound is saturated iff $\mathscr{A}$ is rank 1.

The equality in Eq. (49) was originally derived in Ref. [39] and played an important role in studying information-disturbance relations. The upper bound in Eq. (49) was known even earlier in the context of optimal quantum state estimation [35,38]. Here we are interested in Lemma 15 because it clarifies the estimation fidelities of single-copy measurements and highlights the significance of rank-1 measurements (cf. Proposition 1). If $\mathscr{A}$ is a POVM with m POVM elements, then Lemma 15 yields

$$F(\mathscr{A}) \leq \frac{1}{d+1} + \frac{m}{d(d+1)}, \tag{50}$$

given that $\|A_j\| \leq 1$ for any POVM element A_j. Here the inequality is saturated when $\mathscr{A}$ is a projective measurement, in which case the estimation fidelity is completely determined by the number of measurement outcomes.

The following lemma is a stepping stone for studying two-copy estimation fidelities.

Lemma 16. *Suppose that A and B are nonzero positive operators on $\mathcal{H}$ and that $f = \mathrm{tr}(AB)/[\mathrm{tr}(A)\,\mathrm{tr}(B)]$. Then*

$$\|\mathcal{Q}(A \otimes B)\| \leq 2\,\mathrm{tr}(A)\,\mathrm{tr}(B)(1 + f + \sqrt{f}). \tag{51}$$

The upper bound is saturated iff one of the following two conditions holds:

1. *both A and B are rank 1;*
2. *A and B have orthogonal supports and one of them is rank 1.*

When $A = |\psi\rangle\langle\psi|$ and $B = |\varphi\rangle\langle\varphi|$ are rank-1 projectors, Lemma 16 yields

$$\|\mathcal{Q}(|\psi\rangle\langle\psi| \otimes |\varphi\rangle\langle\varphi|)\| = 2(1 + |\langle\psi|\varphi\rangle|^2 + |\langle\psi|\varphi\rangle|), \tag{52}$$

which in turn implies that

$$\|\mathcal{Q}(|j\rangle\langle j| \otimes |k\rangle\langle k|)\| = \begin{cases} 6, & j = k, \\ 2, & j \neq k. \end{cases} \tag{53}$$

Note that Eq. (53) also follows from Eq. (46). By contrast, Eq. (47) implies that

$$\|\mathcal{Q}(|j\rangle\langle j| \otimes |k\rangle\langle k| \otimes |l\rangle\langle l|)\| = \begin{cases} 24, & j = k = l, \\ 6, & j = k \neq l, \\ 2, & j \neq k, k \neq l, j \neq l. \end{cases} \tag{54}$$

Here $|j\rangle, |k\rangle, |l\rangle$ denote basis states in the computational basis.

By virtue of Eq. (37) and Lemma 16, we can derive a general upper bound for the two-copy estimation fidelity of any product measurement.

Lemma 17. *Let $\mathscr{A}$ and $\mathscr{B}$ be two POVMs on $\mathcal{H}$. Then the two-copy estimation fidelity $F(\mathscr{A} \otimes \mathscr{B})$ satisfies*

$$F(\mathscr{A} \otimes \mathscr{B}) \leq \frac{2d(d+1) + 2\Phi_{1/2}(\mathscr{A}, \mathscr{B})}{d(d+1)(d+2)}, \qquad (55)$$

and the upper bound is saturated iff $\mathscr{A}$ and $\mathscr{B}$ are rank 1.

The following lemma is an immediate corollary of Lemma 17 with $\mathscr{B} = \mathscr{A}$.

Lemma 18. *Let $\mathscr{A}$ be a POVM on $\mathcal{H}$. Then the two-copy estimation fidelity $F(\mathscr{A}^{\otimes 2})$ satisfies*

$$F(\mathscr{A}^{\otimes 2}) \leq \frac{2d(d+1) + 2\Phi_{1/2}(\mathscr{A})}{d(d+1)(d+2)}, \qquad (56)$$

and the upper bound is saturated iff $\mathscr{A}$ is rank 1.

Lemma 18 establishes a precise connection between the two-copy estimation fidelity $F(\mathscr{A}^{\otimes 2})$ and the frame potential $\Phi_{1/2}(\mathscr{A})$ [instead of the frame potential $\Phi_2(\mathscr{A})$ as one may naively expect], thereby endowing the frame potential with a concrete operational meaning in the context of quantum state estimation. Similarly, Lemma 17 endows the cross frame potential with a concrete operational meaning.

C. Impact of coarse graining

Suppose that $\mathscr{A}$ is a rank-1 POVM on $\mathcal{H}$; then any nontrivial coarse graining of $\mathscr{A}$ can only achieve a smaller estimation fidelity according to Lemma 15. The situation is a bit more complicated for the two-copy estimation fidelity. Here we try to shed some light on this problem, which will be useful to studying the connection between the estimation fidelity and quantum incompatibility, as we will see in Sec. VI.

Lemma 19. *Suppose that A, B_1, B_2 are rank-1 positive operators on $\mathcal{H}$ and that $B = B_1 + B_2$. Then*

$$\|\mathcal{Q}(A \otimes B)\| \leq \|\mathcal{Q}(A \otimes B_1)\| + \|\mathcal{Q}(A \otimes B_2)\|, \qquad (57)$$

and the inequality is saturated iff one of the following three conditions holds:

1. B_2 *is proportional to B_1;*
2. A *is orthogonal to both B_1 and B_2;*
3. A, B_1, B_2 *are all supported in a common two-dimensional subspace of $\mathcal{H}$ and A is orthogonal to B_1 or B_2.*

Lemma 20. *Suppose that $\mathscr{A} = \{A_j\}_{j=1}^m$ is a simple rank-1 POVM on $\mathcal{H}$; let $B_1, B_2, \ldots, B_n$ be $n \geq 2$ rank-1 positive*

operators on $\mathcal{H}$ *that are pairwise linearly independent, and let $B = \sum_{k=1}^n B_k$. Then*

$$\sum_{j=1}^m \|\mathcal{Q}(A_j \otimes B)\| \leq \sum_{j=1}^m \sum_{k=1}^n \|\mathcal{Q}(A_j \otimes B_k)\|, \qquad (58)$$

and the inequality is saturated iff $B_1, B_2, \ldots, B_n$ are mutually orthogonal and they commute with all POVM elements in $\mathscr{A}$. In that case, $\mathscr{A}$ contains n rank-1 projectors that are proportional to $B_1, B_2, \ldots, B_n$, respectively, and is thus reducible.

Note that the inequality in Eq. (58) cannot be saturated if $\mathscr{A}$ is irreducible or $B_1, B_2, \ldots, B_n$ are not mutually orthogonal. This observation leads to the following lemma.

Lemma 21. *Suppose that $\mathscr{A}$ and $\mathscr{C}$ are two rank-1 POVMs on $\mathcal{H}$ and that $\mathscr{B}$ is a coarse graining of $\mathscr{C}$. Suppose that $\mathscr{A}$ is irreducible or $\mathscr{C}$ contains no two POVM elements that are mutually orthogonal. Then*

$$F(\mathscr{A} \otimes \mathscr{B}) \leq F(\mathscr{A} \otimes \mathscr{C}), \qquad (59)$$

and the inequality is saturated iff $\mathscr{B}$ is equivalent to $\mathscr{C}$.

Lemma 21 shows that the two-copy estimation fidelity $F(\mathscr{A} \otimes \mathscr{C})$ can only decrease when $\mathscr{C}$ is replaced by a nontrivial coarse graining, assuming that $\mathscr{A}$ is irreducible or $\mathscr{C}$ contains no two POVM elements that are mutually orthogonal. Nevertheless, this conclusion no longer holds if the underlying assumption is dropped; cf. Eq. (63) in the next section.

V. TYPICAL QUANTUM MEASUREMENTS IN THE LIGHT OF QUANTUM STATE ESTIMATION

Lemma 15 in Sec. IV B offers a succinct characterization of rank-1 measurements as optimal single-copy measurements. Here we further demonstrate that the estimation fidelity in Eqs. (35) and (37) is a powerful tool for characterizing typical quantum measurements, including rank-1 projective measurements, MUMs, SICs, and measurements based on tight equiangular lines. Notably, all these elementary quantum measurements are uniquely characterized by extremal one-copy and two-copy estimation fidelities, as summarized in Table I. In other words, all these measurements are uniquely determined by their information-extraction capabilities. To achieve our goal, we completely characterize all quantum measurements that can attain certain extremal estimation fidelities in a number of natural settings. Note that it is not enough to determine one optimal measurement.

TABLE I. Operational characterizations of typical quantum measurements in terms of extremal one-copy and two-copy estimation fidelities. Each measurement (pair of measurements) in the left column is completely determined by the estimation fidelities in bold font in the corresponding row (at most three estimation fidelities are required in each case). Here $\mathscr{A}$ and $\mathscr{B}$ are POVMs on $\mathcal{H}$; $F(\mathscr{A})$ and $F(\mathscr{B})$ are one-copy estimation fidelities, while $F(\mathscr{A}^{\otimes 2})$, $F(\mathscr{B}^{\otimes 2})$, and $F(\mathscr{A} \otimes \mathscr{B})$ are two-copy estimation fidelities. The estimation fidelities F_2^{iid} and F_2^{sep} are defined in Eqs. (65) and (70), respectively.

Quantum measurements	$F(\mathscr{A})$	$F(\mathscr{A}^{\otimes 2})$	$F(\mathscr{B})$	$F(\mathscr{B}^{\otimes 2})$	$F(\mathscr{A} \otimes \mathscr{B})$
Rank 1	$\boldsymbol{\frac{2}{d+1}}$	$\cdots$	$\cdots$	$\cdots$	$\cdots$
Rank-1 projective	$\boldsymbol{\frac{2}{d+1}}$	$\boldsymbol{\frac{2}{d+1}}$	$\cdots$	$\cdots$	$\cdots$
Identical rank-1 projective	$\boldsymbol{\frac{2}{d+1}}$	$\frac{2}{d+1}$	$\boldsymbol{\frac{2}{d+1}}$	$\frac{2}{d+1}$	$\frac{2}{d+1}$
SIC	$\boldsymbol{\frac{2}{d+1}}$	$\boldsymbol{F_2^{\text{iid}}}$	$\cdots$	$\cdots$	$\cdots$
Identical SICs	$\boldsymbol{\frac{2}{d+1}}$	$\boldsymbol{F_2^{\text{iid}}}$	$\frac{2}{d+1}$	F_2^{iid}	$\boldsymbol{F_2^{\text{iid}}}$
MU rank-1 projective	$\boldsymbol{\frac{2}{d+1}}$	$\boldsymbol{\frac{2}{d+1}}$	$\frac{2}{d+1}$	$\frac{2}{d+1}$	$\boldsymbol{F_2^{\text{sep}}}$

A. Optimal collective measurements and *t*-designs

As a generalization of Lemma 15, the following theorem determines tight lower and upper bounds for the estimation fidelity $F(\mathscr{A})$ for N-copy measurements, assuming that all collective measurements are accessible. In addition, optimal N-copy measurements are clarified.

Theorem 2. *Let $\mathscr{A} = \{A_j\}_j$ be any POVM on $\mathcal{H}^{\otimes N}$. Then the N-copy estimation fidelity $F(\mathscr{A})$ satisfies*

$$\frac{1}{d} \leq F(\mathscr{A}) \leq \frac{N+1}{N+d}, \tag{60}$$

and the lower bound is saturated iff $\tilde{\mathcal{Q}}(A_j)$ for each j is proportional to the identity, while the upper bound is saturated iff $P_N A_j P_N$ for each j is proportional to the Nth tensor power of a pure state.

The lower bound in Eq. (60) corresponds to the performance of a random guess; the upper bound is well known in the context of optimal quantum state estimation [31,35,38,41]. A self-contained proof of Theorem 2 is presented in Appendix G. When restricted to the N-partite symmetric subspace, a POVM is optimal iff it has the form

$$\left\{ \frac{D_N}{d} w_j (|\psi_j\rangle\langle\psi_j|)^{\otimes N} \right\}_j, \tag{61}$$

where D_N is determined by Eq. (6) and $\{|\psi_j\rangle, w_j\}_j$ forms a t-design with $t = N$ [41]. This observation establishes a simple connection between optimal collective measurements and quantum measurements based on t-designs.

Incidentally, prominent examples of 2-designs include CMUB [4–8] and SICs [8–12]. When the dimension d is a power of 2, any orbit of the Clifford group is a 3-design. In the case of a qubit, the vertices of the regular tetrahedron, octahedron, cube, icosahedron, and dodecahedron inscribed on the Bloch sphere form t-designs with

$t = 2, 3, 3, 5, 5$, respectively. The vertices of the octahedron also correspond to a CMUB. These platonic solids can be used to construct optimal collective measurements according to Eq. (61) [33]. Note that $D_t = t + 1$ when $d = 2$ by Eq. (6). Suppose that a platonic solid forms a t-design and let $\{\mathbf{r}_j\}_{j=1}^m$ be the set of unit vectors that specify its vertices on the Bloch sphere. Then the corresponding optimal collective measurements on the symmetric subspace of $\mathcal{H}^{\otimes t}$ can be constructed as

$$\left\{ \frac{t+1}{m} \left(\frac{1 + \mathbf{r}_j \cdot \boldsymbol{\sigma}}{2} \right)^{\otimes t} \right\}_{j=1}^m, \tag{62}$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector composed of the three Pauli operators. The optimal two-copy collective measurement based on the regular tetrahedron has already been realized in photonic experiments [75]. Optimal collective measurements based on other platonic solids might also be realized in the near future.

B. Rank-1 projective measurements and SICs

From now on we focus on the estimation fidelities of individual measurements, which are more instructive to understanding quantum measurements on $\mathcal{H}$. Given a POVM $\mathscr{A}$ on $\mathcal{H}$, recall that $F(\mathscr{A}^{\otimes k})$ denotes the k-copy estimation fidelity achieved by the product POVM $\mathscr{A}^{\otimes k}$ built from $\mathscr{A}$. Suppose that $\mathscr{A}$ is a rank-1 projective measurement on $\mathcal{H}$; by virtue of Lemma 15 and Eqs. (53) and (54), it is straightforward to verify that

$$F(\mathscr{A}^{\otimes 2}) = F(\mathscr{A}) = \frac{2}{d+1}, \quad F(\mathscr{A}^{\otimes 3}) = \frac{2(d+5)}{(d+2)(d+3)}. \tag{63}$$

Interestingly, identical projective measurements on two copies can only achieve the same estimation fidelity as a single-copy projective measurement, but identical projective measurements on three copies can enhance the estimation fidelity.
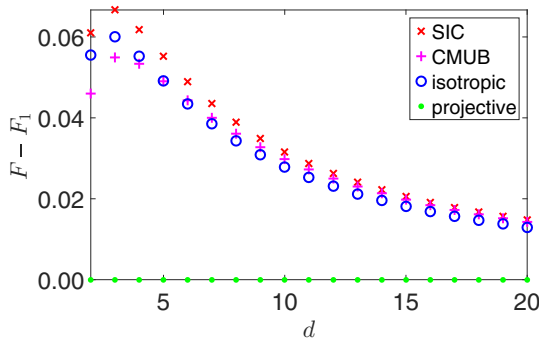
FIG. 2. Shifted two-copy estimation fidelities $F = F(\mathscr{A}^{\otimes 2})$, where $\mathscr{A}$ is a measurement constructed from an orthonormal basis (projective), SIC, CMUB, or Haar random pure states (isotropic). Here $F_1 = 2/(d+1)$ is the one-copy estimation fidelity achieved by a rank-1 projective measurement (or any rank-1 measurement).

When $\mathscr{A}$ is a SIC, by virtue of Lemma 15, Eq. (20), and Lemma 18, we can deduce that

$$F(\mathscr{A}) = \frac{2}{d+1}, \quad F(\mathscr{A}^{\otimes 2}) = F_2^{\text{iid}}, \tag{64}$$

where

$$F_2^{\text{iid}} := \frac{2[d^2 + d + 1 + (d-1)\sqrt{d+1}]}{d(d+1)(d+2)}. \tag{65}$$

On the other hand, $F(\mathscr{A}^{\otimes 3})$ depends on the specific SIC under consideration, as we will see in Sec. VII B. Although rank-1 projective measurements and SICs share the same single-copy estimation fidelity, their two-copy estimation fidelities are quite different, as illustrated in Fig. 2. What is remarkable is that both rank-1 projective measurements and SICs are completely characterized by one-copy and two-copy estimation fidelities, as shown in Theorem 3 and its corollaries below (cf. Table I).

Theorem 3. *Let $\mathscr{A}$ be any rank-1 POVM on $\mathcal{H}$. Then the two-copy estimation fidelity $F(\mathscr{A}^{\otimes 2})$ satisfies*

$$\frac{2}{d+1} \leq F(\mathscr{A}^{\otimes 2}) \leq F_2^{\text{iid}}. \tag{66}$$

If $\mathscr{A}$ is a simple rank-1 POVM, then the lower bound is saturated iff $\mathscr{A}$ is a rank-1 projective measurement, while the upper bound is saturated iff $\mathscr{A}$ is a SIC.

Theorem 3 follows from Lemmas 10 and 18. It highlights special and intriguing roles played by rank-1 projective measurements and SICs in quantum state estimation. Note that rank-1 projective measurements are completely characterized by the lower bound for the two-copy estimation fidelity $F(\mathscr{A}^{\otimes 2})$ as presented in Eq. (66), while SICs

are completely characterized by the upper bound. Furthermore, the assumption of "rank-1" in Theorem 3 can be dropped thanks to Corollaries 1 and 3 below.

Corollary 1. *A simple POVM $\mathscr{A}$ on $\mathcal{H}$ is a rank-1 projective measurement iff it satisfies the condition $F(\mathscr{A}^{\otimes 2}) = F(\mathscr{A}) = 2/(d+1)$.*

Corollary 2. *Two simple POVMs $\mathscr{A}$ and $\mathscr{B}$ on $\mathcal{H}$ are identical rank-1 projective measurements up to relabeling iff they satisfy $F(\mathscr{A} \otimes \mathscr{B}) = F(\mathscr{B}) = F(\mathscr{A}) = 2/(d+1)$.*

Corollary 3. *Any POVM $\mathscr{A}$ on $\mathcal{H}$ satisfies the inequality $F(\mathscr{A}^{\otimes 2}) \leq F_2^{\text{iid}}$. If $\mathscr{A}$ is simple, then the upper bound is saturated iff $\mathscr{A}$ is a SIC.*

Corollary 4. *Suppose that $\mathscr{A}_1, \mathscr{A}_2, \ldots, \mathscr{A}_g$ are g POVMs on $\mathcal{H}$. Then*

$$\sum_{r,s} F(\mathscr{A}_r \otimes \mathscr{A}_s) \leq g^2 F_2^{\text{iid}}. \tag{67}$$

If, in addition, these POVMs are simple, then the upper bound is saturated iff $\mathscr{A}_1, \mathscr{A}_2, \ldots, \mathscr{A}_g$ are identical SICs up to relabeling.

Corollary 5. *Two simple POVMs $\mathscr{A}$ and $\mathscr{B}$ on $\mathcal{H}$ are identical SICs up to relabeling iff they satisfy the condition $F(\mathscr{A} \otimes \mathscr{B}) = F(\mathscr{A}^{\otimes 2}) = F_2^{\text{iid}}$.*

Corollary 1 follows from Lemma 15 and Theorem 3, while Corollary 2 follows from Lemmas 12, 15, and 17 (cf. Theorem 7 below). The two corollaries offer succinct operational characterizations of rank-1 projective measurements and identical rank-1 projective measurements via one-copy and two-copy estimation fidelities. Corollaries 3–5 also follow from Theorem 3, as shown in Appendix H; they offer even more succinct operational characterizations of SICs and identical SICs via two-copy estimation fidelities. Surprisingly, here we do not need any assumption on the rank, purity, or the number of POVM elements. Note that the isotropic measurement and measurements based on CMUB are suboptimal, as illustrated in Fig. 2, although they have (many) more outcomes, in sharp contrast with the conclusion presented in Theorem 2 and the results on traditional quantum state tomography [20,26,27], in which measurements based on higher t-designs cannot perform worse. In addition, here the characterization of SICs is much simpler than most known alternatives, including conventional characterizations based on maximal equiangular lines or minimal 2-designs [9,10,26,74].

The above results demonstrate that both rank-1 projective measurements and SICs are uniquely determined by

their information-extraction capabilities. In other words, these elementary quantum measurements can be defined in purely information theoretic terms, in sharp contrast with traditional algebraic definitions, which lack clear operational meanings. As far as we know, similar results have never been derived or even anticipated before.

C. Measurements based on tight equiangular lines

Here we show that measurements based on tight equiangular lines stand out as optimal measurements when the number of outcomes is limited, which generalizes the optimality result on SICs as stated in Theorem 3.

If $\mathscr{A} = \{A_j\}_{j=1}^m$ is a POVM on $\mathcal{H}$ that is constructed from a set of m tight equiangular lines, then the POVM elements A_j of $\mathscr{A}$ have the form $A_j = d|\psi_j\rangle\langle\psi_j|/m$, where $|\psi_j\rangle$ satisfy Eq. (24). The estimation fidelity of $\mathscr{A}^{\otimes 2}$ can be derived by virtue of Lemmas 11 and 18 [cf. Eq. (37) and Lemma 16], with the result

$$F(\mathscr{A}^{\otimes 2}) = \frac{2}{d+2} + \frac{2d + 2\sqrt{d(m-1)(m-d)}}{m(d+1)(d+2)}. \quad (68)$$

Moreover, such a POVM is optimal among all rank-1 POVMs with m POVM elements, as shown in the following corollary, which is an immediate consequence of Lemmas 11 and 18.

Corollary 6. *Suppose that $\mathscr{A}$ is a rank-1 POVM on $\mathcal{H}$ that is composed of m POVM elements; then the two-copy estimation fidelity $F(\mathscr{A}^{\otimes 2})$ satisfies*

$$F(\mathscr{A}^{\otimes 2}) \leq \frac{2}{d+2} + \frac{2d + 2\sqrt{d(m-1)(m-d)}}{m(d+1)(d+2)}. \quad (69)$$

The upper bound is saturated iff $d \leq m \leq d^2$ and the POVM $\mathscr{A}$ is unbiased and equiangular.

Note that the upper bound in Eq. (69) is strictly monotonically increasing in m, as expected. As an implication of Lemma 15 and Corollary 6, an m-outcome POVM $\mathscr{A}$ is an unbiased rank-1 equiangular POVM iff $F(\mathscr{A}) = 2/(d+1)$ and the inequality in Eq. (69) is saturated.

D. Mutually unbiased measurements

When $\mathscr{A}$ and $\mathscr{B}$ are MU rank-1 projective measurements, the two-copy estimation fidelity $F(\mathscr{A} \otimes \mathscr{B})$ can be computed using Lemmas 12 and 17, with the result

$$F(\mathscr{A} \otimes \mathscr{B}) = F_2^{\text{sep}} := \frac{2(d + 1 + \sqrt{d})}{(d+1)(d+2)}. \quad (70)$$

As illustrated in Fig. 3, this estimation fidelity is very close to the estimation fidelity achieved by independent
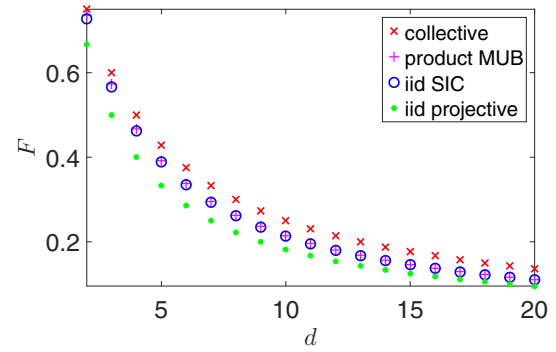

FIG. 3. Two-copy estimation fidelities achieved by optimal collective measurements, optimal product measurements (based on MUB), and optimal independent and identical measurements (based on SICs). As a benchmark, the figure also shows the estimation fidelity achieved by independent and identical rank-1 projective measurements.

and identical measurements based on a SIC. Nevertheless, it turns out that this is the maximum estimation fidelity achievable by separable measurements, including all measurements realized by local operations and classical communication, as manifested in the notation F_2^{sep}. Recall that a POVM is separable if each POVM element is proportional to a separable density operator.

Lemma 22. *Let $\mathscr{A} = \{A_j\}_j$ be any separable POVM on $\mathcal{H}^{\otimes 2}$. Then the two-copy estimation fidelity $F(\mathscr{A})$ satisfies $F(\mathscr{A}) \leq F_2^{\text{sep}}$. If $\mathscr{A}$ is rank 1, then the upper bound is saturated iff each POVM element A_j satisfies the condition $d\,\mathrm{tr}(WA_j) = \mathrm{tr}(A_j)$, where $W = 2P_2 - 1$ is the swap operator.*

When the POVM element A_j is a tensor product, the equality $d\,\mathrm{tr}(WA_j) = \mathrm{tr}(A_j)$ means A_j is a tensor product of two MU positive operators, which is reminiscent of the definition of MUMs. If we only consider product measurements, then only MU rank-1 POVMs can attain the maximum estimation fidelity F_2^{sep}.

Theorem 4. *Suppose that $\mathscr{A}$ and $\mathscr{B}$ are two POVMs on $\mathcal{H}$. Then the two-copy estimation fidelity $F(\mathscr{A} \otimes \mathscr{B})$ satisfies $F(\mathscr{A} \otimes \mathscr{B}) \leq F_2^{\text{sep}}$, and the inequality is saturated iff $\mathscr{A}$ and $\mathscr{B}$ are MU rank-1 POVMs.*

Although optimal product POVMs on $\mathcal{H}^{\otimes 2}$ are necessarily rank 1, it should be noted that optimal separable POVMs are not subjected to this constraint. In the case of a qubit for example, an optimal separable POVM can be

constructed from the four rank-2 operators

$$\frac{|0+\rangle\langle 0+| + |+0\rangle\langle +0|}{2}, \quad \frac{|0-\rangle\langle 0-| + |-0\rangle\langle -0|}{2},$$
$$\frac{|1+\rangle\langle 1+| + |+1\rangle\langle +1|}{2}, \quad \frac{|1-\rangle\langle 1-| + |-1\rangle\langle -1|}{2}, \quad (71)$$

where $|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$.

Corollary 7. *Suppose that $\mathscr{A}$ and $\mathscr{B}$ are two POVMs on $\mathcal{H}$ that satisfy the condition $F(\mathscr{A} \otimes \mathscr{B}) = F_2^{\mathrm{sep}}$. Then $\mathscr{A} \otimes \mathscr{B}$ has at least d^2 POVM elements, and the lower bound is saturated iff $\mathscr{A}$ and $\mathscr{B}$ are MU rank-1 projective measurements.*

Corollary 8. *Suppose that $\mathscr{A}$ and $\mathscr{B}$ are two simple POVMs on $\mathcal{H}$. Then $\mathscr{A}$ and $\mathscr{B}$ are MU rank-1 projective measurements iff they satisfy the conditions $F(\mathscr{A} \otimes \mathscr{B}) = F_2^{\mathrm{sep}}$ and $F(\mathscr{A}^{\otimes 2}) = F(\mathscr{B}^{\otimes 2}) = 2/(d+1)$.*

Corollary 9. *Suppose that $\mathscr{A}_1, \mathscr{A}_2, \ldots, \mathscr{A}_g$ are g POVMs on $\mathcal{H}$. Then*

$$\sum_{r \neq s} F(\mathscr{A}_r \otimes \mathscr{A}_s) \leq g(g-1)F_2^{\mathrm{sep}}, \quad (72)$$

and the upper bound is saturated iff $\mathscr{A}_1, \mathscr{A}_2, \ldots, \mathscr{A}_g$ are MU rank-1 POVMs. If, in addition, these POVMs are simple and $g = d+1$, then the upper bound is saturated iff $\mathscr{A}_1, \mathscr{A}_2, \ldots, \mathscr{A}_{d+1}$ are rank-1 projective measurements, which form a CMUMs.

Thanks to Theorem 4 and its corollaries, MU rank-1 projective measurements are completely characterized by two-copy estimation fidelities as summarized in Table I. Remarkably, we do not even need bases to start with; orthonormal bases appear naturally once the estimation fidelities reach certain extremal values. In addition, Corollaries 8 and 9 do not require any assumption on the rank, purity, or the number of POVM elements. Such simple operational characterizations are not even anticipated in the literature as far as we know. These results are of intrinsic interest to studying quantum estimation theory, quantum measurements, and the complementarity principle.

At this point, it is instructive to compare Corollary 4 with Corollary 9. The former characterizes identical SICs via the maximum of $\sum_{r,s} F(\mathscr{A}_r \otimes \mathscr{A}_s)$, which is a sum of two-copy estimation fidelities, while the latter characterizes (complete sets of) MUMs via the maximum of $\sum_{r \neq s} F(\mathscr{A}_r \otimes \mathscr{A}_s)$. The only difference in the latter summation is that the diagonal terms are absent. Quite surprisingly, this minor change in the summation leads to a jump from SICs to MUMs.

VI. DECODING QUANTUM INCOMPATIBILITY

In addition to characterizing typical quantum measurements, the estimation fidelity encodes valuable information about noncommutativity and incompatibility of quantum measurements. Traditionally, incompatibility is usually understood as a limitation, as embodied in the complementarity principle [13] and uncertainty relations [14–18]. With the development of quantum information science, incompatibility is also recognized as a resource [43,44]. As a byproduct, here we show that incompatibility is a useful resource to enhance the estimation fidelity, thereby offering additional insight on this topic.

A. Quantum incompatibility and the estimation fidelity

Theorem 5. *Suppose that $\mathscr{A}$ and $\mathscr{B}$ are two commuting POVMs on $\mathcal{H}$. Then the two-copy estimation fidelity $F(\mathscr{A} \otimes \mathscr{B})$ satisfies $F(\mathscr{A} \otimes \mathscr{B}) \leq 2/(d+1)$.*

Theorem 5 shows that two-copy measurements based on two commuting POVMs cannot provide any advantage over one-copy measurements. In other words, noncommutativity is necessary to go beyond the single-copy limit on the estimation fidelity. Theorem 7 below further shows that noncommutativity is also sufficient to achieve this goal when one POVM is rank 1, as illustrated in Fig. 4.

Theorem 6. *Suppose that $\mathscr{A}$ and $\mathscr{B}$ are two compatible POVMs on $\mathcal{H}$. Then the two-copy estimation fidelity $F(\mathscr{A} \otimes \mathscr{B})$ satisfies $F(\mathscr{A} \otimes \mathscr{B}) \leq F_2^{\mathrm{iid}}$. If, in addition, both $\mathscr{A}$ and $\mathscr{B}$ are simple, then the upper bound is saturated iff $\mathscr{A}$ and $\mathscr{B}$ are identical SICs up to relabeling.*
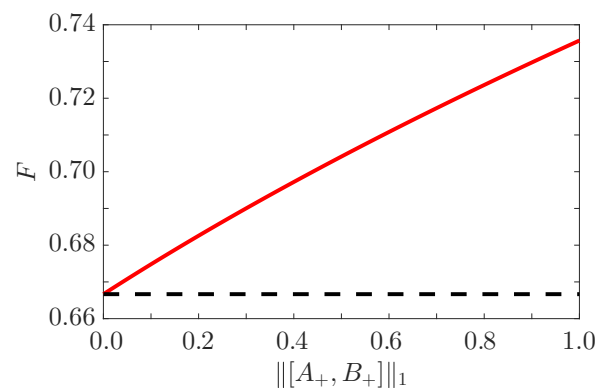

FIG. 4. Relation between the two-copy estimation fidelity and the commutator of POVM elements. Here $F = F(\mathscr{A} \otimes \mathscr{B})$ is the estimation fidelity achieved by the tensor product of two rank-1 projective measurements as shown in Eq. (84), while $\|[A_+, B_+]\|_1$ is the 1-norm of the commutator $[A_+, B_+]$. As a benchmark, the black dashed line denotes the one-copy estimation fidelity achieved by a rank-1 projective measurement.

Here F_2^{iid} is defined in Eq. (65). Theorem 6 shows that two-copy measurements based on two compatible POVMs cannot go beyond the estimation fidelity achieved by product measurements based on identical SICs. It offers another operational characterization of SICs that does not rely on any assumption on the rank, purity, or the number of measurement outcomes; meanwhile, it provides a universal criterion for detecting incompatibility of two POVMs. Such universal criteria are quite rare in the literature [49,50,52]. These results highlight the intriguing connection between SICs and quantum incompatibility, which is of intrinsic interest to foundational studies.

Suppose that $\mathscr{A}_1, \mathscr{A}_2, \ldots, A_g$ are g compatible POVMs. Then Theorem 6 implies that

$$\sum_{r \neq s}^{g} F(\mathscr{A}_r \otimes \mathscr{A}_s) \leq g(g-1) F_2^{\text{iid}}. \qquad (73)$$

In addition, since $\mathscr{A}_1, \mathscr{A}_2, \ldots, A_g$ admit a common refinement, say $\mathscr{B}$, we can also deduce that

$$F(\mathscr{A}_1 \otimes \mathscr{A}_2 \otimes \cdots \otimes \mathscr{A}_r) \leq F(\mathscr{B}^{\otimes g}) \leq F_g^{\text{iid}}, \qquad (74)$$

where F_g^{iid} denotes the maximum estimation fidelity achieved by identical and independent measurements on $\mathcal{H}^{\otimes g}$. This result provides a universal criterion for detecting incompatibility of g arbitrary POVMs. Unfortunately, it is not easy to determine F_g^{iid} for $g \geq 3$; this problem deserves further study.

Theorem 7. *Suppose that $\mathscr{A}$ and $\mathscr{B}$ are POVMs on $\mathcal{H}$ with $\mathscr{A}$ being rank 1. Then the two-copy estimation fidelity $F(\mathscr{A} \otimes \mathscr{B})$ satisfies $F(\mathscr{A} \otimes \mathscr{B}) \geq F(\mathscr{A}) = 2/(d+1)$, and the inequality is saturated iff $\mathscr{A}$ commutes with $\mathscr{B}$. If $\mathscr{A}$ and $\mathscr{B}$ are simple rank-1 POVMs, then the inequality is saturated iff $\mathscr{A}$ and $\mathscr{B}$ are identical rank-1 projective measurements up to relabeling.*

The last statement in Theorem 7 is tied to the characterization of identical rank-1 projective measurements presented in Corollary 2. As an implication of Theorems 4 and 7, any pair of rank-1 POVMs $\mathscr{A}$ and $\mathscr{B}$ on $\mathcal{H}$ satisfies

$$\frac{2}{d+1} \leq F(\mathscr{A} \otimes \mathscr{B}) \leq F_2^{\text{sep}}. \qquad (75)$$

The lower bound is saturated iff $\mathscr{A}$ and $\mathscr{B}$ commute, which means they are equivalent to the same rank-1 projective measurement, while the upper bound is saturated iff $\mathscr{A}$ and $\mathscr{B}$ are MU. Note that MU measurements are often regarded as maximally incompatible measurements [4–7,57]. The above results show that incompatibility is a resource to enhance the estimation fidelity. Although the significance of incompatibility as a resource has been recognized before, results like Theorem 7 are still quite rare

because it is not easy to establish conditions that are both necessary and sufficient.

B. Concrete examples

As an illustration, let us consider two binary POVMs $\mathscr{A} = \{A_+, A_-\}$ and $\mathscr{B} = \{B_+, B_-\}$ acting on a qubit (that is, $d = 2$), where $A_- = 1 - A_+$ and $B_- = 1 - B_+$. Note that the two POVMs are completely determined by the two effect operators A_+ and B_+, respectively, which satisfy the condition $0 \leq A_+, B_+ \leq 1$. Without loss of generality, we can assume that $1 \leq \text{tr}(A_+), \text{tr}(B_+) < 2$. Then $A_\pm$ and $B_\pm$ can be expressed as

$$A_\pm = \frac{1 \pm \alpha \pm \mathbf{a} \cdot \boldsymbol{\sigma}}{2}, \quad B_\pm = \frac{1 \pm \beta \pm \mathbf{b} \cdot \boldsymbol{\sigma}}{2}, \qquad (76)$$

where $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector composed of the three Pauli operators and the parameters $\alpha, \beta, \mathbf{a}, \mathbf{b}$ satisfy the conditions

$$0 \leq \alpha, \beta < 1, \quad |\mathbf{a}| \leq 1 - \alpha, \quad |\mathbf{b}| \leq 1 - \beta. \qquad (77)$$

The parameter α (β) characterizes the bias of the POVM $\mathscr{A}$ ($\mathscr{B}$), while the parameter $|\mathbf{a}|$ ($|\mathbf{b}|$) characterizes the sharpness of $\mathscr{A}$ ($\mathscr{B}$). Notably, $\mathscr{A}$ is unbiased iff $\alpha = 0$, while $\mathscr{A}$ is rank 1 iff $\alpha = 0$ and $|\mathbf{a}| = 1$. Similarly, $\mathscr{B}$ is unbiased iff $\beta = 0$, while $\mathscr{B}$ is rank 1 iff $\beta = 0$ and $|\mathbf{b}| = 1$. In addition, $\mathscr{A}$ and $\mathscr{B}$ are MU iff $\mathbf{a} \cdot \mathbf{b} = 0$.

The single-copy estimation fidelity $F(\mathscr{A})$ can be computed by virtue of Lemma 15, with the result

$$F(\mathscr{A}) = \frac{3 + |\mathbf{a}|}{6}. \qquad (78)$$

The two-copy estimation fidelity $F(\mathscr{A}^{\otimes 2})$ can be computed by virtue of Eqs. (37) and (43), with the result

$$F(\mathscr{A}^{\otimes 2}) = \frac{3 + |\mathbf{a}| + \alpha |\mathbf{a}|}{6}. \qquad (79)$$

Interestingly, the single-copy estimation fidelity of a binary POVM on a qubit is completely determined by its sharpness, while the two-copy estimation fidelity depends on both sharpness and bias. In addition, the parameters α and $|\mathbf{a}|$ are completely determined by $F(\mathscr{A})$ and $F(\mathscr{A}^{\otimes 2})$. Notably, the inequality $F(\mathscr{A}^{\otimes 2}) \geq F(\mathscr{A})$ is saturated iff $\mathscr{A}$ is unbiased ($\alpha = 0$) or trivial ($|\mathbf{a}| = 0$).

To determine the estimation fidelity of the product POVM $\mathscr{A} \otimes \mathscr{B}$, we need to compute $\mathcal{Q}(A_\pm \otimes B_\pm)$. By

virtue of Eq. (43) we can derive the result

$$\mathcal{Q}(A_+ \otimes B_+) = 3(1+\alpha)(1+\beta) + \mathbf{a} \cdot \mathbf{b} + (1+\beta)\mathbf{a} \cdot \boldsymbol{\sigma} \\ + (1+\alpha)\mathbf{b} \cdot \boldsymbol{\sigma}, \tag{80}$$

which implies that

$$\|\mathcal{Q}(A_+ \otimes B_+)\| = 3(1+\alpha)(1+\beta) + \mathbf{a} \cdot \mathbf{b} \\ + |(1+\beta)\mathbf{a} + (1+\alpha)\mathbf{b}|. \tag{81}$$

The norm $\|\mathcal{Q}(A_+ \otimes B_-)\|$ can be derived by replacing β and $\mathbf{b}$ with $-\beta$ and $-\mathbf{b}$, respectively; a similar recipe applies to $\|\mathcal{Q}(A_- \otimes B_\pm)\|$. Now the estimation fidelity $F(\mathscr{A} \otimes \mathscr{B})$ can be calculated using Eq. (37), with the result

$$F(\mathscr{A} \otimes \mathscr{B}) = \tfrac{1}{2} + \tfrac{1}{24}[|(1+\beta)\mathbf{a} + (1+\alpha)\mathbf{b}| \\ + |(1-\beta)\mathbf{a} - (1+\alpha)\mathbf{b}| \\ + |(1+\beta)\mathbf{a} - (1-\alpha)\mathbf{b}| \\ + |(1-\beta)\mathbf{a} + (1-\alpha)\mathbf{b}|]. \tag{82}$$

If $\mathscr{A}$ and $\mathscr{B}$ are unbiased, which means $\alpha = \beta = 0$, then Eq. (82) reduces to

$$F(\mathscr{A} \otimes \mathscr{B}) = \frac{1}{2} + \frac{|\mathbf{a}+\mathbf{b}| + |\mathbf{a}-\mathbf{b}|}{12}. \tag{83}$$

So $F(\mathscr{A} \otimes \mathscr{B}) \leq 2/3$ iff $|\mathbf{a}+\mathbf{b}| + |\mathbf{a}-\mathbf{b}| \leq 2$. It is well known that the latter condition holds iff $\mathscr{A}$ and $\mathscr{B}$ are compatible (jointly measurable) [42,76–78]. Therefore, incompatibility is both necessary and sufficient to enhance the estimation fidelity beyond the single-copy limit in this special case. In addition, we have $F(\mathscr{A} \otimes \mathscr{B}) = \max\{F(\mathscr{A}), F(\mathscr{B})\}$ when $\mathbf{a}$ and $\mathbf{b}$ are parallel or antiparallel, which is consistent with Theorems 5 and 7.

If $\mathscr{A}$ and $\mathscr{B}$ are rank-1 projective measurements, which means $\alpha = \beta = 0$ and $|\mathbf{a}| = |\mathbf{b}| = 1$, then $F(\mathscr{A} \otimes \mathscr{B})$ can be expressed as

$$F(\mathscr{A} \otimes \mathscr{B}) = \frac{3 + \sqrt{1 + |\mathbf{a} \times \mathbf{b}|}}{6} = \frac{3 + \sqrt{1 + |\sin\phi|}}{6} \\ = \frac{3 + \sqrt{1 + \|[A_+, B_+]\|_1}}{6}, \tag{84}$$

where ϕ is the angle between $\mathbf{a}$ and $\mathbf{b}$, and $\|[A_+, B_+]\|_1$ is the Schatten 1-norm (or trace norm) of the commutator $[A_+, B_+] := A_+ B_+ - B_+ A_+$. Note that

$$[A_+, B_+] = [A_-, B_-] = -[A_+, B_-] = -[A_-, B_+]. \tag{85}$$

Therefore, $F(\mathscr{A} \otimes \mathscr{B}) \geq 2/3$, and the lower bound is saturated iff $\mathbf{a}$ and $\mathbf{b}$ are parallel or antiparallel, in which case $\mathscr{A}$ and $\mathscr{B}$ commute and are thus identical rank-1 projective measurements up to relabeling, as shown in Theorem 7 and illustrated in Fig. 4.

C. Connection with entropic uncertainty relations

Entropic uncertainty relations are another important manifestation of quantum incompatibility [17,18]. Given two rank-1 projective measurements $\mathscr{A}$ and $\mathscr{B}$ on $\mathcal{H}$, is there any connection between the two-copy estimation fidelity $F(\mathscr{A} \otimes \mathscr{B})$ and entropic uncertainty relations between $\mathscr{A}$ and $\mathscr{B}$? Here we reveal a precise connection in the case of a qubit. Denote by $H_\rho(\mathscr{A})$ $[H_\rho(\mathscr{B})]$ the entropy of measurement outcomes when the projective measurement $\mathscr{A}$ ($\mathscr{B}$) is performed on a given state ρ. Then the entropy sum $H_\rho(\mathscr{A}) + H_\rho(\mathscr{B})$ satisfies a state-independent entropic uncertainty relation [17,18,45],

$$H_\rho(\mathscr{A}) + H_\rho(\mathscr{B}) \geq H_{\text{MES}}(\mathscr{A}, \mathscr{B}) = H_{\text{MES}}(\phi), \tag{86}$$

where $H_{\text{MES}}(\mathscr{A} \otimes \mathscr{B})$ denotes the minimum entropy sum associated with the two projective measurements $\mathscr{A}, \mathscr{B}$, and ϕ is the angle between $\mathbf{a}$ and $\mathbf{b}$ as in Eq. (84). Note that $H_{\text{MES}}(\mathscr{A}, \mathscr{B})$ is completely determined by ϕ, so we can write $H_{\text{MES}}(\phi)$ in its place.

Let

$$p = \frac{1 + \cos\theta}{2}, \quad q = \frac{1 + \cos(\theta - \phi)}{2}. \tag{87}$$

Then $H_{\text{MES}}(\phi)$ can be expressed as [18,45]

$$H_{\text{MES}}(\phi) = \min_{0 \leq \theta < 2\pi} [h_{\text{bin}}(p) + h_{\text{bin}}(q)], \tag{88}$$

where $h_{\text{bin}}(p)$ is the binary Shannon entropy defined as

$$h_{\text{bin}}(p) := -p\log_2 p - (1-p)\log_2(1-p). \tag{89}$$

When $0 \leq \phi \leq \phi_1$ with $\phi_1 \approx 1.17056$, the minimum in Eq. (88) is attained at $\theta = \phi/2$ [45]; in general, the minimum can be determined by numerical calculation. In addition, it is easy to verify that

$$H_{\text{MES}}(-\phi) = H_{\text{MES}}(\pi + \phi) = H_{\text{MES}}(\phi). \tag{90}$$

So the value of $H_{\text{MES}}(\phi)$ is determined by $|\sin\phi|$. Moreover, it is not difficult to show that $H_{\text{MES}}(\phi)$ is monotonically increasing in $|\sin\phi|$, just like the two-copy estimation fidelity $F(\mathscr{A} \otimes \mathscr{B})$ in Eq. (84). Therefore, the minimum entropy sum $H_{\text{MES}}(\mathscr{A}, \mathscr{B})$ associated with two rank-1 projective measurements on a qubit is determined by the two-copy estimation fidelity $F(\mathscr{A} \otimes \mathscr{B})$, and vice versa, as illustrated in Fig. 5. This observation reveals a surprising connection between quantum state estimation and entropic uncertainty relations.
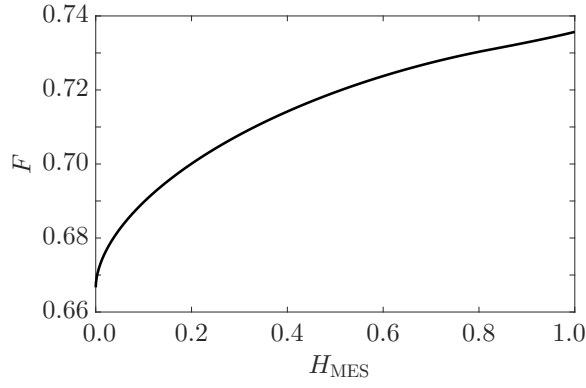
FIG. 5. Relation between the two-copy estimation fidelity and the minimum entropy sum. Here F is the two-copy estimation fidelity associated with two rank-1 projective measurements on a qubit as shown in Eq. (84), and H_{MES} is the minimum entropy sum presented in Eq. (88), which characterizes the entropic uncertainty relation in Eq. (86).

VII. DISTINGUISHING INEQUIVALENT MUB AND SICs

In this section we show that the three-copy estimation fidelity can be used to distinguish inequivalent discrete symmetric structures tied to the quantum state space, including MUB and SICs in particular. This capability is rooted in the fact that the three-copy estimation fidelity encodes valuable information about the triple products of POVM elements, which play important roles in studying SICs [79–81] and discrete Wigner functions [82]. Note that such information cannot be retrieved by considering pairwise overlaps alone.

A. Operational distinction between inequivalent MUB

Let $\{|\alpha_j\rangle\}_j$, $\{|\beta_k\rangle\}_k$, and $\{|\gamma_l\rangle\}_l$ be three orthonormal bases in $\mathcal{H}$; let $\mathscr{A} = \{|\alpha_j\rangle\langle\alpha_j|\}_j$, $\mathscr{B} = \{|\beta_k\rangle\langle\beta_k|\}_k$, and $\mathscr{C} = \{|\gamma_l\rangle\langle\gamma_l|\}_l$ be the corresponding rank-1 projective measurements. In this section we take the convention that $j, k, l \in \{0, 1, \ldots, d - 1\}$. According to Eqs. (37) and (47), the three-copy estimation fidelity $F(\mathscr{A} \otimes \mathscr{B} \otimes \mathscr{C})$ may depend on the triple products

$$f_{jkl} := \mathrm{tr}(|\alpha_j\rangle\langle\alpha_j|\beta_k\rangle\langle\beta_k|\gamma_l\rangle\langle\gamma_l|) \qquad (91)$$

in addition to the pairwise fidelities (transition probabilities) between the basis elements. This dependence can be used to distinguish inequivalent triples of bases that share the same pairwise fidelities.

As an illustration, here we consider triples of MUB in dimension 4 ($d = 4$). In this case, according to Ref. [83], there exists a three-parameter family of triples of MUB. The first basis is chosen to be the computational basis by convention; the second and third bases correspond to the

columns of the two Hadamard matrices

$$\frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & ie^{ix} & -ie^{ix} \\ 1 & -1 & -ie^{ix} & ie^{ix} \end{pmatrix},$$

$$\frac{1}{2}\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ -e^{iy} & e^{iy} & e^{iz} & -e^{iz} \\ e^{iy} & -e^{iy} & e^{iz} & -e^{iz} \end{pmatrix}, \qquad (92)$$

where $x, y, z \in [0, 2\pi)$ are three real parameters. Note that the transformation $x \mapsto x + \pi$ amounts to the permutation of the last two columns of the first Hadamard matrix; similarly, the transformations $y \mapsto y + \pi$ and $z \mapsto z + \pi$ amount to the permutations of the columns of the second Hadamard matrix. So it suffices to consider the parameter range $x, y, z \in [0, \pi)$.

Now suppose that $\{|\alpha_j\rangle\}_j$ coincides with the computational basis $\{|j\rangle\}_j$, while $\{|\beta_k\rangle\}_k$ and $\{|\gamma_l\rangle\}_l$ are determined by the columns of the two Hadamard matrices in Eq. (92), respectively; here the dependencies on the parameters x, y, z are suppressed to simplify the notation. Then the three bases $\{|\alpha_j\rangle\}_j$, $\{|\beta_k\rangle\}_k$, and $\{|\gamma_l\rangle\}_l$ are MU, that is,

$$\begin{aligned} \mathrm{tr}(|\alpha_j\rangle\langle\alpha_j|\beta_k\rangle\langle\beta_k|) &= \mathrm{tr}(|\beta_k\rangle\langle\beta_k|\gamma_l\rangle\langle\gamma_l|) \\ &= \mathrm{tr}(|\alpha_j\rangle\langle\alpha_j|\gamma_l\rangle\langle\gamma_l|) \\ &= \tfrac{1}{4} \quad \text{for all } j, k, l = 0, 1, 2, 3. \quad (93) \end{aligned}$$

By Eqs. (37) and (47), the three-copy estimation fidelity of $\mathscr{A} \otimes \mathscr{B} \otimes \mathscr{C}$, denoted by $F_{\mathrm{MUB}}(x, y, z) := F(\mathscr{A} \otimes \mathscr{B} \otimes \mathscr{C})$ henceforth, can be computed as

$$F_{\mathrm{MUB}}(x, y, z) = \frac{\sum_{j,k,l} \|\mathcal{Q}(|j\rangle\langle j| \otimes |\beta_k\rangle\langle\beta_k| \otimes |\gamma_l\rangle\langle\gamma_l|)\|}{840}. \qquad (94)$$

The variation of the estimation fidelity $F_{\mathrm{MUB}}(x, y, z)$ with x, y, z is shown in Figs. 6 and 7.
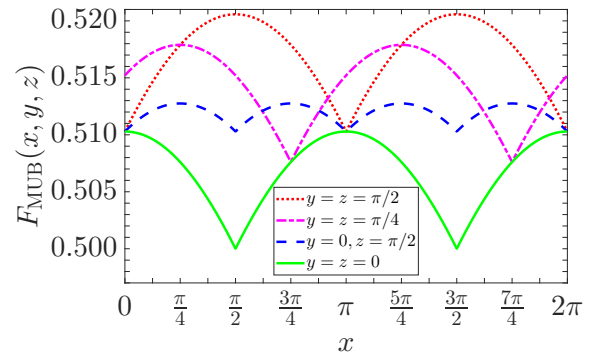

FIG. 6. Three-copy estimation fidelity $F_{\mathrm{MUB}}(x, y, z)$ achieved by the product projective measurement based on a triple of MUB as determined in Eq. (94).

In general, $F_{\mathrm{MUB}}(x,y,z)$ does not have a simple expression because $\|\mathcal{Q}(|j\rangle\langle j| \otimes |\beta_k\rangle\langle\beta_k| \otimes |\gamma_l\rangle\langle\gamma_l|)\|$ depends on the triple product f_{jkl} and in general does not have a simple analytical expression. Nevertheless, analytical formulas for $\|\mathcal{Q}(|j\rangle\langle j| \otimes |\beta_k\rangle\langle\beta_k| \otimes |\gamma_l\rangle\langle\gamma_l|)\|$ can be derived in a few special cases of interest:

$$\|\mathcal{Q}(|j\rangle\langle j| \otimes |\beta_k\rangle\langle\beta_k| \otimes |\gamma_l\rangle\langle\gamma_l|)\|$$
$$= \begin{cases} \frac{15}{2} & \text{if } f_{jkl} = \frac{1}{8}, \\ \frac{15}{4} & \text{if } f_{jkl} = -\frac{1}{8}, \\ 4 + \frac{5}{4}\sqrt{3} & \text{if } f_{jkl} = \pm\frac{i}{8}. \end{cases} \quad (95)$$

In the case $x = \pi/2$ and $y = z = 0$, calculation shows that 48 of the triple products f_{jkl} are equal to $1/8$, while the remaining 16 triple products are equal to $-1/8$. Therefore,

$$F_{\mathrm{MUB}}(x,y,z) = \frac{1}{840}\left(\frac{15}{2} \times 48 + \frac{15}{4} \times 16\right) = \frac{1}{2}. \quad (96)$$

In the case $x = y = z = \pi/2$, calculation shows that 32 of the triple products f_{jkl} are equal to $1/8$, while the remaining

32 triple products are equal to $i/8$ or $-i/8$. Therefore,

$$F_{\mathrm{MUB}}(x,y,z) = \frac{1}{840}\left(\frac{15}{2} \times 32 + \frac{16 + 5\sqrt{3}}{4} \times 32\right)$$
$$= \frac{46 + 5\sqrt{3}}{105} \approx 0.5206. \quad (97)$$

Numerical calculation indicates that $1/2$ is the minimum of $F_{\mathrm{MUB}}(x,y,z)$, while $(46 + 5\sqrt{3})/105$ is the maximum of $F_{\mathrm{MUB}}(x,y,z)$ (cf. Figs. 6 and 7). The difference is about 4.1%, which is quite significant and is amenable to experimental demonstration. Here Haar random pure states involved in the estimation problem can be replaced by any ensemble of pure states that forms a 4-design, which can be constructed from a suitable Clifford orbit, as described in Ref. [63].

B. Operational distinction between inequivalent SICs

The estimation fidelity can also be used to distinguish inequivalent SICs. As an illustration, here we consider SICs in dimension 3. It is known that all SICs in dimension 3 are covariant with respect to the Heisenberg-Weyl group with respect to a suitable basis [9–12,79,84–86]. The standard Heisenberg-Weyl group is generated by the
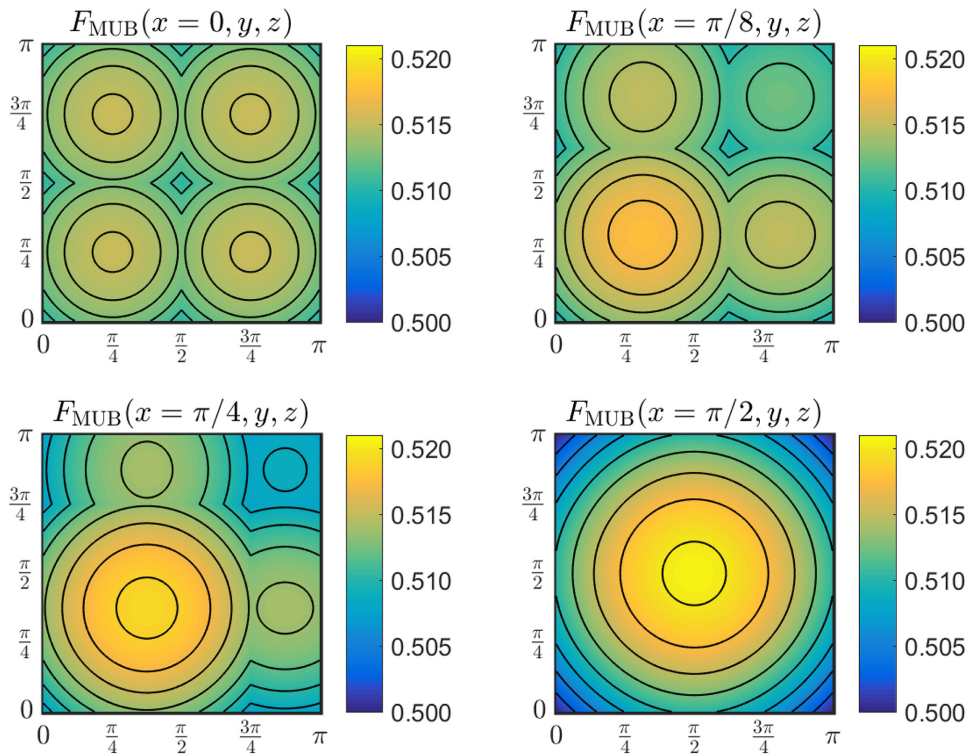

FIG. 7. Contour and color plots of the three-copy estimation fidelity $F_{\mathrm{MUB}}(x,y,z)$ [cf. Eq. (94)] for four cross sections that are parallel to the y-z plane as specified by four different values of x.

cyclic-shift operator X and phase operator Z:

$$X := \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \quad Z := \begin{pmatrix} 1 & 0 & 0 \\ & e^{2\pi i/3} & 0 \\ 0 & 0 & e^{4\pi i/3} \end{pmatrix}. \quad (98)$$

Let

$$|\psi(\phi)\rangle := \frac{1}{\sqrt{2}}(0, 1, -e^{i\phi})^{\mathrm{T}}, \quad 0 \le \phi < 2\pi; \quad (99)$$

for each choice of the phase ϕ, a SIC can be constructed as [9,84]

$$\mathscr{A}_{\mathrm{SIC}}(\phi) := \left\{ \tfrac{1}{3} X^j Z^k |\psi(\phi)\rangle \langle \psi(\phi)| (X^j Z^k)^\dagger \right\}_{j,k=0,1,2}. \quad (100)$$

Note that $\mathscr{A}_{\mathrm{SIC}}(\phi + (2\pi/3))$ and $\mathscr{A}_{\mathrm{SIC}}(\phi)$ are identical up to relabeling.

Moreover, any SIC in dimension 3 is unitarily equivalent to $\mathscr{A}_{\mathrm{SIC}}(\phi)$ for $\phi \in [0, \pi/9]$; given $0 \le \phi_1 \le \phi_2 \le \pi/9$, then $\mathscr{A}_{\mathrm{SIC}}(\phi_1)$ and $\mathscr{A}_{\mathrm{SIC}}(\phi_2)$ are unitarily equivalent iff $\phi_1 = \phi_2$ [28,79]. The two SICs $\mathscr{A}_{\mathrm{SIC}}(\phi = 0)$ and $\mathscr{A}_{\mathrm{SIC}}(\phi = \pi/9)$ are exceptional in the sense that they have larger symmetry groups compared with a generic SIC $\mathscr{A}_{\mathrm{SIC}}(\phi)$ with $0 < \phi < \pi/9$. In particular, the SIC $\mathscr{A}_{\mathrm{SIC}}(\phi = 0)$ has the largest symmetry group and can be regarded as the most symmetric SIC [79,84,87]. However, it is not clear if inequivalent SICs have different operational implications before the current study.

Here we are interested in the estimation fidelity of $\mathscr{A}_{\mathrm{SIC}}(\phi)^{\otimes 3}$, denoted by $F_{\mathrm{SIC}}(\phi) := F(\mathscr{A}_{\mathrm{SIC}}(\phi)^{\otimes 3})$ henceforth. The analytical expression for $F_{\mathrm{SIC}}(\phi)$ is too complicated to be informative, but it is easy to compute its value numerically by virtue of Eqs. (37) and (47). The dependence of $F_{\mathrm{SIC}}(\phi)$ on ϕ is illustrated in Fig. 8, which indicates that $F_{\mathrm{SIC}}(\phi)$ is periodic in ϕ with period $2\pi/9$. In addition, $F_{\mathrm{SIC}}(\phi)$ increases monotonically with ϕ for $\phi \in [0, \pi/9]$, but decreases monotonically for $\phi \in [\pi/9, 2\pi/9]$.
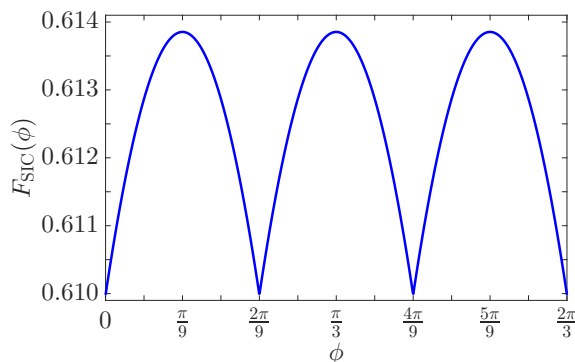

FIG. 8. Three-copy estimation fidelity $F_{\mathrm{SIC}}(\phi)$ achieved by the POVM $\mathscr{A}_{\mathrm{SIC}}(\phi)^{\otimes 3}$, where $\mathscr{A}_{\mathrm{SIC}}(\phi)$ is the SIC defined in Eq. (100).

Notably, $F_{\mathrm{SIC}}(\phi)$ attains its maximum when $\phi = \pi/9$, which corresponds to the exceptional SIC with intermediate symmetry; by contrast, $F_{\mathrm{SIC}}(\phi)$ attains its minimum when $\phi = 0$, which corresponds to the most symmetric SIC. This conclusion seems quite unexpected, and a simple explanation is yet to be found. The estimation fidelities achieved by generic SICs interpolate between the two extreme cases. In conjunction with known results on the equivalent classes of SICs under unitary transformations [79,84,87], Fig. 8 provides strong evidence for the following conjecture.

Conjecture 1. *Two SICs in dimension* 3 *can achieve the same three-copy estimation fidelity iff they are unitarily equivalent.*

VIII. SUMMARY

We proposed a simple but powerful approach for decoding the characteristics of quantum measurements by virtue of a simple problem in quantum state estimation. Based on this approach we provided surprisingly simple characterizations of various typical and important quantum measurements, including rank-1 projective measurements, MUMs, and SICs. Notably, we do not need any assumption on the rank, purity, or the number of POVM elements, and we do not need bases to start with, which seems impossible with all previous approaches. Our work demonstrates that all these elementary quantum measurements are uniquely determined by their information-extraction capabilities. In other words, all these elementary quantum measurements can be defined in purely information theoretic terms, in sharp contrast with traditional algebraic definitions, which lack clear operational meanings. In this way, our work offers a fresh perspective for understanding and exploring quantum measurements from their information-extraction capabilities.

The two-copy estimation fidelity we introduced also offers a new perspective for understanding quantum incompatibility as a resource. In addition, this estimation fidelity can be used to construct a universal criterion for detecting incompatibility of two arbitrary POVMs. Moreover, it has an intimate connection with entropic uncertainty relations. Furthermore, we showed that the three-copy estimation fidelity can be used to distinguish inequivalent MUB and SICs, which cannot be distinguished by pairwise fidelities. Such operational figures of merit are quite rare in the literature and are expected to play an important role in understanding various discrete symmetric structures tied to the quantum state space. In the course of study, we derived a number of results on quantum measurements and (weighted complex projective) t-designs, which are of independent interest. Our work offers valuable insights not only on quantum measurements and quantum estimation theory, but also on

various related research areas, including geometry of quantum states, *t*-designs and random quantum states, quantum incompatibility, and foundational studies. The implications of these results deserve further explorations in the future.

APPENDIX A: PROOFS OF LEMMAS 1 AND 2

Proof of Lemma 1. Without loss of generality we can assume that no POVM element in $\mathscr{A}$ or $\mathscr{B}$ is equal to the zero operator. The inequality $\wp(\mathscr{A}) \leq \wp(\mathscr{B})$ can be proved as follows:

$$
\begin{aligned}
d\wp(\mathscr{A}) &= \sum_j \frac{\mathrm{tr}(A_j^2)}{\mathrm{tr}(A_j)} \\
&= \sum_j \frac{\sum_{k,l} \Lambda_{jk}\Lambda_{jl}\,\mathrm{tr}(B_k B_l)}{\mathrm{tr}(A_j)} \\
&\leq \sum_j \frac{\sum_{k,l} \Lambda_{jk}\Lambda_{jl}\sqrt{\mathrm{tr}(B_k^2)}\sqrt{\mathrm{tr}(B_l^2)}}{\mathrm{tr}(A_j)} \\
&= \sum_j \frac{\left[\sum_k \Lambda_{jk}\sqrt{\mathrm{tr}(B_k^2)}\right]^2}{\sum_k \Lambda_{jk}\,\mathrm{tr}(B_k)} \\
&\leq \sum_k \frac{\mathrm{tr}(B_k^2)}{\mathrm{tr}(B_k)} = d\wp(\mathscr{B}).
\end{aligned}
\tag{A1}
$$

Here the first inequality follows from the Cauchy-Schwarz inequality, and the second inequality follows from Lemma S1 of Ref. [50]. If $\mathscr{A}$ is equivalent to $\mathscr{B}$, then the opposite inequality $\wp(\mathscr{B}) \leq \wp(\mathscr{A})$ holds by the same token, so we have $\wp(\mathscr{A}) = \wp(\mathscr{B})$, which confirms the implication $1 \Rightarrow 2$.

If $\wp(\mathscr{A}) = \wp(\mathscr{B})$, then the two inequalities in Eq. (A1) are saturated. Note that $\mathrm{tr}(B_k B_l) \leq \sqrt{\mathrm{tr}(B_k^2)}\sqrt{\mathrm{tr}(B_l^2)}$, and the inequality is saturated iff B_k and B_l are proportional to each other. The saturation of the first inequality in Eq. (A1) then implies that $\Lambda_{jk}\Lambda_{jl} = 0$ whenever B_k and B_l are linearly independent, which confirms the implication $2 \Rightarrow 3$.

If statement 3 holds, then the product $\Lambda_{jk}\Lambda_{jl}$ can take on a nonzero value only if B_k and B_l are proportional to each other. In this case, $\mathscr{B}$ can be realized by data processing after performing $\mathscr{A}$; in other words, $\mathscr{B}$ is a coarse graining

of $\mathscr{A}$. Since $\mathscr{A}$ is a coarse graining of $\mathscr{B}$ by assumption, it follows that $\mathscr{A}$ is equivalent to $\mathscr{B}$, which confirms the implication $3 \Rightarrow 1$ and completes the proof of Lemma 1. ∎

Proof of Lemma 2. Suppose that $\mathscr{A} = \{A_j\}_j$ and $\mathscr{B} = \{B_k\}_k$ are two simple POVMs. Obviously, $\mathscr{A}$ and $\mathscr{B}$ are equivalent if they are identical up to relabeling.

Conversely, suppose that $\mathscr{A}$ and $\mathscr{B}$ are equivalent; then A_j can be expressed as $A_j = \sum_k \Lambda_{jk} B_k$, where Λ is a stochastic matrix. According to Lemma 1, each row of Λ has only one nonzero entry, given that the POVM elements in $\mathscr{B}$ are pairwise linearly independent, and so are the POVM elements in $\mathscr{A}$. It follows that A_j is proportional B_k whenever $\Lambda_{jk} > 0$. Now the simplicity of $\mathscr{A}$ further implies that each column of Λ has only one nonzero entry, which is necessarily equal to 1. Therefore, Λ is a permutation matrix, which means $\mathscr{A}$ and $\mathscr{B}$ are identical up to relabeling, confirming the first statement in Lemma 2.

To prove the second statement in Lemma 2, let $\mathscr{C} = \{C_j\}_j$ be an arbitrary POVM; then an equivalent simple POVM can be constructed by deleting POVM elements that are equal to the zero operator and combining POVM elements that are proportional to each other. According to the first statement in Lemma 2, such a simple POVM is unique up to relabeling. ∎

APPENDIX B: PROOFS OF LEMMAS 3–5 AND THEOREM 1

Proof of Lemma 3. Suppose that $\mathscr{A} = \{A_j\}_{j=1}^m$, where A_j are rank 1 by assumption. Then we have

$$
\sum_j A_j = 1, \quad \sum_j \mathrm{tr}(A_j) = d,
\tag{B1}
$$

$$
d = \sum_{j,k} \mathrm{tr}(A_j A_k) \geq \sum_{j,k} \mathrm{tr}(A_j^2) = \sum_j (\mathrm{tr}\,A_j)^2 \geq \frac{d^2}{m},
\tag{B2}
$$

which implies that $m \geq d$, so $\mathscr{A}$ has at least d POVM elements. Obviously, the lower bound is saturated if $\mathscr{A}$ is a rank-1 projective measurement.

Conversely, if $\mathscr{A}$ has d POVM elements, that is, $m = d$, then the two inequalities in Eq. (B2) are saturated, which implies that

$$
\mathrm{tr}(A_j A_k) = \delta_{jk}.
\tag{B3}
$$

Therefore, all the POVM elements A_j are mutually orthogonal rank-1 projectors, which means $\mathscr{A}$ is a rank-1 projective measurement, confirming the first statement in Lemma 3. In the above reasoning it is not necessary to assume that $\mathscr{A}$ is simple.

Next, we turn to the second statement in Lemma 3. Let us consider the span of POVM elements in $\mathscr{A}$

and its dimension, assuming that $\mathscr{A}$ is simple. By assumption, each POVM element of $\mathscr{A}$ has the form $A_j = w_j |\psi_j\rangle\langle\psi_j|$ with $0 < w_j \leq 1$; in addition, the corresponding set of kets $\{|\psi_j\rangle\}_j$ spans $\mathcal{H}$. So we can find d kets, say $|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_d\rangle$, that form a basis (not necessarily orthogonal) for $\mathcal{H}$. Then the corresponding set of projectors $\{|\psi_j\rangle\langle\psi_j|\}_{j=1}^d$ is necessarily linearly independent, which implies that

$$\dim(\mathrm{span}(\mathscr{A})) \geq \dim(\mathrm{span}(\{|\psi_j\rangle\langle\psi_j|\}_{j=1}^d)) = d. \quad \text{(B4)}$$

If $\mathscr{A}$ is a rank-1 projective measurement, then the lower bound is saturated.

Conversely, if the lower bound in Eq. (B4) is saturated, then each POVM element of $\mathscr{A}$ is a linear combination of $|\psi_j\rangle\langle\psi_j|$ for $j = 1, 2, \ldots, d$. Note that the rank of such a linear combination is equal to the number of nonzero coefficients. Since $\mathscr{A}$ is rank 1 by assumption, it follows that each POVM element of $\mathscr{A}$ is proportional to $|\psi_j\rangle\langle\psi_j|$ for some $j = 1, 2, \ldots, d$, which implies that $\mathscr{A}$ has d POVM elements given that $\mathscr{A}$ is simple. Therefore, $\mathscr{A}$ is a rank-1 projective measurement according to the first statement in Lemma 3 as proved above. ∎

Proof of Lemma 4. Let $\mathscr{A} = \{A_j\}_{j=1}^m$ and $\mathscr{B} = \{B_k\}_{k=1}^n$. If $\mathscr{B} \subseteq \mathscr{A}$ and the projectors in $\mathscr{B}$ are mutually orthogonal, then $\mathscr{A} \setminus \mathscr{B}$ is orthogonal to $\mathscr{B}$ given that

$$\sum_{j=1}^m A_j = 1, \quad A_j \geq 0 \quad \text{for all } j = 1, 2, \ldots, m, \quad \text{(B5)}$$

so $\mathscr{A}$ and $\mathscr{B}$ commute.

Conversely, suppose that $\mathscr{A}$ and $\mathscr{B}$ commute. Then each $A_j \in \mathscr{A}$ commutes with each $B_k \in \mathscr{B}$, which means A_j is either orthogonal to B_k or proportional to B_k. Since $\mathscr{A}$ is a simple POVM, it follows that, for any given projector $B_k \in \mathscr{B}$, there exists a unique POVM element in $\mathscr{A}$ that is proportional to B_k, and all other POVM elements are orthogonal to B_k. By a suitable relabeling if necessary, we can assume that

$$A_j \propto B_j \quad \text{for all } j = 1, 2, \ldots, n. \quad \text{(B6)}$$

Then the above analysis means

$$B_j B_k = B_j \delta_{jk} \quad \text{for all } j, k = 1, 2, \ldots, n, \quad \text{(B7)}$$

$$A_j A_k = A_j^2 \delta_{jk} \quad \text{for all } j = 1, 2, \ldots, m; \ k = 1, 2, \ldots, n. \quad \text{(B8)}$$

In particular, the rank-1 projectors in $\mathscr{B}$ are mutually orthogonal, and so are the POVM elements $A_1, A_2, \ldots, A_n$. Now Eqs. (B5)–(B8) together further imply that the POVM elements $A_1, A_2, \ldots, A_n$ are mutually orthogonal rank-1

projectors and $A_j = B_j$ for $j = 1, 2, \ldots, n$, which in turn imply that $\mathscr{B} \subseteq \mathscr{A}$. ∎

Proof of Lemma 5. Lemma 5 is a simple corollary of Lemma 4 and can also be proved directly as follows. Suppose that $\mathscr{A} = \{A_j\}_j$ and $\mathscr{B} = \{B_k\}_k$ are two simple rank-1 POVMs. Then $\mathscr{A}$ and $\mathscr{B}$ commute with each other if they are identical projective measurements up to relabeling.

Conversely, if $\mathscr{A}$ and $\mathscr{B}$ commute, then $A_j B_k = B_k A_j$ for any pair j, k. Note that two rank-1 positive operators commute with each other iff they are orthogonal or proportional to each other. In conjunction with the assumption that $\mathscr{A}$ and $\mathscr{B}$ are simple rank-1 POVMs, we conclude that each POVM element in $\mathscr{A}$ ($\mathscr{B}$) is proportional to a unique POVM element in $\mathscr{B}$ ($\mathscr{A}$) and is orthogonal to all other POVM elements in $\mathscr{B}$ ($\mathscr{A}$). In this way, POVM elements in $\mathscr{A}$ have one-to-one correspondence with POVM elements in $\mathscr{B}$; in particular, $\mathscr{A}$ and $\mathscr{B}$ have the same number of POVM elements. By a suitable relabeling if necessary, we can assume that A_j is proportional to B_j and is orthogonal to B_k with $k \neq j$. So all POVM elements in $\mathscr{A}$ are mutually orthogonal, and so are POVM elements in $\mathscr{B}$, which means both $\mathscr{A}$ and $\mathscr{B}$ are rank-1 projective measurements. Moreover, $\mathscr{A}$ and $\mathscr{B}$ are identical up to relabeling given the above correspondence. ∎

Proof of Theorem 1. Let $\{\mathscr{A}_r\}_{r=1}^g$ be an arbitrary set of g MU simple rank-1 POVMs on $\mathcal{H}$, where $\mathscr{A}_r = \{A_{rj}\}_j$. Let $A'_{rj} = A_{rj} - (\mathrm{tr}\, A_{rj}/d)$ and $\mathscr{A}'_r = \{A'_{rj}\}_j$. Then A'_{rj} are traceless and

$$\dim(\mathrm{span}(\mathscr{A}_r)) = \dim(\mathrm{span}(\mathscr{A}'_r)) + 1. \quad \text{(B9)}$$

By assumption, $\mathscr{A}_r$ and $\mathscr{A}_s$ with $r \neq s$ are MU, which implies that

$$\mathrm{tr}(A'_{rj} A'_{sk}) = 0 \quad \text{for all } j, k, \quad \text{(B10)}$$

so A'_{rj} and A'_{sk} are orthogonal with respect to the Hilbert-Schmidt inner product. As a consequence,

$$\begin{aligned} d^2 &\geq \dim\left(\mathrm{span}\left(\bigcup_{r=1}^g \mathscr{A}_r\right)\right) \\ &= \dim\left(\mathrm{span}\left(\bigcup_{r=1}^g \mathscr{A}'_r\right)\right) + 1 \\ &= \sum_{r=1}^g [\dim(\mathrm{span}(\mathscr{A}_r)) - 1] + 1 \\ &= \sum_{r=1}^g \dim(\mathrm{span}(\mathscr{A}_r)) - g + 1 \\ &\geq dg - g + 1, \end{aligned} \quad \text{(B11)}$$

where the second inequality follows from Lemma 3 and is saturated iff each $\mathscr{A}_r$ is a rank-1 projective measurement.

Equation (B11) implies that $g \leq d + 1$. If the upper bound is saturated, then the two inequalities in Eq. (B11) are saturated, which means $\dim(\mathrm{span}(\mathscr{A}_r)) = d$ for each $\mathscr{A}_r$. So all the POVMs $\mathscr{A}_r$ are rank-1 projective measurements by Lemma 3, which implies that $\{\mathscr{A}_r\}_{r=1}^g$ is a CMUMs. ∎

APPENDIX C: PROOFS OF LEMMAS 6–9

1. Main proofs

Proof of Lemma 6. By assumption, $\mathcal{S}$ can be expressed as $\mathcal{S} = \{|\psi_j\rangle, w_j\}_{j=1}^m$, where

$$w_j > 0, \quad \sum_j w_j = d, \quad \sum_j w_j |\psi_j\rangle\langle\psi_j| = 1. \quad \text{(C1)}$$

The lower bound in Eq. (23) can be proved as follows:

$$\Phi_{1/2}(\mathcal{S}) = \sum_{j,k} w_j w_k |\langle\psi_j|\psi_k\rangle| \geq \sum_{j,k} w_j w_k |\langle\psi_j|\psi_k\rangle|^2$$

$$= \mathrm{tr}\left(\sum_j w_j |\psi_j\rangle\langle\psi_j|\right)^2 = d. \quad \text{(C2)}$$

If $\mathcal{S}$ is an orthonormal basis (with uniform weights), which means $m = d$, $w_j = 1$, and $\langle\psi_j|\psi_k\rangle = \delta_{jk}$, then it is straightforward to verify that the lower bound is saturated.

Conversely, if the lower bound in Eq. (C2) is saturated and $\mathcal{S}$ is simple, then $|\langle\psi_j|\psi_k\rangle|$ can take on only two distinct values, namely, 0 and 1, so we have

$$\langle\psi_j|\psi_k\rangle = \delta_{jk} \quad \text{for all } j, k = 1, 2, \ldots m. \quad \text{(C3)}$$

This equation can hold only if $m \leq d$. On the other hand, Eq. (C1) implies that $m \geq d$ [cf. Lemma 3 and Eq. (7) in the main text]. So $m = d$ and $\{|\psi_j\rangle\}_{j=1}^d$ forms an orthonormal basis. Now Eq. (C1) further implies that $w_j = 1$ for all j. Therefore, $\mathcal{S}$ is an orthonormal basis (with uniform weights).

To prove the upper bound in Eq. (23), define $p_{jk} := w_j w_k / d^2$ and $x_{jk} := |\langle\psi_j|\psi_k\rangle|^2$. Then Eq. (C1) implies that

$$\sum_{j,k} p_{jk} = 1, \quad \sum_{j,k} p_{jk} x_{jk} = \frac{1}{d}. \quad \text{(C4)}$$

In addition, from Eq. (10) we can deduce that

$$\sum_{j,k} p_{jk} x_{jk}^2 = \frac{1}{d^2} \sum_{j,k} w_j w_k |\langle\psi_j|\psi_k\rangle|^4$$

$$= \frac{1}{d^2} \mathrm{tr}\left[\sum_j w_j (|\psi_j\rangle\langle\psi_j|)^{\otimes 2}\right]^2$$

$$\geq \frac{2}{d(d+1)}, \quad \text{(C5)}$$

and the lower bound is saturated iff $\{|\psi_j\rangle, w_j\}_{j=1}^m$ forms a 2-design. By virtue of Lemmas 23 and 25 in Appendix C 2, we can now deduce that

$$\Phi_{1/2}(\mathcal{S}) = \sum_{j,k} w_j w_k |\langle\psi_j|\psi_k\rangle| = d^2 \sum_{j,k} p_{jk} \sqrt{x_{jk}}$$

$$\leq d^2 \zeta\left(\frac{1}{d}, \frac{2}{d(d+1)}\right) = 1 + (d-1)\sqrt{d+1}, \quad \text{(C6)}$$

which confirms the upper bound in Eq. (23). Here the function ζ is defined in Eq. (C26) in Appendix C 2. If $\mathcal{S}$ is a SIC (with uniform weights), which means $m = d^2$, $w_j = 1/d$, and $|\langle\psi_j|\psi_k\rangle|^2 = (d\delta_{jk} + 1)/(d+1)$, then it is straightforward to verify that the upper bound is saturated [cf. Eq. (20)].

Conversely, if the upper bound in Eq. (23) is saturated, then the inequality in Eq. (C6) is saturated. According to Lemmas 23 and 25, the lower bound in Eq. (C5) must saturate, so $\{|\psi_j\rangle, w_j\}_{j=1}^m$ forms a 2-design; meanwhile, we have

$$\sum_{j,k:|\langle\psi_j|\psi_k\rangle|^2 = 1/(d+1)} w_j w_k = d^2 - 1, \quad \text{(C7)}$$

$$\sum_{j,k:|\langle\psi_j|\psi_k\rangle|^2 = 1} w_j w_k = 1, \quad \text{(C8)}$$

given that $w_j w_k = d^2 p_{jk}$, so $|\langle\psi_j|\psi_k\rangle|^2$ can take on only two distinct values, namely, 1 and $1/(d+1)$.

If, in addition, $\mathcal{S}$ is simple, then $|\langle\psi_j|\psi_k\rangle|^2 < 1$ whenever $j \neq k$, so Eqs. (C7) and (C8) imply that

$$|\langle\psi_j|\psi_k\rangle|^2 = \frac{d\delta_{jk} + 1}{d + 1} \quad \text{for all } j, k = 1, 2, \ldots m. \quad \text{(C9)}$$

This equation can hold only if $m \leq d^2$. On the other hand, the opposite inequality $m \geq d^2$ has to hold given that $\{|\psi_j\rangle, w_j\}_{j=1}^m$ forms a 2-design [cf. Eq. (7) in the main text]. So $m = d^2$ and the set $\{|\psi_j\rangle\}_{j=1}^{d^2}$ forms a SIC. Furthermore,

from Eq. (C8) we can deduce that

$$\sum_j w_j^2 = \sum_{j,k:|\langle \psi_j | \psi_k \rangle|^2 = 1} w_j w_k = 1. \qquad (C10)$$

Equations (C1) and (C10) together imply that $w_j = 1/d$ for all j. Therefore, $\mathcal{S}$ is a SIC (with uniform weights), which completes the proof of Lemma 6. ∎

Proof of Lemma 7. By assumption, the weighted set $\mathcal{S}$ has the form $\mathcal{S} = \{|\psi_j\rangle, w_j\}_{j=1}^m$ and satisfies the conditions

$$0 \le w_j \le 1, \quad \sum_j w_j = d, \quad \sum_{j,k} w_j w_k |\langle \psi_j | \psi_k \rangle|^2 = d. \qquad (C11)$$

Let $h = \sum_j w_j^2$; then the above equation implies that

$$\frac{d^2}{m} \le h \le d, \qquad (C12)$$

and the lower bound is saturated iff $w_j = d/m$ for all j. Therefore,

$$\begin{aligned}
\Phi_{1/2}(\mathcal{S}) &= \sum_{j,k} w_j w_k |\langle \psi_j | \psi_k \rangle| \\
&= \sum_j w_j^2 + \sum_{j \ne k} w_j w_k |\langle \psi_j | \psi_k \rangle| \\
&\le \sum_j w_j^2 + \sqrt{\sum_{j \ne k} w_j w_k} \sqrt{\sum_{j \ne k} w_j w_k |\langle \psi_j | \psi_k \rangle|^2} \\
&= h + \sqrt{d^2 - h} \sqrt{d - h} \\
&\le \frac{d^2}{m} + \frac{d}{m} \sqrt{d(m-1)(m-d)}, \qquad (C13)
\end{aligned}$$

which confirms the upper bound in Eq. (25). Here the first inequality follows from the Cauchy inequality. The second inequality follows from Eq. (C12) and the fact that the function $h + \sqrt{d^2 - h} \sqrt{d - h}$ is strictly decreasing in h for $0 \le h \le d$ and $d \ge 2$; it is saturated iff $h = d^2/m$.

If $\mathcal{S}$ is composed of m equiangular states (with uniform weights), then Eq. (24) in the main text holds and we have $w_j = d/m$ for $j = 1, 2, \dots, m$. So both inequalities in Eq. (C13) are saturated, which means the upper bound in Eq. (25) is saturated.

Conversely, if the upper bound in Eq. (25) is saturated, then both inequalities in Eq. (C13) are saturated. The saturation of the second inequality implies that $h = d^2/m$, which in turn implies that $w_j = d/m$ for $j = 1, 2, \dots, m$. Then the saturation of the first inequality implies Eq. (24) given Eq. (C11). Therefore, $\mathcal{S}$ is composed of m equiangular states (with uniform weights). Note that any equiangular set in $\mathcal{H}$ can contain at most d^2 states [9,72,74], so

Eq. (25) cannot be saturated when $m > d^2$. This observation completes the proof of Lemma 7. ∎

Proof of Lemma 8. By assumption, $\mathcal{S}$ and $\mathcal{T}$ can be expressed as $\mathcal{S} = \{|\psi_j\rangle, w_j\}_{j=1}^m$ and $\mathcal{T} = \{|\varphi_k\rangle, w_k'\}_{k=1}^n$, which satisfy

$$\begin{aligned}
& w_j, w_k' > 0, \quad \sum_j w_j = \sum_k w_k' = d, \\
& \sum_j w_j |\psi_j\rangle\langle\psi_j| = \sum_k w_k' |\varphi_k\rangle\langle\varphi_k| = 1.
\end{aligned} \qquad (C14)$$

The upper bound in Eq. (26) can be proved as follows:

$$\begin{aligned}
\Phi_{1/2}(\mathcal{S}, \mathcal{T}) &= \sum_{j,k} w_j w_k' |\langle \psi_j | \varphi_k \rangle| \\
&\le \sqrt{\left(\sum_{j,k} w_j w_k'\right)\left(\sum_{j,k} w_j w_k' |\langle \psi_j | \varphi_k \rangle|^2\right)} \\
&= \sqrt{d^2 \times d} = d^{3/2}. \qquad (C15)
\end{aligned}$$

Here the inequality follows from the Cauchy inequality and is saturated iff $|\langle \psi_j | \varphi_k \rangle|^2 = 1/d$ for each pair j, k. Therefore, the upper bound in Eq. (26) is saturated iff $\mathcal{S}$ and $\mathcal{T}$ are MU.

The lower bound in Eq. (26) can be proved following a similar approach used to prove the lower bound in Eq. (23):

$$\begin{aligned}
\Phi_{1/2}(\mathcal{S}, \mathcal{T}) &= \sum_{j,k} w_j w_k' |\langle \psi_j | \varphi_k \rangle| \ge \sum_{j,k} w_j w_k' |\langle \psi_j | \varphi_k \rangle|^2 \\
&= \mathrm{tr}\left[\left(\sum_j w_j |\psi_j\rangle\langle\psi_j|\right)\left(\sum_k w_k' |\varphi_k\rangle\langle\varphi_k|\right)\right] \\
&= d. \qquad (C16)
\end{aligned}$$

If $\mathcal{S}$ and $\mathcal{T}$ are identical orthonormal bases (with uniform weights) up to relabeling, then $n = m = d$, $w_j = w_k' = 1$, and $|\langle \psi_j | \varphi_k \rangle| = \delta_{jk}$ after a suitable relabeling if necessary, so the lower bound is saturated.

Conversely, if the lower bound in Eq. (C16) is saturated, then $|\langle \psi_j | \varphi_k \rangle|$ can take on only two distinct values, namely, 0 and 1. If, in addition, $\mathcal{S}$ and $\mathcal{T}$ are simple 1-designs, which satisfy the normalization condition in Eq. (C14), then, for each j, there exists a unique k such that $|\langle \psi_j | \varphi_k \rangle| = 1$; similarly, for each k, there exists a unique j such that $|\langle \psi_j | \varphi_k \rangle| = 1$. Therefore, $n = m = d$ and

$$\langle \psi_j | \psi_k \rangle = \langle \varphi_j | \varphi_k \rangle = \delta_{jk}; \qquad (C17)$$

in addition, we have $|\langle \psi_j | \varphi_k \rangle| = \delta_{jk}$ after a suitable relabeling if necessary. Now Eq. (C14) further implies that $w_j = w_j' = 1$ for $j = 1, 2, \dots, d$. Therefore, $\mathcal{S}$ and $\mathcal{T}$ are

identical orthonormal bases (with uniform weights) up to relabeling. Note that we identify weighted sets that differ only by overall phase factors, as mentioned in the main text. ∎

Proof of Lemma 9. To prove the upper bound in Eq. (27), we can apply a similar reasoning used to prove the upper bound in Eq. (23). Without loss of generality, we can assume that $\mathcal{S}$ is a 1-design, while $\mathcal{T}$ is a 2-design. Then $\mathcal{S}$ and $\mathcal{T}$ can be expressed as $\mathcal{S} = \{|\psi_j\rangle, w_j\}_{j=1}^m$ and $\mathcal{T} = \{|\varphi_k\rangle, w_k'\}_{k=1}^n$, which satisfy

$$w_j, w_k' > 0, \quad \sum_j w_j = \sum_k w_k' = d,$$

$$\sum_j w_j |\psi_j\rangle\langle\psi_j| = 1, \quad \sum_k w_k'(|\varphi_k\rangle\langle\varphi_k|)^{\otimes 2} = \frac{2P_2}{d+1}, \tag{C18}$$

where P_2 is the projector onto the symmetric subspace in $\mathcal{H}^{\otimes 2}$.

Let $p_{jk} = w_j w_k'/d^2$ and $x_{jk} = |\langle\psi_j|\varphi_k\rangle|^2$. Then the conditions in Eq. (C18) imply that

$$\sum_{j,k} p_{jk} = 1, \quad \sum_{j,k} p_{jk} x_{jk} = \frac{1}{d}; \tag{C19}$$

in addition,

$$\sum_{j,k} p_{jk} x_{jk}^2$$
$$= \frac{1}{d^2} \sum_{j,k} w_j w_k' |\langle\psi_j|\varphi_k\rangle|^4$$
$$= \frac{1}{d^2} \mathrm{tr}\left\{ \left[\sum_j w_j(|\psi_j\rangle\langle\psi_j|)^{\otimes 2}\right]\left[\sum_k w_k'(|\varphi_k\rangle\langle\varphi_k|)^{\otimes 2}\right]\right\}$$
$$= \frac{2}{d^2(d+1)} \mathrm{tr}\left[\sum_j w_j P_2(|\psi_j\rangle\langle\psi_j|)^{\otimes 2}\right]$$
$$= \frac{2}{d^2(d+1)} \sum_j w_j$$
$$= \frac{2}{d(d+1)}. \tag{C20}$$

According to Lemmas 23 and 25 in Appendix C 2, Eqs. (C19) and (C20) imply that

$$\Phi_{1/2}(\mathcal{S},\mathcal{T}) = \sum_{j,k} w_j w_k' |\langle\psi_j|\varphi_k\rangle| = d^2 \sum_{j,k} p_{jk}\sqrt{x_{jk}}$$
$$\leq d^2 \zeta\left(\frac{1}{d}, \frac{2}{d(d+1)}\right) = 1 + (d-1)\sqrt{d+1}, \tag{C21}$$

which confirms the upper bound in Eq. (27). If $\mathcal{S}$ and $\mathcal{T}$ are identical SICs (with uniform weights) up to relabeling, which means $n = m = d^2$, $w_k' = w_j = 1/d$, and $|\langle\psi_j|\varphi_k\rangle|^2 = (d\delta_{jk} + 1)/(d + 1)$ after a suitable relabeling if necessary, then it is straightforward to verify that the upper bound is saturated [cf. Eq. (20)].

Conversely, if the upper bound in Eq. (27) is saturated, then the inequality in Eq. (C21) is saturated. According to Lemmas 23 and 25, we have

$$\sum_{j,k:|\langle\psi_j|\varphi_k\rangle|^2 = 1/(d+1)} w_j w_k' = d^2 - 1, \tag{C22}$$

$$\sum_{j,k:|\langle\psi_j|\varphi_k\rangle|^2 = 1} w_j w_k' = 1, \tag{C23}$$

so $|\langle\psi_j|\varphi_k\rangle|^2$ can take on only two distinct values, namely, 1 and $1/(d + 1)$. If, in addition, $\mathcal{S}$ and $\mathcal{T}$ are simple 1-designs, which satisfy Eq. (C18), then, for each $|\psi_j\rangle$ in $\mathcal{S}$, there exists a unique $|\varphi_k\rangle$ in $\mathcal{T}$ such that $|\langle\psi_j|\varphi_k\rangle|^2 = 1$, and vice versa. It follows that $n = m$ and

$$|\langle\varphi_j|\varphi_k\rangle|^2 = |\langle\psi_j|\psi_k\rangle|^2 = |\langle\psi_j|\varphi_k\rangle|^2 = \frac{d\delta_{jk} + 1}{d + 1} \tag{C24}$$

for $j, k = 1, 2, \ldots, m$ after a suitable relabeling if necessary. This equation can hold only if $m \leq d^2$.

Equations (C18) and (C24) together imply that

$$d = \Phi_1(\mathcal{S}) = \frac{d^2}{d+1} + \frac{d}{d+1}\sum_{j=1}^m w_j^2$$
$$\geq \frac{d^2}{d+1} + \frac{d^3}{m(d+1)}, \tag{C25}$$

which in turn implies that $\sum_{j=1}^m w_j^2 = 1$ and $m \geq d^2$. So we have $m = d^2$ given the opposite inequality $m \leq d^2$ derived above. In conjunction with the normalization conditions in Eq. (C18), we can deduce that $w_j = 1/d$ for $j = 1, 2, \ldots, d^2$. A similar reasoning yields $w_k' = 1/d$ for $k = 1, 2, \ldots, d^2$. Therefore, $\mathcal{S}$ and $\mathcal{T}$ are identical SICs (with uniform weights) up to relabeling, which completes the proof of Lemma 9. ∎

2. Auxiliary results on the 1/2-moment

Here we derive several results on the 1/2-moment of a bounded random variable given the first and second

moments. For $0 < b \leq a < 1$, define

$$
\zeta(a,b) := \frac{b - a^2 + (1-a)\sqrt{(1-a)(a-b)}}{1 - 2a + b}
$$
$$
= \frac{2a - a^2 - b + (1+a)\sqrt{(1-a)(a-b)}}{(\sqrt{1-a} + \sqrt{a-b})^2}.
\tag{C26}
$$

In two special cases, Eq. (C26) reduces to

$$
\zeta(a,a) = a, \quad \zeta(a,a^2) = \sqrt{a}.
\tag{C27}
$$

When $a = 1 - (1-b)r$ with $0 < r \leq 1$, Eq. (C26) yields

$$
\zeta(1 - (1-b)r, b) = 1 - \frac{r(\sqrt{r(1-r)} - r)}{1 - 2r}(1-b).
\tag{C28}
$$

Lemma 23. *Suppose that $0 < b \leq a < 1$. Then $\zeta(a,b)$ is strictly increasing in a and strictly decreasing in b. In addition, $\zeta(a,b)$ is jointly concave in a and b.*

Proof. First we assume that $0 < b < a < 1$. According to the equations

$$
\frac{\partial \zeta(a,b)}{\partial a} = \frac{(1-a)\left[(1 + 4a - 5b)\sqrt{1-a} + 3(1-b)\sqrt{a-b}\right]}{2\sqrt{(1-a)(a-b)}\left(\sqrt{1-a} + \sqrt{a-b}\right)^3} > 0,
\tag{C29}
$$

$$
\frac{\partial \zeta(a,b)}{\partial b} = -\frac{(1-a)^{3/2}\left(a - b + \sqrt{(1-a)(a-b)}\right)}{2(a-b)\left(\sqrt{1-a} + \sqrt{a-b}\right)^3} < 0,
\tag{C30}
$$

$\zeta(a,b)$ is strictly increasing in a and strictly decreasing in b. According to the equations

$$
\frac{\partial^2 \zeta(a,b)}{\partial a^2} = -\frac{(1-b)^2\left[(1 + 2a - 3b) + 4\sqrt{(1-a)(a-b)}\right]}{4(1-a)^{1/2}(a-b)^{3/2}\left(\sqrt{1-a} + \sqrt{a-b}\right)^4} < 0,
\tag{C31}
$$

$$
\frac{\partial^2 \zeta(a,b)}{\partial b^2} = -\frac{(1-a)^{3/2}\left[(1 + 2a - 3b) + 4\sqrt{(1-a)(a-b)}\right]}{4(a-b)^{3/2}\left(\sqrt{1-a} + \sqrt{a-b}\right)^4} < 0,
\tag{C32}
$$

$$
\frac{\partial^2 \zeta(a,b)}{\partial a^2}\frac{\partial^2 \zeta(a,b)}{\partial b^2} - \left(\frac{\partial^2 \zeta(a,b)}{\partial a \partial b}\right)^2 = 0,
\tag{C33}
$$

$\zeta(a,b)$ is jointly concave in a and b. Incidentally, the equality in the last equation is tied to Eq. (C28).

In the general situation $0 < b \leq a < 1$, the conclusions in Lemma 23 follow from the above analysis and the fact that $\zeta(a,b)$ is continuous in the limit $b \to a$,

$$
\lim_{b \to a} \zeta(a,b) = \zeta(a,a) = a.
\tag{C34}
$$

This completes the proof. ∎

The significance of the function $\zeta(a,b)$ is manifested in the following lemma.

Lemma 24. *Suppose that X is a random variable that satisfies the conditions $0 \leq X \leq 1$, $\mathbb{E}[X] = a$, and $\mathbb{E}[X^2] = b$ with $0 < b \leq a < 1$; then*

$$
a\sqrt{\frac{a}{b}} \leq \mathbb{E}[\sqrt{X}] \leq \zeta(a,b).
\tag{C35}
$$

The lower bound is saturated iff

$$
P(X = 0) = 1 - \frac{a^2}{b}, \quad P\left(X = \frac{b}{a}\right) = \frac{a^2}{b},
\tag{C36}
$$

while the upper bound is saturated iff

$$P\left(X = \frac{a-b}{1-a}\right) = \frac{(1-a)^2}{1-2a+b}, \quad P(X = 1) = \frac{b-a^2}{1-2a+b}.$$
(C37)

The assumptions in Lemma 24 imply the inequalities $0 < a^2 \le b \le a < 1$. Equation (C36) means X can only take on the values of 0 and b/a, while Eq. (C37) means X can only take on the values of 1 and $(a-b)/(1-a)$. Lemma 24 is a corollary of Lemma 25 below.

Lemma 25. *Suppose that a and b are positive constants that satisfy $0 < a^2 \le b \le a < 1$. Suppose that $x_1, x_2, \ldots, x_m$ and $p_1, p_2, \ldots, p_m$ are nonnegative numbers that satisfy*

$$0 \le x_j \le 1, \quad 0 \le p_j \le 1, \quad \text{for all } j,$$
$$\sum_j p_j = 1, \quad \sum_j p_j x_j = a, \quad \sum_j p_j x_j^2 = b; \quad \text{(C38)}$$

then

$$a\sqrt{\frac{a}{b}} \le \sum_j p_j \sqrt{x_j} \le \zeta(a,b).$$
(C39)

The lower bound in Eq. (C39) is saturated iff

$$\sum_{j \mid x_j=0} p_j = 1 - \frac{a^2}{b}, \quad \sum_{j \mid x_j=b/a} p_j = \frac{a^2}{b}, \quad \text{(C40)}$$

while the upper bound is saturated iff

$$\sum_{j \mid x_j=(a-b)/(1-a)} p_j = \frac{(1-a)^2}{1-2a+b}, \quad \sum_{j \mid x_j=1} p_j = \frac{b-a^2}{1-2a+b}.$$
(C41)

Proof. When $m = 2$, Lemma 25 follows from Lemma 26 below. When $b = a^2$, we have

$$\zeta(a,b) = \sqrt{a}, \quad \sum_{j \mid x_j=a} p_j = 1, \quad \sum_{j \mid x_j \ne a} p_j = 0, \quad \text{(C42)}$$

so Lemma 25 also holds.

It remains to consider the case with $m > 2$ and $b > a^2$, which means not all x_j with $p_j > 0$ are equal to each other given the constraints in Eq. (C38). Suppose that the minimum of $\sum_j p_j \sqrt{x_j}$ is attained when $p_j = p_j^*$ and $x_j = x_j^*$.

Without loss of generality, we can assume that

$$p_j^* > 0 \quad \text{for all } j \le l, \quad p_j^* = 0 \quad \text{for all } j \ge l+1,$$
$$x_j^* < x_k^* \quad \text{for all } 1 \le j < k \le l,$$
(C43)

where $2 \le l \le m$. Then we have

$$p_j\sqrt{x_j} + p_k\sqrt{x_k} \ge p_j^*\sqrt{x_j^*} + p_k^*\sqrt{x_k^*} \quad \text{for all } 1 \le j < k \le l,$$
(C44)

as long as

$$p_j + p_k = p_j^* + p_k^*, \quad p_j x_j + p_k x_k = p_j^* x_j^* + p_k^* x_k^*,$$
$$p_j x_j^2 + p_k x_k^2 = p_j^* x_j^{*2} + p_k^* x_k^{*2}.$$
(C45)

By virtue of Lemma 26 below applied to the set of parameters $x_j, x_k, p_j/(p_j + p_k), p_k/(p_j + p_k)$, we can now deduce that $x_j^* = 0$, which in turn implies that $l = 2$ given the assumptions in Eq. (C43). According to Lemma 26 again, $\sum_j p_j \sqrt{x_j}$ is bounded from below by $a\sqrt{a/b}$, which confirms the lower bound in Eq. (C39), and the bound is saturated iff Eq. (C40) holds. The upper bound in Eq. (C39) and the saturation condition can be established by a similar reasoning. ∎

Lemma 26. *Suppose that a and b are positive constants that satisfy $0 < a^2 \le b \le a < 1$. Suppose that p_1, p_2, x_1, x_2 are nonnegative numbers that satisfy*

$$0 \le x_1 \le x_2 \le 1, \quad 0 \le p_1, p_2 \le 1,$$
$$p_1 + p_2 = 1, \quad p_1 x_1 + p_2 x_2 = a, \quad p_1 x_1^2 + p_2 x_2^2 = b;$$
(C46)

then

$$a\sqrt{\frac{a}{b}} \le p_1\sqrt{x_1} + p_2\sqrt{x_2} \le \zeta(a,b).$$
(C47)

If $b = a^2$, then $p_1\sqrt{x_1} + p_2\sqrt{x_2} = \sqrt{a} = \zeta(a,b)$ and $x_j = a$ whenever $p_j \ne 0$ for $j = 1, 2$. If $b > a^2$, then the lower bound in Eq. (C47) is saturated iff

$$x_1 = 0, \quad p_1 = 1 - \frac{a^2}{b}, \quad x_2 = \frac{b}{a}, \quad p_2 = \frac{a^2}{b}, \quad \text{(C48)}$$

while the upper bound is saturated iff

$$x_1 = \frac{a-b}{1-a}, \quad p_1 = \frac{(1-a)^2}{1-2a+b},$$
$$x_2 = 1, \quad p_2 = \frac{b-a^2}{1-2a+b}.$$
(C49)

Proof. If $b = a^2$, then $\zeta(a, b) = \sqrt{a}$. In addition, Eq. (C46) implies that

$$p_1 p_2 (x_1 - x_2)^2 = 0, \tag{C50}$$

which means $p_1 p_2 = 0$ or $x_1 = x_2$. So $x_j = a$ whenever $p_j \neq 0$, and we have $p_1 \sqrt{x_1} + p_2 \sqrt{x_2} = \sqrt{a} = \zeta(a, b)$, in which case Eq. (C47) holds automatically.

If $b > a^2$, then the assumptions in Lemma 26 imply that $0 < p_1, p_2 < 1$ and $0 \leq x_1 < a < x_2 \leq 1$. In addition, x_2, p_1, p_2 are determined by x_1 as

$$x_2 = \frac{b - ax_1}{a - x_1}, \quad p_1 = \frac{b - a^2}{x_1^2 - 2ax_1 + b},$$

$$p_2 = \frac{(a - x_1)^2}{x_1^2 - 2ax_1 + b}. \tag{C51}$$

Note that x_2 increases monotonically with x_1. In addition, the assumption that $b > a^2$ implies that

$$x_1^2 - 2ax_1 + b > 0, \tag{C52}$$

so the requirement $0 < p_1, p_2 < 1$ is automatically guaranteed given that $0 \leq x_1 < a$. Together with the requirement $0 \leq x_1 < x_2 \leq 1$, Eq. (C51) also implies that

$$0 \leq x_1 \leq \frac{a - b}{1 - a} < a < \frac{b}{a} \leq x_2 \leq 1. \tag{C53}$$

By virtue of Eq. (C51) we can further deduce that

$$p_1 \sqrt{x_1} + p_2 \sqrt{x_2} = h(x_1, a, b), \tag{C54}$$

where

$$h(x_1, a, b) := \frac{(b - a^2)\sqrt{x_1} + (a - x_1)\sqrt{(a - x_1)(b - ax_1)}}{x_1^2 - 2ax_1 + b}, \tag{C55}$$

which is continuous in x_1 for $0 \leq x_1 \leq (a - b)/(1 - a)$ given the assumption that $0 < a^2 < b \leq a < 1$ together with Eqs. (C52) and (C53).

When $0 < x_1 \leq (a - b)/(1 - a)$, the derivative of $h(x_1, a, b)$ over x_1 reads

$$\frac{\partial h(x_1, a, b)}{\partial x_1} = \frac{(b - a^2)(y_2 \sqrt{x_2} - y_1 \sqrt{x_1})}{2\sqrt{x_1 x_2}(x_1^2 - 2ax_1 + b)^2}$$

$$= \frac{(b - a^2)(x_1^2 - 2ax_1 + b)}{2(a - x_1)\sqrt{x_1 x_2}(y_2 \sqrt{x_2} + y_1 \sqrt{x_1})}$$

$$> 0, \tag{C56}$$

where x_2 is given in Eq. (C51) and

$$y_1 = 3b - 2ax_1 - x_1^2, \quad y_2 = b + 2ax_1 - 3x_1^2. \tag{C57}$$

The second equality in Eq. (C56) follows from the facts that $y_1, y_2 > 0$ and

$$\left(y_2 \sqrt{x_2} - y_1 \sqrt{x_1}\right)\left(y_2 \sqrt{x_2} + y_1 \sqrt{x_1}\right)$$

$$= (y_2^2 x_2 - y_1^2 x_1) = \frac{(x_1^2 - 2ax_1 + b)^3}{a - x_1}. \tag{C58}$$

Equation (C56) implies that $h(x_1, a, b)$ is strictly monotonically increasing in x_1 for $0 \leq x_1 \leq (a - b)/(1 - a)$ given that $h(x_1, a, b)$ is continuous in x_1 in this range. In conjunction with Eq. (C53) we can now deduce that

$$a\sqrt{\frac{a}{b}} = h(0, a, b) \leq p_1 \sqrt{x_1} + p_2 \sqrt{x_2}$$

$$\leq h\left(\frac{a - b}{1 - a}, a, b\right) = \zeta(a, b), \tag{C59}$$

which confirms Eq. (C47).

If Eq. (C48) holds, then it is easy to verify that the lower bound in Eq. (C47) [identical to the lower bound in Eq. (C59)] is saturated. Conversely, if the lower bound in Eq. (C47) is saturated, then $x_1 = 0$ given that $h(x_1, a, b)$ is strictly increasing in x_1 for $0 \leq x_1 \leq (a - b)/(1 - a)$, so Eq. (C48) holds according to Eq. (C51). By a similar reasoning, the upper bound in Eq. (C47) is saturated iff Eq. (C49) holds. ∎

APPENDIX D: PROOF OF LEMMA 14

Equation (38) in the lemma follows from Eq. (37) and the equality

$$\left\| \mathcal{Q}\left(U^{\otimes N} A U^{\dagger \otimes N}\right) \right\| = \|\mathcal{Q}(A)\|, \tag{D1}$$

which holds for any positive operator A on $\mathcal{H}^{\otimes N}$.

Equation (39) follows from Eq. (35) and the equation

$$\|\tilde{\mathcal{Q}}(A \otimes 1^{\otimes k})\| = \max_\rho \text{tr}[P_{N+k+1}(A \otimes 1^{\otimes k} \otimes \rho)]$$

$$= \frac{D_{N+k+1}}{D_{N+1}} \max_\rho \text{tr}[P_{N+1}(A \otimes \rho)]$$

$$= \frac{D_{N+k+1}}{D_{N+1}} \|\tilde{\mathcal{Q}}(A)\|, \tag{D2}$$

which holds for any positive operator A on $\mathcal{H}^{\otimes N}$.

To prove Eq. (40), let $\mathscr{A} = \{A_j\}_j$ and $\mathscr{B} = \{B_k\}_k$. By assumption, $\mathscr{A}$ is a coarse graining of $\mathscr{B}$, which means

$A_j = \sum_k \Lambda_{jk} B_k$ for some stochastic matrix Λ. Therefore,

$$\sum_j \|\mathcal{Q}(A_j)\|$$

$$= \sum_j \left\|\mathcal{Q}\left(\sum_k \Lambda_{jk} B_k\right)\right\| = \sum_j \left\|\sum_k \Lambda_{jk} \mathcal{Q}(B_k)\right\|$$

$$\leq \sum_j \sum_k \Lambda_{jk} \|\mathcal{Q}(B_k)\| = \sum_k \|\mathcal{Q}(B_k)\|, \qquad (D3)$$

which implies Eq. (40) in view of Eq. (37).

The equality $F(\mathscr{A} \otimes \mathscr{C}) = F(\mathscr{C} \otimes \mathscr{A})$ in Eq. (41) follows from Eq. (37) and the equality

$$\|\mathcal{Q}(A \otimes C)\| = \|\mathcal{Q}(C \otimes A)\|, \qquad (D4)$$

which holds for any positive operator A on $\mathcal{H}^{\otimes N}$ and any positive operator C on $\mathcal{H}^{\otimes k}$. The inequality in Eq. (41) follows from Eqs. (39) and (40) together with the facts that

$$\mathscr{A} \otimes \mathscr{I}^{\otimes k} \preceq \mathscr{A} \otimes \mathscr{C}, \quad \mathscr{I}^{\otimes N} \otimes \mathscr{C} \preceq \mathscr{A} \otimes \mathscr{C}. \quad (D5)$$

APPENDIX E: PROOFS OF LEMMAS 15–17

Proof of Lemma 15. According to Eq. (37) with $N = 1$ and Eq. (48) we have

$$F(\mathscr{A}) = \sum_j \frac{\|\mathcal{Q}(A_j)\|}{2D_2}$$

$$= \frac{1}{d(d+1)} \sum_j [\mathrm{tr}(A_j) + \|A_j\|]$$

$$= \frac{1}{d+1} + \frac{1}{d(d+1)} \sum_j \|A_j\|, \qquad (E1)$$

which confirms the equality in Eq. (49) in Lemma 15. Here the third equality follows from the normalization condition $\sum_j A_j = 1$. The lower bound in Eq. (49) follows from the inequality $\|A_j\| \geq \mathrm{tr}(A_j)/d$, which is saturated iff A_j is proportional to the identity; so the lower bound is saturated iff $\mathscr{A}$ is trivial. The upper bound in Eq. (49) follows from the inequality $\|A_j\| \leq \mathrm{tr}(A_j)$, which is saturated iff A_j is rank 1; so the upper bound is saturated iff $\mathscr{A}$ is rank 1. ∎

Proof of Lemma 16. Since both sides of Eq. (51) are homogeneous in A and B, to prove this equation, we can assume that $\mathrm{tr}(A) = \mathrm{tr}(B) = 1$ without loss of generality, which means $f = \mathrm{tr}(AB)$.

If A and B are rank 1, then we can further assume that $\mathcal{H}$ has dimension 2 without loss of generality. In this case

A and B have the forms

$$A = \frac{1 + \mathbf{a} \cdot \boldsymbol{\sigma}}{2}, \quad B = \frac{1 + \mathbf{b} \cdot \boldsymbol{\sigma}}{2}, \qquad (E2)$$

where $\mathbf{a}$ and $\mathbf{b}$ are two real unit vectors in dimension 3, and $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ is the vector composed of the three Pauli operators. So we have $f = \mathrm{tr}(AB) = (1 + \mathbf{a} \cdot \mathbf{b})/2$, and Eq. (46) in the main text implies that

$$\mathcal{Q}(A \otimes B) = 3 + \mathbf{a} \cdot \mathbf{b} + (\mathbf{a} + \mathbf{b}) \cdot \boldsymbol{\sigma}, \qquad (E3)$$

$$\|\mathcal{Q}(A \otimes B)\| = 3 + \mathbf{a} \cdot \mathbf{b} + |\mathbf{a} + \mathbf{b}|$$

$$= 3 + \mathbf{a} \cdot \mathbf{b} + \sqrt{2 + 2\mathbf{a} \cdot \mathbf{b}}$$

$$= 2(1 + f + \sqrt{f}), \qquad (E4)$$

which confirms Eq. (51) with equality.

In general, suppose that A and B have convex decompositions $A = \sum_j \lambda_j |\psi_j\rangle\langle\psi_j|$ and $B = \sum_k \mu_k |\varphi_k\rangle\langle\varphi_k|$, respectively, where $\lambda_j, \mu_k > 0$; let $f_{jk} = |\langle\psi_j|\varphi_k\rangle|^2$. Then we have

$$\sum_j \lambda_j = \sum_k \mu_k = 1, \quad \sum_{j,k} \lambda_j \mu_k f_{jk} = \mathrm{tr}(AB) = f. \quad (E5)$$

Therefore,

$$\|\mathcal{Q}(A \otimes B)\| \leq \sum_{j,k} \lambda_j \mu_k \|\mathcal{Q}(|\psi_j\rangle\langle\psi_j| \otimes |\varphi_k\rangle\langle\varphi_k|)\|$$

$$= \sum_{j,k} 2\lambda_j \mu_k (1 + f_{jk} + \sqrt{f_{jk}})$$

$$\leq 2(1 + f + \sqrt{f}), \qquad (E6)$$

which confirms Eq. (51). Here the first inequality follows from the triangle inequality for the operator norm; the second inequality follows from Eq. (E5) and the (strict) concavity of the square-root function.

If both A and B are rank 1, then the upper bound in Eq. (51) is saturated according to Eq. (E4). If A and B have orthogonal supports and one of them is rank 1, then the upper bound is also saturated, which can be verified by virtue of Eq. (43) or (46).

Conversely, if the upper bound in Eq. (51) is saturated, then the two inequalities in Eq. (E6) are saturated. The saturation of the second inequality implies that $f_{jk} = f$ for all j, k. Since this result holds irrespective of the convex decompositions of A and B, it follows that $|\langle\psi|\varphi\rangle|^2 = f$ for any pure state $|\psi\rangle$ in the support of A and any pure state $|\varphi\rangle$ in the support of B. Therefore, both A and B are rank 1, or A and B have orthogonal supports. In the former case, the upper bound in Eq. (51) is indeed saturated according to Eq. (E4). In the latter case, we have $f = 0$ and the upper

bound in Eq. (51) is equal to 2. In addition, from Eq. (43) or (46) we can deduce that

$$\mathcal{Q}(A \otimes B) = 1 + A + B, \tag{E7}$$

which implies that

$$\|\mathcal{Q}(A \otimes B)\| = 1 + \max\{\|A\|, \|B\|\} \leq 2$$
$$= 2(1 + f + \sqrt{f}). \tag{E8}$$

The upper bound is saturated iff $\|A\| = 1$ or $\|B\| = 1$, which means A is rank 1 or B is rank 1 given the assumption that $\mathrm{tr}(A) = \mathrm{tr}(B) = 1$. This observation completes the proof of Lemma 16. ∎

Proof of Lemma 17. In general, $\mathscr{A}$ and $\mathscr{B}$ can be expressed as $\mathscr{A} = \{A_j\}_j$ and $\mathscr{B} = \{B_k\}_k$, where $A_j, B_k \neq 0$ and $\sum_j A_j = \sum_k B_k = 1$. Let $a_j = \mathrm{tr}(A_j)$, $b_k = \mathrm{tr}(B_k)$, and $f_{jk} = \mathrm{tr}(A_j B_k)/(a_j b_k)$. Then we have

$$\sum_j a_j = \sum_j \mathrm{tr}(A_j) = \sum_k b_k = \sum_k \mathrm{tr}(B_k) = d,$$
$$\sum_{j,k} a_j b_k f_{jk} = \sum_{j,k} \mathrm{tr}(A_j B_k) = d. \tag{E9}$$

In addition, Lemma 16 yields the inequality

$$\|\mathcal{Q}(A_j \otimes B_k)\| \leq 2 a_j b_k (1 + f_{jk} + \sqrt{f_{jk}}). \tag{E10}$$

By virtue of Eq. (37) we can now deduce that

$$F(\mathscr{A} \otimes \mathscr{B}) = \frac{1}{d(d+1)(d+2)} \sum_{j,k} \|\mathcal{Q}(A_j \otimes B_k)\|$$
$$\leq \frac{2}{d(d+1)(d+2)} \sum_{j,k} a_j b_k (1 + f_{jk} + \sqrt{f_{jk}})$$
$$= \frac{2d(d+1) + 2\Phi_{1/2}(\mathscr{A}, \mathscr{B})}{d(d+1)(d+2)}, \tag{E11}$$

which confirms the upper bound in Eq. (55). Here the last equality follows from the definition of $\Phi_{1/2}(\mathscr{A}, \mathscr{B})$ in Eq. (18) and the normalization conditions in Eq. (E9).

If $\mathscr{A}$ and $\mathscr{B}$ are rank-1 POVMs, then the upper bound in Eq. (E10) is saturated for each pair j, k, so the upper bound in Eq. (E11) [identical to the upper bound in Eq. (55)] is saturated.

Conversely, if the upper bound in Eq. (55) is saturated, then the upper bound in Eq. (E10) is saturated for each pair j, k. Suppose on the contrary that $\mathscr{A}$ is not rank 1; then it contains a POVM element, say A_1, of rank at least 2. According to Lemma 16, all POVM elements in $\mathscr{B}$ are rank 1 and are orthogonal to A_1, which is impossible. Therefore, $\mathscr{A}$ is rank 1, and so is $\mathscr{B}$ by the same token. In a word, the upper bound in Eq. (55) is saturated iff $\mathscr{A}$ and $\mathscr{B}$ are rank 1. ∎

APPENDIX F: PROOFS OF LEMMAS 19–21

Proof of Lemma 19. The inequality in Eq. (57) follows from the triangle inequality for the operator norm given that $\mathcal{Q}(A \otimes B) = \mathcal{Q}(A \otimes B_1) + \mathcal{Q}(A \otimes B_2)$. The inequality is saturated iff there exists a ket $|\psi\rangle \in \mathcal{H}$ such that

$$\mathcal{Q}(A \otimes B_1)|\psi\rangle = \|\mathcal{Q}(A \otimes B_1)\| |\psi\rangle,$$
$$\mathcal{Q}(A \otimes B_2)|\psi\rangle = \|\mathcal{Q}(A \otimes B_2)\| |\psi\rangle. \tag{F1}$$

If condition 1 in Lemma 19 holds, that is, B_2 is proportional to B_1, then $\mathcal{Q}(A \otimes B_2)$ is proportional to $\mathcal{Q}(A \otimes B_1)$, so the inequality in Eq. (57) is saturated. If condition 2 or 3 in Lemma 19 holds, then the inequality is also saturated according to Eq. (43) [cf. Eq. (E3)] and the above observation. Note that the eigenspace associated with the maximum eigenvalue of $\mathcal{Q}(A \otimes B_j)$ is twofold degenerate when A and B_j are orthogonal, but nondegenerate otherwise.

Next, we suppose that none of the three conditions in Lemma 19 holds. Then B_2 is not proportional to B_1, and A is not orthogonal to one of the two operators B_1, B_2. If A, B_1, B_2 are not supported in any common two-dimensional subspace of $\mathcal{H}$, then there does not exist any ket $|\psi\rangle$ that satisfies Eq. (F1), so the inequality in Eq. (57) is not saturated.

If A, B_1, B_2 are all supported in a common two-dimensional subspace of $\mathcal{H}$, then A is orthogonal to neither B_1 nor B_2. Therefore, the eigenspace of $\mathcal{Q}(A \otimes B_j)$ associated with the maximum eigenvalue is nondegenerate for $j = 1, 2$ according to Eq. (43) [cf. Eq. (E3)], and there does not exist any ket $|\psi\rangle$ that satisfies Eq. (F1) either, so the inequality in Eq. (57) is not saturated. This observation completes the proof of Lemma 19. ∎

Proof of Lemma 20. The inequality in Eq. (58) follows from the triangle inequality for the operator norm. If $B_1, B_2, \ldots, B_n$ are mutually orthogonal and they commute with all POVM elements in $\mathscr{A}$, then it is easy to verify that the inequality is saturated according to Eq. (43).

To prove the converse, let $C = B - B_1 - B_2$; then

$$
\begin{aligned}
\sum_{j=1}^{m} &\| \mathcal{Q}(A_j \otimes B) \| \\
&\leq \sum_{j=1}^{m} \| \mathcal{Q}(A_j \otimes (B_1 + B_2)) \| + \sum_{j=1}^{m} \| \mathcal{Q}(A_j \otimes C) \| \\
&\leq \sum_{j=1}^{m} \sum_{k=1}^{n} \| \mathcal{Q}(A_j \otimes B_k) \|.
\end{aligned} \tag{F2}
$$

If the final upper bound is saturated, then

$$
\sum_{j=1}^{m} \| \mathcal{Q}(A_j \otimes (B_1 + B_2)) \| = \sum_{j=1}^{m} \sum_{k=1}^{2} \| \mathcal{Q}(A_j \otimes B_k) \|, \tag{F3}
$$

which implies that

$$
\| \mathcal{Q}(A_j \otimes (B_1 + B_2)) \| = \sum_{k=1}^{2} \| \mathcal{Q}(A_j \otimes B_k) \| \tag{F4}
$$

for $j = 1, 2, \ldots, m$.

Let $\mathcal{V}_{12}$ be the two-dimensional subspace of $\mathcal{H}$ that contains the supports of B_1 and B_2, and let $\mathcal{V}_{12}^{\perp}$ be its orthogonal complement; let P_{12} be the orthogonal projector onto $\mathcal{V}_{12}$. Then Eq. (F4) implies that each A_j is either supported in $\mathcal{V}_{12}$ or supported in $\mathcal{V}_{12}^{\perp}$ according to Lemma 19, given that B_2 is not proportional to B_1. In the first case, each A_j is orthogonal to either B_1 or B_2; in the second case, each A_j is orthogonal to and commutes with both B_1 and B_2. Denote by $\mathcal{A}_1$ ($\mathcal{A}_2$) the set of POVM elements in $\mathcal{A}$ that belong to the first (second) category. Then $\mathcal{A}_1$ is a POVM on $\mathcal{V}_{12}$, while $\mathcal{A}_2$ is a POVM on $\mathcal{V}_{12}^{\perp}$, that is,

$$
\sum_{A_j \in \mathcal{A}_1} A_j = P_{12}, \quad \sum_{A_j \in \mathcal{A}_2} A_j = 1 - P_{12}. \tag{F5}
$$

If B_1 is not orthogonal to B_2, then the first equality cannot hold. This contradiction shows that B_1 and B_2 are orthogonal. Consequently, each A_j in $\mathcal{A}_1$ is proportional to either B_2 or B_1 and commutes with both B_1 and B_2. In conjunction with the above conclusion, we conclude that all POVM elements in $\mathcal{A}$ commute with B_1 and B_2.

The above reasoning is still applicable if B_1, B_2 are replaced by B_j, B_k with $1 \leq j < k \leq n$. In this way we can deduce that $B_1, B_2, \ldots, B_n$ are mutually orthogonal and they commute with all POVM elements in $\mathcal{A}$. According to Lemma 4, $\mathcal{A}$ contains n rank-1 projectors that are proportional to $B_1, B_2, \ldots, B_n$, respectively. ∎

Proof of Lemma 21. The inequality in Eq. (59) follows from Lemma 14, which also implies that the inequality is saturated if $\mathcal{B}$ is equivalent to $\mathcal{C}$.

To prove the converse, we can assume that $\mathcal{A}$ and $\mathcal{C}$ are simple rank-1 POVMs without loss of generality. Suppose that $\mathcal{B} = \{B_j\}_{j=1}^{n}$ and $\mathcal{C} = \{C_k\}_{k=1}^{o}$. By assumption, B_j can be expressed as

$$
B_j = \sum_{k=1}^{o} \Lambda_{jk} C_k, \tag{F6}
$$

where Λ is a stochastic matrix, which means $\Lambda_{jk} \geq 0$ and $\sum_{j=1}^{n} \Lambda_{jk} = 1$ for $k = 1, 2, \ldots, o$. Therefore,

$$
\sum_{A \in \mathcal{A}} \| \mathcal{Q}(A \otimes B_j) \| \leq \sum_{A \in \mathcal{A}} \sum_{k=1}^{o} \Lambda_{jk} \| \mathcal{Q}(A \otimes C_k) \| \tag{F7}
$$

for $j = 1, 2, \ldots, n$. This equation implies that

$$
\sum_{A \in \mathcal{A}} \sum_{j=1}^{n} \| \mathcal{Q}(A \otimes B_j) \| \leq \sum_{A \in \mathcal{A}} \sum_{k=1}^{o} \| \mathcal{Q}(A \otimes C_k) \|, \tag{F8}
$$

which is equivalent to Eq. (59) according to Eq. (37).

If $\mathcal{B}$ is not equivalent to $\mathcal{C}$, then $\mathcal{B}$ is not rank 1 according to Lemma 1 and Proposition 2 and thus contains at least one POVM element, say B_1, with rank at least 2. Consequently, the corresponding inequality in Eq. (F7) is strict according to Lemma 20 given that $\mathcal{A}$ is irreducible or $\mathcal{C}$ contains no two POVM elements that are mutually orthogonal by assumption. Therefore, the inequality in Eq. (F8) is also strict and we have

$$
F(\mathcal{A} \otimes \mathcal{B}) < F(\mathcal{A} \otimes \mathcal{C}) \tag{F9}
$$

by Eq. (37). In conclusion, the inequality in Eq. (59) is saturated iff $\mathcal{B}$ is equivalent to $\mathcal{C}$. ∎

APPENDIX G: PROOF OF THEOREM 2

1. Main proof

Proof of Theorem 2. By virtue of Eq. (35) in the main text and Lemma 27 below, the lower bound in Eq. (60) can be proved as follows:

$$
\begin{aligned}
F(\mathcal{A}) &= \frac{1}{D_{N+1}} \sum_j \| \tilde{\mathcal{Q}}(A_j) \| \\
&\geq \frac{N+d}{d(N+1)D_{N+1}} \sum_j \mathrm{tr}(P_N A_j) \\
&= \frac{\mathrm{tr}(P_N)}{d D_N} = \frac{D_N}{d D_N} = \frac{1}{d}. \tag{G1}
\end{aligned}
$$

Here the inequality is saturated iff $\tilde{\mathcal{Q}}(A_j)$ for each j is proportional to the identity.

The upper bound in Eq. (60) can be derived from Eq. (35) and Lemma 27 as follows:

$$
\begin{aligned}
F(\mathscr{A}) &= \frac{1}{D_{N+1}} \sum_j \|\tilde{\mathcal{Q}}(A_j)\| \leq \frac{1}{D_{N+1}} \sum_j \mathrm{tr}(P_N A_j) \\
&= \frac{\mathrm{tr}(P_N)}{D_{N+1}} = \frac{D_N}{D_{N+1}} = \frac{N+1}{N+d}.
\end{aligned} \tag{G2}
$$

Here the inequality is saturated iff $P_N A_j P_N$ for each j is proportional to the Nth tensor power of a pure state. This observation completes the proof of Theorem 2. ∎

2. Auxiliary lemmas

Lemma 27. *Any positive operator A on $\mathcal{H}^{\otimes N}$ satisfies*

$$
\frac{N+d}{d(N+1)} \mathrm{tr}(P_N A) \leq \|\tilde{\mathcal{Q}}(A)\| \leq \mathrm{tr}(P_N A), \tag{G3}
$$

and the lower bound is saturated iff $\tilde{\mathcal{Q}}(A)$ is proportional to the identity, while the upper bound is saturated iff $P_N A P_N$ is proportional to the Nth tensor power of a pure state.

Proof. The lower bound in Eq. (G3) can be proved as follows:

$$
\begin{aligned}
\|\tilde{\mathcal{Q}}(A)\| &\geq \frac{1}{d} \mathrm{tr}[\tilde{\mathcal{Q}}(A)] = \frac{1}{d} \mathrm{tr}[P_{N+1}(A \otimes 1)] \\
&= \frac{D_{N+1}}{d D_N} \mathrm{tr}(P_N A) = \frac{N+d}{d(N+1)} \mathrm{tr}(P_N A).
\end{aligned} \tag{G4}
$$

Here the inequality is saturated iff $\tilde{\mathcal{Q}}(A)$ is proportional to the identity.

The upper bound in Eq. (G3) and the saturation condition follow from Lemma 28 and the equation

$$
\|\tilde{\mathcal{Q}}(A)\| = \max_\rho [P_{N+1}(A \otimes \rho)], \tag{G5}
$$

where the maximization is taken over all normalized pure states. ∎

Lemma 28. *Suppose that ρ is a pure sate on $\mathcal{H}$ and that A is a positive operator acting on $\mathcal{H}^{\otimes N}$. Then*

$$
\mathrm{tr}[P_{N+1}(A \otimes \rho)] \leq \mathrm{tr}(P_N A), \tag{G6}
$$

and the upper bound is saturated iff $P_N A P_N$ is proportional to the Nth tensor power of ρ.

Proof. The upper bound in Eq. (G6) can be derived as follows:

$$
\begin{aligned}
\mathrm{tr}[P_{N+1}(A \otimes \rho)] &= \mathrm{tr}[P_{N+1}(A \otimes \rho)P_{N+1}] \\
&= \mathrm{tr}[P_{N+1}(P_N A P_N \otimes \rho)P_{N+1}] \\
&\leq \mathrm{tr}(P_N A P_N) \mathrm{tr}(\rho) \\
&= \mathrm{tr}(P_N A).
\end{aligned} \tag{G7}
$$

If $P_N A P_N$ is proportional to the Nth tensor power of ρ, then $P_N A P_N \otimes \rho$ is supported in the symmetric subspace in $\mathcal{H}^{\otimes(N+1)}$, so the inequality in Eq. (G7) is saturated, which means the upper bound in Eq. (G6) is saturated.

Conversely, if the inequality in Eq. (G7) is saturated, then $P_N A P_N \otimes \rho$ is supported in the symmetric subspace in $\mathcal{H}^{\otimes(N+1)}$. Let $\mathrm{tr}_{\bar{j}}(\cdot)$ denote the partial trace over all the parties except for party j. Then all the operators $\mathrm{tr}_{\bar{j}}(P_N A P_N)$ for $j = 1, 2, \ldots, N$ have the same support as ρ, which implies that $P_N A P_N$ is proportional to the Nth tensor power of ρ. ∎

APPENDIX H: PROOFS OF THEOREM 3 AND COROLLARIES 1–5

Proof of Theorem 3. Theorem 3 is a simple corollary of Lemmas 10 and 18. ∎

Proof of Corollary 1. If $\mathscr{A}$ is a rank-1 projective measurement, then $F(\mathscr{A}^{\otimes 2}) = F(\mathscr{A}) = 2/(d+1)$ by Eq. (63). Conversely, if $F(\mathscr{A}^{\otimes 2}) = F(\mathscr{A}) = 2/(d+1)$, then $\mathscr{A}$ is rank 1 by Lemma 15. Furthermore, Theorem 3 implies that $\mathscr{A}$ is a rank-1 projective measurement. ∎

Proof of Corollary 2. If $\mathscr{A}$ and $\mathscr{B}$ are identical rank-1 projective measurements up to relabeling, then Eq. (63) implies that

$$
F(\mathscr{A} \otimes \mathscr{B}) = F(\mathscr{B}) = F(\mathscr{A}) = \frac{2}{d+1}. \tag{H1}
$$

Conversely, if this equation holds, then both $\mathscr{A}$ and $\mathscr{B}$ are rank 1 according to Lemma 15. By virtue of Lemma 17 we can further deduce that

$$
\frac{2}{d+1} = F(\mathscr{A} \otimes \mathscr{B}) = \frac{2d(d+1) + 2\Phi_{1/2}(\mathscr{A}, \mathscr{B})}{d(d+1)(d+2)}, \tag{H2}
$$

which implies that $\Phi_{1/2}(\mathscr{A}, \mathscr{B}) = d$. Therefore, $\mathscr{A}$ and $\mathscr{B}$ are identical rank-1 projective measurements up to relabeling according to Lemma 12. ∎

Proof of Corollary 3. If $\mathscr{A}$ is a rank-1 POVM, then the conclusions in Corollary 3 follow from Theorem 3.

If $\mathscr{A}$ is not a rank-1 POVM, let $\mathscr{B}$ be a rank-1 POVM that refines $\mathscr{A}$. Then $\mathscr{B}^{\otimes 2}$ is a refinement of $\mathscr{A}^{\otimes 2}$, so Lemma 14 and Theorem 3 imply that

$$F(\mathscr{A}^{\otimes 2}) \leq F(\mathscr{B}^{\otimes 2}) \leq F_2^{\mathrm{iid}}. \qquad \text{(H3)}$$

To attain the upper bound F_2^{iid}, any rank-1 refinement of $\mathscr{A}$ must attain the bound F_2^{iid} and is thus equivalent to a SIC according to Theorem 3. However, this condition is impossible when $\mathscr{A}$ is not rank 1. So the upper bound F_2^{iid} cannot be attained except for rank-1 POVMs. This observation completes the proof of Corollary 3. ∎

Proof of Corollary 4. Let

$$\mathscr{A} = \bigcup_{r=1}^{g} \frac{\mathscr{A}_r}{g}; \qquad \text{(H4)}$$

then $\mathscr{A}$ is a POVM on $\mathcal{H}$. By virtue of Eq. (37) and Corollary 3 we can derive that

$$\sum_{r,s} F(\mathscr{A}_r \otimes \mathscr{A}_s) = g^2 F(\mathscr{A}^{\otimes 2}) \leq g^2 F_2^{\mathrm{iid}}, \qquad \text{(H5)}$$

which confirms Eq. (67). If $\mathscr{A}_1, \mathscr{A}_2, \ldots, \mathscr{A}_g$ are identical SICs up to relabeling, then $\mathscr{A}$ is equivalent to a SIC, so the inequality is saturated according to Eq. (64).

Conversely, if the inequality in Eq. (H5) is saturated, then $\mathscr{A}$ is equivalent to a SIC by Corollary 3. Let $\mathscr{A}'$ be a simple POVM that is equivalent to $\mathscr{A}$; then $\mathscr{A}'$ is a SIC. Suppose that $\mathscr{A}'$ is composed of the POVM elements $A_1, A_2, \ldots, A_{d^2}$. Then these POVM elements form a basis in the operator space, and a linear combination of them is equal to the identity operator iff all the coefficients are equal to 1. In addition, each POVM element in $\mathscr{A}_r$ for $r = 1, 2, \ldots, g$ is proportional to a POVM element in $\mathscr{A}'$. Since $\mathscr{A}_r$ is a simple POVM by assumption, it follows that $\mathscr{A}_r$ is identical to $\mathscr{A}'$ up to relabeling for $r = 1, 2, \ldots, g$, so $\mathscr{A}_1, \mathscr{A}_2, \ldots, \mathscr{A}_g$ are identical SICs up to relabeling. ∎

Proof of Corollary 5. Corollary 5 would follow from Corollary 4 if the condition $F(\mathscr{A} \otimes \mathscr{B}) = F(\mathscr{A}^{\otimes 2}) = F_2^{\mathrm{iid}}$ is replaced by

$$F(\mathscr{A} \otimes \mathscr{B}) = F(\mathscr{B}^{\otimes 2}) = F(\mathscr{A}^{\otimes 2}) = F_2^{\mathrm{iid}}. \qquad \text{(H6)}$$

Without this stronger condition we need to devise a different proof.

If $\mathscr{A}$ and $\mathscr{B}$ are identical SICs up to relabeling, then Eq. (H6) holds according to Eq. (64) and Theorem 3.

Conversely, if $F(\mathscr{A} \otimes \mathscr{B}) = F(\mathscr{A}^{\otimes 2}) = F_2^{\mathrm{iid}}$, then $\mathscr{A}$ is a SIC by Corollary 3 given that $\mathscr{A}$ and $\mathscr{B}$ are simple POVMs. So $\mathscr{A}$ is constructed from a 2-design. Let $\mathscr{B}'$ be

any simple rank-1 POVM that refines $\mathscr{B}$; then by virtue of Lemma 14 we can deduce that

$$F(\mathscr{A} \otimes \mathscr{B}') \geq F(\mathscr{A} \otimes \mathscr{B}) = F_2^{\mathrm{iid}}, \qquad \text{(H7)}$$

which implies that

$$\Phi_{1/2}(\mathscr{A}, \mathscr{B}') \geq 1 + (d-1)\sqrt{d+1} \qquad \text{(H8)}$$

by Lemma 17. Thanks to Lemma 13, this inequality is necessarily saturated; moreover, $\mathscr{B}'$ is identical to the SIC $\mathscr{A}$ up to relabeling. The last conclusion holds for any simple rank-1 POVM $\mathscr{B}'$ that refines $\mathscr{B}$, which is impossible if $\mathscr{B}$ is not rank 1. Therefore, $\mathscr{B}$ is rank 1; moreover, $\mathscr{A}$ and $\mathscr{B}$ are identical SICs up to relabeling. ∎

APPENDIX I: PROOFS OF LEMMA 22, THEOREM 4, AND COROLLARIES 7–9

Proof of Lemma 22. Thanks to Lemma 14, to prove the inequality $F(\mathscr{A}) \leq F_2^{\mathrm{sep}}$ in Lemma 22, we can assume that $\mathscr{A}$ is a rank-1 POVM. Then each POVM element A_j of $\mathscr{A}$ is a tensor product of two rank-1 positive operators. Let $a_j = \mathrm{tr}(A_j)$ and $f_j = \mathrm{tr}(WA_j)/a_j$. Then the normalization condition $\sum_j A_j = 1^{\otimes 2}$ implies that

$$\sum_j a_j = \sum_j \mathrm{tr}(A_j) = d^2, \qquad \text{(I1)}$$

$$\sum_j a_j f_j = \sum_j \mathrm{tr}[(2P_2 - 1)A_j] = d, \qquad \text{(I2)}$$

from which we can deduce that

$$\sum_j a_j \sqrt{f_j} \leq d\sqrt{d}. \qquad \text{(I3)}$$

In addition, Lemma 16 implies that

$$\|\mathcal{Q}(A_j)\| = 2a_j(1 + f_j + \sqrt{f_j}). \qquad \text{(I4)}$$

By virtue of Eq. (37) we can now deduce that

$$
\begin{aligned}
F(\mathscr{A}) &= \frac{1}{d(d+1)(d+2)} \sum_j \|\mathcal{Q}(A_j)\| \\
&= \frac{2}{d(d+1)(d+2)} \sum_j a_j(1 + f_j + \sqrt{f_j}) \\
&\leq \frac{2(d+1+\sqrt{d})}{(d+1)(d+2)} = F_2^{\mathrm{sep}}.
\end{aligned}
\qquad \text{(I5)}
$$

Here the inequality is saturated iff the inequality in Eq. (I3) is saturated, which is the case iff each f_j is equal to $1/d$, that is, $d\,\mathrm{tr}(WA_j) = \mathrm{tr}(A_j)$. ∎

Proof of Theorem 4. The inequality $F(\mathscr{A} \otimes \mathscr{B}) \leq F_2^{\text{sep}}$ in the theorem follows from Lemma 22 (cf. Lemmas 12 and 17). When $\mathscr{A}$ and $\mathscr{B}$ are rank 1, Lemma 22 also implies that the upper bound is saturated iff $\mathscr{A}$ and $\mathscr{B}$ are MU. To complete the proof, it suffices to prove that the upper bound can never be saturated if $\mathscr{A}$ or $\mathscr{B}$ is not rank 1.

According to Lemmas 14 and 22, to saturate the inequality $F(\mathscr{A} \otimes \mathscr{B}) \leq F_2^{\text{sep}}$, any rank-1 refinement of $\mathscr{A}$ and any rank-1 refinement of $\mathscr{B}$ are necessarily MU. So the fidelity between any state vector in the support of each POVM element in $\mathscr{A}$ and any state vector in the support of each POVM element in $\mathscr{B}$ is equal to $1/d$. However, this condition can never hold if $\mathscr{A}$ or $\mathscr{B}$ is not rank 1. This observation completes the proof of Theorem 4 ∎

Proof of Corollary 7. According to Theorem 4, the assumption that $F(\mathscr{A} \otimes \mathscr{B}) = F_2^{\text{sep}}$ implies that $\mathscr{A}$ and $\mathscr{B}$ are rank 1 and MU. Therefore, both $\mathscr{A}$ and $\mathscr{B}$ have at least d POVM elements according to Lemma 3, which implies that $\mathscr{A} \otimes \mathscr{B}$ has at least d^2 POVM elements. The lower bound is saturated if $\mathscr{A}$ and $\mathscr{B}$ are MU rank-1 projective measurements. Conversely, if $\mathscr{A} \otimes \mathscr{B}$ has d^2 POVM elements, then both $\mathscr{A}$ and $\mathscr{B}$ have d POVM elements and are thus rank-1 projective measurements according to Lemma 3. In addition, the two measurements are MU according to Theorem 4, as mentioned above. ∎

Proof of Corollary 8. If $\mathscr{A}$ and $\mathscr{B}$ are MU rank-1 projective measurements, then we have $F(\mathscr{A} \otimes \mathscr{B}) = F_2^{\text{sep}}$ by Eq. (70) and $F(\mathscr{A}^{\otimes 2}) = F(\mathscr{B}^{\otimes 2}) = 2/(d+1)$ by Eq. (63).

Conversely, if $F(\mathscr{A} \otimes \mathscr{B}) = F_2^{\text{sep}}$, then $\mathscr{A}$ and $\mathscr{B}$ are MU rank-1 POVMs according to Theorem 4. If, in addition, $F(\mathscr{A}^{\otimes 2}) = F(\mathscr{B}^{\otimes 2}) = 2/(d+1)$, then $\mathscr{A}$ and $\mathscr{B}$ are rank-1 projective measurements according to Theorem 3. Therefore, $\mathscr{A}$ and $\mathscr{B}$ are MU rank-1 projective measurements if both conditions hold. ∎

Proof of Corollary 9. The upper bound in Eq. (72) follows from the inequality $F(\mathscr{A} \otimes \mathscr{B}) \leq F_2^{\text{sep}}$ in Theorem 4.

If $\mathscr{A}_1, \mathscr{A}_2, \ldots, \mathscr{A}_g$ are MU rank-1 POVMs, then the upper bound is saturated according to Theorem 4 again.

Conversely, if the upper bound in Eq. (72) is saturated, then Theorem 4 implies that

$$F(\mathscr{A}_r \otimes \mathscr{A}_s) = F_2^{\text{sep}} \quad \text{for all } r \neq s; \tag{I6}$$

moreover, $\mathscr{A}_1, \mathscr{A}_2, \ldots, \mathscr{A}_g$ are g MU rank-1 POVMs. If, in addition, these POVMs are simple and $g = d + 1$, then $\mathscr{A}_1, \mathscr{A}_2, \ldots, \mathscr{A}_{d+1}$ are rank-1 projective measurements according to Theorem 1 and thus form a CMUMs. ∎

APPENDIX J: PROOF OF THEOREM 5

Proof of Theorem 5. Let $\mathscr{A} = \{A_j\}_j$ and $\mathscr{B} = \{B_k\}_k$ be two commuting POVMs. Then the estimation fidelity $F(\mathscr{A} \otimes \mathscr{B})$ can be computed by virtue of Eq. (37), with the result

$$\begin{aligned} F(\mathscr{A} \otimes \mathscr{B}) &= \frac{1}{d(d+1)(d+2)} \sum_{j,k} \|\mathcal{Q}(A_j \otimes B_k)\| \\ &\leq \frac{1}{d(d+1)(d+2)} \sum_j 2(d+2) \operatorname{tr}(A_j) \\ &= \frac{2}{d+1}, \end{aligned} \tag{J1}$$

which confirms Theorem 5. Here the inequality follows from Lemma 29 below. ∎

Lemma 29. *Suppose that A is a positive operator on $\mathcal{H}$ and that $\mathscr{B}$ is a POVM that commutes with A. Then*

$$\sum_{B \in \mathscr{B}} \|\mathcal{Q}(A \otimes B)\| \leq 2(d+2) \operatorname{tr}(A). \tag{J2}$$

Proof. To prove Eq. (J2), first consider the case in which A is a projector of rank r. By assumption, each POVM element B in $\mathscr{B}$ commutes with A and is thus block diagonal with respect to the eigenspaces of A.

If $\mathscr{B}$ is rank 1, then $\|B\| = \operatorname{tr}(B)$ and B is supported in the support of A or in its orthogonal complement. So either the condition $AB = B$ or the condition $AB = 0$ holds. According to Eq. (43) we have

$$\begin{aligned} \mathcal{Q}(A \otimes B) &= \operatorname{tr}(A) \operatorname{tr}(B) + \operatorname{tr}(AB) + \operatorname{tr}(B)A + \operatorname{tr}(A)B + AB + BA \\ &= \begin{cases} (r+1) \operatorname{tr}(B) + \operatorname{tr}(B)A + (r+2)B & \text{if } AB = B, \\ r \operatorname{tr}(B) + \operatorname{tr}(B)A + rB & \text{if } AB = 0, \end{cases} \end{aligned} \tag{J3}$$

which implies that

$$\|\mathcal{Q}(A \otimes B)\| = \begin{cases} 2(r+2)\operatorname{tr}(B) & \text{if } AB = B, \\ 2r\operatorname{tr}(B) & \text{if } AB = 0. \end{cases} \quad \text{(J4)}$$

Therefore,

$$\sum_{B \in \mathscr{B}} \|\mathcal{Q}(A \otimes B)\| = 2r \sum_{B \in \mathscr{B}} \operatorname{tr}(B) + 4 \sum_{B \in \mathscr{B} | AB = B} \operatorname{tr}(B)$$

$$= 2rd + 4r = 2(d+2)\operatorname{tr}(A), \quad \text{(J5)}$$

which confirms Eq. (J2) with equality. Here the second equality follows from the facts that

$$\sum_{B \in \mathscr{B}} B = 1, \qquad \sum_{B \in \mathscr{B} | AB = B} B = A. \quad \text{(J6)}$$

If $\mathscr{B}$ is not rank 1, then we can find a rank-1 refinement $\mathscr{B}'$ of $\mathscr{B}$ that commutes with A given that $\mathscr{B}$ commutes with A. Therefore,

$$\sum_{B \in \mathscr{B}} \|\mathcal{Q}(A \otimes B)\| \leq \sum_{B \in \mathscr{B}'} \|\mathcal{Q}(A \otimes B)\| = 2(d+2)\operatorname{tr}(A),$$

$$\text{(J7)}$$

which confirms Eq. (J2) again.

Next, we drop the assumption that A is a projector. Let $A = \sum_j \lambda_j P_j$ be the spectral decomposition of A, where λ_j are distinct eigenvalues and P_j are the corresponding eigenprojectors. By assumption, each $B \in \mathscr{B}$ commutes with A and thus also commutes with all eigenprojectors P_j. Therefore,

$$\sum_{B \in \mathscr{B}} \|\mathcal{Q}(A \otimes B)\| = \sum_{B \in \mathscr{B}} \left\| \sum_j \lambda_j \mathcal{Q}(P_j \otimes B) \right\|$$

$$\leq \sum_j \sum_{B \in \mathscr{B}} \lambda_j \|\mathcal{Q}(P_j \otimes B)\|$$

$$\leq \sum_j 2\lambda_j (d+2)\operatorname{tr}(P_j)$$

$$= 2(d+2)\operatorname{tr}(A), \quad \text{(J8)}$$

which confirms Eq. (J2) and completes the proof of Lemma 29. ∎

APPENDIX K: PROOF OF THEOREM 6

Let $\mathscr{C}$ be a simple POVM that refines both $\mathscr{A}$ and $\mathscr{B}$. Then $\mathscr{C} \otimes \mathscr{C}$ is a refinement of $\mathscr{C} \otimes \mathscr{B}$, which is in turn a refinement of $\mathscr{A} \otimes \mathscr{B}$, so

$$F(\mathscr{A} \otimes \mathscr{B}) \leq F(\mathscr{C} \otimes \mathscr{B}) \leq F(\mathscr{C} \otimes \mathscr{C}) \leq F_2^{\text{iid}}, \quad \text{(K1)}$$

where the first two inequalities follow from Lemma 14 and the third inequality follows from Corollary 3. If $\mathscr{A}$

and $\mathscr{B}$ are identical SICs up to relabeling, then the upper bound is saturated according to Eq. (64) (cf. Theorem 3 and Corollary 3).

Conversely, if the final upper bound in Eq. (K1) is saturated, then all three inequalities are saturated simultaneously, that is,

$$F(\mathscr{A} \otimes \mathscr{B}) = F(\mathscr{C} \otimes \mathscr{B}) = F(\mathscr{C} \otimes \mathscr{C}) = F_2^{\text{iid}}. \quad \text{(K2)}$$

Here the third equality implies that $\mathscr{C}$ is a SIC according to Corollary 3 and is thus irreducible. Then the second equality implies that $\mathscr{B}$ is equivalent to $\mathscr{C}$ according to Lemma 21 and is thus also irreducible. Finally, the first equality implies that $\mathscr{A}$ is equivalent to $\mathscr{C}$ according to Lemma 21 again. If both $\mathscr{A}$ and $\mathscr{B}$ are simple, then they are both identical to $\mathscr{C}$ up to relabeling according to Lemma 2 and are thus identical SICs up to relabeling.

APPENDIX L: PROOF OF THEOREM 7

The inequality $F(\mathscr{A} \otimes \mathscr{B}) \geq F(\mathscr{A})$ and equality $F(\mathscr{A}) = 2/(d+1)$ follow from Lemmas 14 and 15, respectively, given that $\mathscr{A}$ is rank 1 by assumption. If $\mathscr{A}$ and $\mathscr{B}$ commute, then $F(\mathscr{A} \otimes \mathscr{B}) \leq 2/(d+1)$ by Theorem 5. So the inequality $F(\mathscr{A} \otimes \mathscr{B}) \geq F(\mathscr{A})$ is saturated.

To further clarify the saturation condition of the inequality $F(\mathscr{A} \otimes \mathscr{B}) \geq F(\mathscr{A})$, note that $\mathscr{A}$ can be expressed as $\mathscr{A} = \{A_j\}_j$, where $A_j = a_j |\psi_j\rangle\langle\psi_j|$ with $a_j = \operatorname{tr}(A_j)$, and $\mathscr{B}$ can be expressed as $\mathscr{B} = \{B_k\}_k$. By virtue of Eq. (37) we can deduce that

$$F(\mathscr{A}) = \frac{1}{d(d+1)} \sum_j \|Q_j\| = \frac{2}{d+1}, \quad \text{(L1)}$$

$$F(\mathscr{A} \otimes \mathscr{B}) = \frac{1}{d(d+1)(d+2)} \sum_{j,k} \|Q_{jk}\|, \quad \text{(L2)}$$

where

$$Q_j = \mathcal{Q}(A_j) = a_j (|\psi_j\rangle\langle\psi_j| + 1), \quad \text{(L3)}$$

$$Q_{jk} = \mathcal{Q}(A_j \otimes B_k)$$
$$= a_j [\operatorname{tr}(B_k) + \langle\psi_j|B_k|\psi_j\rangle + B_k + \operatorname{tr}(B_k)|\psi_j\rangle\langle\psi_j|$$
$$+ |\psi_j\rangle\langle\psi_j|B_k + B_k|\psi_j\rangle\langle\psi_j|]. \quad \text{(L4)}$$

Note that $|\psi_j\rangle$ is the eigenstate of Q_j corresponding to the largest eigenvalue, which is nondegenerate. In addition, Q_j

and Q_{jk} satisfy the relations

$$\sum_k Q_{jk} = (d+2)Q_j, \quad \sum_k \|Q_{jk}\| \geq (d+2)\|Q_j\|. \quad \text{(L5)}$$

By Eqs. (L1) and (L2), the inequality $F(\mathscr{A} \otimes \mathscr{B}) \geq F(\mathscr{A})$ is saturated iff the inequality in Eq. (L5) is saturated for each j.

If $\mathscr{A}$ commutes with $\mathscr{B}$, then $|\psi_j\rangle\langle\psi_j|$ commutes with B_k, and $|\psi_j\rangle$ is an eigenstate of B_k. Consequently, $|\psi_j\rangle$ is an eigenstate of Q_{jk} associated with the largest eigenvalue $\|Q_{jk}\|$, so that

$$\begin{aligned}
\sum_k \|Q_{jk}\| &= \sum_k \langle\psi_j|Q_{jk}|\psi_j\rangle \\
&= \langle\psi_j|(d+2)Q_j|\psi_j\rangle \\
&= (d+2)\|Q_j\|, \quad \text{(L6)}
\end{aligned}$$

which implies that $F(\mathscr{A} \otimes \mathscr{B}) = F(\mathscr{A})$ given Eqs. (L1) and (L2). This derivation reproduces the conclusion derived above, which is based on Theorem 5.

Conversely, if the inequality $F(\mathscr{A} \otimes \mathscr{B}) \geq F(\mathscr{A})$ saturates, then the inequality in Eq. (L5) is saturated for each j, which implies that

$$\langle\psi_j|Q_{jk}|\psi_j\rangle = \|Q_{jk}\| \quad \text{for all } j, k, \quad \text{(L7)}$$

so $|\psi_j\rangle$ is an eigenstate of Q_{jk} with eigenvalue $\|Q_{jk}\|$. By virtue of Eq. (L4), we can further deduce that $|\psi_j\rangle$ is an eigenstate of B_k. Therefore, each $|\psi_j\rangle\langle\psi_j|$ commutes with each B_k, which means $\mathscr{A}$ commutes with $\mathscr{B}$.

Next, suppose that both $\mathscr{A}$ and $\mathscr{B}$ are simple rank-1 POVMs. By Lemma 5 and the first conclusion in Theorem 7 as proved above, the inequality $F(\mathscr{A} \otimes \mathscr{B}) \geq F(\mathscr{A})$ is saturated iff $\mathscr{A}$ and $\mathscr{B}$ are identical rank-1 projective measurements up to relabeling. Alternatively, this conclusion follows from Lemmas 12, 15, and 17 (cf. the proof of Corollary 2).

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Correction: Several minor proof correction requests were not implemented properly and have now been applied.