Certainty relations, mutual entanglement, and nondisplaceable manifolds

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(Received 15 July 2015; published 9 September 2015)

We derive explicit bounds for the average entropy characterizing measurements of a pure quantum state of size N in L orthogonal bases. Lower bounds lead to novel entropic uncertainty relations, while upper bounds allow us to formulate universal certainty relations. For $L = 2$ the maximal average entropy saturates at $\log N$ because there exists a mutually coherent state, but certainty relations are shown to be nontrivial for $L \geqslant 3$ measurements. In the case of a prime power dimension, $N = p^k$, and the number of measurements $L = N + 1$, the upper bound for the average entropy becomes minimal for a collection of mutually unbiased bases. An analogous approach is used to study entanglement with respect to L different splittings of a composite system linked by bipartite quantum gates. We show that, for any two-qubit unitary gate $U \in \mathrm{U}(4)$ there exist states being mutually separable or mutually entangled with respect to both splittings (related by U) of the composite system. The latter statement follows from the fact that the real projective space $\mathbb{R}P^3 \subset \mathbb{C}P^3$ is nondisplaceable by a unitary transformation. For $L = 3$ splittings the maximal sum of L entanglement entropies is conjectured to achieve its minimum for a collection of three mutually entangled bases, formed by two mutually entangling gates.

DOI: 10.1103/PhysRevA.92.032109 PACS number(s): 03.65.Ta, 03.65.Aa, 03.67.Mn

I. INTRODUCTION

Quantum uncertainty relations characterizing the ultimate limitations [1,2] which nature puts on the preparation and measurements of any quantum state continuously attract significant attention. Much of it is focused on the entropic formulation of uncertainty [3–14], since the information entropy function is a clever collection of the information contained in all the moments of the probability distribution. Standard entropic uncertainty relations [15–17] provide a lower bound for the sum of entropies characterizing information obtained in two arbitrary orthogonal measurements. Various generalizations including positive-operator valued-measures (POVM) [12], coarse graining [18–21], quantum memory [22,23], different trade-off relations [24,25], or even quasi-Hermitian operators [26] and elaborate studies devoted to quantum protocols [27], can be found in the literature related to the topic discussed in this paper.

Conversely, no comparable effort had been made to establish relevant *certainty relations* [28,29] given as an upper bound for the sum of the two entropies in question. Even though, for more than two measurements described in terms of mutually unbiased bases (MUBs), almost optimal entropic certainty relations have been derived [28–32], there were no corresponding results valid for two arbitrary measurements. Two very recent contributions [33,34] independently solved that long-standing problem.

To show that, in the case of two orthogonal measurements, the upper bound for the sum of the two entropies can be saturated, Korzekwa *et al.* [33] utilized the mathematical notion of a *nondisplaceable manifold*. Such a type of manifold (necessarily embedded in a larger space) has a special feature that it cannot be displaced into any other position in a way that the original manifold and the displaced one do not intersect.

Consider, for instance, an equator of a standard two-sphere. It is easy to imagine that this particular manifold is nondisplaceable in S^2, because any two great circles of a sphere do intersect. There always exist two mutually antipodal points belonging simultaneously to both circles. Such a statement can be generalized in various ways for higher dimensions. Making use of the fact that a great torus T_{N-1} embedded in a complex projective space $\mathbb{C}P^{N-1}$ is nondisplaceable with respect to transformations by a unitary $U \in \mathrm{U}(N)$ [35], it is possible to show that there exists a quantum state *mutually unbiased* with respect to both bases. We shall further refer to such kind of state as being *mutually coherent*.

In this work we analyze upper bounds for the average entropy involving an arbitrary number of orthogonal measurements. We derive a universal certainty relation valid for any set of L measurements in an N-dimensional Hilbert space. Assuming that N is a power of prime, we further analyze the case of mutually unbiased bases, for which we conjecture that the difference between the upper and the lower limits is the smallest among all orthogonal measurements in $N + 1$ bases. An analogous statement that the variance of the Shannon entropy is minimal for MUBs is based on numerical results, while a counterpart proposition for the Tsallis entropy of order two (also called the linear entropy) is analytically proven.

The parallel aim of the paper is to analyze certain properties of quantum entanglement. Usually one discusses bipartite entanglement with respect to a given splitting of the composite Hilbert space, $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, naturally motivated by a concrete physical scenario. On the other hand, from a mathematical perspective, it is legitimate to analyze entanglement with respect to any different splitting of the Hilbert space, $\mathcal{H} = \mathcal{H}_{A'} \otimes \mathcal{H}_{B'}$. This point of view becomes very natural in the case of multipartite systems. For instance, in the case of four subsystems [36] one can investigate entanglement with

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respect to the splitting AB and CD, but also with respect to the splittings AC and BD or AD and BC.

In our current investigations, however, we focus on bipartite $N \times N$ systems [37]. For a given splitting $\mathcal{H}_A \otimes \mathcal{H}_B$ one defines the standard product basis, $|\phi_{ij}\rangle = |e_i^A\rangle \otimes |f_j^B\rangle$ and, making use of an arbitrary global unitary matrix U, introduces the rotated basis $U|\phi_{ij}\rangle$, with $i,j = 1,\dots,N$. One may now study entanglement with respect to both splittings of $\mathcal{H}$, determined by the two separable orthogonal bases. A quantum state separable with respect to any splitting of the Hilbert space is called absolutely separable [37] and, in the case of two-qubit systems, the structure of this set is well understood [38,39].

In this work we thus study the entanglement of a given quantum pure state with respect to several splittings of the composite Hilbert space. In a close analogy to the problem of uncertainty relations, in which one analyzes the average measurement entropy, we analyze here the average entanglement of a pure quantum state, computed with respect to an arbitrary collection of L splittings of the Hilbert space, related by global unitary matrices. Relaying on the fact that the real projective space $\mathbb{R}P^3$ is nondisplaceable in $\mathbb{C}P^3$ by a unitary transformation, we show that, for any two splittings of $\mathcal{H}_4$ into two subspaces of size two, there exists a *mutually entangled state*, maximally entangled with respect to both partitions. Numerical results allow us to conjecture that the same statement can be true for $N \times N$ systems.

This work is organized as follows: In Sec. II we introduce necessary notation and discuss trivial certainty relations for two orthogonal measurements. Some consequences of this result are further investigated in Sec. III. In Sec. IV we discuss mutual coherence in the situation with more than two measurements and derive the certainty and uncertainty relations relevant for any choice of L and N. The second part of the work is devoted to entanglement of a given pure state, quantified with respect to several different splittings of the composite Hilbert space. In Secs. V and VI we explore connections between the concept of mutually coherent states and quantum entanglement by searching for mutually entangled states and mutually entangling gates.

II. CERTAINTY RELATIONS AND MUTUALLY COHERENT STATES

Consider a quantum state $|\psi\rangle \in \mathcal{H}_N$ belonging to an N-dimensional Hilbert space $\mathcal{H}_N$ which is measured in several orthonormal bases determined by unitary matrices $\{U_k\}$. These bases (each of them forms the columns of a particular U_k) are eigenbases of some observables standing behind the measurements. Information gained in that process can be described by the Ingarden–Urbanik entropy [40]

$$S^{IU}(|\psi\rangle, U_k) = S_k = -\sum_{i=1}^{N} p_i^{(k)} \log p_i^{(k)}, \qquad (1)$$

which is the Shannon entropy calculated for the probability distribution $p_i^{(k)} = |\langle i|U_k|\psi\rangle|^2$. The choice of the base of the logarithm is arbitrary, but in numerical calculations we will use natural logarithms. The entropy S_k is a non-negative quantity upper-bounded by $\log N$. The question about the uncertainty and certainty relations for the two measurements (given in terms of U_1 and U_2) is devoted to the two numbers (or rather functions of N and $U_2U_1^\dagger$) $B_{\min}$ and $B_{\max}$ to be determined, such that

$$0 \leqslant B_{\min} \leqslant \frac{S_1 + S_2}{2} \leqslant B_{\max} \leqslant \log N. \qquad (2)$$

The matrix $U_2U_1^\dagger$ is a single quantity that matters here because, by the transformation $|\psi\rangle \mapsto U_1^\dagger|\psi'\rangle$, one can always bring the first unitary to be the identity $\mathbb{1}$, while all other matrices become multiplied by $U_1^\dagger$. A profound (although very rarely close to optimal) example of a valid $B_{\min}$ is $-\max_{i,j} \log c_{ij}$, with c_{ij} denoting the modulus of the matrix element of $U_2U_1^\dagger$, situated in the ith row and the jth column. This is the well-known Maassen–Uffink result [17].

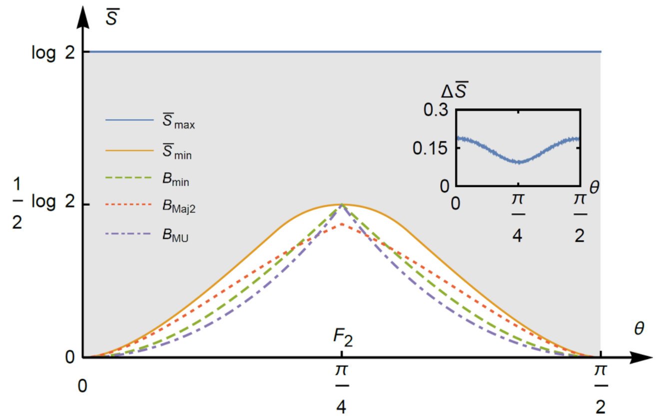

FIG. 1. (Color online) Average entropy $\bar{S}$ for two single-qubit measurements related by an orthogonal matrix $O \in O(2)$ as a function of the rotation angle θ. Solid lines denote numerical lower and upper bounds which limit the allowed region (shaded), while dotted lines represent Maassen–Uffink and majorization lower bounds. Dashed line corresponds to the bound $B_{\min}$ derived in this paper. The inset shows root mean square of the entropy $\Delta\bar{S}$ averaged over the set of pure states as a function of the angle θ.

In Fig. 1 we show behavior of the minimal and maximal average entropy $\bar{S} = (S_1 + S_2)/2$ for an orthogonal matrix $O = [\cos\theta, \sin\theta; -\sin\theta, \cos\theta]$ as a function of the rotation angle θ. Note that the case of any unitary matrix of order $N = 2$ is equivalent to a certain orthogonal matrix [5]. Even for this simple family, the minimal values $\bar{S}_{\min}$ are rather cumbersome [41]. $\bar{S}_{\min}$ lays obviously above the Maassen–Uffink bound [17] as well as the majorization bound B_{Maj2} derived in Ref. [8]. In Fig. 1 we also plot in advance our candidate for $B_{\min}$, which in Sec. IV is derived for an arbitrary setting described in general by L unitaries $U_1,\dots,U_L \in \mathrm{U}(N)$. The lower bound assumes the largest value for $\theta = \pi/4$, for which the matrix O coincided with the Hadamard matrix.

On the other hand, the upper bound occurs to be trivial, as the maximal value is always saturated, $B_{\max} = \bar{S}_{\max} = \log 2$. This is a direct consequence of a more general statement mentioned already in the introduction, saying that for any choice of a unitary matrix $U \in \mathrm{U}(N)$ one can always find a state $|\psi_{\mathrm{coh}}\rangle$ of the form $(1, e^{i\phi_2}, \dots, e^{i\phi_N})/\sqrt{N}$ such that all probabilities are equal, $|\langle i|\psi_{\mathrm{coh}}\rangle|^2 = |\langle i|U|\psi_{\mathrm{coh}}\rangle|^2 = 1/N$ [33,34]. This leads to the upper bound $B_{\max} = \log N$. Hence for any two orthogonal measurements in any dimension N there exist

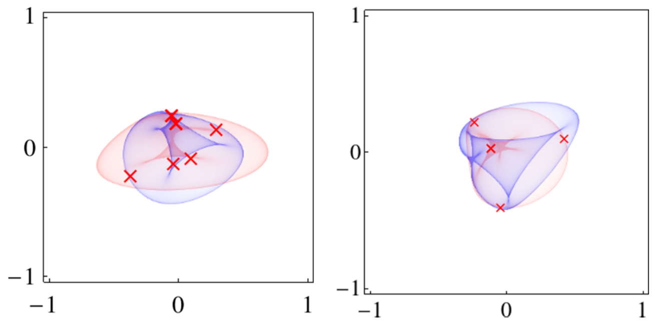

FIG. 2. (Color online) Two examples of projections of two tori T^2 and $U(T^2)$ embedded in $\mathbb{C}P^2$ on a plane. Here $U \in \mathrm{U}(3)$ and the crosses denote the intersection points.

no nontrivial upper bounds and certainty relations. This counterintuitive statement follows from the fact that the great tori T^{N-1} embedded in the set of pure states $\mathbb{C}P^{N-1}$ is nondisplaceable with respect to action of $\mathrm{U}(N)$ [35,42]. More intuitively, it is a generalization of an easy fact that any two great circles on a sphere do intersect. Therefore the torus T^{N-1} of basis coherent states [43] ($\phi_1 \equiv 0$)

$$|\psi_{\rm coh}^{\phi}\rangle = \frac{1}{\sqrt{N}}\sum_{j=1}^{N} e^{i\phi_j}|j\rangle,$$

and the torus $U|\psi_{\rm coh}^{\phi}\rangle$, defined in terms of any unitary matrix U (which in the above scheme is equal to $U_2U_1^{\dagger}$), of states coherent with respect to the transformed basis do intersect [33]. An arbitrary point from the intersection represents a *mutually coherent state*, coherent with respect to both bases, also called a "zero-noise, zero-disturbance state" [33]. Recent investigations show [44] that, for $N = 3$, both two-tori generically cross in six or four discrete points—see Fig. 2

Note that the density matrix $|\psi_{\rm coh}^{\phi}\rangle\langle\psi_{\rm coh}^{\phi}|$ written in both bases is *contradiagonal* [45] because it has all diagonal elements equal. Hence, taking into account permutations of the spectrum, the basis coherent states are as distant from the diagonal density matrices as possible at a single orbit of unitarily similar states. It is important to emphasize here the difference between the set of basis coherent states, which forms a torus, and the set of *spin coherent states* [46] or, more generally, $\mathrm{SU}(K)$ coherent states, producing a complex projective space $\mathbb{C}P^{K-1} \subset \mathbb{C}P^{N-1}$.

III. FURTHER CONSEQUENCES OF TRIVIAL CERTAINTY RELATION

The fact that $B_{\max} = \log N$ implies few interesting consequences. Assume that Alice possesses a maximally coherent (with respect to her computational basis $|1\rangle,\ldots,|N\rangle$) quantum state $|\psi_{\rm coh}^{\phi}\rangle$ with tunable parameters $\phi_2,\ldots,\phi_N$. Two immediate corollaries follow:

Corollary 1 (Sharing). For any choice of the basis on the Bob side, Alice can always tune the phases in a way that she can share the maximal coherence of the state $|\psi_{\rm coh}^{\phi}\rangle$ with Bob.

Corollary 2 (Recovering). In the presence of the unitary evolution given by an arbitrary unitary operator $U(t)$, so that the considered quantum state at any time moment T is equal to $U(T)|\psi_{\rm coh}^{\phi}\rangle$, Alice can always tune the phases in a way that she can recover the maximally coherent state, i.e., $U(T)|\psi_{\rm coh}^{\phi}\rangle$ is maximally coherent.

A physically relevant question related to the potential usefulness of the above corollaries concerns imperfections, i.e., the case when the angles $\phi_2,\ldots,\phi_N$ are not ideally tuned. What is then the coherence of the second (in Bob's basis or after the evolution) quantum state? In order to answer that question we need to quantify the coherence. To this end we resort to the l_1 norm of coherence

$$C_{l_1}(\rho) = \sum_{i\neq j}|\rho_{ij}| = \left(\sum_i |\langle i|\psi\rangle|\right)^2 - 1, \tag{3}$$

which is a proper measure [43,47] of the discussed resource. The second equality in (3) is valid only in the case when ρ is pure. For the maximally coherent state the measure attains its maximum equal to $N - 1$.

We start with the following simple lemma:

Lemma 1. Let $|\psi_{\rm coh}^{\phi}\rangle$ be a maximally coherent state and let $|\xi\rangle$ be any pure state such that

$$|\langle\psi_{\rm coh}^{\phi}|\xi\rangle|^2 = 1 - \varepsilon, \tag{4}$$

with some error ε. Then

$$C_{l_1}(|\xi\rangle) \geqslant N - 1 - \varepsilon N. \tag{5}$$

To prove this lemma we only notice that

$$\begin{aligned}\sqrt{1-\varepsilon} &= |\langle\psi_{\rm coh}^{\phi}|\xi\rangle| \\ &= \frac{1}{\sqrt{N}}\left|\xi_1 + \sum_{j=2}^{N} e^{-i\phi_j}\xi_j\right| \leqslant \frac{1}{\sqrt{N}}\sum_j|\xi_j|,\end{aligned} \tag{6}$$

where $\xi_j = \langle j|\xi\rangle$, and rearrange the resulting inequality by using (3).

We know that the angles in question can be tuned in a way that, for any unitary U, the state

$$|\tilde{\psi}_{\rm coh}^{\phi}\rangle = U|\psi_{\rm coh}^{\phi}\rangle \tag{7}$$

is maximally coherent. Moreover, if we prepare the state $|\psi_{\rm coh}^{\phi}\rangle$ imperfectly, so that instead of it we have at our disposal a state $|\xi\rangle$ satisfying (4), then also

$$|\langle\tilde{\psi}_{\rm coh}^{\phi}|U|\xi\rangle|^2 = 1 - \varepsilon. \tag{8}$$

The bound (5), which is linear in the error ε, thus immediately applies to the transformed state $U|\xi\rangle$. We observe that a general preparation imperfection described by ε linearly decreases the coherence of the quantum state. In the next part, we show that, whenever the imperfections are provided only by the phase mismatch ($\phi_1 = 0$),

$$|\xi\rangle = |\psi_{\rm coh}^{\phi+\chi}\rangle, \tag{9}$$

with $|\chi_j| \leqslant \varepsilon$, then the coherence decreases by a term quadratic in ε. We have the chain of relations

$$|\langle\psi_{\rm coh}^{\phi}|\xi\rangle|^2 = \frac{1}{N^2}\left|\sum_j e^{i\chi_j}\right|^2 \geqslant \frac{1}{N^2}\left|\sum_j e^{\pm i\varepsilon}\right|^2, \tag{10}$$

which directly lead to

$$\left|\langle\psi_{\mathrm{coh}}^{\boldsymbol{\phi}}|\xi\rangle\right|^2 \geqslant 1-\sin^2(\varepsilon) \quad \text{for even } N,$$
$$\left|\langle\psi_{\mathrm{coh}}^{\boldsymbol{\phi}}|\xi\rangle\right|^2 \geqslant 1-c_N\sin^2(\varepsilon) \quad \text{for odd } N, \tag{11}$$

with $c_N = 1 - 1/N^2$. These bounds, together with Lemma III show that the difference between $N-1$ and $C_{l_1}(U|\xi\rangle)$ is proportional to ε^2.

IV. MUTUAL COHERENCE FOR SEVERAL MEASUREMENTS

A. *Uncertainty and certainty relations*

In a more general setup, one studies L orthogonal measurements determined by a collection of L unitary matrices $\{U_1 \equiv \mathbb{1}, U_2, \dots, U_L\}$. The mutual coherence together with related concepts while described in terms of the information entropies is captured by the uncertainty and certainty relations

$$0 \leqslant B_{\min} \leqslant \frac{1}{L}\sum_{j=1}^{L} S_j \leqslant B_{\max} \leqslant \log N, \tag{12}$$

where, as before, S_j is the Shannon entropy of the probability distribution $p_i^{(j)} = |\langle i|U_j|\psi\rangle|^2$. In general, it is not an easy task to provide nontrivial bounds $B_{\min}$ and $B_{\max}$ valid for a broad class of measurements. Several lower bounds, leading to uncertainty relations, were recently studied in the literature [5,6,8,48], but we present below an alternative lower bound. Furthermore, we derive in Sec. IV B a universal upper bound which leads to a *certainty* relation. Note that the information acquired in the set of measurements can also be characterized by the average entropy of Rényi or Tsallis [49], which reduce to the Shannon entropy in particular cases.

For a given set of bases defining orthogonal measurements, the natural question appears of whether the average entropy can achieve the maximal value $\log N$. This is the case if there exists a mutually coherent state, i.e., the state $|\psi_{\mathrm{coh}}^{\boldsymbol{\phi}}\rangle$ such that

$$\frac{1}{L}\sum_{j=1}^{L} C_{l_1}\left(U_j|\psi_{\mathrm{coh}}^{\boldsymbol{\phi}}\rangle\right) = N-1 \tag{13}$$

is maximal. In order to answer the above question, we use the decomposition of unitary matrices [34,50], being a corollary of the fact that $|\psi_{\mathrm{coh}}^{\boldsymbol{\phi}}\rangle$ exists for $L=2$:

$$U_j = D(\boldsymbol{\omega}^{(j)})\mathcal{F}_N(1\oplus Y_j)\mathcal{F}_N^{\dagger}D(-\boldsymbol{\phi}^{(j)}). \tag{14}$$

This parametrization involves the phase gate

$$D(\boldsymbol{\alpha}^{(j)}) = \mathrm{diag}\left(e^{i\alpha_1^{(j)}}, e^{i\alpha_2^{(j)}}, \dots, e^{i\alpha_N^{(j)}}\right), \tag{15}$$

and the Fourier matrix $(\mathcal{F}_N)_{kl} = e^{2i\pi(k-1)(l-1)/N}/\sqrt{N}$. The matrices Y_j represent arbitrary $(N-1)$-dimensional unitary operations acting on the subspace spanned by $|2\rangle, \dots, |N\rangle$.

The phase gate $D(-\boldsymbol{\phi}^{(j)})$ acting on the state $|\psi_{\mathrm{coh}}^{\boldsymbol{\phi}^{(j)}}\rangle$ produces the dephased maximally coherent state of the form $|\psi_{\mathrm{coh}}^{\mathbf{0}}\rangle = \sum_{j=1}^{N}|j\rangle/\sqrt{N}$. Further application of the Fourier gate $\mathcal{F}_N^{\dagger}$ transforms the state $|\psi_{\mathrm{coh}}^{\mathbf{0}}\rangle$ into $|1\rangle$. The latter state remains unchanged if one applies $1\oplus Y_j$ with an arbitrary Y_j. In the final steps, the inverse Fourier transform together with the second phase gate in (14) leads to the final maximally coherent state $|\psi_{\mathrm{coh}}^{\boldsymbol{\omega}^{(j)}}\rangle$. We are now in position to answer the major question of this section.

Corollary 3. The unitary matrices $\mathbb{1}, U_2, \dots, U_L$ given by the decomposition (14), such that at least one $Y_j \neq \mathbb{1}$, possess a mutually coherent state if the phase gates $D(-\boldsymbol{\phi}^{(j)})$ are the same for all matrices in question, i.e., they do not depend on the index $j = 2, \dots, L$.

The above corollary is an immediate consequence of the involved decomposition. It does not exclude other possibilities with special $\boldsymbol{\phi}^{(j)}$-dependent internal unitaries Y_j allowing for different right phase gates, but the situation described by Corollary 3 seems to be generic.

We note in passing that the concept of mutual coherence is related to nonextensibility of mutually unbiased bases [51]. The set of MUBs is called extensible if there exists an additional basis formed by the states being mutually coherent with respect to the MUBs in question [52]. Thus, if the analyzed bases possess no mutually coherent state they are nonextensible.

B. Generally valid bounds

Our major aim is to derive the bounds $B_{\min}$ and $B_{\max}$ relevant for a general setting (arbitrary L and N) described in terms of a collection of unitaries $U_1, \dots, U_L$. To achieve this goal, we need to briefly introduce the Bloch representation of a quantum state. Denote by σ_i, $i = 1, \dots, N^2-1$, the traceless and Hermitian generators of the group SU(N) fulfilling $\mathrm{Tr}\sigma_i\sigma_{i'} = 2\delta_{i'i}$, which are given by Pauli matrices for $N=2$. Any quantum state can be spanned by a basis formed by the identity $\mathbb{1}_N$ and the matrices $\{\sigma_i\}$. In particular, the density matrix of the state $|\psi\rangle$ can be written as

$$|\psi\rangle\langle\psi| = \frac{1}{N}\left(\mathbb{1}_N + \sqrt{\frac{N(N-1)}{2}}\sum_{i=1}^{N^2-1} x_i\sigma_i\right). \tag{16}$$

The Bloch vector $\boldsymbol{x}$ is constrained by $\boldsymbol{x}\cdot\boldsymbol{x} = 1$ and [53,54]

$$2(N-2)\boldsymbol{x} = \sqrt{N(N-1)/2}\,\mathrm{Tr}((\boldsymbol{x}\cdot\boldsymbol{\sigma})\boldsymbol{\sigma}). \tag{17}$$

Let us now rescale the original probabilities $p_i^{(k)}$ to be

$$\tilde{p}_{i,k} = L^{-1}p_i^{(k)} \equiv \frac{1}{L}|\langle i|U_k|\psi\rangle|^2, \tag{18}$$

so that $\tilde{p}_{i,k}$ sum up (with respect to both $1\leqslant i\leqslant N$ and $1\leqslant k\leqslant L$) to 1. In other words, we treat L orthogonal measurements as a single POVM involving $N\cdot L$ Kraus operators.

Define the "purity" coefficient

$$\mathcal{P} = \sum_{k=1}^{L}\sum_{i=1}^{N}\tilde{p}_{i,k}^2, \quad \frac{1}{LN} \leqslant \mathcal{P} \leqslant \frac{1}{L}. \tag{19}$$

We now prove a statement crucial in the derivation of the general bounds.

Theorem 1. The coefficient $\mathcal{P}$ is bounded,

$$\mathcal{P}_{\min} \leqslant \mathcal{P} \leqslant \mathcal{P}_{\max}, \tag{20}$$

by

$$\mathcal{P}_{\min} = \frac{1}{LN} + \left(\frac{N-1}{2NL^2}\right)\mathcal{M}_{\min},$$
$$\mathcal{P}_{\max} = \frac{1}{LN} + \left(\frac{N-1}{2NL^2}\right)\mathcal{M}_{\max}, \tag{21}$$

where $\mathcal{M}_{\min}$ and $\mathcal{M}_{\max}$ respectively denote the minimal and the maximal eigenvalues of the matrix

$$M_{j'j} = \sum_{k=1}^{L}\sum_{i=1}^{N} \mathrm{Tr}(U_k^\dagger|i\rangle\langle i|U_k\sigma_{j'})\mathrm{Tr}(U_k^\dagger|i\rangle\langle i|U_k\sigma_j). \tag{22}$$

We start the proof with the chains of inequalities defining $\mathcal{P}_{\min}$ and $\mathcal{P}_{\max}$:

$$\mathcal{P} \leqslant \max_{|\psi\rangle}\mathcal{P} \leqslant \max_{\boldsymbol{x}\cdot\boldsymbol{x}=1}\mathcal{P} = \mathcal{P}_{\max}, \tag{23}$$

$$\mathcal{P} \geqslant \min_{|\psi\rangle}\mathcal{P} \geqslant \min_{\boldsymbol{x}\cdot\boldsymbol{x}=1}\mathcal{P} = \mathcal{P}_{\min}. \tag{24}$$

In other words, optimization with respect to $|\psi\rangle$ is equivalent to optimization made for the Bloch vector $\boldsymbol{x}$ constrained by $\boldsymbol{x}\cdot\boldsymbol{x} = 1$ and (17). We obtain the desired bounds by skipping the second constraint. Due to the fact that all matrices σ_i are traceless, we have the identity

$$\sum_{i=1}^{N} \mathrm{Tr}(U_k^\dagger|i\rangle\langle i|U_k\sigma_j) = 0, \tag{25}$$

leading to the dependence of $\mathcal{P}$ on $\boldsymbol{x}$, of the form

$$\mathcal{P}(\boldsymbol{x}) = \frac{1}{LN} + \frac{N-1}{2NL^2}\sum_{j',j=1}^{N^2-1} M_{j'j}x_j x_{j'}. \tag{26}$$

The last step of the proof is the direct optimization with respect to $\boldsymbol{x}$ which, since the matrix M is Hermitian, picks up its relevant eigenvalues.

We are now in position to present the major result of this section, which leads to *purity-optimized* entropic uncertainty and certainty relations.

Theorem 2. The valid bounds $B_{\min}$ and $B_{\max}$ are of the form

$$B_{\min} = L\mathcal{P}_{\max}[a(K+1)\log(K+1) + (1-a)K\log K], \tag{27}$$

where $K = \lfloor (L\mathcal{P}_{\max})^{-1}\rfloor$, $a = (L\mathcal{P}_{\max})^{-1} - K$, $\lfloor\cdot\rfloor$ denotes the floor function, and

$$B_{\max} = S(Q) - \log L, \tag{28}$$

with $S(Q)$ being the Shannon entropy of the probability vector

$$Q = \frac{1}{LN}\Big\{1 + (LN-1)\sqrt{r}, \underbrace{1-\sqrt{r},\ldots,1-\sqrt{r}}_{LN-1}\Big\}, \tag{29}$$

given by $r = (LN\mathcal{P}_{\min} - 1)/(LN-1)$.

The lower bound $B_{\min}$ is a direct extension of Theorem 2 established for mutually unbiased bases by Wu, Yu, and Mølmer in Ref. [30]. Because our Theorem IV B generalizes and extends Theorem 1 from Ref. [30], $B_{\min}$ is given as in Theorem 2 therein with their C being set to $L\mathcal{P}_{\max}$. Note that the results of Wu *et al.* were based on the detailed analysis performed by Harremoës and Topsøe [31]. To derive $B_{\max}$ we can directly rely on Ref. [31], using their Theorem II.5 part i. This result provides an upper bound for the sum of the Shannon entropies as a function of the coefficient $\mathcal{P}$. Since this bound is a decreasing function of $\mathcal{P}$, it remains valid when $\mathcal{P}$ becomes substituted by its lower bound, namely $\mathcal{P}_{\min}$. Note that the bound $B_{\max}$ is the genuinely first result of that kind, while the alternative lower bounds can also be obtained by averaging the pairwise bounds (for $L = 2$) or by multi-observable majorization [8]. There is no possibility to get the pairwise counterpart of $B_{\max}$ because, for $L = 2$, one has $\mathcal{M}_{\min} = 0$, $r = 0$ and consequently $S(Q) = \log N$.

In the following sections we study several numerical examples showing the behavior of the optimal bounds in comparison with the analytical results at hand, including the progress described above.

C. Three measurements for qubits

A great circle is nondisplaceable in a sphere, so any two such circles will always intersect. However, three great circles belonging to a sphere will generically not cross in a single point—see Fig. 5. Therefore one can expect that, for three orthogonal measurements of a qubit in three bases, the average entropy of the probability vectors representing the measurement outcomes will be less than the maximal value.

To investigate this issue we analyze a one-parameter family of three measurements, determined by three unitary matrices, depending on an angle θ:

$$U_1 = \mathbb{1}_2,\quad U_2 = \begin{pmatrix}\cos\theta & \sin\theta\\ \sin\theta & -\cos\theta\end{pmatrix},$$
$$U_3 = \begin{pmatrix}\cos\theta & \sin\theta\\ i\sin\theta & -i\cos\theta\end{pmatrix}. \tag{30}$$

Note that, for $\theta = 0$, all three bases coincide, while in the case of $\theta = \pi/4$ they become mutually unbiased. Figure 3 shows the average entropy of measurement in these three bases as a function of the angle θ: the shaded area shows the allowed region bounded by solid lines, where dotted (or dashed-dotted) lines denote bounds obtained by using the

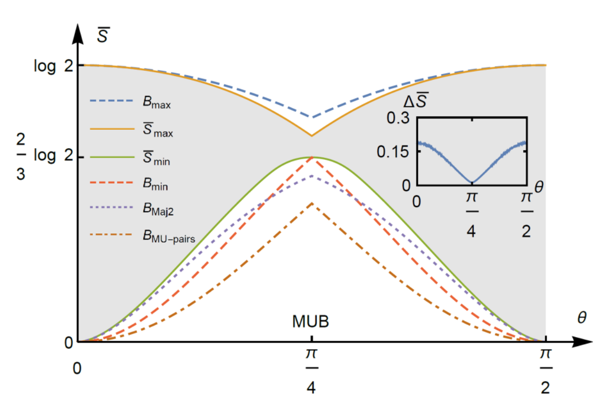

FIG. 3. (Color online) As in Fig. 1 for $L = 3$ measurements of a qubit. Note the upper bound $B_{\max}$ (28) represented by the upper dashed curve, which provides a nontrivial entropic certainty relation, and the lower bound $B_{\min}$ (27), which becomes tight at $\theta = \pi/4$ for MUBs.

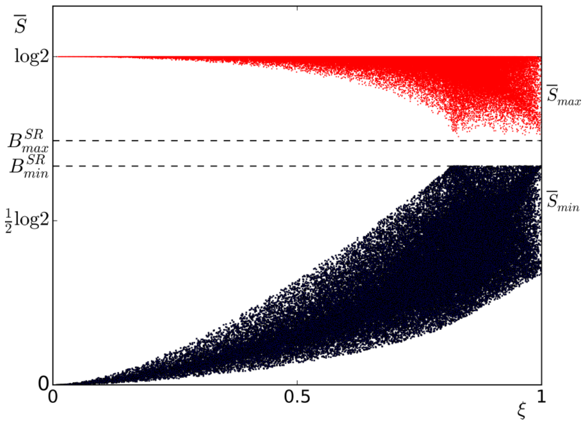

FIG. 4. (Color online) Maximal and minimal value of the averaged entropy $\bar{S}$ for a triple of random unitary gates of size $N = 2$ as a function of the parameter ξ, which characterizes the average deviation of unitary matrices from identity, and equals unity for MUBs.

Maassen–Uffink relation [17] and the majorization bound [8]. Dashed lines correspond to the bounds (27) and (28) provided by Theorem 2. Note that the difference between the upper and the lower limits, computed numerically and represented by solid lines, is the smallest for $\theta = \pi/4$, corresponding to MUBs. A similar property holds for the root-mean-square deviation of the entropy, $\Delta\bar{S}$, presented in the inset.

In order to explore the generic case of three arbitrary orthogonal measurements of a qubit, we work in the first basis once more by setting $U_1 = \mathbb{1}_2$ and draw the remaining two matrices U_2 and U_3 according to the Haar measure on the unitary group $\mathcal{U}(2)$. In Fig. 4 we present the maximal and minimal values of the average entropy $\bar{S}$ optimized over the set of all pure states for collection of three randomly chosen bases. The variable ξ on the horizontal axis characterizes the average deviation of the unitary transformation matrices from identity and is normalized as $0 \leqslant \xi \leqslant 1$. It is defined by

$$\xi^2 = \frac{4}{3}\sum_{j=1}^{3} v_j(1 - v_j), \tag{31}$$

where the probabilities: $v_1 = |(U_2)_{11}|^2 = \cos^2\theta_1$, $v_2 = |(U_3)_{11}|^2 = \cos^2\theta_2$, and $v_3 = |(U_2U_3^\dagger)_{11}|^2 = |\cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2 e^{i(\beta_1-\beta_2)}|^2$, are expressed as functions of phases entering the parametrization of unitary matrices $U_2 = [\cos\theta_1, \sin\theta_1; -\sin\theta_1, \cos\theta_1]$ and $U_3 = [e^{-i\beta_2}\cos\theta_2, -e^{-i\beta_1}\sin\theta_2; e^{i\beta_1}\sin\theta_2, e^{i\beta_2}\cos\theta_2]$.

The value $\xi = 0$ corresponds to the trivial case $\theta_1 = 0 = \theta_2$, for which $U_2 = \mathbb{1}$ and U_3 is a phase gate. The opposite value $\xi = 1$ describes the case of MUBs, for which $\theta_1 = \pi/4 = \theta_2$ and $\beta_1 = \pi/4 = \beta_2$. For $L = 3$ MUBs of size $N = 2$ the known bounds for the average entropy [28] are tight: $B^{\rm SR}_{\min} = \frac{2}{3}\log 2$ and

$$B^{\rm SR}_{\max} = \frac{1}{2}\log(6) - \frac{1}{2\sqrt{3}}\log(2+\sqrt{3}) \approx 0.516, \tag{32}$$

respectively. Note that $\log 2 \approx 0.693$, giving in this case that the ultimate upper bound attained by mutually coherent states is larger than the optimal value (32). In other words, the collection of three MUBs for $N = 2$ does not share any mutually coherent state. The bound $B_{\max}$, (28), provides a reliable upper limitation, especially beyond the MUB case.

A closer look at Fig. 4 reveals that the trivial lower bound equal to 0 is attained only if $\xi = 0$, as for other values of ξ the nontrivial entropic uncertainty relations apply. On the other hand, the maximal upper bound log 2, being the signature of mutual coherence, is saturated for every allowed value of ξ. This asymmetry is a major qualitative difference between mutual coherence and the 0-entropy case or, in different terms, between certainty and uncertainty relations. While the latter situation is typically forbidden by quantum mechanics, the former case is rather common. When one comes closer to mutual unbiasedness of the bases in question, it is however more likely to find examples which possess no mutually coherent state at all.

Observe that the difference between the upper and the lower limits is the smallest for $\xi = 1$, corresponding to MUBs. Numerical results show that a similar property holds for the variance of the entropy. We are not in position to prove this fact analytically for the Shannon entropy. However, a related statement formulated in terms of the variance of the Tsallis entropy of order two holds for any dimension N, for which a complete set of $N + 1$ MUBs exists—see Appendix C.

Geometrical intuition on the Bloch sphere

Any orthogonal basis in $\mathcal{H}_2$ can be represented as a pair of antipodal points on the Bloch sphere. With three bases (three pairs of antipodal points) one can thus associate (generically) eight spherical triangles laying on the Bloch sphere. Let $A_\blacktriangle$ and $P_\blacktriangle$ denote, respectively, the smallest area and the smallest perimeter calculated among all these triangles. Both parameters are equal to zero if all three bases do coincide and achieve the maximum if the three bases in question are mutually unbiased. Such a MUB case with $A_{\blacktriangle\,\max} = \pi/2$ and $P_{\blacktriangle\,\max} = 3\pi/2$ is sketched in Fig. 5. Moreover, we observe that the geometric parameters $A_\blacktriangle$ and $P_\blacktriangle$ are invariant with respect to any unitary rotation of the reference frame.

For any triple of random unitary matrices of order $N = 2$ we found (repeating the calculations leading to Fig. 4) the parameters $A_\blacktriangle$ and $P_\blacktriangle$, and further computed extremal values of the mean entropy $\bar{S}$ optimized over the set of pure states. Results presented in Fig. 6 show that the area of the minimal triangle carries information concerning the upper bound for the mean entropy while the smallest perimeter characterizes the lower bound. We observe that the proposed geometrical invariants (area and perimeter) reliably capture the property of mutual unbiasedness visible as the narrow entropy window on the right-hand side of the plot.

D. $N + 1$ measurements in N dimensions

Consider a family of four bases in $\mathcal{H}_3$ determined by the following unitary matrices:

$$U_1 = \mathbb{1}_3, \quad U_2 = (\mathcal{F}_3)^{4\theta/\pi}, \tag{33}$$

$$U_3 = D(\mathcal{F}_3)^{4\theta/\pi}, \quad U_4 = D^2(\mathcal{F}_3)^{4\theta/\pi}. \tag{34}$$

Here $\mathcal{F}_3$ represents the Fourier matrix of size three, while $D = \mathrm{diag}(1, \exp(i2\pi/3), \exp(i2\pi/3))$. As in the one-qubit case, all

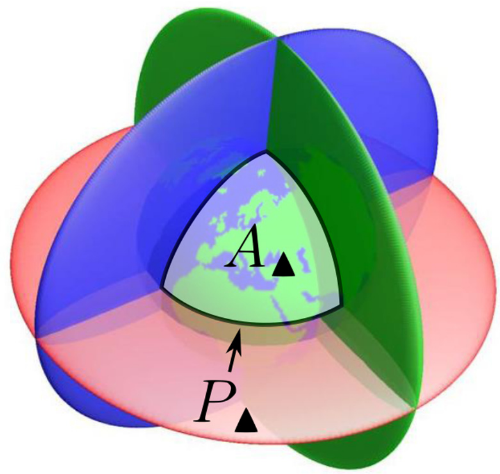

FIG. 5. (Color online) Three equators on the sphere usually do not cross at a single point as shown in the figure based on the logo of the International Conference on Squeezed States and Uncertainty Relations (ICSSUR) held in Gdańsk in 2015, which can be interpreted as a triple of MUBs for one qubit. Any collection of three orthogonal bases in $\mathcal{H}_2$ can be associated with triangles on a sphere characterized by the minimal area $A_\blacktriangle$ or the minimal perimeter $P_\blacktriangle$. In the case of the MUBs shown here, all eight spherical triangles are of equal shape and size.

matrices become diagonal for $\theta = 0$ and correspond to the same basis, while for $\theta = \pi/4$ the bases are mutually unbiased.

Figure 7 presents the behavior of numerically computed maximal and minimal values of the average entropy $\bar{S}$ compared with analytical bounds. Note that the difference between the numerical upper and the lower limits, which are represented by solid lines, is once more the smallest for $\theta = \pi/4$, corresponding to MUBs. A similar property holds as well for the root-mean-square deviation of the entropy, $\Delta\bar{S}$, presented in the inset.

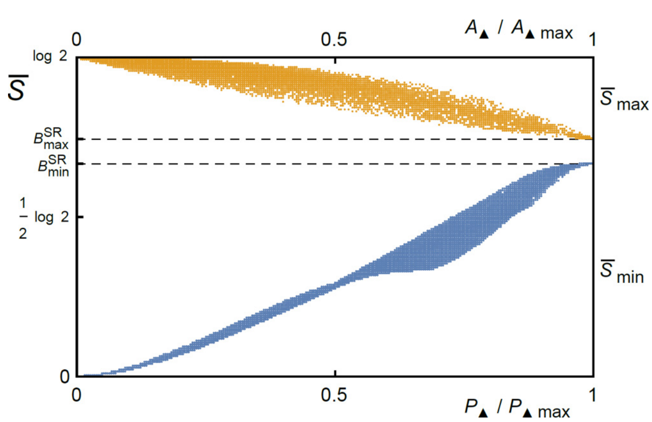

FIG. 6. (Color online) Limits of the average entropy $\bar{S}$ for $L = 3$ measurements optimized over pure states from $\mathcal{H}_2$. The parameter $\bar{S}_{\max}$ (upper abscissa; yellow) is depicted as a function of the smallest area $A_\blacktriangle$ of the spherical triangle while $\bar{S}_{\min}$ (lower abscissa; blue) is a function of the smallest perimeter $P_\blacktriangle$. Both parameters equal zero if the three bases coincide and they attain their maximal values $A_{\blacktriangle\,\max}$ and $P_{\blacktriangle\,\max}$ for a set of MUBs.

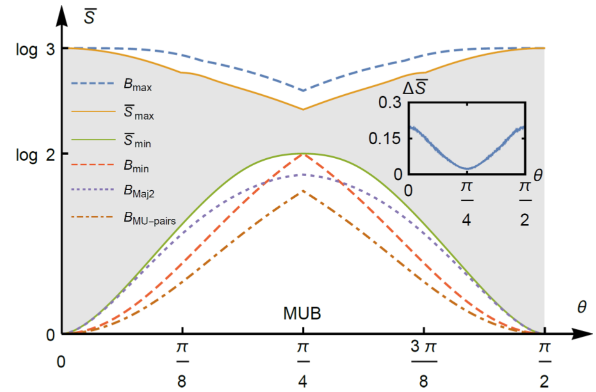

FIG. 7. (Color online) As in Fig. 3 for $L = 4$ orthogonal measurements in $N = 3$ dimensions. Note the nontrivial behavior of the maximal value $\bar{S}_{\max}$ and the upper bound $B_{\max}$, which attain their minima for $\theta = \pi/4$ corresponding to MUBs.

Let us now proceed to larger dimensions of the Hilbert space. In this place we are going to restrict our attention to prime-power dimensions, $N = p^k$, for which a set of $N+1$ MUBs is known [55,56]. In this very case concrete upper and lower bounds for the average entropy $\bar{S}$ were obtained by Sanchez–Ruiz [28,29],

$$B^{\mathrm{SR}}_{\min} = \begin{cases} \log \frac{N+1}{2} & \text{for } N \text{ odd} \\ \frac{N}{2(N+1)} \log \frac{N}{2} + \frac{N/2+1}{N+1} \log\left(\frac{N}{2}+1\right) & \text{for } N \text{ even,} \end{cases}$$

$$B^{\mathrm{SR}}_{\max} = \log N + \frac{(N-1)^2 \log (N-1)}{(N+1)N(N-2)}. \tag{35}$$

and later generalized by Wu, Yu, and Mølmer in Ref. [30]. Observe that both bounds asymptotically behave as $\log N -$ const., where the constant reads $a^{\mathrm{SR}}_{\min} = \log 2 \approx 0.693$ for the lower bound and it vanishes for the upper bound, i.e., $a^{\mathrm{SR}}_{\max} = 0$.

Figure 8 shows both bounds (dashed lines) compared with numerically obtained lower and upper limits $\bar{S}_{\min}$ and $\bar{S}_{\max}$. The central curve shows the behavior of the mean value $\langle \bar{S}\rangle_\psi$, averaged over entire set of pure states in $\mathcal{H}_N$ with respect to the unitarily invariant Haar measure. For dimensions N of the

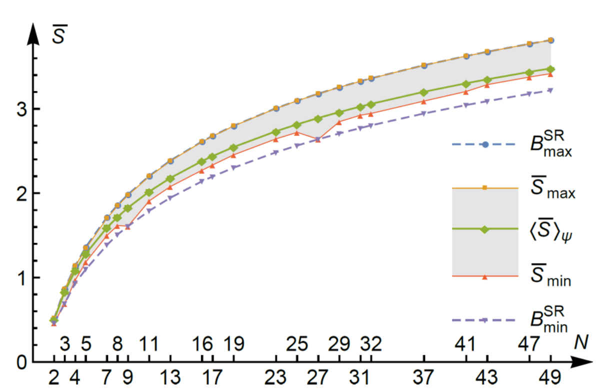

FIG. 8. (Color online) Behavior of the average entropy $\bar{S}$ over a set MUBs in $\mathcal{H}_N$ as a function of the dimensions N for power of primes. Upper and lower bounds of Sanchez–Ruiz are compared with numerical maximum and minimum taken over the set of all pure states.

order of 20 the error bars, marked in the graph, are smaller than the symbol size. Note that the allowed, shaded region, is very close to the upper bound of Sanchez. This suggests that the bound $B_{\max}^{\mathrm{SR}}$ is close to optimal, while it is more likely to improve the lower bound $B_{\min}^{\mathrm{SR}}$.

The mean Ingarden–Urbanik entropy of a random pure state is given by [57]

$$\langle S^{IU}\rangle = \Psi(N+1) - \Psi(2) \underset{N\to\infty}{\simeq} \log N - (1-\gamma), \quad (36)$$

where Ψ is the digamma function and $\gamma \approx 0.577$ is the Euler gamma constant. Unitary invariance of a random state $|\psi\rangle$ gives us that, for a complete set of MUBs in dimension $N = p^k$, we have

$$\left\langle \frac{1}{N+1}\sum_{i=1}^{N+1} S^{IU}(|\psi\rangle, U_i)\right\rangle = \Psi(N+1) - \Psi(2) \underset{N\to\infty}{\simeq} \log N - (1-\gamma). \quad (37)$$

Even though we were in a position to study the problem for dimensions not exceeding 50, we found it interesting to analyze limiting behavior of our results. All three numerical curves can be fit with the general relation $S_j \approx \log N - \text{const.}$, where the fit values are $a_{\min} \approx 0.48$, $a_{\max} \approx 0.07$, and $a_{\mathrm{av}} \approx 0.42$ for the average over all pure states. The latter value coincides well with the asymptotic result $a_\infty = 1 - \gamma \approx 0.422$, while the former values contribute to the conjecture that the lower analytical bound (35) of Sanchez might be easier to improve.

V. MUTUALLY ENTANGLED STATES

In the second part of this work we link uncertainty and certainty relations for the average measurement entropy with quantum entanglement related to different splittings of the composite Hilbert space. Although quantum entanglement is usually analyzed with respect to a fixed splitting of the Hilbert space, $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, distinguished by strong physical arguments, following Refs. [37–39] we analyze also entanglement with respect to any other splitting, say $\mathcal{H} = \mathcal{H}_{A'} \otimes \mathcal{H}_{B'}$, linked to the original splitting by a global unitary matrix U. Asking about an average entanglement of a given pure state with respect to several splittings of a composite space $\mathcal{H}$ we arrive at a problem closely related with the standard entropic uncertainty relations discussed above.

Entanglement of any pure state of a bipartite system $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ can be characterized by its *entropy of entanglement* equal to the von Neumann entropy of the partial trace $E(|\psi\rangle) := S(\rho_A)$, where $\rho_A = \mathrm{Tr}_B|\psi\rangle\langle\psi|$. In analogy with the notions presented in the previous sections we discuss the *mutual entanglement* of a given pure state with respect to an arbitrary number of L different splittings of the $N \times N$ composite system, determined by global unitary matrices $W_j \in U(N^2)$ with $j = 1,\dots,L$. We assume here that both Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ are N dimensional. A direct counterpart of the uncertainty relations (12) is

$$0 \leqslant E_{\min} \leqslant \bar{E} \leqslant E_{\max} \leqslant \ln N, \quad (38)$$

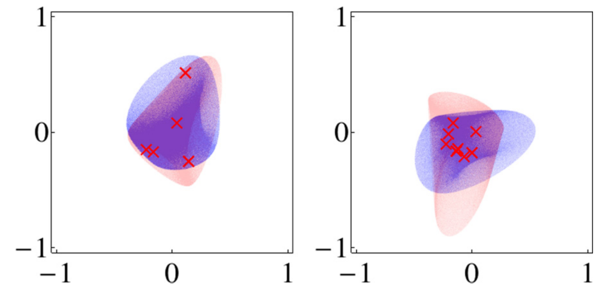

FIG. 9. (Color online) Two examples of projections of $\mathbb{R}P^3$ and $U(\mathbb{R}P^3)$ embedded in $\mathbb{C}P^3$ on a plane. Projection of intersection points marked by crosses correspond to the mutually entangled states.

where the mutual entanglement, averaged with respect to L different splittings of the Hilbert space, reads

$$\bar{E} := \frac{1}{L}\sum_{j=1}^{L} E(W_j|\psi\rangle), \quad (39)$$

and $\{W_j\}$ with $j = 1,\dots,L$ denotes a collection of L bipartite unitary gates, i.e., unitary matrices of order N^2. Note that similarly to the case of ordinary uncertainty relations it is convenient to set $W_1 = \mathbb{1}$.

We are now going to study the simplest case of $N = 2$ and $L = 2$, which deals with two splittings only. Apart from the original splitting given by the computational product basis $|i,j\rangle$ $(i,j = 1,2)$, there is the second splitting described by the transformed basis $W_2|i,j\rangle$. We have the following:

Proposition 1. Consider the case $N = 2$ and $L = 2$, and an arbitrary unitary matrix $W_2 \in \mathrm{U}(4)$. Then (a) the upper bound in (38) is saturated because there exists a *mutually entangled* state $|\psi_{\mathrm{ent}}\rangle$, so that $E_{\max} = \log 2$; and (b) the lower bound in (38) is saturated as well and there exists a *mutually separable* state $|\psi_{\mathrm{sep}}\rangle$, so that $E_{\min} = 0$.

A proof of this proposition based on canonical form of a two-qubit gate [58,59] is provided in Appendix A. To show part (b) of the above proposition one can also rely on geometric properties of projective spaces. Let us recall that in the two-qubit case the manifold of maximally entangled states is $\mathrm{U}(2)/\mathrm{U}(1) = \mathbb{R}P^3$. As it is known that $\mathbb{R}P^M$ is nondisplaceable in $\mathbb{C}P^M$ with respect to transformations by $\mathrm{U}(M+1)$ [42,60], two real manifolds embedded into a complex one have to intersect—see Fig. 9. In the particular case $M = 3$, the presence of the intersection points directly implies that for any choice of $W_2 \in \mathrm{U}(4)$ there exists a *mutually entangled state* $|\psi_{\mathrm{ent}}\rangle$ maximally entangled with respect to the partition of the Hilbert space in the computational basis $W_1 = \mathbb{1}$ and in the basis rotated by W_2.

For any family of $L = 2$ unitary matrices W_1, W_2 of order four, the upper bound for the averaged entanglement is saturated: $\bar{E} = \log 2$. Therefore we show in Fig. 10 the averaged entanglement $\bar{E}$ for a family of $L = 3$ unitary matrices of order four explicitly given later in (50). This plot, analogous to Fig. 3, displays nontrivial upper bounds for $\bar{E}$. Moreover, these results suggest that there exists a state mutually separable with respect to all three splittings of $\mathcal{H}_4$ into $\mathcal{H}_2 \otimes \mathcal{H}_2$.

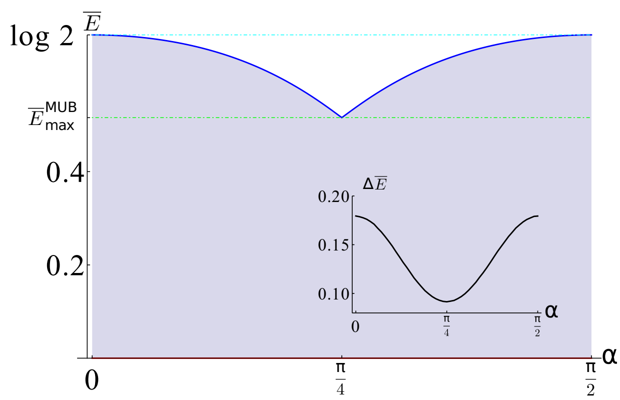

FIG. 10. (Color online) Average entanglement $\bar{E}$ for family of three unitary gates (50) of size four as a function of the phase α. For $\alpha = \pi/4$ corresponding to MEBs, the upper bound for $\bar{E}$ attains its minimum, as well as the root-square deviation $\Delta\bar{E}$ shown in the inset.

Numerical results obtained for the dimension $N = 3$ suggest that, *for any* unitary gate W_2 of order nine, there exists a related mutually entangled state, so that we conjecture that, in general, $E_{\max} = \log N$. To prove this conjecture it would be enough to show that the space of maximally entangled states $\mathrm{U}(N)/\mathrm{U}(1)$ is nondisplaceable in $\mathbb{C}P^{N^2-1}$ with respect to action of $\mathrm{U}(N^2)$. Note that the dimension of this space is $N^2 - 1$, and equals the *half* of the dimension of the embedding space, because it forms a Lagrangian manifold. Since the similar scenario occurred for quantum coherences, it is thus tempting to conjecture that the above statement, true if $N = 2$, holds also for any $N \geqslant 3$.

VI. MUTUALLY ENTANGLING GATES

In the previous section we introduced the concept of mutual entanglement and studied this notion in the simplest case of two different splittings of the composite Hilbert space. Now we consider an arbitrary number of $L \geqslant 3$ bipartite unitary matrices W_j, $j = 1,\dots,L$ (with $W_1 = \mathbb{1}$), which define different tensor-product structures. Since one copes with L different splittings of the entire system into subsystems, one can define the notion of separable and maximally entangled states with respect to these partitions and ask about the quantum states for which $\bar{E}$ given in (39) is minimal or maximal.

The same approach can be applied, for instance, in the particular case $N = 4$, as the system consists of two ququarts or rather four qubits A,B,C,D. For instance, setting $L = 3$ and choosing W_2 and W_3 to be suitable permutation matrices, which define bipartite splittings $AB|CD$, $AC|BD$ and $AD|BC$, respectively, one can study the mutual entanglement with respect to different partitions and look for maximally entangled multipartite states [61–64] such that all their reductions are maximally mixed. In the case of four qubits, there are no pure states maximally entangled with respect to the three above partitions [36,65].

In the case of bipartite unitary gates one distinguishes *special perfect entanglers*, which transform a product basis into maximally entangled basis [66]. More formally, a unitary matrix W acting on $\mathcal{H}_N \otimes \mathcal{H}_N$ will be briefly called an *entangling gate*, if all its columns are maximally entangled [67], so it transforms separable basis states into maximally entangled states

$$E(W|i,j\rangle) = \log N \quad \text{for} \quad i,j = 1,\dots,N. \tag{40}$$

Such gates are known for any N [68,69], so for $L = 2$ there exists a gate for which the minimal mutual entanglement $\bar{E}_{\min}$ will not be smaller than $\frac{1}{2}\log N$. Quite interestingly, for two-qubit systems such gates are especially distinguished, because they maximize the *entangling power*, i.e., the average entropy of entanglement produced from a generic separable state [70].

Analyzing the case of a larger number of unitaries $L \geqslant 3$, we are going to demonstrate the existence of *mutually entangling gates*, which are able to transform product states into states maximally entangled with respect to all L splittings in question. In other words, these unitary matrices are formed out of maximally entangled vectors, which remain maximally entangled in any transformed splitting. In a direct analogy to the notion of mutually unbiased bases [56] we define *mutually entangled gates*.

Definition 1. We say that a collection of unitary matrices $W_1 = \mathbb{1}, W_2,\dots,W_L \in \mathcal{U}(N^2)$ is *mutually entangled* if, for $i \neq j$, the gates $W_i^\dagger W_j$ satisfy condition (40), i.e., the columns of the matrix W_j are maximally entangled in the basis given by W_i and vice versa.

We shall also say that the columns of these unitary matrices form *mutually entangled bases* (MEBs). As shown below, both concepts happen to be closely related.

Theorem 3. If there exists a set of m MUBs in $\mathcal{H}_N$, then there also exists a set of m MEBs in $\mathcal{H}_N \otimes \mathcal{H}_N$.

In other words, Theorem 3 states that m mutually unbiased bases provide the set of m mutually entangling gates, for which the average entanglement $\bar{E}$ satisfies

$$\frac{m-1}{m}\log N \leqslant \bar{E} \leqslant \log N. \tag{41}$$

We prove the above theorem by constructing the relevant entangling gates. First we recall the construction of unitary bases by Werner [68], called "shift and multiply." For a given Latin square $\{\lambda(j,k)\}_{j,k=1}^N$ and a collection of Hadamard matrices $H^{(1)},H^{(2)},\dots,H^{(N)}$ one constructs unitary matrices

$$U^{(i,j)} = \sum_{k=1}^N H^{(j)}_{i,k}|\lambda(j,k)\rangle\langle k|, \tag{42}$$

which form an orthogonal basis of the Hilbert–Schmidt space of complex matrices of order N. Thus the columns of a matrix

$$V = \frac{1}{\sqrt{N}}\sum_{k,i,j=1}^N H^{(j)}_{i,k}|\lambda(j,k),k\rangle\langle i,j| \tag{43}$$

form a maximally entangled basis in $\mathbb{C}^{N^2}$. Note that V can be written as (T denotes the transposition)

$$V = P(H^{(1)T} \oplus H^{(2)T} \oplus \cdots \oplus H^{(N)T})U_{\mathrm{SWAP}}, \tag{44}$$

where U_{SWAP} is a swap permutation matrix and P is a permutation matrix given by

$$P = \sum_{k,l}|\lambda(l,k),k\rangle\langle l,k|. \tag{45}$$

The rows of the matrix V do not generate a maximally entangled basis, but if we permute its columns and define

$$W = P(H^{(1)T} \oplus H^{(2)T} \oplus \cdots \oplus H^{(N)T})P^T, \quad (46)$$

then the rows and columns of the matrix W generate a maximally entangled basis. The above reasoning leads to the following explicit construction of mutually entangled gates.

Assume that we are given a Latin square $\{\lambda(j,k)\}_{j,k=1}^{N}$ and a collection of k mutually unbiased bases $M_1, M_2, \ldots, M_k$ of size N. The bases are unbiased, that is

$$M_i^\dagger M_j \text{ is a rescaled Hadamard matrix for } i \neq j. \quad (47)$$

Using these matrices we introduce a collection of bases:

$$W^{(i)} = P(\mathbb{1} \otimes M_i)P^T. \quad (48)$$

We have the following:

Corollary 4. Let λ be a Latin square of size N and let P be defined as in (45). Then the bases $W^{(i)}$ are mutually entangled.

Proof. We write for $i \neq j$:

$$\begin{aligned} W^{(i)\dagger} W^{(j)} &= (P(\mathbb{1} \otimes M_i)P^T)^\dagger P(\mathbb{1} \otimes M_j)P^T \\ &= P(\mathbb{1} \otimes M_i^\dagger M_j)P^T. \end{aligned} \quad (49)$$

Since $M_i^\dagger M_j$ is a rescaled Hadamard matrix we obtain that $W^{(i)\dagger} W^{(j)}$ is a unitary basis. ∎

To demonstrate how the above construction works in action we provide in Appendix B the two collections of mutually entangled bases, respectively, for 2×2 and 3×3 systems.

A. Mutual entanglement for two-qubit system

Let us consider a family of matrices defined in (30) which interpolates between $\{\mathbb{1}, \mathbb{1}, \mathbb{1}\}$ for $\alpha = 0$ and MUBs for $\alpha = \pi/4$. From the above family we construct bases of $\mathbb{C}^4$ as

$$\left\{ W_0 = \mathbb{1}_4,\ W_1 = \begin{pmatrix} \cos(\alpha) & 0 & 0 & \sin(\alpha) \\ 0 & \cos(\alpha) & \sin(\alpha) & 0 \\ 0 & \sin(\alpha) & -\cos(\alpha) & 0 \\ \sin(\alpha) & 0 & 0 & -\cos(\alpha) \end{pmatrix}, \right.$$

$$\left. W_2 = \begin{pmatrix} \cos(\alpha) & 0 & 0 & \sin(\alpha) \\ 0 & \cos(\alpha) & \sin(\alpha) & 0 \\ 0 & i\sin(\alpha) & -i\cos(\alpha) & 0 \\ i\sin(\alpha) & 0 & 0 & -i\cos(\alpha) \end{pmatrix} \right\}. \quad (50)$$

In the case of $\alpha = \pi/4$ the above family forms mutually entangled bases. We analyzed lower and upper bounds for the average entanglement $\bar{E}$ with respect to three splittings of $\mathcal{H}_4$, as defined in (39). In the case of $L = 2$ splittings the upper bound, $\bar{E}_{\max} = \log 2$, can be saturated, but for $L = 3$ the upper bound becomes not trivial—see Fig. 10. The average entanglement $\bar{E}$ attains its minimal value, $\bar{E}_{\max}^{\mathrm{MEB}}$ given by (32), for three mutually entangled bases corresponding to $\alpha = \pi/4$.

VII. CONCLUDING REMARKS

A lot of work was recently done to improve and generalize entropic uncertainty relations, which provide lower bounds for the average entropy of probability vectors describing measurements in several orthogonal bases. Following the ideas of Sanchez [28] in this work we analyzed in parallel also upper bounds for the average entropy and obtained entropic uncertainty (27) and certainty (28) relations valid for an arbitrary number of measurements of any pure state in $\mathcal{H}_N$. The main motivation for such a study stems from a search of states which are simultaneously unbiased with respect to bases determining orthogonal measurements. Such states display the effects of quantum coherence with respect to all these bases, so that the average entropy becomes maximal.

In the case of any $L = 2$ measurements in an arbitrary N-dimensional Hilbert space, mutually coherent states exist, so the upper bound for the average entropy is saturated, $\bar{S} = \log N$. This result, related to nondisplaceability of the great torus in complex projective space $\mathbb{C}P^{N-1}$ [35], does not hold for a larger number of $L \geqslant 3$ measurements, for which certainty relations become nontrivial. Numerical results show that the analytic upper bound derived for MUBs by Sanchez [28] is rather precise, so it would be desirable to generalize them for other collections of orthogonal bases.

Analyzing probabilities obtained in sequence of L orthogonal measurements of a quantum state one can also interpreted them as a result of a single generalized measurement P, called a positive-operator-valued measure (POVM), which consists of $N \cdot L$ projection operators. Hence the averaged entropy (12) of L orthogonal measurements is equal, up to an additive constant $\log L$, to the entropy of the probability vector describing the POVM. Furthermore, the so-called *informational power* of P [71] associated with the set of MUBs, is closely related with the minimal entropy $\bar{S}_{\min}$, averaged over $L = N + 1$ measurements and minimized over the set of all pure states. This quantity occurs to be equal to $\log N - \bar{S}_{\min}$ [72–74], while the quantity $\log N - \bar{S}_{\max}$ coincides with the minimal relative entropy.

A complete set of $L = N + 1$ mutually unbiased bases in $\mathcal{H}_N$ forms an optimal scheme of a quantum measurement distinguished be several statistical properties [56]. Our numerical results allow us to conjecture that the complete set of MUBs minimizes fluctuations of the average entropy while varying the pure state investigated.

Conjecture 1. For any choice of $L = N + 1$ measurements in a dimension $N = p^k$ the lower bound for the averaged entropy $\bar{S}$ achieves its maximum and the upper bound achieves its minimum if L unitary matrices form a MUB.

Conjecture 2. The standard deviation of the averaged entropy $\Delta\bar{S} = (\langle \bar{S}^2 \rangle_\psi - \langle \bar{S} \rangle_\psi^2)^{1/2}$, averaged over the entire set of pure states of size N is minimal if the collection of $L = N + 1$ unitary matrices forms a MUB.

Not being able to prove Conjecture 2 for the Shannon entropy we provide in Appendix C a proof of an analogous proposition formulated in terms of the Tsallis entropy of order two. This result contributes to our understanding of the special role mutually unbiased bases play in the theory of quantum measurement.

The second key goal of this work was to establish a closer link between entropic uncertainty relations and the theory of quantum entanglement. While one usually investigates entanglement with respect to a fixed splitting of the Hilbert space, we study here also entanglement with respect to different splittings of the composite Hilbert space, related by a global unitary transformation.

For any composed Hilbert space $\mathcal{H} = \mathcal{H}_N \otimes \mathcal{H}_N$, the corresponding product basis $|i,j\rangle$ and a global unitary gate $U \in \mathrm{U}(N^2)$ one can investigate entanglement with respect to the transformed bases, $U|i,j\rangle$, with $i,j = 1,\ldots N$. For any pure state $|\psi\rangle$ of a bipartite system we analyzed its average entanglement $\bar{E}$ with respect to several choices of the separable bases, linked by unitaries $U_1,\ldots,U_L$, and investigated lower and upper bounds for this quantity.

In the case of two-qubit systems, the average entanglement for $L = 2$ can attain the limiting value $\log 2$ because a state *mutually entangled* with respect to both splittings exists. This result follows from the fact that the set of two-qubit maximally entangled states, equivalent to the real projective space $\mathbb{R}P^3$, is nondisplaceable in $\mathbb{C}P^3$ with respect to the action of U(4). Numerical results allow us to conjecture that a similar statement holds also in higher dimensions.

It is worth emphasizing that nondisplaceability of real projective spaces in the corresponding complex projective space [42] admits other applications. Consider $(N = 3)$-dimensional space corresponding to angular momentum $j = (N-1)/2 = 1$ and the set $\mathcal{C}$ of SU(2)-coherent states obtained by rotating the maximal-weight state $|j,j\rangle = |1,1\rangle$ by the Wigner rotation matrix [46]. In the stellar representation these states are described by two stars coinciding with a single point of the sphere. The set $\mathcal{A}$ of "anticoherent states," which are as far from $\mathcal{C}$ as possible, contains the state $|1,0\rangle$ represented by two stars in antipodal points at the sphere. Hence the set $\mathcal{A}$ has the form of the real projective space $\mathbb{R}P^2$, which is nondisplaceable in $\mathbb{C}P^2$ with respect to the action of U(3). This implies that the sets $\mathcal{A}$ and $\mathcal{A}' = U(\mathcal{A})$ do intersect, so there exists a pure state anticoherent with respect to any two choices of the maximal-weight state.

Let us conclude the paper with a short list of open questions. It is a challenge to improve explicit "certainty relations": *upper* bounds for the average entropy obtained for $L \geqslant 3$ measurements with respect to arbitrary orthogonal bases. In the case of MUB the upper bounds of Sanchez [28] occur to be rather precise, so it is more likely to improve his lower bounds. It would be interesting to derive analogous lower and upper bounds for the averaged entanglement of a bipartite state with respect to $L \geqslant 3$ different splittings of the Hilbert space and to prove existence of mutually entangled states for the general $N \times N$ problem.

ACKNOWLEDGMENTS

It is our pleasure to thank I. Bengtsson, P. Horodecki, K. Korzekwa, M. Kuś, P. Nurowski, M. Plenio, W. Słomczyński, A. Szymusiak, and L. Vaidman for fruitful discussions. We are grateful to M. Stobińska and M. Żukowski for giving us an opportunity to present these results during the International Conference on Squeezed States and Uncertainty Relations ICSSUR15 held in Gdańsk and for allowing us to modify the inspiring logo of the conference to prepare Fig. 5. We acknowledge financial support by the Polish National Science Centre (NCN) under Grant No. DEC-2012/04/S/ST6/00400 (Z.P.) and the John Templeton Foundation (K.Ż). Ł.R. acknowledges financial support from Grant No. 2014/13/D/ST2/01886 of the Polish National Science Centre. Research in Freiburg is supported by the Excellence Initiative of the German Federal and State Governments (Grant ZUK 43), the Research Innovation Fund of the University of Freiburg, the ARO under contracts W911NF-14-1-0098 and W911NF-14-1-0133 (Quantum Characterization, Verification, and Validation), and the DFG (GR 4334/1-1).

APPENDIX A: MUTUALLY ENTANGLED STATES AND MUTUALLY SEPARABLE STATES FOR TWO QUBITS

In this Appendix we demonstrate existence of mutually entangled states and mutually separable states in the two-qubit case. Without loss of generality we may consider two matrices $\mathbb{1}$ and $W_2 \in \mathrm{U}(4)$, which is brought by local unitary transformations into its canonical form [58,59],

$$W_2 = \begin{pmatrix} e^{ib_3}\cos(b1) & 0 & 0 & ie^{ib_3}\sin(b_1) \\ 0 & e^{-ib_3}\cos(b_2) & ie^{-ib_3}\sin(b_2) & 0 \\ 0 & ie^{-ib_3}\sin(b_2) & e^{-ib_3}\cos(b_2) & 0 \\ ie^{ib_3}\sin(b_1) & 0 & 0 & e^{ib_3}\cos(b_1) \end{pmatrix}, \tag{A1}$$

parametrized by three real parameters b_1,b_2,b_3. Next, we find vectors $|x\rangle$ and $|y\rangle$ such that

$$\begin{aligned} \tfrac{1}{2}E(|x\rangle) + \tfrac{1}{2}E(W_2|x\rangle) &= 0, \\ \tfrac{1}{2}E(|y\rangle) + \tfrac{1}{2}E(W_2|y\rangle) &= \log 2, \end{aligned} \tag{A2}$$

i.e., $|x\rangle$ is separable in both bases and $|y\rangle$ is maximally entangled in both bases.

We see immediately that we can take $|y\rangle = (|0,0\rangle + |1,1\rangle)/\sqrt{2}$. To show the existence of a mutually separable vector we consider two cases: If $b_2 = 0$ we may take $|x\rangle = |0,1\rangle$ and in opposite case we may take $|x\rangle$ to be proportional to

$$|x\rangle \simeq |0\rangle \otimes \left(|0\rangle + e^{2ib_3}\sqrt{\frac{\sin(b_1)\cos(b_1)}{\sin(b_2)\cos(b_2)}}\,|1\rangle\right). \tag{A3}$$

APPENDIX B: EXAMPLES OF MUTUALLY ENTANGLED BASES

We provide here exemplary collections of three unitary matrices of order 2^2 and four unitary matrices of order 3^2, which form mutually entangled bases (see Definition VI).

A collection of three mutually entangled bases for two qubits reads

$$W_1 = \mathbb{1}_4, \quad W_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & 1 & -1 & 0 \\ 1 & 0 & 0 & -1 \end{pmatrix}, \quad W_3 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \\ 0 & i & -i & 0 \\ i & 0 & 0 & -i \end{pmatrix}. \tag{B1}$$

In the case of two-qutrit systems, four mutually entangled bases are

$$W_1 = \mathbb{1}_9,$$

$$W_2 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & \omega & 0 & 0 & 0 & \omega^2 & 1 & 0 & 0 \\ 0 & 0 & \omega & 1 & 0 & 0 & 0 & \omega^2 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & \omega & 0 & 0 & 0 & \omega^2 \\ 0 & \omega^2 & 0 & 0 & 0 & \omega & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & \omega^2 & 1 & 0 & 0 & 0 & \omega & 0 \\ 1 & 0 & 0 & 0 & \omega^2 & 0 & 0 & 0 & \omega \end{pmatrix},$$

$$W_3 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & \omega^2 & 0 & 0 & 0 & 1 & \omega & 0 & 0 \\ 0 & 0 & \omega^2 & \omega & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ \omega & 0 & 0 & 0 & \omega^2 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & \omega^2 & \omega & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & \omega & 0 & 0 & 0 & \omega^2 & 0 \\ \omega & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \omega^2 \end{pmatrix},$$

$$W_4 = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & \omega & \omega^2 & 0 & 0 \\ 0 & 0 & 1 & \omega^2 & 0 & 0 & 0 & \omega & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ \omega^2 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & \omega \\ 0 & \omega & 0 & 0 & 0 & 1 & \omega^2 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & \omega & \omega^2 & 0 & 0 & 0 & 1 & 0 \\ \omega^2 & 0 & 0 & 0 & \omega & 0 & 0 & 0 & 1 \end{pmatrix}, \tag{B2}$$

where $\omega = e^{2\pi i/3}$ is the cubic root of unity.

APPENDIX C: VARIANCE OF MEASUREMENT OUTCOMES

Consider L orthogonal measurements performed on a quantum state of size N. Numerical results suggest that the variance of the average entropy characterizing the measurements is minimal if all measurement bases are mutually unbiased. In this Appendix we prove this statement for the Tsallis entropy or order two, earlier used for purpose of uncertainty relations [25,75].

The Tsallis entropy T_β of order $\beta > 0$ is defined as

$$T_\beta(p) = \frac{1}{\beta - 1}\Big(1 - \sum p_i^\beta\Big) \tag{C1}$$

and reduces to the Shannon entropy as $\alpha \to 1$.

Consider an arbitrary unitary matrix $U_i \in \mathrm{U}(N)$ defining a bases, in which an orthogonal measurement is performed. For any pure state $|\psi\rangle$ we introduce the corresponding vector of probabilities,

$$p_j^{(i)} = |\langle j|U_i|\psi\rangle|^2, \tag{C2}$$

described by the Tsallis entropy T_2,

$$T^{(i)} = T_2(p^{(i)}) = 1 - \sum_j \big(p_j^{(i)}\big)^2. \tag{C3}$$

Assume now that $|\psi\rangle$ is a random pure state distributed according to the unitary invariant Haar measure. We can now average the mean Tsallis entropy over the entire set of pure states and analyze its variance.

Theorem 4. Let $U_1 = \mathbb{1}, U_2, \ldots, U_L$ be a collection of L unitary matrices of order N, which for any state $|\psi\rangle$ leads to the set of probability vectors (C2) described by the Tsallis entropy (C3) and its mean value $\bar{T} = (T^{(1)} + T^{(2)} + \cdots + T^{(L)})/L$. If the set of L MUBs in dimension N exists then the variance of the mean entropy, $\mathrm{var}(\bar{T})$ averaged over the set of all pure states in $\mathcal{H}_N$ is minimal if matrices $\{U_j\}_{j=1}^L$ are mutually unbiased.

Proof. Note that, to prove this we can restrict our attention to the case of two unitary matrices. For convenience we denote $U_1 \equiv \mathbb{1}$, $U_2 \equiv U$ and

$$p_i = |\langle i|\psi\rangle|^2, \quad q_j = |\langle j|U|\psi\rangle|^2. \tag{C4}$$

Next we write

$$\begin{aligned} &\mathrm{var}(T_2(p) + T_2(q)) \\ &\quad = \langle (T_2(p) + T_2(q))^2\rangle - \langle T_2(p) + T_2(q)\rangle^2 \\ &\quad = \big\langle T_2^2(p)\big\rangle + \big\langle T_2^2(q)\big\rangle - \langle T_2(p) + T_2(q)\rangle^2 + 2\langle T_2(p)T_2(q)\rangle. \end{aligned} \tag{C5}$$

Unitary invariance of the distribution of $|\psi\rangle$ implies that the first three terms do not depend on U, so to get the minimum value of the variance one has to minimize the last term $\langle T_2(p)T_2(q)\rangle$. Let us rewrite it in the form

$$\begin{aligned} \langle T_2(p)T_2(q)\rangle &= \Big\langle \Big(1 - \sum p_i^2\Big)\Big(1 - \sum q_i^2\Big)\Big\rangle \\ &= 1 - \Big\langle \sum p_i^2\Big\rangle - \Big\langle \sum q_i^2\Big\rangle + \Big\langle \sum p_i^2 \sum q_j^2\Big\rangle. \end{aligned} \tag{C6}$$

To get the minimum one should minimize the average $\langle \sum p_i^2 \sum q_j^2\rangle$, which consists of the following terms:

$$\big\langle p_i^2 q_j^2\big\rangle = \langle |\psi_i|^4 |(U|\psi\rangle)_j|^4\rangle. \tag{C7}$$

Treating the vector $|\psi\rangle$ as a first column of a random unitary matrix distributed according to the Haar measure, we can use

Weingarten calculus [76] and obtain the following value:

$$\langle|\psi_i|^4|(U|\psi\rangle)_j|^4\rangle = \frac{(N-1)!4!}{(N+3)!}\left(|u_{ji}|^4 + |u_{ji}|^2\sum_{k\neq i}|u_{jk}|^2 + \frac{1}{6}\sum_{k=1}^{N}|u_{jk}|^4 + \frac{1}{6}\sum_{\substack{k\neq l\\ k,l\neq i}}^{N}|u_{jk}|^2|u_{jl}|^2\right). \tag{C8}$$

The above result implies that

$$\begin{aligned}\left\langle\sum_i p_i^2\sum_j q_j^2\right\rangle &= \frac{(N-1)!4!}{(N+3)!}\left(\left(1+\frac{(N-1)}{6}\right)\sum_{ij}|u_{ij}|^4 + \left(1+\frac{(N-2)}{6}\right)\sum_i\sum_{k\neq l}|u_{ik}|^2|u_{il}|^2\right)\\ &= \frac{(N-1)!4!}{(N+3)!}\left(\frac{1}{6}\sum_{ij}|u_{ij}|^4 + \left(1+\frac{N-2}{6}\right)\sum_i\sum_{kl}|u_{ik}|^2|u_{il}|^2\right)\\ &= \frac{(N-1)!4!}{(N+3)!}\left(\frac{1}{6}\sum_{ij}|u_{ij}|^4 + \left(1+\frac{N-2}{6}\right)N\right).\end{aligned} \tag{C9}$$

It is now easy to conclude that the above expression is minimized for $|u_{ij}|^2 = 1/N$, i.e., for U being unbiased with identity. The same reasoning applied for $L(L-1)/2$ pairs of measurements gives us that the variance of the sum of all measurements will be minimal if all matrices are mutually unbiased. ■

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