Geometric approach to extend Landau-Pollak uncertainty relations for positive operator-valued measures

G.M. Bosyk[1,2], S. Zozor[2,1], M. Portesi[1,2], T.M. Osán[3], and P.W. Lamberti[3]

[1] *Instituto de Física La Plata (IFLP), CONICET, and Departamento de Física, Facultad de Ciencias Exactas, Universidad Nacional de La Plata, 1900 La Plata, Argentina,*

[2] *Laboratoire Grenoblois d'Image, Parole, Signal et Automatique (GIPSA-Lab, CNRS), 11 rue des Mathématiques, 38402 Saint Martin d'Hères, France, and*

[3] *Facultad de Matemática, Astronomía y Física (FaMAF), Universidad Nacional de Córdoba, and CONICET, Avenida Medina Allende S/N, Ciudad Universitaria, X5000HUA, Córdoba, Argentina*

(Dated: January 1, 2018)

We provide a twofold extension of Landau–Pollak uncertainty relations for mixed quantum states and for positive operator-valued measures, by recourse to geometric considerations. The generalization is based on metrics between pure states, having the form of a function of the square of the inner product between the states. The triangle inequality satisfied by such metrics plays a crucial role in our derivation. The usual Landau–Pollak inequality is thus a particular case (derived from Wootters metric) of the family of inequalities obtained, and, moreover, we show that it is the most restrictive relation within the family.

PACS numbers: 03.65.Ca, 03.65.Ta, 02.50.-r, 05.90.+m
Keywords: Landau–Pollak inequality, uncertainty relations, metrics, mixed states, POVM

I. INTRODUCTION

The uncertainty principle is one of the most important principles in quantum mechanics. Originally stated by Heisenberg [1], it establishes a limitation on the simultaneous predictability of incompatible observables. Uncertainty relations constitute the quantitative expressions of this principle. The first formulations, due to Heisenberg, Robertson and Schrödinger [1, 2], are the most popular ones. However, they exhibit a state-dependent lower bound for the product of the variances of a pair of noncommuting observables. Thus, a drawback of this formulation is that it is not universal; moreover, the universal bound (the minimum over the states) is trivial, i.e., it equals zero. Several alternatives have been studied, such as those using the sum of the variances instead of the product [3], or those using information-theoretic measures as quantifiers of lack of information (see Refs. [4–6], and [7] for recent reviews). Recently, some of us [8] extended entropic formulations of the uncertainty principle to the case of a pair of observables with nondegenerate discrete N-dimensional spectra, using generalized informational entropies. The proposed formulation makes use of the Landau–Pollak inequality (LPI) which has been introduced in time-frequency analysis [9], and later on adapted to the quantum mechanics' language [4]. In this last case, the inequality is itself a (geometric) formulation of the uncertainty principle and applies for pure states and nondegenerate observables. The goal of this paper is precisely to extend the scope of Landau–Pollak-type inequalities.

Let us consider a pure state $|\Psi\rangle$ belonging to an N-dimensional Hilbert space $\mathcal{H}$, and two observables with discrete, nondegenerate spectra and corresponding eigenbases $\{|a_i\rangle\}_{i=1,\ldots,N}$ and $\{|b_j\rangle\}_{j=1,\ldots,N}$, described by the operators $A=\sum_{i=1}^N a_i\,|a_i\rangle\langle a_i|$ and $B=\sum_{j=1}^N b_j\,|b_j\rangle\langle b_j|$. The LPI [4, 9] reads:

$$\arccos\Big(\max_i|\langle a_i|\Psi\rangle|\Big)+\arccos\Big(\max_j|\langle b_j|\Psi\rangle|\Big)\geq\arccos c \tag{1}$$

where $c=\max_{ij}|\langle a_i|b_j\rangle|$ is the so-called overlap between the eigenbases of the observables. The overlap ranges from $\frac{1}{\sqrt{N}}$ (complementary observables) to 1 (the observables share at least an eigenstate). The quantity $|\langle a_i|\Psi\rangle|^2$ (resp. $|\langle b_j|\Psi\rangle|^2$) is interpreted as the probability that observable A (resp. B), for a system in preparation $|\Psi\rangle$, takes the eigenvalue a_i (resp. b_j). The LPI (1) is a meaningful expression of the strong uncertainty principle for nondegenerate observables and pure states. On the one hand, unlike standard approaches, the right hand side of (1) is a state-independent lower bound on the probability distributions associated with observables A and B. The bound is nontrivial whenever $c<1$, i.e., when the observables A and B do not share a common eigenstate. On the other hand, when $\max_i|\langle a_i|\Psi\rangle|^2=1$, i.e., when the probability distribution associated to observable A is concentrated, LPI implies that $\max_i|\langle b_i|\Psi\rangle|^2\leq c^2<1$ that means that the probability distribution associated with observable B cannot be concentrated; Furthermore, in the complementary case $c=\frac{1}{\sqrt{N}}$, the probability distribution associated with observable B must be uniform. Besides, LPI has been used to improve Maassen–Uffink entropic uncertainty relation [5], and a weak version has been used to obtain entanglement criteria [10, 11].

The extraction of information from a quantum system inevitably requires to perform a measurement. The simplest one is a projection valued measure (PVM), also known as von Neumann measurement. However, a description of a measurement by PVM is in general insufficient because most of the observations that can be performed are not of this type. Besides, for many applications one is only interested in the probability distributions associated to the observables but not in the post-measurement state. Fortunately, there exists a simple mathematical tool known as positive operator-valued measures (POVM) formalism which provides a generalization of standard projective measurements and also a description of any possible measurement to be performed [13, 14].

Until recently, LPI had only been demonstrated for pure quantum states. However, in a recent contribution [12], inequality (1) was generalized to deal with mixed states for the case of nondegenerate observables, and was indeed extended (based on geometric concepts) using a family of uncertainty measures other than the arccosine (which is related to Wootters metric). Here we go a step further, extending the LPI (1) and its generalization given in Ref. [12], in order to deal with degenerate observables described by POVM sets. In Sec. II, we first resume the framework, namely that of two observables described by two POVM sets, and we describe measures of uncertainty based on a class of metric between pure states. Then we formulate our main results, namely: (i) extension of the LPI in the context of POVM using a class of generalized uncertainty measures, (ii) determination of the most restrictive measure within the class considered, and (iii) analysis of the uncertainty intrinsic to a given POVM set. In Sec. III we provide some numerical illustrations. We analyze the consequences of the extended LPI in the context of POVM, and we also discuss the optimality or not of the uncertainty relations obtained. Some conclusions are drawn in Sec. IV. The proof of the extended LPI is made in several steps, developed in detail in App. A; whereas in App. B the algorithms used for the simulations are presented.

II. GENERALIZED LANDAU–POLLAK INEQUALITIES: MAIN RESULTS

Let us consider two observables A and B described by the POVM sets $\mathcal{A} = \{A_i\}_{i=1,\dots,N_A}$ and $\mathcal{B} = \{B_j\}_{j=1,\dots,N_B}$, respectively, i.e., $\mathcal{A}$ and $\mathcal{B}$ are sets of Hermitian (or self-adjoint) positive semi-definite operators acting on an N-dimensional Hilbert space $\mathcal{H}$, that satisfy the completeness relation or resolution of the identity: $\sum_{i=1}^{N_A} A_i = I = \sum_{j=1}^{N_B} B_j$, where I is the identity operator on $\mathcal{H}$, and N_A and N_B are not necessarily equal to one another, or equal to N. In some sense, the A_i's (resp. B_j's) allow to represent the possible outcomes of observable A (resp. B). Also, let us consider a system whose state is described by a density operator ρ acting on $\mathcal{H}$, where ρ is Hermitian, positive semi-definite, and normalized ($\operatorname{Tr}\rho = 1$). We denote by $\mathcal{D}$ the set of density operators. The quantity

$$p_i(A;\rho) = \operatorname{Tr}(A_i \rho)$$

represents the probability of measuring the ith outcome of A when the system is in the state ρ [13]. In the context of observables with nondegenerate spectra and pure states, the operators take the form of rank one projectors, $A_i = |a_i\rangle\langle a_i|$ and $\rho = |\Psi\rangle\langle\Psi|$.

Let us now turn to the consideration of a measure of uncertainty that allows us for the generalization of the LPI. We start with continuous functions $f : [0\,;\,1] \mapsto \mathbb{R}_+$, that are strictly decreasing and satisfy $f(1) = 0$, and such that for two (normalized) pure states $|\Psi\rangle$ and $|\Phi\rangle$, $f\left(|\langle\Psi|\Phi\rangle|^2\right) = d_f\left(|\Psi\rangle, |\Phi\rangle\right)$ defines a metric between them. This kind of metrics is interesting as they depend on the inner product between two quantum states and, hence, they are invariant under unitary transformations. Some well-known cases are:

- $f(x) = \arccos\sqrt{x}$, leading to the Wootters metric, or Bures angle [15],
- $f(x) = \sqrt{2\left(1-\sqrt{x}\right)}$, leading to the Bures metric [13, 16],
- $f(x) = \sqrt{1-x}$, related to the root-infidelity metric [17], or Hilbert–Schmidt or trace distance [13].

We notice that these metrics extend to (or, indeed, were defined for) mixed states, with function f being applied to the fidelity between two mixed states [13, 18]. From such metrics d_f, the quantity

$$\mathcal{U}_f\left(\mathcal{A};\rho\right) = f\left(P_{\mathcal{A};\rho}\right) \tag{2}$$

with

$$P_{\mathcal{A};\rho} = \max_i \operatorname{Tr}\left(A_i\rho\right) = \max_i p_i(A;\rho) \tag{3}$$

defines an uncertainty measure corresponding to the measurement of a set $\mathcal{A}$ of operators that describe observable A, for a system in a state ρ, in the sense that [12]

- $\mathcal{U}_f\left(\mathcal{A};\rho\right) \ge 0$ for all $P_{\mathcal{A};\rho} \in \left[\frac{1}{N_A}, 1\right]$, and
- $\mathcal{U}_f\left(\mathcal{A};\rho\right)$ is decreasing in terms of the maximal probability $P_{\mathcal{A};\rho}$, with
  - ⋄ $\mathcal{U}_f\left(\mathcal{A};\rho\right)$ is maximum iff $P_{\mathcal{A};\rho} = \frac{1}{N_A}$, that is equivalent to the equiprobability situation $p_i(A;\rho) = \frac{1}{N_A}$ for all i,
  - ⋄ $\mathcal{U}_f\left(\mathcal{A};\rho\right)$ vanishes iff $P_{\mathcal{A};\rho} = 1$, that is equivalent to the certainty situation $p_i(A;\rho) = \delta_{ik}$ for a given k.

Our main result in the present contribution is a twofold generalization of Landau–Pollak-type uncertainty relations, comprising the cases of mixed states and of POVM descriptions. We establish the following theorem, whose proof is postponed until Apps. A 1–A 3, and give a discussion below.

Theorem 1. *Let $\mathcal{A} = \{A_i\}_{i=1,\dots,N_A}$ and $\mathcal{B} = \{B_j\}_{j=1,\dots,N_B}$ be two positive operator valued measures describing discrete observables A and B, respectively, and acting on an N-dimensional Hilbert space $\mathcal{H}$. Then for an arbitrary density operator $\rho \in \mathcal{D}$ acting on $\mathcal{H}$, the following relation holds:*

$$\mathcal{U}_f\left(\mathcal{A};\rho\right) + \mathcal{U}_f\left(\mathcal{B};\rho\right) \geq f\left(c_{\mathcal{A},\mathcal{B}}^{\,2}\right) \tag{4}$$

where

$$c_{\mathcal{A},\mathcal{B}} = \max_{ij} \left\| \sqrt{A_i}\,\sqrt{B_j} \right\| \;=\; \max_{ij} \left\| \sqrt{B_j}\,\sqrt{A_i} \right\| \tag{5}$$

is the generalized overlap between the two POVM sets.

The overlap (5) is given in terms of an operator norm. For the sake of completeness, we recall here its definition: for any operator O on $\mathcal{H}$, $\|O\| = \max_{|\varphi\rangle\in\mathcal{H}} \frac{\|O|\varphi\rangle\|}{\||\varphi\rangle\|} = \max_{|\varphi\rangle\in\mathcal{H}} \frac{\langle\varphi|O^\dagger O|\varphi\rangle^{\frac{1}{2}}}{\langle\varphi|\varphi\rangle^{\frac{1}{2}}} = \max_{|\Psi\rangle\in\mathcal{H}:\||\Psi\rangle\|=1} \|O|\Psi\rangle\|$, where $O^\dagger$ is the adjoint operator of O [19].

Notice that, in the case of observables with nondegenerate spectra, letting $A_i = |a_i\rangle\langle a_i|$ and $B_j = |b_j\rangle\langle b_j|$ then one has $c_{\mathcal{A},\mathcal{B}} = \max_{ij} |\langle a_i|b_j\rangle| = c$. The generalization of LPI to mixed states proved in Ref. [12] is then recovered from Theorem 1. Moreover, in this case, inequality (4) is sharp whatever f, in the sense that there exists at least one state that renders equality. Indeed, denoting by (i', j') the pair of indices such that $c_{\mathcal{A},\mathcal{B}} = \|\sqrt{A_{i'}}\,\sqrt{B_{j'}}\|$, and choosing $|\Psi\rangle = |a_{i'}\rangle$ or $|\Psi\rangle = |b_{j'}\rangle$, together with the fact that $f(1) = 0$, allows to prove the assertion.

A way to look at the family of inequalities (4) is in the sense that they establish a restriction to the values that the pair of maximal probabilities $(P_{\mathcal{A};\rho}\,,\,P_{\mathcal{B};\rho})$ can take jointly, within the rectangle $\left[\frac{1}{N_A}\,;\,1\right] \times \left[\frac{1}{N_B}\,;\,1\right]$. We point out that the fact discussed in the preceding paragraph for the context of nondegenerate observables, does not mean that the whole family of inequalities renders the same permitted domain for the pair; that is neither the case in the POVM context. And, in fact, the restriction imposed by (4) manifests in a reduced rectangle. Indeed, if $P_{\mathcal{A};\rho} \leq c_{\mathcal{A},\mathcal{B}}^{\,2}$ (resp. $P_{\mathcal{B};\rho} \leq c_{\mathcal{A},\mathcal{B}}^{\,2}$), then $f(P_{\mathcal{A};\rho}) \geq f(c_{\mathcal{A},\mathcal{B}}^{\,2})$ [resp. $f(P_{\mathcal{B};\rho}) \geq f(c_{\mathcal{A},\mathcal{B}}^{\,2})$] and thus inequality (4) is satisfied whatever $P_{\mathcal{B};\rho} \in \left[\frac{1}{N_B}\,;\,1\right]$ $\left(\text{resp. } P_{\mathcal{A};\rho} \in \left[\frac{1}{N_A}\,;\,1\right]\right)$. But if (and only if) the pair $(P_{\mathcal{A};\rho}, P_{\mathcal{B};\rho})$ is within the square $(c_{\mathcal{A},\mathcal{B}}^{\,2}\,;\,1]^2$, the inequality becomes restrictive. A careful look at (4) suggests us to define the function

$$\begin{aligned} h_c^f &\;:\; [c^2\,;\,1] \to [c^2\,;\,1] \\ h_c^f(x) &\;=\; f^{-1}\left(f(c^2) - f(x)\right) \end{aligned} \tag{6}$$

Thus, the restriction due to inequality (4) writes down as

$$P_{\mathcal{B};\rho} \leq h_{c_{\mathcal{A},\mathcal{B}}}^f(P_{\mathcal{A};\rho}) \qquad \text{for} \qquad P_{\mathcal{A};\rho} \in (c_{\mathcal{A},\mathcal{B}}^{\,2}\,;\,1] \tag{7}$$

(a similar relation is valid exchanging the roles of $\mathcal{A}$ and $\mathcal{B}$).

In the case of nondegenerate spectra, the fact that the lower bound to the uncertainty sum can be reached whatever f, is evidenced in the maximum-probabilities plane in the fact that the points $(c^2, 1)$ and $(1, c^2)$ coincide for all curves $y = h_c^f(x)$, as already mentioned in Ref. [12], and there do exist states for which $(P_{\mathcal{A};\rho}, P_{\mathcal{B};\rho}) = (1, c^2)$ and those for which $(P_{\mathcal{A};\rho}, P_{\mathcal{B};\rho}) = (c^2, 1)$. The question that had remained open, was to know which function f of the family considered leads to the most restrictive inequality (7), i.e., which f minimizes $h_c^f(P)$ when c and $P \in (c^2\,;\,1)$ are fixed. The answer is given in the following theorem, the proof of which is presented in App. A 4:

Theorem 2. *Within the whole family of uncertainty inequalities given by Theorem 1, the strongest restriction for the pair of maximal probabilities $(P_{\mathcal{A};\rho}, P_{\mathcal{B};\rho})$, rewritten as inequality (7), and its counterpart changing $\mathcal{A}$ with $\mathcal{B}$, corresponds to Wootters case, namely for the function $f(x) = \arccos\sqrt{x}$.*

It is important also to address the following situation: when considering only one observable, in the general POVM context, there exists a possible uncertainty that is intrinsic to the POVM representation itself [20]. Indeed a POVM set $\mathcal{A}$ can be such that whatever the state of the system is, no outcome appears with certainty. This situation arises when no operator in $\mathcal{A}$ has an eigenvalue equal to unity. An inequality quantifying such an intrinsic uncertainty is given in the following corollary to Theorem 1, whose proof is presented in App. A 5:

Corollary 1. *Let $\mathcal{A} = \{A_i\}_{i=1,\dots,N_A}$ be a POVM set describing an observable A, and acting on an N-dimensional Hilbert space $\mathcal{H}$. Then for an arbitrary density operator $\rho \in \mathcal{D}$ acting on $\mathcal{H}$, the following relation holds:*

$$\mathcal{U}_f\left(\mathcal{A};\rho\right) \geq f\left(c_{\mathcal{A}}^{\,2}\right), \tag{8}$$

where

$$c_{\mathcal{A}} = \max_i \left\| \sqrt{A_i} \right\| \;\in\; \left[\frac{1}{\sqrt{N_A}}, 1\right] \tag{9}$$

is a generalized intrinsic overlap of the POVM set. The bound is nontrivial (only) when the eigenvalues of any operator A_i are different from unity.

Combining Theorem 1 and Corollary 1, it appears that the lower bound for the sum of metric-based uncertainties of the form (2) can be improved as follows:

Corollary 2. *Let $\mathcal{A} = \{A_i\}_{i=1,\dots,N_A}$ and $\mathcal{B} = \{B_j\}_{j=1,\dots,N_B}$ be two POVM sets describing observables A and B respectively, and acting on an N-dimensional Hilbert space $\mathcal{H}$. Then for an arbitrary density operator $\rho \in \mathcal{D}$ acting on $\mathcal{H}$, the following relation holds:*

$$\mathcal{U}_f(\mathcal{A};\rho) + \mathcal{U}_f(\mathcal{B};\rho) \geq \max\left\{ f\left(c_{\mathcal{A}}^{\,2}\right) + f\left(c_{\mathcal{B}}^{\,2}\right),\, f\left(c_{\mathcal{A},\mathcal{B}}^{\,2}\right)\right\} \tag{10}$$

where $c_{\mathcal{A}}$, $c_{\mathcal{B}}$ and $c_{\mathcal{A},\mathcal{B}}$ are the intrinsic and joint generalized overlaps.

We notice that the overlap $c_{\mathcal{A},\mathcal{B}}$ is bounded from below and above in the following way (see App. A 6 for the proof):

$$\max\left\{ \frac{c_{\mathcal{A}}}{\sqrt{N_B}}\,,\, \frac{c_{\mathcal{B}}}{\sqrt{N_A}} \right\} \,\leq\, c_{\mathcal{A},\mathcal{B}} \,\leq\, c_{\mathcal{A}}\, c_{\mathcal{B}} \tag{11}$$

Consequently, from the last inequality and since $c_{\mathcal{A}} c_{\mathcal{B}} \leq \min\{c_{\mathcal{A}},\, c_{\mathcal{B}}\}$, we get $f(c_{\mathcal{A},\mathcal{B}}^{\,2}) \geq f\left(\min\{c_{\mathcal{A}}^{\,2}\,,\, c_{\mathcal{B}}^{2}\}\right) = \max\left\{f(c_{\mathcal{A}}^{\,2})\,,\, f(c_{\mathcal{B}}^{2})\right\}$. When at least one operator A_i (and/or B_j) of the POVM set $\mathcal{A}$ (and/or of $\mathcal{B}$) has an eigenvalue equal to unity, $c_{\mathcal{A}} = 1$ (and/or $c_{\mathcal{B}} = 1$), thus we get $f(c_{\mathcal{A},\mathcal{B}}^{\,2}) \geq f(c_{\mathcal{B}}^{2})$ (and/or $f(c_{\mathcal{A},\mathcal{B}}^{\,2}) \geq f(c_{\mathcal{A}}^{\,2})$): together with $f(1) = 0$, $f(c_{\mathcal{A},\mathcal{B}}^{\,2}) \geq f(c_{\mathcal{A}}^{\,2}) + f(c_{\mathcal{B}}^{2})$, i.e., the bound in Eq. (10) reduces to that of Eq. (4).

It turns out that the allowed domain for the pair of maximal probabilities $(P_{\mathcal{A};\rho}, P_{\mathcal{B};\rho})$ is constrained as given in the following corollary, the proof of which is given in App. A 7:

Corollary 3. *Let $\mathcal{A} = \{A_i\}_{i=1,\dots,N_A}$ and $\mathcal{B} = \{B_j\}_{j=1,\dots,N_B}$ be two POVM sets describing observables A and B respectively, and acting on an N-dimensional Hilbert space $\mathcal{H}$. Then for an arbitrary density operator ρ acting on $\mathcal{H}$, the pair of maximal probabilities $(P_{\mathcal{A};\rho}, P_{\mathcal{B};\rho})$ is constrained to the domain*

$$\mathbb{D}_{\mathrm{LP}}(c_{\mathcal{A}}, c_{\mathcal{B}}, c_{\mathcal{A},\mathcal{B}}) = \left\{ (P_{\mathcal{A}}, P_{\mathcal{B}}) \in \left[\frac{1}{N_A}\,;\, c_{\mathcal{A}}^{\,2}\right] \times \left[\frac{1}{N_B}\,;\, c_{\mathcal{B}}^{2}\right] \;:\; P_{\mathcal{B}} \leq h_{c_{\mathcal{A},\mathcal{B}}}(P_{\mathcal{A}}) \text{ when } P_{\mathcal{A}} \geq c_{\mathcal{A},\mathcal{B}}^{\,2} \right\} \tag{12}$$

where $h_{c_{\mathcal{A},\mathcal{B}}}$ is given by (6) for $f(x) = \arccos\sqrt{x}$. If $c_{\mathcal{B}}^{2} \leq h_{c_{\mathcal{A},\mathcal{B}}}(c_{\mathcal{A}}^{\,2})$, i.e., $c_{\mathcal{A},\mathcal{B}} \geq c_{\mathcal{A}} c_{\mathcal{B}} - \sqrt{(1-c_{\mathcal{A}})(1-c_{\mathcal{B}})}$, the allowed domain becomes $\left[\frac{1}{N_A}\,;\, c_{\mathcal{A}}^{\,2}\right] \times \left[\frac{1}{N_B}\,;\, c_{\mathcal{B}}^{2}\right]$.

Let us now illustrate both theorems by simulated POVM sets and simulated states. These simulations allow us to comment on the uncertainty relations and, in particular, on Corollary 3 in various contexts.

III. NUMERICAL ILLUSTRATIONS

This section aims at illustrating the constraints imposed on the simultaneous predictability of two observables as expressed by the uncertainty relations (4) in Theorem 1. To this end, we draw randomly several POVM pairs; and for any given pair $(\mathcal{A}_k, \mathcal{B}_k)$ of POVM ($k = 1, \dots$), we draw randomly mixed states $\{\rho_l\}_{l=1,\dots}$. Then we calculate the uncertainty sums $\mathcal{U}_f(\mathcal{A}_k;\rho_l) + \mathcal{U}_f(\mathcal{B}_k;\rho_l)$ and the corresponding bounds $f\left(c_{\mathcal{A}_k,\mathcal{B}_k}^{\,2}\right)$ for different functions f (see App. B for technical details on the simulation of POVM and states). In order to illustrate Corollary 3, we analyze not only $\mathcal{U}_f(\mathcal{A}_k;\rho_l) + \mathcal{U}_f(\mathcal{B}_k;\rho_l)$, but also the cloud of points $\{(P_{\mathcal{A}_k;\rho_l}\,,\, P_{\mathcal{B}_k;\rho_l})\}_{l=1,\dots}$ where $(\mathcal{A}_k, \mathcal{B}_k)$ is fixed, together with their allowed domain $\mathbb{D}_{\mathrm{LP}}(c_{\mathcal{A}_k}, c_{\mathcal{B}_k}, c_{\mathcal{A}_k,\mathcal{B}_k})$.

Figures 1.(a)–(c) represent the simultaneous uncertainty $\mathcal{U}_f(\mathcal{A}_k;\rho_l) + \mathcal{U}_f(\mathcal{B}_k;\rho_l)$ versus the overlap $c_{\mathcal{A}_k,\mathcal{B}_k}$, compared to the lower bound $f\left(c_{\mathcal{A}_k,\mathcal{B}_k}^{\,2}\right)$ for: (a) Wootters metric given by $f(x) = \arccos\sqrt{x}$, (b) Bures metric with $f(x) = \sqrt{2\,(1-\sqrt{x})}$, and (c) root-infidelity metric with $f(x) = \sqrt{1-x}$, in the context of observables with nondegenerate spectra, and for both pure and mixed states. Here, the operators written as $A_i = |a_i\rangle\langle a_i|, i = 1, \dots, N$, are built from the column vectors $|a_i\rangle$ of a unitary matrix (and similarly for the B_j). The dimension is chosen to be $N = 3$. These figures illustrate Theorem 1 and the fact that, in the nondegenerate case, the bounds that we find are optimal. Figure 1.(d) depicts the domain $\mathbb{D}_{\mathrm{LP}}(1, 1, 0.75)$ and functions $h_{c_{\mathcal{A},\mathcal{B}}}^{f}$ for the Bures and root-infidelity metrics, together with snapshots of pairs $(P_{\mathcal{A};\rho_l}\,,\, P_{\mathcal{B};\rho_l})$: this clearly illustrates that the case corresponding to Wootters metric gives the most restrictive domain within the family of uncertainty inequalities (Theorem 2). It also suggests that, in the nondegenerate context, $\mathbb{D}_{\mathrm{LP}}$ is the best domain in the sense that it coincides with $\{(P_{\mathcal{A};\rho}\,,\, P_{\mathcal{B};\rho}) : \rho \in \mathcal{D}\}$. This assertion remains however to be proved.

Figure 2 depicts some examples of domains $\mathbb{D}_{\mathrm{LP}}(c_{\mathcal{A}}, c_{\mathcal{B}}, c_{\mathcal{A},\mathcal{B}})$, Eq. (12), together with snapshots of pairs $(P_{\mathcal{A};\rho_l}, P_{\mathcal{B};\rho_l})$, in various contexts. The dimensions chosen are $N = 3$, $N_A = 4$ and $N_B = 5$. In Figs. 2.(a) and (b), $c_{\mathcal{A},\mathcal{B}} < c_{\mathcal{A}} c_{\mathcal{B}} - \sqrt{(1-c_{\mathcal{A}})(1-c_{\mathcal{B}})}$, and in

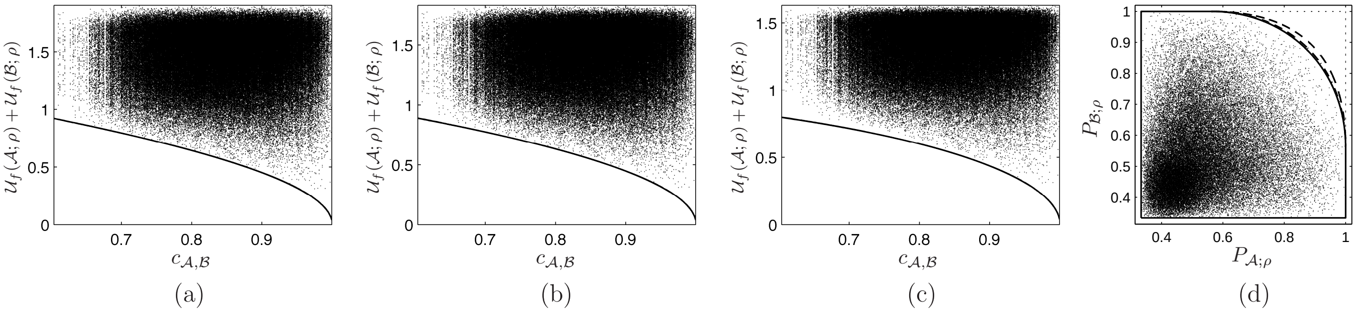


FIG. 1: Illustration of the uncertainty relations given in Theorem 1 in the case of nondegenerate observables and $N = 3$. Snapshots of the uncertainty sum $\mathcal{U}_f(\mathcal{A}_k;\rho_l)+\mathcal{U}_f(\mathcal{B}_k;\rho_l)$ vs. the corresponding generalized overlap $c_{\mathcal{A}_k,\mathcal{B}_k}$ (points), and comparison to the bound $f(c^{\,2}_{\mathcal{A},\mathcal{B}})$ (solid line) for: (a) $f(x) = \arccos\sqrt{x}$ (Wootters); (b) $f(x) = \sqrt{2\,(1-\sqrt{x})}$ (Bures); (c) $f(x) = \sqrt{1-x}$ (root-infidelity). In the simulation, $k = 1,\dots,10^4$ and $l = 1,\dots,25$. (d) Domain $\mathbb{D}_{\mathrm{LP}}(1,1,0.75)$ that corresponds to Wootters metric (solid line), and functions $h^f_{c_{\mathcal{A},\mathcal{B}}}$ for the Bures (dashed-dotted line) and root-infidelity (dashed line) metrics; the points represent the pairs $(P_{\mathcal{A},\rho_l}, P_{\mathcal{B},\rho_l})$ with $(\mathcal{A},\mathcal{B})$ fixed and $l = 1,\dots,5\times10^4$.

Figs. 2.(c) and (d) $c_{\mathcal{A},\mathcal{B}} > c_\mathcal{A} c_\mathcal{B} - \sqrt{(1-c_\mathcal{A})(1-c_\mathcal{B})}$, illustrating situations where $\mathbb{D}_{\mathrm{LP}}$ restricts to $\left[\frac{1}{N_A}\,;\,c_\mathcal{A}^{\,2}\right] \times \left[\frac{1}{N_B}\,;\,c_\mathcal{B}^{\,2}\right]$ or not. In Figs. 2.(a) and (b) [resp. Figs. 2.(c) and (d)], the overlaps are equal, but the pairs of POVM are different. It can be seen that the domain where the pairs $(P_{\mathcal{A}_k;\rho_l}\,,\,P_{\mathcal{B}_k;\rho_l})$ live does not depend only on the overlaps, but also depend on the pair of POVM itself. To be more precise, dealing with optimality, two notions have to be considered:

- $(\mathcal{A},\mathcal{B})-$optimal domain $\mathbb{D}_{\mathrm{POVM}}(\mathcal{A},\mathcal{B}) = \{(P_{\mathcal{A};\rho}\,,\,P_{\mathcal{B};\rho}) : \rho\in\mathcal{D}\}$ is the smallest domain containing all pairs $(P_{\mathcal{A};\rho}\,,\,P_{\mathcal{B};\rho})$ for any mixed state $\rho\in\mathcal{D}$ acting on $\mathcal{H}$.

- $(c_\mathcal{A}, c_\mathcal{B}, c_{\mathcal{A},\mathcal{B}})-$optimal set $\mathbb{D}_{\mathrm{c}}(c_\mathcal{A}, c_\mathcal{B}, c_{\mathcal{A},\mathcal{B}}) = \displaystyle\bigcup_{(\mathcal{A},\mathcal{B}) \text{ s.t. } (c_\mathcal{A},c_\mathcal{B},c_{\mathcal{A},\mathcal{B}})} \mathbb{D}_{\mathrm{POVM}}(\mathcal{A},\mathcal{B})$, is the union of sets $\mathbb{D}_{\mathrm{POVM}}(\mathcal{A},\mathcal{B})$ with $(\mathcal{A},\mathcal{B})$ sharing the same triplet $(c_\mathcal{A}, c_\mathcal{B}, c_{\mathcal{A},\mathcal{B}})$ of overlaps.

These two domains are probably not equal. Moreover, at this step, the illustrations seem to indicate that $\mathbb{D}_{\mathrm{LP}} \neq \mathbb{D}_{\mathrm{POVM}}$, but it remains to be proved formally. The $(c_\mathcal{A}, c_\mathcal{B}, c_{\mathcal{A},\mathcal{B}})-$optimality or not of $\mathbb{D}_{\mathrm{LP}}$ remains also to be investigated, but the illustrations seem to indicate that this last optimality is probable.

IV. CONCLUDING REMARKS

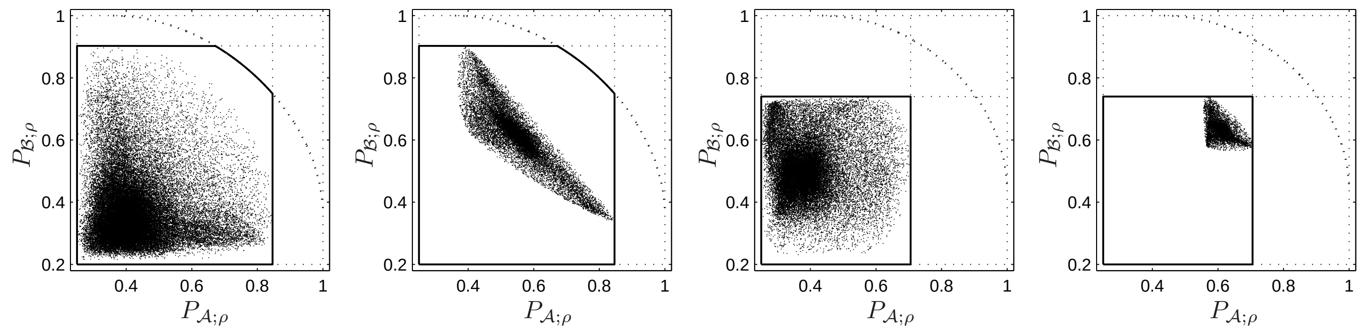
In summary, in this work we have been able to extend the Landau–Pollak inequality for degenerate observables described by the most general formalism of positive operator-valued measures. We derived a family of uncertainty relations, given in Theorem 1, in the most general context of observables described by POVM sets and for mixed quantum states. The relations obtained extend and generalize the well-known Landau–Pollak inequality in the general context and provide a whole family of inequalities. The starting point that gives rise to this set of relations is the assimilation of measures of uncertainty in terms of a conveniently defined metric, which satisfies the triangle inequality. We adopt metrics that lie on decreasing functions of the square of the inner product between pure states. It comes out that Wootters metric, leading to the usual Landau–Pollak inequality (its extension to mixed states and POVM descriptions) is the most restrictive within the family of inequalities we obtain (Theorem 2). From these theorems, we recover that in general, in the POVM representation context, there exists an uncertainty intrinsic to the representation itself (Corollary 1), and thus, that the allowable domain for the pair of maximal probabilities corresponding to two observables is constrained by both the joint uncertainty relation and the intrinsic one (Corollary 2).

A direct consequence of our results is that a previous work [8] dealing with generalized entropies of probability vectors extends very easily in the most general case of POVM representations of observables.

Finally, the simulated numerical results suggest that for a given pair of POVM $\mathcal{A}$ and $\mathcal{B}$, the allowable domain for the pair $(P_{\mathcal{A};\rho}, P_{\mathcal{B};\rho})$ is tighter that domain $\mathbb{D}_{\mathrm{LP}}(c_\mathcal{A}, c_\mathcal{B}, c_{\mathcal{A},\mathcal{B}})$ given by Corollary 3: the questions of finding the tightest domain for $(P_{\mathcal{A};\rho}, P_{\mathcal{B};\rho})$, given POVM sets $\mathcal{A}$ and $\mathcal{B}$ [$(\mathcal{A},\mathcal{B})-$ optimal set $\mathbb{D}_{\mathrm{POVM}}(\mathcal{A},\mathcal{B})$] or given $(c_\mathcal{A}, c_\mathcal{B}, c_{\mathcal{A},\mathcal{B}})$ [$(c_\mathcal{A}, c_\mathcal{B}, c_{\mathcal{A},\mathcal{B}})-$ optimal set $\mathbb{D}_{\mathrm{c}}(c_\mathcal{A}, c_\mathcal{B}, c_{\mathcal{A},\mathcal{B}})$], remain open. The structure of the tight domains (convex or not?) and the properties of the states (pure or not?) reaching the border of these domains are also open questions. These points give possible directions for further investigation in the field.

Acknowledgments

SZ and MP are very grateful to the Région Rhône-Alpes (France) for the grants that enabled this work.



(a) (b) (c) (d)

FIG. 2: Illustration of Corollary 3: domain $\mathbb{D}_{\mathrm{LP}}(c_{\mathcal{A}}, c_{\mathcal{B}}, c_{\mathcal{A},\mathcal{B}})$ and snapshots of pairs $(P_{\mathcal{A};\rho_l}\,,\, P_{\mathcal{B};\rho_l})$ (points). In each figure, $N = 3$, $N_A = 4$, $N_B = 5$, and the dotted lines represent respectively $P_{\mathcal{A};\rho} = \frac{1}{N_A}$, $P_{\mathcal{B};\rho} = \frac{1}{N_B}$, $P_{\mathcal{A};\rho} = c_{\mathcal{A}}^2$, $P_{\mathcal{B};\rho} = c_{\mathcal{B}}^2$, and $P_{\mathcal{B};\rho} = h_{c_{\mathcal{A},\mathcal{B}}}(P_{\mathcal{A};\rho})$. The domain $\mathbb{D}_{\mathrm{LP}}(c_{\mathcal{A}}, c_{\mathcal{B}}, c_{\mathcal{A},\mathcal{B}})$ is delimited by the solid line. In (a) and (b): $(c_{\mathcal{A}}\,,\, c_{\mathcal{B}}\,,\, c_{\mathcal{A},\mathcal{B}}) = (0.92\,,\, 0.95\,,\, 0.60)$; in (c) and (d): $(c_{\mathcal{A}}\,,\, c_{\mathcal{B}}\,,\, c_{\mathcal{A},\mathcal{B}}) = (0.84\,,\, 0.86\,,\, 0.84)$. The number of snapshots is of the order of 10^4.

MP and GMB also acknowledge financial support from CONICET (Argentina), and warm hospitality during their stays at GIPSA-Lab. PWL and TMO are grateful to SECyT-UNC (Argentina) for financial support. We warmly thank Pr. Pierre Comon from GIPSA-lab for the useful discussion about the simulation of sets of self-adjoint semidefinite matrices adding up to unity.

Appendix A: Proofs of the theorems and corollaries

1. Landau–Pollak-type uncertainty relation for sets of projectors and pure states

The first step in our demonstration is to consider pure states $|\Psi\rangle$ and sets of projectors $\mathcal{P} = \{P_i\}_{i=1,\ldots,N_P}$, being $P_i^2 = P_i$. The case of PVM sets is a particular case, where $P_i P_{i'} = P_i \delta_{ii'}$. The following lemma extends the LPI for these particular measurements.

Lemma 1. *Let $\mathcal{P} = \{P_i\}_{i=1,\ldots,N_P}$ and $\mathcal{Q} = \{Q_j\}_{j=1,\ldots,N_Q}$ be two sets of projectors acting on an N-dimensional Hilbert space $\mathcal{H}$. Then for an arbitrary pure state $|\Psi\rangle \in \mathcal{H}$, the following relation holds:*

$$\mathcal{U}_f\left(\mathcal{P}; |\Psi\rangle\langle\Psi|\right) + \mathcal{U}_f\left(\mathcal{Q}; |\Psi\rangle\langle\Psi|\right) \geq f(c_{\mathcal{P},\mathcal{Q}}^2) \qquad \text{(A1)}$$

where $c_{\mathcal{P},\mathcal{Q}} = \max_{ij} \left\| \sqrt{P_i}\,\sqrt{Q_j} \right\| = \max_{ij} \left\| \sqrt{Q_j}\,\sqrt{P_i} \right\|$.

Proof. Note first that for any operator O, the operator norm satisfies $\|O\| = \|O^\dagger\|$ [19]. This property together with the Hermitian property of operators P_i and Q_j justifies the equality $\left\|\sqrt{P_i}\,\sqrt{Q_j}\right\| = \left\|\sqrt{Q_j}\,\sqrt{P_i}\right\|$. Consider now the two normalized pure states:

$$|\psi_i\rangle = \frac{P_i|\Psi\rangle}{\|P_i|\Psi\rangle\|} \quad \text{and} \quad |\varphi_j\rangle = \frac{Q_j|\Psi\rangle}{\|Q_j|\Psi\rangle\|} \qquad \text{(A2)}$$

for $\|P_i|\Psi\rangle\| \neq 0$ and $\|Q_j|\Psi\rangle\| \neq 0$, then

$$|\langle\Psi|\psi_i\rangle|^2 = \langle\Psi|P_i|\Psi\rangle \quad \text{and} \quad |\langle\Psi|\varphi_j\rangle|^2 = \langle\Psi|Q_j|\Psi\rangle \qquad \text{(A3)}$$

using that $P_i^2 = P_i$ and $Q_j^2 = Q_j$.

Now, the triangle inequality fulfilled by the metric d_f applied to the triplet $|\psi_i\rangle, |\varphi_j\rangle$ and $|\Psi\rangle$ reads:

$$f\left(\langle\Psi|P_i|\Psi\rangle\right) + f\left(\langle\Psi|Q_j|\Psi\rangle\right) \geq f\left(\frac{|\langle\Psi|P_i Q_j|\Psi\rangle|^2}{\|P_i|\Psi\rangle\|^2 \|Q_j|\Psi\rangle\|^2}\right). \qquad \text{(A4)}$$

Notice that

$$\begin{aligned} |\langle\Psi|P_i Q_j|\Psi\rangle| &= \left|\langle\Psi|\,\sqrt{P_i}\,\sqrt{P_i}\,\sqrt{Q_j}\,\sqrt{Q_j}\,|\Psi\rangle\right| \\ &\leq \left\|\sqrt{P_i}\,|\Psi\rangle\right\| \left\|\sqrt{P_i}\,\sqrt{Q_j}\,\sqrt{Q_j}\,|\Psi\rangle\right\| \\ &\leq \left\|\sqrt{P_i}\,|\Psi\rangle\right\| \left\|\sqrt{Q_j}\,|\Psi\rangle\right\| \left\|\sqrt{P_i}\,\sqrt{Q_j}\right\| \\ &\leq \left\|\sqrt{P_i}\,|\Psi\rangle\right\| \left\|\sqrt{Q_j}\,|\Psi\rangle\right\| c_{\mathcal{P},\mathcal{Q}}, \end{aligned} \qquad \text{(A5)}$$

where the first inequality follows from the Cauchy–Schwartz inequality, the second one from the definition of the operator norm, and the third one from the definition of $c_{\mathcal{P},\mathcal{Q}}$. The proof ends noting that $\sqrt{P_i} = P_i$ and $\sqrt{Q_j} = Q_j$, choosing i' and j' so that $\langle\Psi|P_{i'}|\Psi\rangle = \max_i \langle\Psi|P_i|\Psi\rangle$ (necessarily nonzero) and $\langle\Psi|Q_{j'}|\Psi\rangle = \max_j \langle\Psi|Q_j|\Psi\rangle$, together with the decreasing property of the function f and the definition of $\mathcal{U}_f$ given by Eq. (2). Let us mention that the interchange of the roles of P_i and Q_j leads to the same result due to $|\langle\psi_i|\varphi_j\rangle|^2 = |\langle\varphi_j|\psi_i\rangle|^2$ and the symmetry satisfied by the operator norm. □

Note that the sets $\mathcal{P}$ and $\mathcal{Q}$ do not need to satisfy the resolution of the identity, i.e., the inequality applies beyond the scope of the complete description of observables by sets of projectors.

2. Landau–Pollak-type uncertainty relation for POVM pairs and pure states

We can extend now the previous result to general POVM sets.

Lemma 2. *Let $\mathcal{A} = \{A_i\}_{i=1,\dots,N_A}$ and $\mathcal{B} = \{B_j\}_{j=1,\dots,N_B}$ be two POVM sets describing observables A and B and acting on an N-dimensional Hilbert space $\mathcal{H}$. Then for an arbitrary pure state $|\Psi\rangle \in \mathcal{H}$, the following relation holds:*

$$\mathcal{U}_f\left(\mathcal{A};|\Psi\rangle\langle\Psi|\right) + \mathcal{U}_f\left(\mathcal{B};|\Psi\rangle\langle\Psi|\right) \geq f(c_{\mathcal{A},\mathcal{B}}^{\,2}) \tag{A6}$$

where $c_{\mathcal{A},\mathcal{B}} = \max_{ij}\left\|\sqrt{A_i}\,\sqrt{B_j}\right\| = \max_{ij}\left\|\sqrt{B_j}\,\sqrt{A_i}\right\|$.

Proof. Let us consider the pure state $|\Phi\rangle = |\Psi\rangle \oplus 0 \oplus 0$ belonging to the extended Hilbert space which is the direct sum $\mathcal{H}\oplus\mathcal{H}^{\mathrm{aux}}\oplus\mathcal{H}^{\mathrm{aux}}$, where $\mathcal{H}^{\mathrm{aux}}$ has the same dimension as $\mathcal{H}$. Consider also projectors P_i and Q_j of the form [10]

$$P_i = \begin{pmatrix} A_i & \sqrt{A_i(I-A_i)} & 0 \\ \sqrt{A_i(I-A_i)} & I-A_i & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

$$Q_j = \begin{pmatrix} B_j & 0 & \sqrt{B_j(I-B_j)} \\ 0 & 0 & 0 \\ \sqrt{B_j(I-B_j)} & 0 & I-B_j \end{pmatrix}.$$

Using that

$$\begin{aligned} \langle\Phi|P_i|\Phi\rangle &= \langle\Psi|A_i|\Psi\rangle, \\ \langle\Phi|Q_j|\Phi\rangle &= \langle\Psi|B_j|\Psi\rangle, \\ \frac{|\langle\Phi|P_iQ_j|\Phi\rangle|}{\|P_i|\Phi\rangle\|\|Q_j|\Phi\rangle\|} &= \frac{|\langle\Psi|A_iB_j|\Psi\rangle|}{\|\sqrt{A_i}|\Psi\rangle\|\|\sqrt{B_j}|\Psi\rangle\|}, \end{aligned}$$

then inequality (A4) applied to any triplet P_i, Q_j and $|\Phi\rangle$ so that $\langle\Phi|P_i|\Phi\rangle \neq 0 \neq \langle\Phi|Q_j|\Phi\rangle$, leads to

$$\begin{aligned} f\left(\langle\Psi|A_i|\Psi\rangle\right) &+ f\left(\langle\Psi|B_j|\Psi\rangle\right) \\ &\geq f\left(\frac{|\langle\Psi|A_iB_j|\Psi\rangle|^2}{\|\sqrt{A_i}|\Psi\rangle\|^2\|\sqrt{B_j}|\Psi\rangle\|^2}\right). \end{aligned} \tag{A7}$$

Now, as done in (A5), we have $\frac{|\langle\Psi|A_iB_j|\Psi\rangle|}{\|\sqrt{A_i}|\Psi\rangle\|\|\sqrt{B_j}|\Psi\rangle\|} \leq c_{\mathcal{A},\mathcal{B}}$. The end of the proof is similar to that of Lemma 1. □

Note that, here again, the sets $\mathcal{A}$ and $\mathcal{B}$ do not need to fulfill the resolution of the identity. Thus, Lemma 2 applies in a more general context than that of the description of observables by POVM.

3. Landau–Pollak-type uncertainty relation for POVM sets and mixed states

We are ready now to prove inequality (4) in Theorem 1. To this end, let us consider a density operator ρ acting on $\mathcal{H}$. Since it is Hermitian and positive semidefinite, it can be diagonalized on an orthonormal basis $\{|l\rangle\}$ of $\mathcal{H}$, i.e., $\rho = \sum_{l=1}^N \rho_l\,|l\rangle\langle l|$ with $\rho_l \geq 0$ and $\sum_l \rho_l = \mathrm{Tr}\,\rho = 1$. Let us then consider a purification $|\Phi'\rangle$ of ρ, belonging to a product Hilbert space $\mathcal{H}\otimes\widetilde{\mathcal{H}}^{\mathrm{aux}}$,

$$|\Phi'\rangle = \sum_{l=1}^N \sqrt{\rho_l}\;|l\rangle\otimes|l^{\mathrm{aux}}\rangle, \tag{A8}$$

where $\{|l^{\mathrm{aux}}\rangle\}$ is an arbitrary orthonormal basis of $\widetilde{\mathcal{H}}^{\mathrm{aux}}$ (without loss of generality, we assume $\widetilde{\mathcal{H}}^{\mathrm{aux}}$ of the same dimension as $\mathcal{H}$). The mixed state on $\mathcal{H}$ is recovered by the partial trace, that is

$$\mathrm{Tr}_{\,\mathrm{aux}}\left(|\Phi'\rangle\langle\Phi'|\right) = \sum_{l=1}^N \rho_l|l\rangle\langle l| = \rho. \tag{A9}$$

It can be verified that

$$\langle\Phi'|A_i\otimes I|\Phi'\rangle = \mathrm{Tr}\,(A_i\rho)\,, \quad \langle\Phi'|B_j\otimes I|\Phi'\rangle = \mathrm{Tr}\,(B_j\rho)\,,$$

and that

$$\begin{aligned} \left\|\left(\sqrt{A_i\otimes I}\right)\left(\sqrt{B_j\otimes I}\right)\right\| &= \left\|\left(\sqrt{A_i}\otimes I\right)\left(\sqrt{B_j}\otimes I\right)\right\| \\ = \left\|\left(\sqrt{A_i}\,\sqrt{B_j}\right)\otimes I\right\| &= \left\|\sqrt{A_i}\,\sqrt{B_j}\right\|. \end{aligned}$$

Applying inequality (A6) to the triplet $A_i\otimes I$, $B_j\otimes I$ and $|\Phi'\rangle$, leads to inequality (4), that concludes the proof of Theorem 1.

4. Proof of Theorem 2: Wootters metric gives the most restrictive domain for $(P_{\mathcal{A};\rho}, P_{\mathcal{B};\rho})$

The inner product defines the cosine of an angle between two states of $\mathcal{H}$. Thus, in the context of pure states, since $P_{\mathcal{A};\rho}$ and $P_{\mathcal{B};\rho}$ are closely linked to inner products, it can be intuitively guessed that within the family of inequalities (4), the most restrictive one occurs when $f = \arccos\sqrt{x}$. Indeed, in this case inequality (4) links the angles between the possible pairs among three vectors of $\mathcal{H}$. In the general context of Theorem 1, this guess turns out to be true.

First of all, recall that inequality (4) is restrictive only when the pair $(P_{\mathcal{A};\rho}, P_{\mathcal{B};\rho})$ belongs to $(c_{\mathcal{A},\mathcal{B}}^{\,2}\,;1]^2$ under the form (7):

$$P_{\mathcal{B};\rho} \leq h^f_{c_{\mathcal{A},\mathcal{B}}}\left(P_{\mathcal{A};\rho}\right) \qquad \text{for} \qquad P_{\mathcal{A};\rho} \in [c_{\mathcal{A},\mathcal{B}}^{\,2}\,;1]$$

where $h^f_c(x) = f^{-1}\big(f(c^2) - f(x)\big)$. Note now that Wootters metric, given by $f(x) = \arccos\sqrt{x}$, leads to

$h_c(x) = \left(c\sqrt{x}+\sqrt{1-c^2}\sqrt{1-x}\right)^2$ (the superscript arccos has been suppressed for the sake of simplicity). Thus, denoting

$$\gamma = \arccos c \qquad \text{and} \qquad x = \cos^2\theta \quad \text{with} \quad \theta \in [0\,;\,\gamma],$$

we can write

$$h_c(\cos^2\theta) = \cos^2(\gamma - \theta).$$

Fix now a decreasing function f and assume that there is a $\theta_f \in [0\,;\,\gamma]$ such that

$$h_c^f(\cos^2\theta_f) < h_c(\cos^2\theta_f) = \cos^2(\gamma - \theta_f).$$

From the definition (6) of h_c^f and the decreasing property of f, this inequality becomes

$$f\big(\cos^2\theta_f\big) + f\big(\cos^2(\gamma-\theta_f)\big) < f(\cos^2\gamma) \qquad \text{(A10)}$$

Let us then consider two orthogonal pure states $|\psi_1\rangle$ and $|\Psi\rangle$ of $\mathcal{H}$ and let us define the pure states:

$$\begin{aligned} |\phi\rangle &= \cos\theta_f\,|\psi_1\rangle + \sin\theta_f\,|\Psi\rangle, \\ |\psi_2\rangle &= \cos\gamma\,|\psi_1\rangle + \sin\gamma\,|\Psi\rangle. \end{aligned}$$

It can be verified that $|\langle\phi|\psi_1\rangle|^2 = \cos^2\theta_f$, $|\langle\phi|\psi_2\rangle|^2 = \cos^2(\gamma-\theta_f)$ and $|\langle\psi_2|\psi_1\rangle|^2 = \cos^2\gamma$, such that inequality (A10) writes

$$f\big(|\langle\phi|\psi_1\rangle|^2\big) + f\big(|\langle\phi|\psi_2\rangle|^2\big) < f\big(|\langle\psi_2|\psi_1\rangle|^2\big)$$

For such a function f, $d_f\big(|\Phi\rangle,|\Psi\rangle\big) = f\big(|\langle\Phi|\Psi\rangle|^2\big)$ is *not* a metric since it does not satisfy the triangle inequality. In conclusion, for any function f defining a metric d_f between pure states, $h_c^f(x) \geq h_c(x)$ in $[c^2\,;\,1]$, proving that Wootters metric gives the most restrictive inequality of the family (4), as stated in Theorem 2.

5. Proof of Corollary 1: Intrinsic uncertainty relation for POVM representations

The proof of (8) is immediate from Theorem 1, taking $\mathcal{B} = \mathcal{I} \equiv \{I\}$. It can also be proved directly by noting that $p_i(A;|\Psi\rangle\langle\Psi|) = \langle\Psi|A_i|\Psi\rangle \leq \||\Psi\rangle\|\;\|A_i|\Psi\rangle\| \leq \||\Psi\rangle\|^2\;\|A_i\| = \|A_i\|$ for any (normalized) pure state. Writing a mixed state as a convex combination of pure-states density matrices, we get again $p_i(A;\rho) \leq \|A_i\| = \|\sqrt{A_i}\|^2$. The proof ends by choosing the index i' that maximizes $p_i(A;\rho)$ together with the decreasing property of f.

Regarding the interval for the intrinsic overlap in (9), by definition $c_{\mathcal{A}}^{\,2} \geq \left\|\sqrt{A_i}\right\|^2 \geq \langle\Psi\,|A_i|\,\Psi\rangle$ for any i and normalized state $|\Psi\rangle$. Summing over i, from the resolution of the identity and since $|\Psi\rangle$ is normalized, it yields $N_A\,c_{\mathcal{A}}^{\,2} \geq 1$. Moreover, $\langle\Psi\,|A_i|\,\Psi\rangle \leq 1$ implies that $\left\|\sqrt{A_i}\right\| \leq 1$ for all i, and thus $c_{\mathcal{A}} \leq 1$.

6. Proof of the bounds for the overlap $c_{\mathcal{A},\mathcal{B}}$ in (11)

The first inequality in (11) comes from $c_{\mathcal{A},\mathcal{B}}^{\,2} \geq \left\|\sqrt{A_i}\;\sqrt{B_j}\right\|^2 \geq \left\langle\Psi\left|\sqrt{A_i}\;B_j\;\sqrt{A_i}\right|\Psi\right\rangle$ for any i,j and unitary $|\Psi\rangle$. Summing over j, from the resolution of the identity, and taking the maximum over $|\Psi\rangle$ and then over i, leads to $N_B c_{\mathcal{A},\mathcal{B}}^{\,2} \geq c_{\mathcal{A}}^{\,2}$. By inverting A_i and B_j in the expression of $c_{\mathcal{A},\mathcal{B}}$ the overlap also satisfies $N_A c_{\mathcal{A},\mathcal{B}}^{\,2} \geq c_{\mathcal{B}}^{\,2}$. The second inequality is a consequence of the submultiplicative property $\left\|\sqrt{A_i}\;\sqrt{B_j}\right\| \leq \left\|\sqrt{A_i}\right\|\left\|\sqrt{B_j}\right\| \leq c_{\mathcal{A}}\;c_{\mathcal{B}}$ (see Ref. [19]).

7. Proof of Corollary 3: Allowed domain for the pair of maximal probabilities $(P_{\mathcal{A};\rho}, P_{\mathcal{B};\rho})$

The proof is immediate from Theorems 1 and 2, Corollary 2, and the definition $h_c(x) = \cos^2\left(\arccos c - \arccos\sqrt{x}\right) = \left(c\sqrt{x}+\sqrt{1-c^2}\sqrt{1-x}\right)^2$. By symmetry, the roles of $\mathcal{A}$ and $\mathcal{B}$ can be interchanged, leading naturally to the same domain.

Appendix B: Simulation of states and of POVM

Here, we present the algorithms used in Sec. III to simulate quantum states (pure or mixed) and POVM.

Pure states can be simulated as $|\Psi\rangle = \Phi(\vartheta)\frac{|\varphi\rangle}{\||\varphi\rangle\|}$ where $\frac{|\varphi\rangle}{\||\varphi\rangle\|}$ has a uniform distribution on the unit sphere $\mathbb{S}^N$ by drawing $|\varphi\rangle$ according to a zero-mean Gaussian law with identity covariance matrix [21]; $\Phi(\vartheta)$ is a diagonal matrix of phases $\mathrm{e}^{\imath\vartheta_i}$ where the ϑ_i $(i = 1,\ldots,N)$ are mutually independent and uniformly distributed on $[0\,;\,2\pi)$, and independent of $|\varphi\rangle$.

In order to simulate mixed states, we can use the fact that an Hermitian, positive semidefinite operator can be diagonalized on an orthonormal basis, $\rho = \sum_{m=1}^N \alpha_m|\Psi_m\rangle\langle\Psi_m|$ where $\alpha_m \geq 0$ are the eigenvalues of ρ, with $\sum_m \alpha_m = 1$ because of the normalization of ρ [22]. Thus, we can simulate orthonormal bases $\{|\Psi_m\rangle\}_{m=1,\ldots,N}$ as the columns of a randomly drawn unitary matrix [23]; the coefficients α_m can be drawn independently according to a uniform law on $[0\,;\,1]$, and normalized to add to unity. Another way of making should be to generate a complex Gaussian random matrix M and to compute $\rho = \frac{MM^\dagger}{\operatorname{Tr}(MM^\dagger)}$ as proposed for instance in Ref. [22], or from a pure state in a higher dimensional space and taking the partial trace (see App. A 3 and Refs. [22, 24]).

As far as we know, there are no ways to simulate POVM sets with a specific distribution. For $\mathcal{A}$ (and similarly for $\mathcal{B}$), a simple approach may consist in drawing a unitary matrix U [23] and a set of N_A diagonal matrices D_i of positive elements, and to consider the set of matrices $A_i = U\left(\sum_{j=1}^{N_A} D_j\right)^{-1} D_i U^\dagger$ that satisfies the resolution of identity. In this case the A_i give a resolution to the identity, but they share the same eigenspace. To avoid this drawback, we simulate sets of N_A self-adjoint matrices in the following way, that can be viewed as an extension of the previous approach [25]. Let

$$A_i = R_i\, U_i\, \Delta_i\, U_i^\dagger\, R_i^\dagger \quad \text{for} \quad i = 1, \ldots, N_A - 1$$

and

$$A_{N_A} = R_{N_A-1}\, U_{N_A-1}\, (I - \Delta_{N_A-1})\, U_{N_A-1}^\dagger\, R_{N_A-1}^\dagger$$

where

- U_i are unitary matrices independently drawn according to the Haar (uniform) distribution on the set of unitary matrices [23],
- Δ_i are diagonal matrices, where the components are independently drawn according to a uniform distribution on $[0\,;\,1]$,
- $R_1 = I$, and $R_i = R_{i-1}\, U_{i-1}\, \sqrt{I - \Delta_{i-1}}$ for $i = 2, \ldots, N_A - 1$.

It can be verified recursively that the A_i form a resolution of the identity, evaluating the sum $((A_{N_A} + A_{N_A-1}) + A_{N_A-2}) + \ldots + A_1$ step by step. Moreover, the A_i do not share the same eigenspace.

[1] W. Heisenberg, Z. Phys. **43**, 172 (1927).
[2] H.P. Robertson, Phys. Rev. **34**, 163 (1929); E. Schrödinger, Sitzungsber. Preuss. Akad. Wiss. Phys. Math. Kl. **19**, 296 (1930).
[3] H.F Hofmann, and S. Takeuchi, Phys. Rev. A **68**, 032103 (2003); Y. Huang, Phys. Rev. A **86**, 024101 (2012).
[4] H. Maassen, and J.B.M. Uffink, Phys. Rev. Lett. **60**, 1103 (1988).
[5] J.L. de Vicente, and J. Sánchez-Ruiz, Phys. Rev. A **77**, 042110 (2008); G.M. Bosyk, M. Portesi, A.L. Plastino, and S. Zozor, Phys. Rev. A **84**, 056101 (2011).
[6] I.I. Hirschman, Am. J. Math. **79**, 152 (1957); I. Bialynicki-Birula, and J. Mycielski, Commun. Math. Phys. **44**, 129 (1975); D. Deutsch, Phys. Rev. Lett. **50**, 631 (1983); K. Kraus, Phys. Rev. D **35**, 3070 (1987); M. Berta, M. Christandl, R. Colbeck, J.M. Renes, and R. Renner, Nat. Phys. **6**, 659 (2010); A.E. Rastegin, J. Phys. A: Math. Theor. **43**, 155302 (2010); A.E. Rastegin, J. Phys. A: Math. Theor. **44**, 095303 (2011); Y. Huang, Phys. Rev. A **83**, 052124 (2011); A. Luis, Phys. Rev. A **84**, 034101 (2011); A.E. Rastegin, Int. J. Theo. Phys. **51** 1300 (2012); P. J. Coles, R. Colbeck, L. Yu, and M. Zwolak, Phys. Rev. Lett. **108**, 210405 (2012); G.M. Bosyk, M. Portesi, and A.L. Plastino, Phys. Rev. A **85**, 012108 (2012); Z. Puchała, Ł. Rudnicki, and K. Życzkowski, J. Phys. A: Math. Theor. **44**, 272002 (2013); Ł. Rudnicki, Z. Puchała, and K. Życzkowski, Phys. Rev. A. **89**, 052115 (2014); P.J. Coles and M. Piani, Phys. Rev. A **89**, 022112(2014).
[7] I. Bialynicki-Birula and Ł. Rudnicki, in: *Statistical complexity*, Ch.1, Ed. by K.D. Sen (Springer, Berlin, 2011); S. Wehner, and A. Winter, New J. Phys. **12**, 025009 (2010).
[8] S. Zozor, G.M. Bosyk, and M. Portesi, arXiv:1311.5602v2 [quant-ph] (2014).
[9] H.J. Landau and H.O. Pollak, Bell Syst. Tech. J. **40**, 65 (1961).
[10] T. Miyadera and H. Imai, Phys. Rev. A **76**, 062108 (2007).
[11] J.L. de Vicente and J. Sánchez-Ruiz, Phys. Rev. A **71**, 052325 (2005); Y. Huang, Phys. Rev. A **82**, 012335 (2010).
[12] G.M. Bosyk, T.M. Osán, P.W. Lamberti, and M. Portesi, Phys. Rev. A **89**, 034101 (2014).
[13] I. Bengtsson and K. Życzkowski. *Geometry of Quantum States: An Introduction to Quantum Entanglement* (Cambridge University Press, 2006).
[14] M.A. Nielsen and I.L. Chuang. *Quantum Computation and Quantum Information* (Cambridge University Press, 2010).
[15] W.K. Wootters, Phys. Rev. D **23**, 357 (1981); M.A. Nielsen, and I.L. Chuang. *Quantum Computation and Quantum Information* (Cambridge University Press, 2000).
[16] D. Bures, Trans. Amer. Math. Soc. **135**, 199 (1969).
[17] A. Gilchrist, N. K. Langford, and M. A. Nielsen, Phys. Rev. A **71**, 062310 (2005).
[18] A. Uhlmann, Rep. Math. Phys. **9**, 273 (1976); R. Jozsa, J. Mod. Opt. **41**, 2315 (1994).
[19] M. Reed and B. Simon. Methods of Modern Mathematical Physics, vol I: Functional Analysis. Academic Press Inc., 1980; J. B. Conway. A Course in Functional Analysis. Graduate Texts in Mathematics. Springer Verlag, New-York, 2nd edition, 1990.
[20] S. Massar, Phys. Rev. A **76**, 042114 (2007).
[21] D.E. Knuth, The Art of Computer Programming, volume 2 / Seminumerical algorithms. Addison Wesley Longman, Reading, 3rd edition, 1998.
[22] K. Życzkowski and H.J. Sommers, J. Phys. A **36**, 10115 (2003).
[23] K. Życzkowski and M. Kuś, J. Phys. A **27**,4235 (1994); F. Mezzadri, Notices of the AMS **54**, 592 (2007).
[24] K. Życzkowski and H.J. Sommers, Phys. Rev. A **71**, 032313 (2005).
[25] P. Comon. Unpublished. 2014.