

Multistate imaginarity and coherence in qubit systems

Mao-Sheng Li ¹, Rafael Wagner ^{2,3,4,*} and Lin Zhang ⁵

¹*School of Mathematics, South China University of Technology, Guangzhou 510640, China*

²*Institut für Theoretische Physik, Universität Ulm, Ulm, Germany*

³*INL—International Iberian Nanotechnology Laboratory, Braga, Portugal*

⁴*Centro de Física, Universidade do Minho, Braga, Portugal*

⁵*School of Science, Hangzhou Dianzi University, Hangzhou 310018, China*



(Received 13 August 2025; accepted 5 January 2026; published 20 January 2026)

Traditionally, the characterization of quantum resources has focused on individual quantum states. Recent literature, however, has increasingly explored the characterization of resources in *multistates*—ordered collections of states indexed by a varying parameter. In this work, we provide a unitary-invariant framework to pinpoint imaginarity and coherence in sets of qubit states: We prove that Bloch vectors must be coplanar to be imaginarity free and collinear to be incoherent, yielding exact rank-based tests of coherence and imaginarity and closed-form bounds for existing robustness quantifiers, all based on two-state overlaps only. We also show that the set of imaginarity-free multistates is not convex, and that third-order invariants completely characterize multistate imaginarity of single-qubits but not of higher-dimensional systems. As our main technical result, we show that *every* Bargmann invariant of single-qubit states is determined (up to conjugation) by two-state overlaps. Beyond qubits, we give purity and system-agnostic coherence witnesses from equality constraints on higher-order invariants and connect our results to practical protocols—characterization of partial distinguishability, spin-chirality detection, and subchannel discrimination.

DOI: [10.1103/tpgw-v6ht](https://doi.org/10.1103/tpgw-v6ht)

I. INTRODUCTION

Quantum resources [1–3] are typically defined and characterized with respect to individual quantum states or quantum channels. While this has been a successful approach, it arguably overlooks many well-known phenomena that call for a concrete understanding of the *collective* properties of quantum states. Numerous examples in the literature, spanning a wide range of applications in quantum information science, support this perspective.

One example is the collective behavior of a set of single photons entering a linear-optical multiport interferometer [4–7]: In this case, the *indistinguishability* of the states encoding each photon’s internal degrees of freedom decisively impacts the output-port statistics of the interferometer. Another example is provided by *quantum pseudorandomness*, which is a property defined relative to a parameterized set of quantum states $\{\rho_i\}_i$ [8–10]. One can then investigate the resources present in said collections of states and infer intriguing aspects about the relationship between pseudorandomness and the amount of quantum resources present in such sets [11–14]. Yet another example, from the perspective of

quantum channels, is the notion of *non-Markovianity* [15]. This is best understood as a property depending on a fine-grained, time-dependent evolution (i.e., of a collection of maps $\{\mathcal{E}_t\}_t$) rather than a coarse-grained description by a single quantum map.

This plurality of examples is motivating the study of quantum resources defined not by individual elements but by *sets* or *collections* of quantum objects [16–28]. Of particular relevance to our work are the collective quantum resources described by *set coherence*, as introduced by Designolle *et al.* [16] (previously investigated by Refs. [25,29–32] under different names) and *set imaginarity*, as introduced by Miyazaki and Matsumoto [17].

Quantum coherence [33,34] is the paradigmatic quantum resource—essential (though not sufficient) for computational [35,36] or informational [37] advantage. A related—but less explored—resource is quantum imaginarity [38–42], which is a type of coherence requiring nonzero imaginary parts of off-diagonal elements. Imaginarity has been shown to yield communication advantages [43] and to be connected with hiding and masking quantum information [44], quantum pseudorandom states and unitaries [12], enhanced sensing via weak measurements [45–48], work extraction through complex-valued quasiprobabilities [49,50], and scrambling applied to quantum machine learning [51].

Moving to such a collective description naturally introduces a basis-independent perspective, since one considers the resource not of a single quantum state in a fixed basis but of the overall structure and behavior of the ensemble. As multivariate traces are known to capture all unitary-invariant

*Contact author: rafael.wagner@uni-ulm.de

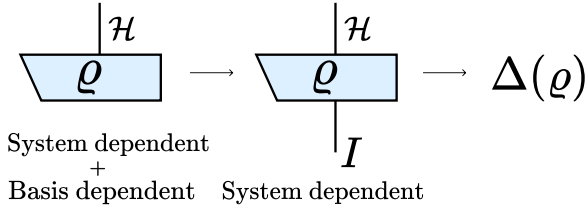


FIG. 1. States, multistates, and Bargmann invariants. Left: A single quantum state ϱ , whose coherence is defined relative to a specific basis and system. Middle: A multistate $\varrho : I \rightarrow \mathcal{D}(\mathcal{H})$, which can be viewed operationally as a state preparator assigning a quantum state $\varrho(i)$ to each index $i \in I$. Its coherence is a collective, basis-independent property of the set $\{\varrho(i)\}_{i \in I}$. Right: A Bargmann invariant $\Delta(\varrho) = \text{Tr}[\prod_{i \in I} \varrho(i)]$ whose value is invariant under changes of basis. Its value can reflect the coherence present in every multistate that realizes it.

properties of a collection of operators, because they form a complete list of generating invariants [52–55], one is naturally led—when considering density matrices as the relevant operators—to view *Bargmann invariants* [56] as relevant tools.

Bargmann invariants are multivariate traces of states $\text{Tr}(\rho_1 \cdots \rho_n)$ that can be experimentally measured in various ways [55, 57–61]. These have recently been connected with Kirkwood-Dirac (KD) quasiprobability distributions [57, 62–66], out-of-time-order correlators [57, 58, 67], weak values [68, 69], quantum speed limits [70], geometric phases [71–74], multiphoton indistinguishability [6, 7, 76, 75–83], overlap uncertainty relations [84], quantum thermodynamics [49, 85–89], and the certification of quantum resources [24, 90–94].

In this work, we exploit Gram matrix methods and Bargmann invariant theory to characterize the simplest nontrivial instances of basis-independent imaginarity and coherence for collections of states: the case where we only consider states of a single qubit. Since we are interested in finite ordered collections of states, relative to a varying parameter, these are elegantly captured by the operational notion of a *multistate* [27, 28] (see Fig. 1), i.e., a function $\varrho : I \rightarrow \mathcal{D}(\mathcal{H})$ which to every index $i \in I$ associates a quantum state $\varrho(i) \equiv \rho_i$ in some Hilbert space $\mathcal{H}$. The image of ϱ is given by sets of states $\{\rho_i\}_{i \in I}$ and, moreover, each such multistate has an associated ordered set $\varrho = (\rho_1, \dots, \rho_n)$ when $I = \{1, \dots, n\} =: [n]$ for some fixed number $n \in \mathbb{N}$.

Our main contributions are the following:

(1) We derive necessary and sufficient conditions for single-qubit multistates $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^2)$ to be imaginarity-free (see Theorem III.3) or incoherent (see Theorem VI.1), expressed solely in terms of two-state overlaps $\text{Tr}(\rho_i \rho_j)$ of the states in the multistates. Our results formalize the following geometric intuition: a set of states is incoherent exactly when all Bloch vectors lie on a common line and imaginarity-free exactly when they lie in a common plane.

(2) These simple criteria have a few immediate implications. To mention one, we show that a multistate $\varrho : \{1, 2, 3\} \rightarrow \mathcal{D}(\mathbb{C}^2)$ has imaginarity if and only if (iff) the imaginary part of its associated third-order Bargmann invariant is nonzero, i.e., $\text{Im}[\text{Tr}(\rho_1 \rho_2 \rho_3)] \neq 0$. This is, however,

not the case for multistates relative to higher-dimensional systems. We construct a counterexample of a multistate $\varrho : \{1, 2, 3\} \rightarrow \mathcal{D}(\mathbb{C}^4)$ for which $\text{Im}[\text{Tr}(\rho_1 \rho_2 \rho_3)] = 0$ but that, nevertheless, has imaginarity. This follows from the results in Refs. [57, 90] as the imaginarity of this multistate is witnessed by the fact that $\text{Im}[\text{Tr}(\rho_1^2 \rho_2 \rho_3)] \neq 0$.

(3) We furthermore use this characterization to show that the set of all imaginarity-free multistates is not convex. The nonconvexity of the incoherent multistates had been previously shown by Designolle *et al.* [16].

(4) Beyond providing a necessary and sufficient condition for single-qubit multistate coherence, our main technical contribution is a more powerful result: Take any single-qubit multistate $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^2)$ and write its associated Bargmann invariant as

$$\Delta(\varrho) := \text{Tr}(\rho_1 \cdots \rho_n) = \text{Re}[\Delta(\varrho)] + i\text{Im}[\Delta(\varrho)].$$

Then both $\text{Re}[\Delta(\varrho)]$ and $|\text{Im}[\Delta(\varrho)]|$ are completely characterized by polynomials over the complete list of two-state overlaps $(\text{Tr}(\rho_i \rho_j))_{i,j}$ (see Theorem V.1). In other words, the only nontrivial unitary-invariant information that is not already encoded in the overlaps is the *sign* of the imaginary part of the invariant. This result is a generalization to every $n \in \mathbb{N}$ of the cases $n = 3, 4$, and 5 explored in Ref. [95]. The polynomials mentioned above are constructed inductively.

(5) We express set-coherence and set-imaginarity *quantifiers*—restricted to the single-qubit case—as functions of two-state overlaps and show that imaginarity quantifiers in particular can be written as a semidefinite optimization problem. We then relate these quantifiers to our rank conditions, deriving explicit upper and lower bounds (see Theorem IV.1 for the case of set imaginarity and Theorem VII.1 for the case of set coherence).

(6) We also discuss simple extensions of our tools beyond the single-qubit case. Following Refs. [24, 90], we propose simple *equality constraints* on Bargmann invariants that serve as operational witnesses for multi-state coherence and imaginarity in systems of arbitrary dimension.

(7) We illustrate how our quantifiers yield operational advantages in subchannel discrimination and discuss implications of our results for multiphoton indistinguishability and spin chirality. These examples demonstrate the physical relevance of the resources we investigate.

The remainder of this document is structured as follows. In Sec. II we review the relevant background. Section III characterizes single-qubit multistate imaginarity, with Theorem III.3 establishing simple and intuitive rank-based criteria. Section VI characterizes single-qubit multistate coherence via Theorem VI.1. Section V has our main technical contribution, where we provide a characterization of the real and imaginary parts of *all* Bargmann invariants of single-qubit states. Section VIII discusses the physical relevance of our results and possible applications. Section IX provides discussion and future directions.

II. BACKGROUND

A. Set coherence and set imaginarity

We denote by $\mathcal{H}$ the Hilbert space associated to a quantum system of finite dimension $d = \dim(\mathcal{H})$. Moreover, we

also denote by $\mathcal{D}(\mathcal{H})$ the set of all positive trace-one operators which we refer to as quantum states and by $\mathcal{P}_1(\mathcal{H}) = \{|\psi\rangle\langle\psi| \mid \langle\psi|\psi\rangle = 1\}$ the extremal elements of $\mathcal{D}(\mathcal{H})$, i.e., the set of all pure quantum states.

A *multistate* is a function $\varrho : I \rightarrow \mathcal{D}(\mathcal{H})$ from an index set I to the set of density matrices of some Hilbert space [26–28,96]. Operationally, we can view a multistate as a “state preparator” or “preparation box” having classical inputs chosen from an index set I and to each i it outputs a quantum state $\varrho(i) = \rho_i$. The image of a multistate is a set of states $\varrho(I) = \{\rho_i\}_i$. If the index set is discrete (and finite) the multistate corresponds to a (finite) sequence $\varrho = (\varrho(i))_{i \in I}$. For example, $\varrho : \{1, 2, 3\} \rightarrow \mathcal{D}(\mathcal{H})$ corresponds to $\varrho = (\varrho(1), \varrho(2), \varrho(3))$. Note that since the tuple and the function are bijectively related, we use the same notation for both.

We start by introducing the notions of set coherence and set imaginarity, which are concepts defined relative to the image of a multistate. Recall that a state $\rho \in \mathcal{H}$, with $d = \dim(\mathcal{H}) < \infty$, is said to be incoherent with respect to an orthonormal basis $\mathbb{A} = \{|a_i\rangle\}_{i=1}^d$ iff for every $i \neq j$ we have $\langle a_i | \rho | a_j \rangle = 0$. Set coherence can then be defined as follows:

Definition II.1 (Set coherence). A set of states $\{\rho_i\}_i \subseteq \mathcal{D}(\mathcal{H})$ is *incoherent* if there exists a unitary $U : \mathcal{H} \rightarrow \mathcal{H}$ such that, for all i , $U\rho_i U^\dagger$ is a diagonal density matrix with respect to some orthonormal basis $\mathbb{A}$. If this does not hold, we say that $\{\rho_i\}_i$ is *coherent*.

Alternatively, if we denote the set of all incoherent states with respect to a basis $\mathbb{A}$ as

$$\mathcal{I}(\mathcal{H}, \mathbb{A}) := \{\rho \in \mathcal{D}(\mathcal{H}) \mid \forall i, j. i \neq j \Rightarrow \langle a_i | \rho | a_j \rangle = 0\},$$

then we can define set coherence as follows: A set $\{\rho_i\}_i$ is incoherent if there exists *some* basis $\mathbb{A}$ with respect to which $\{\rho_i\}_i \subseteq \mathcal{I}(\mathcal{H}, \mathbb{A})$ and coherent otherwise.

While this definition is usually credited to Ref. [16], it is worth mentioning that there the authors consider set coherence as a notion defined with respect to finite *tuples* (i.e., to multistates whose index set is finite) as opposed to *sets* (i.e., as opposed to the image of a multistate). Moreover, it is obvious that a set $\{\rho_i\}_i$ is incoherent iff $[\rho_i, \rho_j] = 0$ for all i, j .

We thus note that set coherence is a feature of the whole set (not of individual members only) and independent of the number of states present in the set. This is distinct with saying that a certain set has coherent states relative to a certain basis which is in line with the standard basis-dependent description. For example, the set $\{|+\rangle\langle+|, \mathbb{1}/2\}$ has a coherent state with respect to $\{|0\rangle, |1\rangle\}$ yet, according to Definition II.1 the set is *incoherent* given that there exists a basis (namely $\{|+\rangle, |-\rangle\}$) with respect to which all states are incoherent.

Similarly, we define the notion of set imaginarity lifting the definition of basis-dependent imaginarity of a single state [39,40] to the basis-independent definition of imaginarity for a set of states [17]. Recall that a state $\rho \in \mathcal{D}(\mathcal{H})$, with $d = \dim(\mathcal{H}) < \infty$, is imaginarity free with respect to an orthonormal basis $\mathbb{A} = \{|a_i\rangle\}_{i=1}^d$ iff for every i, j we have that $\langle a_i | \rho | a_j \rangle \in \mathbb{R}$. Otherwise, we say that ρ has nonzero imaginarity or that it is not imaginarity free. With that, we can define set imaginarity as follows.

Definition II.2 (Set imaginarity). A set of states $\{\rho_i\}_i \subseteq \mathcal{D}(\mathcal{H})$ is *imaginarity free* if there exists a unitary $U : \mathcal{H} \rightarrow \mathcal{H}$ such that, for all i , $U\rho_i U^\dagger$ is a real density matrix with respect

to some basis $\mathbb{A}$. If this does not hold, we then say that $\{\rho_i\}_i$ is *not imaginarity free*.

We say that a set of states that is not imaginarity free *has* imaginarity. If we denote the set of all imaginarity-free states with respect to the basis $\mathbb{A}$ as

$$\mathcal{R}(\mathcal{H}, \mathbb{A}) := \{\rho \in \mathcal{D}(\mathcal{H}) \mid \forall i, j. \langle a_i | \rho | a_j \rangle \in \mathbb{R}\},$$

then we can equivalently define set imaginarity as follows: A set $\{\rho_i\}_{i \in I}$ is imaginarity free if there exists *some* basis $\mathbb{A}$ with respect to which $\{\rho_i\}_i \subseteq \mathcal{R}(\mathcal{H}, \mathbb{A})$ and not imaginarity free otherwise.

In what follows, we will use the same terminology of set imaginarity and set coherence applied to the multistates ϱ . We will then say that a multistate $\varrho : I \rightarrow \mathcal{D}(\mathcal{H})$ has coherence (imaginarity) iff the image $\varrho(I)$ is set coherent (not imaginarity free).

The set of all incoherent multistates $\varrho : I \rightarrow \mathcal{D}(\mathcal{H})$ will be denoted as

$$\mathcal{I}_I(\mathcal{H}) = \{\varrho : I \rightarrow \mathcal{D}(\mathcal{H}) \mid \exists \mathbb{A} \text{ s.t. } \varrho(I) \subseteq \mathcal{I}(\mathcal{H}, \mathbb{A})\} \quad (1)$$

and similarly the set of all imaginarity-free multistates

$$\mathcal{R}_I(\mathcal{H}) = \{\varrho : I \rightarrow \mathcal{D}(\mathcal{H}) \mid \exists \mathbb{A} \text{ s.t. } \varrho(I) \subseteq \mathcal{R}(\mathcal{H}, \mathbb{A})\}. \quad (2)$$

When $I = [n] \equiv \{1, \dots, n\}$ we write $\mathcal{I}_n(\mathcal{H})$ and $\mathcal{R}_n(\mathcal{H})$ instead.

We remark that this is a straightforward manner to lift basis-dependent definitions relative to a single state (in our case, coherence and imaginarity) to basis-independent definitions relative to multistates. As another example, Refs. [91,97] considered *set magic*—whenever the image of a multistate cannot be unitarily mapped to elements inside the stabilizer polytope—and characterized two-state overlap inequality witnesses of this property for generic multistates.

Changing from a single-state to a multistate description allows us to straightforwardly “lift” basis-dependent notions into basis-independent ones. However, this approach still retains an inherent *system dependence*—that is, a reference to the specific Hilbert space in which the states are defined. To go further, we can also “lift” this system dependence to a system (and basis) independent notion. We do so by drawing on the theory of Bargmann invariants and by framing the discussion in terms of quantum realization problems [98], an approach which was also considered by Ref. [90].

B. Sets of Bargmann invariants

As mentioned in the Introduction, Bargmann invariants play a crucial role in the characterization of basis-independent resources of multistates, as they generate all unitary-invariant polynomial functions of tuples of states [54,55]. More formally, estimating sufficiently many Bargmann invariants provides a complete solution to a unitary equivalence decision problem of the following form:

Given two multistates $\varrho, \varsigma : [n] \rightarrow \mathcal{D}(\mathcal{H})$, is there a unitary $U : \mathcal{H} \rightarrow \mathcal{H}$ such that $U\varrho U^\dagger = \varsigma$?

Above, we have used the notation $U\varrho U^\dagger = (U\rho_1 U^\dagger, \dots, U\rho_n U^\dagger)$. In finite dimensions ($d = \dim \mathcal{H} < \infty$), the existence of a unitary U with $U\varrho U^\dagger = \varsigma$ is equivalent to the requirement that all Bargmann invariants

agree. Concretely, such a unitary U exists iff for every $1 \leq m \leq d^2$ and every sequence $i_1, \dots, i_m$ from $\{1, \dots, n\}$ the corresponding Bargmann invariants *coincide*:

$$\text{Tr}(\rho_{i_1} \dots \rho_{i_m}) = \text{Tr}(\sigma_{i_1} \dots \sigma_{i_m}). \quad (3)$$

It turns out, based on the findings of Refs. [52,55], that considering all the exponentially many Bargmann invariants mentioned above is often *unnecessary*. Identifying minimal (or at least reduced) sets of invariants that suffice to solve these decision problems remains an active area of research. In fact, one of our results shows that in the case of single-qubit multistate imaginarity, estimating a *single* Bargmann invariant is sufficient (see Corollary III.7). Moreover, Ref. [55] presents an algorithm for identifying a minimal set of necessary and sufficient Bargmann invariants, under the assumption that the multistate consists exclusively of pure states.

Besides completely characterizing the unitary-invariant properties of multistates of fixed Hilbert space dimension, Bargmann invariants can also be used to relax the requirement of system dependence, as we now discuss.

Let us assume that the index set of a multistate is a finite set, so that $I \simeq \{1, \dots, n\} \equiv [n]$. In this case, we describe the set of all Bargmann invariants as an instance of a specific *quantum realizability problem* [98]:

Given a value $\Delta \in \mathbb{C}$, is there some multistate $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^d)$ such that $\Delta = \text{Tr}(\rho_1 \dots \rho_n) \equiv \Delta(\varrho)$?

If the answer is yes, then we say that $\Delta \in \mathfrak{B}_n^{(d)}$. Succinctly, we define this set as

$$\mathfrak{B}_n^{(d)} := \{\Delta \in \mathbb{C} \mid \exists \varrho \in \mathcal{D}(\mathbb{C}^d)^n \text{ s. t. } \Delta = \Delta(\varrho)\}.$$

If for a certain Δ there exists ϱ such that $\Delta = \Delta(\varrho)$, then we say that Δ is *realized by* ϱ in the Hilbert space $\mathcal{H} = \mathbb{C}^d$. More generally, we say that a complex number $\Delta \in \mathbb{C}$ is quantum realizable if there exists some multistate $\varrho = (\rho_1, \dots, \rho_n)$ with respect to some Hilbert space $\mathcal{H}$ such that $\Delta = \Delta(\varrho)$. References [57,90] have pointed out the simple (yet useful) remark that $\text{Im}[\text{Tr}(\rho_1 \dots \rho_n)] \neq 0$ implies that $\{\rho_i\}_i$ has imaginarity as by Definition II.2.

An important subset of $\mathfrak{B}_n^{(d)}$ is the set of all values Δ realizable by multistates of *pure states*, that we denote as $\Psi : [n] \rightarrow \mathcal{P}_1(\mathbb{C}^d)$. Therefore, we define

$$\mathfrak{B}_n^{(d)}|_{\text{pure}} := \{\Delta \in \mathbb{C} \mid \exists \Psi \in \mathcal{P}_1(\mathbb{C}^d)^n \text{ s. t. } \Delta = \Delta(\Psi)\}.$$

These definitions lead to the following ascending chain of sets:

$$\mathfrak{B}_n^{(2)} \subseteq \mathfrak{B}_n^{(3)} \subseteq \dots \subseteq \mathfrak{B}_n^{(d)} \subseteq \dots \subseteq \mathfrak{B}_n^{(n)} = \mathfrak{B}_n,$$

where we define

$$\mathfrak{B}_n = \bigcup_{d=2}^{\infty} \mathfrak{B}_n^{(d)}.$$

Ultimately, the set $\mathfrak{B}_n$ for a given fixed n is the subset of complex values that Bargmann invariants can reach. We can give a specific example to make this discussion more concrete while also highlighting the system independence we have mentioned earlier. For a more careful and comprehensive discussion we refer to Ref. [99], Chapter 7].

Fix $\Delta = i/6$, and consider third-order Bargmann invariant realizability. Every multistate $\varrho : [3] \rightarrow \mathcal{D}(\mathcal{H})$ (in any Hilbert-space dimension) that attains this value must contain imaginarity. More operationally, suppose one visits a laboratory that reports they are estimating a third-order Bargmann invariant. Even without any knowledge of the laboratory's Hilbert-space description of these quantum states, observing $\Delta = i/6$ already certifies that the prepared states exhibit imaginarity.

Notably, Valentine Bargmann [56] presented a pure multistate $\Psi : [3] \rightarrow \mathcal{P}_1(\mathbb{C}^2)$ defined by the vectors

$$|\psi_1\rangle = |0\rangle, \quad \psi_2 = |-\rangle, \quad \psi_3 = \frac{1}{\sqrt{3}}(|0\rangle + (1-i)|1\rangle), \quad (4)$$

achieving $\Delta(\Psi) = i/6$, where $\Psi(i) = |\psi_i\rangle\langle\psi_i| \equiv \psi_i$. This implies that Ψ has basis-independent imaginarity *and* $\Delta(\Psi) \in \mathfrak{B}_3^{(2)}$. Regardless of whether the states being prepared are these or instead $|\phi_i\rangle = F|\psi_i\rangle$ defined by an isometry $F : \mathbb{C}^2 \rightarrow \mathbb{C}^d$ the conclusion would have stayed the same (a concrete example might be given by applying the 3×3 discrete quantum Fourier transform matrix on the states $|\psi_i\rangle + 0 \cdot |2\rangle$). Thus, it is simple to see that by choosing such isometries, $\Delta \in \mathfrak{B}_3^{(2)} \Rightarrow \Delta \in \mathfrak{B}_3^{(d)}$, for any Hilbert space dimension $d < \infty$. Naturally, one can thus argue that nonzero imaginary values of numbers in $\mathfrak{B}_n$ probe the imaginarity of any realization, relative to any Hilbert space, leading to the notion of system independence illustrated in Fig. 1.

The discussion above motivates the investigation of the possible attainable values of Bargmann invariants, i.e., of the geometry of the set $\mathfrak{B}_n$. On a series of recent results these sets have been completely characterized [90,95,100–102] and it has been showed that the above ascending chain of sets *collapses*, i.e., that

$$\mathfrak{B}_n = \mathfrak{B}_n^{(2)} = \mathfrak{B}_n|_{\text{pure}}$$

for all $n \in \mathbb{N}$. Moreover, there is a *structure theorem* for Bargmann invariants in $\mathfrak{B}_n$ [100,102], which states that

$$\mathfrak{B}_n = \mathfrak{B}_n^{(3)}|_{\text{circ}}, \quad (5)$$

namely, that to every Bargmann invariant $\Delta(\varrho) = \text{Tr}(\rho_1 \dots \rho_n) \in \mathfrak{B}_n$ there exists a *pure* multistate $\Psi = (\psi_1, \dots, \psi_n) \in \mathcal{D}(\mathbb{C}^3)$ such that the associated Gram matrix $(G_{(|\psi_1\rangle, \dots, |\psi_n\rangle)})_{ij} = \langle\psi_i|\psi_j\rangle$ is a *circulant* matrix.

C. Sets of tuples of two-state overlaps

There are other sets of Bargmann invariants that have been investigated in the literature. For example, Refs. [24,25,57,80,81,91,92,94] have also considered more structured sets of tuples of second-order Bargmann invariants. In fact, in this case, Refs. [24,25] have introduced a graph-theoretic framework—connected to Kochen-Specker contextuality [103]—where we can link the index sets of multistates to vertices of a graph and describe the quantum realizability problem relative to this graph.

The formalism from Ref. [24] is built from the following simple idea. To organize which overlaps matter in a given experimentally relevant situation, it is convenient to label the states by a set and select only the pairs whose overlaps enter

the constraints. These labels and pairs form the vertices and edges of a simple graph, where each edge carries the corresponding label associated to an overlap value. We now make this precise.

Let $V = [n]$ and $E \subseteq \{\{i, j\} \mid i, j \in V\}$. We call a function $\Delta : E \rightarrow [0, 1]$ an *edge-weighting* since, formally, the elements $e \in E$ can be viewed as edges in the simple graph defined by $G = (V, E)$. A multistate $\varrho : V \rightarrow \mathcal{D}(\mathcal{H})$ is then a function returning a quantum state in $\mathcal{H}$ for each vertex V of the graph G . This graph-theoretic view will not be necessary in what follows, so we can simply view V as a specification of an index set and E as the specification of which two-state overlaps are relevant.

We say that $\Delta : E \rightarrow [0, 1]$ is *quantum realizable* in a Hilbert space $\mathcal{H}$ if there exists a multistate $\varrho : V \rightarrow \mathcal{D}(\mathcal{H})$ such that

$$\Delta(\{i, j\}) = \Delta_{ij} = \text{Tr}(\varrho(i)\varrho(j))$$

for every $\{i, j\} \in E$. Note that, from this perspective, Δ_{ij} are merely scalars with no reference (*a priori*) to quantum states, while $\text{Tr}(\varrho(i)\varrho(j))$ is the overlap that reaches the value of that scalar for $\{i, j\}$. Whenever there exists such a multistate, we write $\Delta = \Delta(\varrho)$. In this case, we have then a set of quantum correlations defined by such a quantum realization problem:

Definition II.3 (Adapted from Ref. [24]). Let $G = (V, E)$ be a simple graph. The set of quantum-realizable edge weightings is defined as

$$\Omega(G) := \{\Delta \in [0, 1]^E \mid \exists \varrho \text{ s.t. } \Delta = \Delta(\varrho)\}, \quad (6)$$

where $\varrho : V \rightarrow \mathcal{D}(\mathcal{H})$ for some Hilbert space $\mathcal{H}$.

In simple terms, $\Omega(G)$ is the set of all possible tuples of the form $(\text{Tr}(\rho_i \rho_j))_{\{i, j\} \in E}$. If we let $E = \{\{1, 2\}, \{1, 3\}, \{2, 3\}\}$ —which is the edge-set of a three-cycle graph—then $\Omega(G)$ is equivalent to the set of all possible tuples,

$$\Delta(\varrho) = (\text{Tr}(\rho_1 \rho_2), \text{Tr}(\rho_1 \rho_3), \text{Tr}(\rho_2 \rho_3)),$$

for all possible multistates $\varrho : \{1, 2, 3\} \rightarrow \mathcal{D}(\mathcal{H})$ with respect to all possible Hilbert spaces $\mathcal{H}$.

Similarly to the case of the sets of Bargmann invariants $\mathfrak{B}_n$, we can also consider restrictions of these sets. The most relevant to us are the restrictions to pure states,

$$\Omega(G)|_{\text{pure}} := \{\Delta \mid \exists \Psi : V \rightarrow \mathcal{P}_1(\mathcal{H}) \text{ s.t. } \Delta = \Delta(\Psi)\}, \quad (7)$$

and the restriction to imaginarity-free states,

$$\Omega(G)|_{\text{real}} := \{\Delta \mid \exists \varrho : V \rightarrow \mathcal{R}(\mathcal{H}, \mathbb{A}) \text{ s.t. } \Delta = \Delta(\varrho)\}. \quad (8)$$

Provided we have the function $\Delta : E \rightarrow [0, 1]$ and its notion of quantum realization, we can apply it to notions of quantum realizations of any function $f(\Delta)$. For example, if we let

$$P(x_1, x_2, x_3) = x_1^2 + x_2^2 + x_3^2,$$

then we can talk about all values P can take provided that $x_1 = \Delta_{12}(\varrho) \equiv \text{Tr}(\rho_1 \rho_2)$, $x_2 = \Delta_{13}(\varrho) \equiv \text{Tr}(\rho_1 \rho_3)$, $x_3 = \Delta_{23}(\varrho) \equiv \text{Tr}(\rho_2 \rho_3)$ in which case we write

$$P(\Delta(\varrho)) = (\text{Tr}(\rho_1 \rho_2))^2 + (\text{Tr}(\rho_1 \rho_3))^2 + (\text{Tr}(\rho_2 \rho_3))^2.$$

This notion will be relevant to us later on in Sec. VI, when stating and interpreting Theorem V.1.

D. Gram matrix of Bloch vectors

Let $\rho \in \mathcal{D}(\mathbb{C}^2)$ be any single-qubit state, there exists a unique vector $\mathbf{r} = (x, y, z) \in \mathbb{R}^3$ such that $\|\mathbf{r}\|^2 = x^2 + y^2 + z^2 \leq 1$, and

$$\rho = \frac{\mathbb{1} + \mathbf{r} \cdot \boldsymbol{\sigma}}{2}.$$

The vector $\mathbf{r}$ is known as the *Bloch vector* of the state ρ . Given an n -tuple of single qubit states $\varrho = (\rho_1, \rho_2, \dots, \rho_n) \in \mathcal{D}(\mathbb{C}^2)^n$, we can construct the $n \times n$ Gram matrix associated to the related tuple of Bloch vectors $\mathbf{r}_\varrho := (\mathbf{r}_1, \dots, \mathbf{r}_n)$ given by

$$G_{\mathbf{r}_\varrho} := (\langle \mathbf{r}_k, \mathbf{r}_l \rangle)_{kl}.$$

The overlap between two single-qubit states $\rho_i, \rho_j \in \varrho$ is a function of the scalar product between the two Bloch vectors,

$$\text{Tr}[\rho_i \rho_j] = \text{Tr} \left[\frac{(\mathbb{1} + \mathbf{r}_i \cdot \boldsymbol{\sigma}) (\mathbb{1} + \mathbf{r}_j \cdot \boldsymbol{\sigma})}{2} \right] = \frac{1 + \langle \mathbf{r}_i, \mathbf{r}_j \rangle}{2}. \quad (9)$$

So

$$\langle \mathbf{r}_i, \mathbf{r}_j \rangle = 2\text{Tr}[\rho_i \rho_j] - 1, \quad (10)$$

which implies that each entry of the Gram matrix $G_{\mathbf{r}_\varrho}$ is in one-to-one correspondence with some Bargmann invariant of order 2.

We can make this construction more general [104,105], given an orthogonal (with respect to the Hilbert-Schmidt inner product) basis of $d \times d$ matrices, e.g., the set of (generalized) Gell-Mann matrices together with the identity, where $U_0 = \mathbb{1}_d$, U_i are traceless and Hermitian matrices satisfying $\text{Tr}[U_i U_j] = d\delta_{i,j}$.

Each density matrix $\rho \in \mathcal{D}(\mathbb{C}^d)$ can be written as

$$\rho = \frac{1}{d} \left(\mathbb{1}_d + \sum_{j=1}^{d^2-1} r_j U_j \right),$$

where $r_j = \text{tr}[\rho U_j]$. If we are given a multistate $\varrho = (\rho_1, \dots, \rho_n) \in \mathcal{D}(\mathbb{C}^d)$, then each $\varrho(i) = \rho_i$ corresponds to an $d^2 - 1$ -dimensional real vector $\mathbf{r}_i$. Given the related tuple of associated generalized Bloch vectors $\mathbf{r}_\varrho$ we define the $n \times n$ Gram matrix

$$G_{\mathbf{r}_\varrho} := (\langle \mathbf{r}_k, \mathbf{r}_l \rangle)_{k,l}$$

as before, where the vectors $\mathbf{r}_i$ lie in a $d^2 - 1$ -dimensional real vector space. Similarly to Eq. (10), we find that

$$\langle \mathbf{r}_i, \mathbf{r}_j \rangle = d \text{Tr}(\rho_i \rho_j) - 1. \quad (11)$$

III. CHARACTERIZATION OF SINGLE-QUBIT MULTISTATE IMAGINARITY

A. Rank-based criteria

We start by considering the quantum imaginarity of a finite set of single-qubit quantum states. Reference [90] has shown that assuming *purity* it is possible to witness imaginarity using only two-state overlaps. Here we show that we can trade the assumption of purity by that of Hilbert space dimension.

Given an n -tuple of qubit states $\varrho = (\rho_1, \rho_2, \dots, \rho_n) \in \mathcal{D}(\mathbb{C}^2)^n$, let $\mathbf{r}_k = (x_k, y_k, z_k) \in \mathbb{R}^3$ be the Bloch vector of $\rho_k \in$

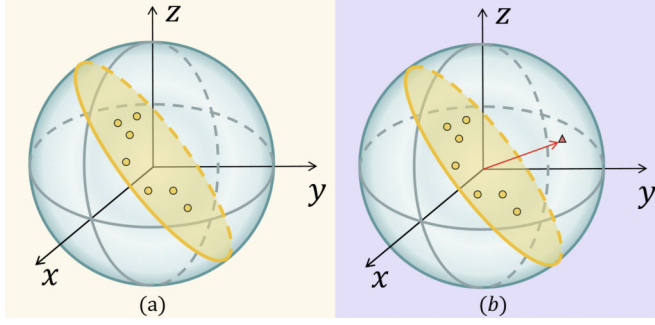


FIG. 2. Geometric interpretation of single-qubit multistate imaginarity. (a) Any set of states lying within a plane defined by a great circle of the Bloch sphere is imaginarity free. (b) If, for every possible such choice of plane, there exists at least one state (represented by a red triangle) that never lies within it, then the set of states has imaginarity.

$\varrho([n])$ for any $k \in [n]$. Our goal is to show that the image of ϱ is imaginarity free *iff* the Gram matrix of Bloch vectors

$$(G_{\mathbf{r}_\varrho})_{kl} := \langle \mathbf{r}_k, \mathbf{r}_l \rangle$$

is at most *rank* 2.

From the point of view of the Bloch sphere representation, our goal is motivated by a simple geometric intuition illustrated in Fig. 2. Any set of states lying entirely within the X - Z plane of the Bloch sphere is clearly real-represented with respect to the canonical basis $\mathbb{A}_{\text{st}} = \{|0\rangle, |1\rangle\}$. Due to unitary invariance, any set of states lying within a plane formed by a great circle of the Bloch sphere should be imaginarity free, since one can unitarily rotate that plane—along with all the states it contains—into the X - Z plane. This geometric intuition is so compelling that one is naturally led to conjecture that this is *the only way* a set of single-qubit states can be imaginarity free. In what follows, we rigorously prove that this intuition is indeed correct.

We start by showing the simple direction:

Lemma III.1. If $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^2)^n$ is an imaginarity-free single-qubit multistate, i.e., $\varrho \in \mathcal{R}_n(\mathbb{C}^2)$, then $\text{rank}(G_\varrho) \leq 2$.

Proof. For each $U \in \text{SU}(2)$, we define the action of U on the multistate ϱ as

$$U\varrho U^\dagger := (U\rho_1 U^\dagger, U\rho_2 U^\dagger, \dots, U\rho_n U^\dagger).$$

The Gram matrix of Bloch vectors is invariant under this map, i.e., for all $U \in \text{SU}(2)$ we have that

$$G_{\mathbf{r}_\varrho} = G_{\mathbf{r}_{U\varrho U^\dagger}}. \quad (12)$$

This follows easily from the fact that, to every fixed choice of unitary U , the map $\rho \mapsto U\rho U^\dagger$ induces an orthogonal (i.e., inner-product preserving) map $\Phi_U : \mathbb{R}^3 \rightarrow \mathbb{R}^3$ given by $\mathbf{r} \mapsto \mathbf{r}_U$ where $\rho = \frac{1+\mathbf{r}\cdot\boldsymbol{\sigma}}{2}$ and $U\rho U^\dagger = \frac{1+\mathbf{r}_U\cdot\boldsymbol{\sigma}}{2}$. To see this, let $\tau = \frac{1+\mathbf{s}\cdot\boldsymbol{\sigma}}{2}$, we have Eq. (9) and

$$\begin{aligned} \text{Tr}[U\rho U^\dagger U\tau U^\dagger] &= \text{Tr}\left[\frac{(1+\mathbf{r}_U\cdot\boldsymbol{\sigma})(1+\mathbf{s}_U\cdot\boldsymbol{\sigma})}{2}\right] \\ &= \frac{1 + \langle \mathbf{r}_U, \mathbf{s}_U \rangle}{2}. \end{aligned}$$

As $\text{Tr}[U\rho U^\dagger U\tau U^\dagger] = \text{Tr}[U\rho\tau U^\dagger] = \text{Tr}[\rho\tau]$, we conclude

$$\frac{1 + \langle \mathbf{r}, \mathbf{s} \rangle}{2} = \text{Tr}[\rho\tau] = \text{Tr}[U\rho U^\dagger U\tau U^\dagger] = \frac{1 + \langle \mathbf{r}_U, \mathbf{s}_U \rangle}{2}.$$

Therefore,

$$\langle \mathbf{r}, \mathbf{s} \rangle = \langle \mathbf{r}_U, \mathbf{s}_U \rangle = \langle \Phi_U(\mathbf{r}), \Phi_U(\mathbf{s}) \rangle.$$

We conclude the argument acknowledging that if $\varrho = (\rho_1, \rho_2, \dots, \rho_n)$ is imaginarity free, there exists some basis $\mathbb{A}$ with respect to which all the density matrices are real-only. This implies that there exists a unitary $U \in \text{U}(2)$ —describing the change of basis from $\mathbb{A}$ to the standard basis $\mathbb{A}_{\text{st}} = \{|0\rangle, |1\rangle\}$ —such that each element in $U\varrho U^\dagger$ lie within the great-circle plane of the Bloch sphere given by the X - Z plane, from which we have that $\text{rank}(G_{\mathbf{r}_{U\varrho U^\dagger}}) \leq 2$. From unitary-invariance of this Gram matrix $G_{\mathbf{r}_\varrho} = G_{\mathbf{r}_{U\varrho U^\dagger}}$, we have

$$\text{rank}(G_{\mathbf{r}_\varrho) \leq 2.$$

This concludes the proof. $\blacksquare$

Noting that for all $\varrho \in \mathcal{D}(\mathbb{C}^2)^n$ implies that $\text{rank}(G_{\mathbf{r}_\varrho) \leq 3$ we obtain a *sufficient* condition for $\varrho \in \mathcal{D}(\mathbb{C}^2)^n$ to have quantum imaginarity: $\text{rank}(G_{\mathbf{r}_\varrho) = 3$. In the following, we will show that this rank condition is also a necessary condition.

First, recall that elements $U \in \text{SU}(2)$ (i.e., U is a 2×2 unitary with $\det[U] = 1$) can be written as

$$U = \begin{bmatrix} \alpha & \beta \\ -\bar{\beta} & \bar{\alpha} \end{bmatrix},$$

where $\alpha = a + ib, \beta = c + id \in \mathbb{C}$ and $a^2 + b^2 + c^2 + d^2 = |\alpha|^2 + |\beta|^2 = 1$. Therefore, this identifies elements of $\text{SU}(2)$ with the 3-sphere $\mathbb{S}^3 = \{\mathbf{r} \in \mathbb{R}^4 \mid \|\mathbf{r}\| = 1\} \subset \mathbb{R}^4$. With respect to this representation, the matrix form of Φ_U is given by

$$\begin{bmatrix} a^2 - b^2 - c^2 + d^2 & 2(ab + cd) & 2(bd - ac) \\ 2(cd - ab) & a^2 - b^2 + c^2 - d^2 & 2(bc + ad) \\ 2(bd + ac) & 2(bc - ad) & a^2 + b^2 - c^2 - d^2 \end{bmatrix}. \quad (13)$$

Moreover, $\det[\Phi_U] = (a^2 + b^2 + c^2 + d^2)^3 = 1$. Therefore, Φ_U is in fact in $\text{SO}(3)$. This is a well-known matrix construction, and Φ as defined describes the (surjective Lie group) homomorphism between $\text{SU}(2)$ and

$\text{SO}(3)$. This result is known as the *double cover lemma* since the mapping $U \mapsto \Phi_U$ maps both $U(\alpha, \beta)$ and $U(-\alpha, -\beta)$ to the same element in $\text{SO}(3)$, hence the “double.”

Lemma III.2 (Double cover lemma, see Theorem 2.6 of Ref. [106]). The map $\Phi : \text{SU}(2) \rightarrow \text{SO}(3)$ defined by $U \mapsto \Phi_U$, with Φ_U given by Eq. (13), is a two-to-one surjective (Lie group) homomorphism.

With this technical ingredient in hand, we are ready to show the following:

Theorem III.3. A single-qubit multistate $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^2)$ has imaginarity, i.e., $\varrho \notin \mathcal{R}_n(\mathbb{C}^2)$, iff $\text{rank}(G_{\mathbf{r}_\varrho}) = 3$.

Proof. From Lemma III.1 we have that $\varrho \notin \mathcal{R}_n(\mathbb{C}^2) \Rightarrow \text{rank}(G_{\mathbf{r}_\varrho}) = 3$. Note that for every single-qubit multistate $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^2)$ we have that $\text{rank}(G_{\mathbf{r}_\varrho}) \leq 3$. Therefore, we proceed to show that $\text{rank}(G_{\mathbf{r}_\varrho}) \leq 2$ implies $\varrho \in \mathcal{R}_n(\mathbb{C}^2)$.

If $\text{rank}(G_{\mathbf{r}_\varrho}) = 1$, then one has $\text{span}_{\mathbb{R}}\{\mathbf{r}_k\}_{k=1}^n = 1$. Assume, without loss of generality, that $\mathbf{r}_1 \neq \mathbf{0}$ and set a reference Bloch vector to be the normalized vector $\mathbf{r} := \frac{\mathbf{r}_1}{\|\mathbf{r}_1\|}$. Since the rank is 1, for each k there exists some real number $x_k \in \mathbb{R}$ such that $\mathbf{r}_k = x_k \mathbf{r}$. Clearly, there exist some orthogonal rotation $R \in \text{SO}(3)$ setting $\mathbf{r}$ to $\mathbf{e}_1 = (1, 0, 0)^T$, i.e., $R\mathbf{r} = \mathbf{e}_1$. As Φ is surjective, we have some $U \in \text{SU}(2)$ such that $\Phi_U = R$. Therefore, $\Phi_U \mathbf{r}_k = x_k \Phi_U \mathbf{r} = x_k R\mathbf{r} = x_k \mathbf{e}_1 = (x_k, 0, 0)^T$. Hence

$$U \rho_k U^\dagger = \frac{\mathbb{1} + (\Phi_U \mathbf{r}_k) \cdot \boldsymbol{\sigma}}{2} = \frac{\mathbb{1} + r_k \sigma_1}{2}$$

is a real density matrix with respect to $\mathbb{A}_{\text{st}} = \{|0\rangle, |1\rangle\}$ for all $k = 1, 2, \dots, n$.

If $\text{rank}(G_{\mathbf{r}_\varrho}) = 2$, then one has $\text{span}_{\mathbb{R}}\{\mathbf{r}_k\}_{k=1}^n = 2$. There exist two orthogonal unit vectors $\mathbf{s}, \mathbf{t} \in \mathbb{R}^3$ such that

$$\text{span}_{\mathbb{R}}\{\mathbf{r}_k\}_{k=1}^n = \text{span}_{\mathbb{R}}\{\mathbf{s}, \mathbf{t}\}.$$

Therefore, for each $\mathbf{r}_k$ there exists $x_k, z_k \in \mathbb{R}$ such that

$$\mathbf{r}_k = x_k \mathbf{s} + z_k \mathbf{t}.$$

There are two unit vectors $\pm \frac{\mathbf{s} \times \mathbf{t}}{\|\mathbf{s} \times \mathbf{t}\|}$ orthogonal to both $\mathbf{s}$ and $\mathbf{t}$. We now choose $\mathbf{u} \in \{\frac{\mathbf{s} \times \mathbf{t}}{\|\mathbf{s} \times \mathbf{t}\|}, -\frac{\mathbf{s} \times \mathbf{t}}{\|\mathbf{s} \times \mathbf{t}\|}\}$ such that $\{\mathbf{s}, \mathbf{u}, \mathbf{t}\}$ forms a right-hand frame for $\mathbb{R}^3$, i.e., a spanning set of vectors such that $\mathbf{s} \times \mathbf{u} = \mathbf{t}$. In this case, we can construct a matrix R which rotates our frame to the standard orthonormal basis

$$R := \mathbf{e}_1 \mathbf{s}^T + \mathbf{e}_2 \mathbf{u}^T + \mathbf{e}_3 \mathbf{t}^T.$$

From the fact that $\{\mathbf{s}, \mathbf{u}, \mathbf{t}\}$ forms a right-hand frame we have that $\det(R) = +1$ which, by construction, implies that $R \in \text{SO}(3)$.

By construction, $R\mathbf{s} = \mathbf{e}_1$ and $R\mathbf{t} = \mathbf{e}_3$. So for each k ,

$$R\mathbf{r}_k = R(x_k \mathbf{s} + z_k \mathbf{t}) = x_k (R\mathbf{s}) + z_k (R\mathbf{t}) = (x_k, 0, z_k)^T.$$

As Φ is surjective, we have some $U \in \text{SU}(2)$ such that $\Phi_U = R$. For this U and each $k \in [n]$:

$$U \rho_k U^\dagger = \frac{\mathbb{1} + (R\mathbf{r}_k) \cdot \boldsymbol{\sigma}}{2} = \frac{\mathbb{1} + x_k \sigma_1 + z_k \sigma_3}{2},$$

which is a real density matrix relative to $\mathbb{A}_{\text{st}}$ since $\sigma_1 = \sigma_x$, $\sigma_3 = \sigma_z$ are also. Therefore, the image of ϱ is imaginarity free.

B. A simple remark beyond single-qubit states

Using the generalized Bloch vector representation of d -dimensional states, it is simple to generalize Lemma III.1.

Proposition III.4. If $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^d)$ is an imaginarity-free multistate, i.e., $\varrho \in \mathcal{R}_n(\mathbb{C}^d)$, then $\text{rank}(G_{\mathbf{r}_\varrho}) \leq \frac{d(d+1)}{2} - 1$, where $\mathbf{r}_\varrho$ are generalized Bloch vectors given by the generalized Gell-Mann matrices.

Proof. If ϱ is imaginarity free, then there exists U such that $U \varrho U^\dagger$ are all real matrices relative to some basis $\mathbb{A}$ for $\mathcal{H}$. Because all matrices $\{U \varrho(i) U^\dagger\}_i$ are Hermitian and have only real entries, they are also equal to their transpose and hence lie in the subspace of real symmetric matrices. (In other words, relative to their Gell-Mann representation, all the components along the imaginary (antisymmetry) generalized Gell-Mann basis vanish.) The subspace of real symmetric $d \times d$ matrices has dimension $d(d+1)/2$. Subtracting the identity, we are left with $d(d+1)/2 - 1$ components of generalized Bloch vectors spanning at most $d(d+1)/2 - 1$ dimensions. Therefore, $\text{rank}(G_{\mathbf{r}_{U \varrho U^\dagger}}) = \text{rank}(G_{\mathbf{r}_\varrho}) \leq d(d+1)/2 - 1$. ■

Note that whenever $d = 2$ we recover Lemma III.1 since in this case $\text{rank}(G_{\mathbf{r}_\varrho}) \leq \frac{2(2+1)}{2} - 1 = 2$ and the generalized Bloch vectors reduce to the usual ones.

We can, furthermore, comment on what prevents us to obtaining a result similar to Theorem III.3. As before, there exists a mapping Φ_d from $\text{SU}(d)$ to $\text{SO}(d^2 - 1)$. However, the dimension gap

$$\begin{aligned} \dim_{\mathbb{R}}[\text{SU}(d)] &= d^2 - 1 < \frac{(d^2 - 1)(d^2 - 2)}{2} \\ &= \dim_{\mathbb{R}}[\text{SO}(d^2 - 1)] \end{aligned}$$

for all $d \geq 3$ makes the map Φ_d fail to be surjective. This prevents this to be a sufficient condition as well.

We can also provide an explicit counterexample. Let us consider $d = 3$ and $\{\lambda_i\}_{i=1}^8$ to be the Gell-Mann matrices (Table I in Ref. [107]). Note that, in this case, $\text{Tr}(\lambda_i \lambda_j) = 2\delta_{ij}$ so that $\langle \mathbf{r}_i, \mathbf{r}_j \rangle = \frac{9\text{Tr}(\rho_i \rho_j) - 3}{2}$. [108] Take three qutrits given by

$$\rho_1 = \frac{1}{3}(\mathbb{1}_3 + \lambda_1), \quad \rho_2 = \frac{1}{3}(\mathbb{1}_3 + \lambda_4), \quad \rho_3 = \frac{1}{3}(\mathbb{1}_3 + \lambda_7). \quad (14)$$

Above, λ_1, λ_4 are two symmetric matrices while λ_7 is an anti-symmetric matrix. A simple calculation shows that $\text{Tr}(\rho_i^2) = 5/9$ and $\text{Tr}(\rho_i \rho_j) = 1/3$ for $i \neq j$. Therefore, $\text{rank}(G_{\mathbf{r}_\varrho}) = 3 < 3(3+1)/2 - 1 = 5$. Nevertheless, the associated multistate $\varrho = (\rho_1, \rho_2, \rho_3)$ has imaginarity since

$$\Delta(\varrho) = \text{Tr}(\rho_1 \rho_2 \rho_3) = \frac{1}{27}(3 + \text{Tr}(\lambda_1 \lambda_4 \lambda_7)) = \frac{1}{27}(3 + i), \quad (15)$$

and therefore $\text{Im}[\Delta(\varrho)] \neq 0$.

Moreover, it is trivial to see that every multistate $\varrho : \{1, 2\} \rightarrow \mathcal{D}(\mathcal{H})$ is imaginarity free for all possible Hilbert spaces $\mathcal{H}$. We state this as a lemma for future reference:

Lemma III.5. Every multistate $\varrho : \{1, 2\} \rightarrow \mathcal{D}(\mathcal{H})$ is imaginarity free.

C. Implications for Bargmann invariants realizable by imaginarity-free multistates

We can use Theorem III.3 to show a few structural results about sets of tuples of Bargmann invariants $\Omega(G)^{(d)}$ when we restrict realizations to a certain Hilbert space dimension d . We start by showing that for any graph $G = (V, E)$ where $|V| = n \geq 3$ not all two-state overlaps (provided that we restrict the

Hilbert space dimension) can be reached by real-only single-qubit states.

Corollary III.6. Let $G = (V, E)$ be a simple graph of n nodes. Then

(1) for $n \in \{1, 2\}$, it holds that $\Omega(G)^{(d)}|_{\text{real}} = \Omega(G)^{(d)}$ for all integers $d \geq 2$.

(2) for $n \geq 3$, it holds that $\Omega(G)^{(2)}|_{\text{real}} \subsetneq \Omega(G)^{(2)}$.

(3) for $n \geq 3$, $d \geq 2$, and $\Delta : E \rightarrow [0, 1]$ it holds that $\Delta(\varrho) \in \Omega(G)^{(d)}|_{\text{real}}$ for all multistates $\varrho : \{1, 2\} \rightarrow \mathcal{D}(\mathcal{H})$.

Proof. The first and third part follow from Lemma III.5, i.e., from the fact that two states in any finite-dimensional Hilbert space span at most a two-dimensional space, which is isometrically isomorphic to qubit space.

As for the second part, from $\text{Tr}[\rho_k \rho_l] = \frac{1 + \langle \mathbf{r}_k, \mathbf{r}_l \rangle}{2}$ and Theorem III.3 it suffices to show that for every $n \geq 3$ there exists $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^2)$ such that $\text{rank}(G_\varrho) = 3$, which is trivially true. ■

Reference [90] had previously shown that for $n = 3$ these two sets are equal, i.e.,

$$\Omega(K_3) = \Omega(K_3)|_{\text{real}},$$

and that for $n = 4$ there is a gap between the sets if we restrict to the pure states. Symbolically,

$$\Omega(K_4)|_{\text{pure}} \cap \Omega(K_4)|_{\text{real}} \subsetneq \Omega(K_4)|_{\text{pure}}.$$

Corollary III.6 implies that a single two-state overlap cannot witness imaginarity. It also implies that in order to experimentally witness imaginarity semidevice independently by measuring two-state overlaps one can choose between two assumptions: either an assumption on the *purity* of the states and then follow the proposal from Ref. [90] or an assumption on their underlying Hilbert space dimension and then experimentally estimate the rank of $G_{\mathbf{r}_\varrho}$.

Another interesting aspect is that third-order invariants *completely* characterize the imaginarity of single-qubit (possibly mixed) states. Let $\rho_k = \frac{\mathbb{I} + \mathbf{r}_k \cdot \boldsymbol{\sigma}}{2}$. The condition $\text{rank}(G_{\mathbf{r}_\varrho}) = 3$ is satisfied iff $\text{span}_{\mathbb{R}}\{\mathbf{r}_k\}_{k=1}^n = 3$ which holds iff there exists k, l, m such that $\mathbf{r}_k, \mathbf{r}_l, \mathbf{r}_m$ are *linearly independent*. Hence $\det[(\mathbf{r}_k, \mathbf{r}_l, \mathbf{r}_m)] \neq 0$. It has been noted in Appendix B in Ref. [95] that

$$\text{Im}(\text{Tr}[\rho_k \rho_l \rho_m]) = \frac{1}{4} \det[(\mathbf{r}_k, \mathbf{r}_l, \mathbf{r}_m)].$$

So we obtain that ϱ has quantum imaginarity *iff* there exists some k, l, m such that $\text{Tr}[\rho_k \rho_l \rho_m] \notin \mathfrak{B}_3|_{\text{real}} \subseteq \mathbb{R}$.

Corollary III.7. Fix $n \in \mathbb{N}$. $\varrho \notin \mathcal{R}_n(\mathbb{C}^2) \iff \text{Tr}(\rho_k \rho_l \rho_m) \notin \mathfrak{B}_3|_{\text{real}}$ for some triplet of labels $k, l, m \in [n]$.

In particular, $\varrho \notin \mathcal{R}_3(\mathbb{C}^2)$ *iff* $\Delta(\varrho) = \text{Tr}(\rho_1 \rho_2 \rho_3) \notin \mathfrak{B}_3|_{\text{real}} = [-1/8, 1]$. In other words, the quantum imaginarity of a set of three quantum states in a single-qubit system is completely characterized by their third-order Bargmann invariant *alone*.

Interestingly, for higher-dimensional systems third-order invariants are *not* sufficient to characterize multistate imaginarity as we now show with an example. Choose $\mathcal{H} = \mathbb{C}^4$. We want to construct a multistate $\varphi : \{1, 2, 3\} \rightarrow \mathcal{D}(\mathbb{C}^2)$ such that $\varphi \notin \mathcal{R}_3(\mathbb{C}^4)$ but that, nevertheless, $\text{Tr}(\varphi_1 \varphi_2 \varphi_3) \in \mathfrak{B}_3|_{\text{real}}$.

First, we consider two multistates $\varrho, \varsigma : \{1, 2, 3\} \rightarrow \mathcal{D}(\mathbb{C}^2)$ given by

$$\begin{aligned} \rho_1 &= \begin{bmatrix} \frac{1}{3} & \frac{i}{3} \\ -\frac{i}{3} & \frac{2}{3} \end{bmatrix}, & \rho_2 &= \begin{bmatrix} \frac{1}{4} & \frac{i}{5} \\ -\frac{i}{5} & \frac{3}{4} \end{bmatrix}, & \rho_3 &= \begin{bmatrix} \frac{1}{6} & \frac{1}{7} \\ \frac{1}{7} & \frac{5}{6} \end{bmatrix}, \\ \sigma_1 &= \begin{bmatrix} \frac{3}{4} & \frac{i}{4} \\ -\frac{i}{4} & \frac{1}{4} \end{bmatrix}, & \sigma_2 &= \begin{bmatrix} \frac{4}{5} & \frac{1}{8} \\ \frac{1}{8} & \frac{1}{5} \end{bmatrix}, & \sigma_3 &= \begin{bmatrix} \frac{1}{6} & \frac{i}{7} \\ -\frac{i}{7} & \frac{5}{6} \end{bmatrix}. \end{aligned}$$

In this case, we have that

$$\text{Tr}[\rho_1 \rho_2 \rho_3] = \frac{1}{3 \times 4 \times 5 \times 6 \times 7} (1253 + 36i),$$

$$\text{Tr}[\sigma_1 \sigma_2 \sigma_3] = \frac{1}{4 \times 5 \times 6 \times 7 \times 8} (1192 - 200i),$$

which implies that each of these multistates has imaginarity. Now, we define a new multistate

$$\varphi_i = \lambda \rho_i \oplus (1 - \lambda) \sigma_i \equiv \begin{bmatrix} \lambda \rho_i & \mathbb{0}_2 \\ \mathbb{0}_2 & (1 - \lambda) \sigma_i \end{bmatrix},$$

for all $i = 1, 2, 3$. The third-order invariant in this case is given by

$$\text{Tr}[\varphi_1 \varphi_2 \varphi_3] = \lambda^3 \text{Tr}[\rho_1 \rho_2 \rho_3] + (1 - \lambda)^3 \text{Tr}[\sigma_1 \sigma_2 \sigma_3].$$

If we choose $\lambda \in (0, 1)$ such that

$$\lambda^3 \frac{36i}{3 \times 4 \times 5 \times 6 \times 7} + (1 - \lambda)^3 \frac{-200i}{4 \times 5 \times 6 \times 7 \times 8} = 0, \quad (16)$$

then we obtain by construction that $\text{Tr}[\varphi_1 \varphi_2 \varphi_3] \in \mathfrak{B}_3|_{\text{real}} \subseteq \mathbb{R}$. However, higher-order invariants are capable to witness the fact that the multistate φ as constructed *has* imaginarity. Since

$$\text{Tr}[\rho_1^2 \rho_2 \rho_3] = \frac{1}{3^2 \times 4 \times 5 \times 6 \times 7} (3199 + 108i),$$

$$\text{Tr}[\sigma_1^2 \sigma_2 \sigma_3] = \frac{1}{4^2 \times 5 \times 6 \times 7 \times 8} (3760 - 800i),$$

we have the fourth-order invariant

$$\text{Tr}[\varphi_1^2 \varphi_2 \varphi_3] = \lambda^4 \text{Tr}[\rho_1^2 \rho_2 \rho_3] + (1 - \lambda)^4 \text{Tr}[\sigma_1^2 \sigma_2 \sigma_3] \notin \mathbb{R}$$

that witnesses the imaginarity of $\varphi : \{1, 2, 3\} \rightarrow \mathcal{D}(\mathbb{C}^4)$. The invariant $\text{Tr}[\varphi_1^2 \varphi_2 \varphi_3] \notin \mathfrak{B}_4|_{\text{real}}$ cannot be real since otherwise

$$\lambda^4 \frac{36i}{3 \times 4 \times 5 \times 6 \times 7} + (1 - \lambda)^4 \frac{-200i}{4 \times 5 \times 6 \times 7 \times 8} = 0,$$

which is in contradiction with Eq. (16).

This construction provides a concrete example to a broad result from Ref. [55], where the authors showed that Bargmann invariants of repeated entries are, in general, necessary to completely characterize the unitary-invariant properties of a set of *mixed* states.

D. On the geometry of the set of imaginarity-free multistates

For the case of quantum coherence, Designolle *et al.* [16] had previously showed that $\mathcal{I}_n(\mathcal{H})$ is not convex. Here we show that $\mathcal{R}_n(\mathcal{H})$ is also, in general, not a convex set.

Corollary III.8. The set $\mathcal{R}_3(\mathbb{C}^2)$ is nonconvex. In other words, there exist $\varrho, \varsigma \in \mathcal{R}_3(\mathbb{C}^2)$ and $p \in (0, 1)$ such that the new multistate defined by

$$\xi = p\varrho + (1-p)\varsigma \quad (17)$$

has imaginarity.

Proof. Let us consider $\varrho : \{1, 2, 3\} \rightarrow \mathcal{D}(\mathbb{C}^2)$ such that $\varrho(i) := \frac{\mathbb{1} + \mathbf{r}_i \cdot \boldsymbol{\sigma}}{2}$ defined by the Bloch vectors

$$\mathbf{r}_1 = (1, 0, 0), \quad \mathbf{r}_2 = (0, 1, 0), \quad \mathbf{r}_3 = (1/\sqrt{2}, 1/\sqrt{2}, 0),$$

and $\varsigma : \{1, 2, 3\} \rightarrow \mathcal{D}(\mathbb{C}^2)$ such that $\varsigma(i) := \frac{\mathbb{1} + \mathbf{s}_i \cdot \boldsymbol{\sigma}}{2}$ defined instead by the vectors

$$\mathbf{s}_1 = (0, 1/\sqrt{2}, 1/\sqrt{2}), \quad \mathbf{s}_2 = (0, 1, 0), \quad \mathbf{s}_3 = (0, 0, 1).$$

Let $A = [\mathbf{r}_1; \mathbf{r}_2; \mathbf{r}_3]$ and $B = [\mathbf{s}_1; \mathbf{s}_2; \mathbf{s}_3]$. We now note that $\text{rank}(G_{\mathbf{r}_\varrho}) = \text{rank}(A)$ and $\text{rank}(G_{\mathbf{s}_\varsigma}) = \text{rank}(B)$ [this follows from the fact that $G_{\mathbf{r}_\varrho} = AA^T$ and $\text{rank}(AA^T) = \text{rank}(A)$]. From Theorem III.3, we have that $\varrho, \varsigma \in \mathcal{R}_3(\mathbb{C}^2)$. Nevertheless, for every $p \in (0, 1)$ if we write ξ as the convex combination of ϱ and ς with weight p we have that $\text{rank}(G_{\mathbf{r}_\xi}) = \text{rank}(C_p)$, where

$$C_p = \begin{pmatrix} 1-p & p/\sqrt{2} & p/\sqrt{2} \\ 0 & 1 & 0 \\ (1-p)/\sqrt{2} & (1-p)/\sqrt{2} & p \end{pmatrix}, \quad (18)$$

which has determinant $\det(C_p) = (1-p)p/2 \neq 0$ for all $p \in (0, 1)$. From this we conclude that $\text{rank}(G_{\mathbf{r}_\xi}) = 3$ for every $0 < p < 1$. Due to Theorem III.3, we conclude that $\xi \notin \mathcal{R}_3(\mathbb{C}^2)$ and therefore that $\mathcal{R}_3(\mathbb{C}^2)$ is not convex. ■

Indeed, our constructive proof not only demonstrates that the set is nonconvex but also provides an explicit example of a line segment whose interior lies entirely outside the imaginarity-free set while its extremal points lie inside.

IV. BOUNDING QUANTIFIERS OF MULTISTATE IMAGINARITY

We now move from the characterization of multistate imaginarity to the quantification of this resource. Following the work by Miyazaki and Matsumoto [17], we can define a function $\text{Im}_{R_1} : \mathcal{D}(\mathcal{H})^n \rightarrow \mathbb{R}_{\geq 0}$ aimed to quantify the imaginarity of a multistate:

$$\text{Im}_{R_1}(\varrho) := \min_U \frac{1}{n} \sum_{j=1}^n \text{Im}_R(U \rho_j U^\dagger),$$

where, for the case of single-qubit multistates, the minimization ranges over all unitaries $U \in \text{U}(2)$ and $\text{Im}_R(\rho)$ is the generalized robustness of imaginarity of a single-state [40–42] relative to the standard basis $\mathbb{A}_{\text{st}} = \{|0\rangle, |1\rangle\}$:

$$\text{Im}_R(\rho) := \min_{\tau \in \mathcal{D}(\mathbb{C}^2)} \left\{ s \geq 0 \left| \frac{\rho + s\tau}{s+1} \in \mathcal{R}(\mathbb{C}^2, \mathbb{A}_{\text{st}}) \right. \right\}.$$

Since $\text{Im}_R(\rho) = 1/2 \|\rho - \rho^T\|_1$ [40,41], using the Bloch vector decomposition of a state $\rho(\mathbf{r}) = \frac{\mathbb{1} + \mathbf{r} \cdot \boldsymbol{\sigma}}{2}$, where $\mathbf{r} = (r_x, r_y, r_z)$ we have that for the single-qubit case the robustness of imaginarity relative to the standard basis becomes simply

$$\text{Im}_R(\rho) = |r_y|. \quad (19)$$

With that, the multistate function $\text{Im}_{R_1}(\varrho)$ becomes

$$\begin{aligned} \text{Im}_{R_1}(\varrho) &= \min_{\mathbf{p} \in \mathbb{S}^2} \frac{1}{n} \sum_{j=1}^n \|\mathbf{r}_j\| \cdot |\cos(\mathbf{r}_j, \mathbf{p})| \\ &= \min_{\mathbf{p} \in \mathbb{S}^2} \frac{1}{n} \sum_{j=1}^n |\langle \mathbf{r}_j, \mathbf{p} \rangle|, \end{aligned} \quad (20)$$

where $\mathbb{S}^2 = \{\mathbf{r} \in \mathbb{R}^3 \mid \|\mathbf{r}\| = 1\}$ is the unit sphere. Moreover, can we write $\text{Im}_{R_1}(\varrho)$ as

$$\text{Im}_{R_1}(\varrho) = \min_{\psi \in \mathcal{P}_1(\mathbb{C}^2)} \frac{1}{n} \sum_{i=1}^n |2\text{Tr}(\varrho(i)\psi) - 1| \quad (21)$$

so that Im_{R_1} becomes a function of two-state overlaps only. We can then frame this as a semidefinite programming (SDP) optimization problem [109]: Given $\varrho = (\rho_1, \dots, \rho_n)$ we need to solve

$$\begin{aligned} &\text{minimize } \frac{1}{n} \sum_{i=1}^n |2\text{Tr}(\rho_i X) - 1|, \\ &\text{subject to } X \geq 0 \\ &\quad \text{Tr}(X) = 1, \end{aligned}$$

which is a semidefinite program (up to a standard trick of transforming an optimization over $|\cdot|$ into a linear program).

Given that one can experimentally infer $G_{\mathbf{r}_\varrho}$ via the measurement of two-state overlaps, it is also interesting to see whether we can bound the possible values $\text{Im}_{R_1}(\varrho)$ can take dependent on properties of the Gram matrix $G_{\mathbf{r}_\varrho}$.

We now show that the eigenvalues of $G_{\mathbf{r}_\varrho}$ provide upper and lower bounds for $\text{Im}_{R_1}(\varrho)$:

Theorem IV.1. Fix $n \geq 3$, and any n -tuple of states $\varrho = (\rho_1, \rho_2, \dots, \rho_n) \in \mathcal{D}(\mathbb{C}^2)^n$. Then

$$\frac{\lambda_3(G_{\mathbf{r}_\varrho})}{n} \leq \text{Im}_{R_1}(\varrho) \leq \sqrt{\frac{\lambda_3(G_{\mathbf{r}_\varrho})}{n}} \leq \frac{1}{\sqrt{3}},$$

where $\lambda_1(G_{\mathbf{r}_\varrho}) \geq \lambda_2(G_{\mathbf{r}_\varrho}) \geq \lambda_3(G_{\mathbf{r}_\varrho}) \geq \lambda_4(G_{\mathbf{r}_\varrho}) = \dots = \lambda_n(G_{\mathbf{r}_\varrho}) = 0$ denote the eigenvalues of $G_{\mathbf{r}_\varrho}$ in decreasing order.

Proof. It is elementary to see (using the Cauchy-Schwarz inequality) that the following inequality always hold:

$$\sum_{j=1}^n |\langle \mathbf{r}_j, \mathbf{p} \rangle|^2 \leq \sum_{j=1}^n |\langle \mathbf{r}_j, \mathbf{p} \rangle| \leq \sqrt{n} \sqrt{\sum_{j=1}^n |\langle \mathbf{r}_j, \mathbf{p} \rangle|^2}.$$

Taking minimum over the unit sphere $\mathbf{p} \in \mathbb{S}^2$ we obtain

$$m \leq \min_{\mathbf{p} \in \mathbb{S}^2} \sum_{j=1}^n |\langle \mathbf{r}_j, \mathbf{p} \rangle| \leq \sqrt{nm}, \quad (22)$$

where $m = \min_{\mathbf{p} \in \mathbb{S}^2} \sum_{j=1}^n |\langle \mathbf{r}_j, \mathbf{p} \rangle|^2$. Moreover, one finds that

$$m = \min_{\mathbf{p} \in \mathbb{S}^2} \sum_{j=1}^n |\langle \mathbf{r}_j, \mathbf{p} \rangle|^2 = \lambda_3(G_{\mathbf{r}_\varrho}). \quad (23)$$

In fact,

$$\sum_{j=1}^n |\langle \mathbf{r}_j, \mathbf{p} \rangle|^2 = \langle \mathbf{p} | \left(\sum_{j=1}^n |\mathbf{r}_j\rangle\langle \mathbf{r}_j| \right) | \mathbf{p} \rangle$$

and if we minimize the right-hand side we get that m is equal to the smallest eigenvalue of the 3×3 matrix $\sum_{j=1}^n |\mathbf{r}_j\rangle\langle \mathbf{r}_j|$.

If we denote $A = [\mathbf{r}_1; \dots; \mathbf{r}_n]$ as a $3 \times n$ matrix, then

$$AA^\dagger = \sum_{j=1}^n |\mathbf{r}_j\rangle\langle \mathbf{r}_j|, \quad \text{and} \quad A^\dagger A = G_{\mathbf{r}_e}.$$

Note that $AA^\dagger$ and $A^\dagger A$ share the same nonzero eigenvalues. So the minimal eigenvalue of $\sum_{j=1}^n |\mathbf{r}_j\rangle\langle \mathbf{r}_j|$, which is 3×3 and therefore has only three eigenvalues, is equal to the third largest eigenvalue of $G_{\mathbf{r}_e}$ in decreasing order, since all others need to be equal to zero as the Gram matrix has rank 3. Therefore, by Eqs. (22) and (23), we have the upper and lower bounds on $\text{Im}_{R_1}(\varrho)$.

To conclude, note that $G_{\mathbf{r}_e}$ is at most rank 3, so at most three eigenvalues are nonzero,

$$\lambda_1 + \lambda_2 + \lambda_3 = \lambda_1 + \lambda_2 + \lambda_3 + \dots + \lambda_n = \text{Tr}[G_{\mathbf{r}_e}] \leq n.$$

Hence

$$3\lambda_3 \leq \lambda_1 + \lambda_2 + \lambda_3 \leq n,$$

which implies

$$\sqrt{\frac{\lambda_3(G_{\mathbf{r}_e})}{n}} \leq \frac{1}{\sqrt{3}}.$$

V. CHARACTERIZING ALL BARGMANN INVARIANTS OF SINGLE-QUBIT STATES

We now proceed to investigate multistate coherence in general, moving beyond the specific case of imaginarity discussed so far. From the perspective of unitary invariance, the results of Ref. [55] reviewed in Sec. II show that estimating sufficiently many Bargmann invariants associated to a multistate ϱ yield necessary and sufficient information for determining whether $\varrho \in \mathcal{I}_n(\mathcal{H})$. This follows since membership in this set can be viewed as an instance of a unitary equivalence problem.

In this section we present one of the main results of our work. When restricted to single-qubit multistates $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^2)$, the collection of two-state overlaps $\Delta(\varrho) = (\text{Tr}(\rho_i \rho_j))_{i,j}$ encode *almost all* the necessary and sufficient unitary-invariant information to characterize this notion of basis-independent coherence.

Theorem V.1. For any n th order Bargmann invariant $\text{Tr}(\rho_1 \dots \rho_n) \in \mathfrak{B}_n^{(2)}$ where $\rho_i \in \mathcal{D}(\mathbb{C}^2)$, its value is completely determined by the overlaps $(\text{Tr}(\rho_i \rho_j))_{i,j \in [n]}$ up to complex conjugation. More precisely, there exist polynomials $P_n, Q_n \in \mathbb{Q}[\Delta_{11}, \Delta_{12}, \dots, \Delta_{nn}]$ such that the Bargmann invariant satisfies the quadratic equation:

$$[\text{Tr}(\rho_1 \dots \rho_n)]^2 - 2P_n(\Delta(\varrho)) \text{Tr}(\rho_1 \dots \rho_n) + Q_n(\Delta(\varrho)) = 0,$$

where $P_n(\Delta(\varrho))$ is the quantum realization of a polynomial obtained by substituting Δ_{ij} with $\Delta_{ij}(\varrho) = \text{Tr}[\rho_i \rho_j]$.

We prove this theorem in Appendix. We can view this result as a generalization for all possible integer values $n \geq 3$

of the results from Ref. [95]. Consider the case $n = 3$. Reference [95] has shown that

$$\begin{aligned} \text{Re}[\Delta_3(\varrho)] &= \frac{1}{4} \left(1 + \sum_{1 \leq i < j \leq 3} \langle \mathbf{r}_i, \mathbf{r}_j \rangle \right), \\ \text{Im}[\Delta_3(\varrho)] &= \frac{1}{4} \det(\mathbf{r}_1; \mathbf{r}_2; \mathbf{r}_3). \end{aligned}$$

This translates to polynomials that read

$$\begin{aligned} P_3(\Delta) &= \frac{1}{2}(\Delta_{12} + \Delta_{13} + \Delta_{23} - 1), \\ Q_3(\Delta) &= \frac{1}{16} \det \begin{pmatrix} 2\Delta_{11} - 1 & 2\Delta_{12} - 1 & 2\Delta_{13} - 1 \\ 2\Delta_{21} - 1 & 2\Delta_{22} - 1 & 2\Delta_{23} - 1 \\ 2\Delta_{31} - 1 & 2\Delta_{32} - 1 & 2\Delta_{33} - 1 \end{pmatrix} \\ &\quad + \underbrace{\frac{1}{4}(\Delta_{12} + \Delta_{13} + \Delta_{23} - 1)^2}_{= P_3(\Delta)^2}. \end{aligned}$$

In Ref. [95] (see also Appendix) the cases $n = 4$ and $n = 5$ are also provided. As a matter of fact, the proof of Theorem V.1 provides an iterative algorithm for updating the polynomials P_n and Q_n that yield the real and imaginary part of a (single-qubit) Bargmann invariant $\text{Tr}(\rho_1 \dots \rho_n)$ provided that one knows P_{n-1} and Q_{n-1} .

As a corollary, real-valued Bargmann invariants defined relative to single-qubit multistates are completely determined by tuples of two-state overlaps alone. These are invariants preserved under

$$(\rho_{i_1}, \rho_{i_2}, \dots, \rho_{i_{n-1}}, \rho_{i_n}) \mapsto (\rho_{i_n}, \rho_{i_{n-1}}, \dots, \rho_{i_2}, \rho_{i_1}). \quad (24)$$

The simplest example is the two-state overlap $\text{Tr}(\rho_1 \rho_2) = \text{Tr}(\rho_2 \rho_1)$. Another example is

$$\begin{aligned} \text{Tr}(\rho_1 \rho_2 \rho_1 \rho_2)^* &= \text{Tr}((\rho_1 \rho_2 \rho_1 \rho_2)^\dagger) \\ &= \text{Tr}(\rho_2 \rho_1 \rho_2 \rho_1) \\ &= \text{Tr}(\rho_1 \rho_2 \rho_1 \rho_2). \end{aligned} \quad (25)$$

Corollary V.2. Let $\rho_i \in \mathcal{D}(\mathbb{C}^2)$ for $i \in [n]$. If $\text{Tr}(\rho_1 \dots \rho_n)$ is real, then its value is completely determined by a polynomial of the overlaps $(\text{Tr}(\rho_i \rho_j))_{i,j \in [n]}$.

Note also that it is simple to see that two-state overlaps *cannot* characterize the sign of complex-valued Bargmann invariants, i.e., cannot be used to distinguish $\text{Tr}(\rho_1 \dots \rho_n)$ from its complex conjugate. This missing information truly needs to be provided by higher-order invariants.

This follows from a similar discussion present in Ref. [57], Sec. 5.2]. Suppose that overlaps alone could characterize the information of the sign of a Bargmann invariant. In this case, we would be able to write for a given single-qubit multistate $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^2)$ the following:

$$\text{Tr}(\rho_1 \dots \rho_n) = A(\Delta(\varrho)) + i(-1)^{C(\Delta(\varrho))} |B(\Delta(\varrho))|, \quad (26)$$

where A , B , and C are functions on tuples of two-state overlap $\Delta(\varrho) = (\text{Tr}(\rho_i \rho_j))_{i,j \in [n]}$, with $(-1)^{C(\Delta(\varrho))} \in \{-1, 1\}$, which implies we can take $C(\Delta(\varrho)) \in \{0, 1\}$ for all $\Delta(\varrho)$ without loss of generality. Let us consider the two multistates $\varrho = (|0\rangle\langle 0|, |+\rangle\langle +|, |+\rangle\langle +|)$ and $\varsigma =$

$(|0\rangle\langle 0|, |+\rangle\langle +|, |+\rangle\langle +|)$. Note that $\Delta_3(\varrho) = \Delta_3(\varsigma)^*$. However, the two tuples of overlaps $\Delta(\varrho) = \Delta(\varsigma)$ are equal, which means that $C(\Delta(\varrho)) = C(\Delta(\varsigma))$ thus showing that this pair of tuples is a counterexample for that formula to hold in general.

This is not specific to that example (nor to single-qubit multistates): One can always construct such a counterexample whenever the Bargmann invariant is complex valued, as the following no-go result shows.

Proposition V.3. Let $\mathcal{H}$ be a finite-dimensional Hilbert space and $\varrho : [n] \rightarrow \mathcal{D}(\mathcal{H})$ be any multistate such that $\text{Im}[\Delta(\varrho)] = \text{Im}[\text{Tr}(\rho_1 \cdots \rho_n)] \neq 0$. Then two-state overlaps cannot determine the sign of this imaginary part.

Proof. The proof is simple. Let us assume a stronger form of Eq. (26) but instead we simply require that the sign is given by a function of two-state overlaps alone. In other words, we assume that (letting $\Delta(\varrho) = \text{Tr}(\rho_1 \cdots \rho_n)$)

$$\Delta(\varrho) = \text{Re}[\Delta(\varrho)] + i(-1)^{C(\Delta(\varrho))}|\text{Im}[\Delta(\varrho)]|, \quad (27)$$

where $C : \mathbb{R}^{n(n+1)/2} \rightarrow \{0, 1\}$ is a function of two-state overlaps $\Delta(\varrho) \equiv (\text{Tr}(\rho_i \rho_j))_{i,j \in [n]}$ alone [110]. Let us fix an arbitrary basis $\mathbb{A}$. Then note that antiunitary operations [111] Θ act on density matrices as

$$\Theta \rho \Theta^\dagger = U \rho^T U^\dagger \quad (28)$$

relative to some unitary matrix U (and transposition relative to $\mathbb{A}$). Because of that, complex-valued invariants get conjugated while real-valued invariants are preserved. Thus, this implies

$$Q_4(\Delta) = P_4(\Delta)^2 + \frac{1}{64} \det \begin{pmatrix} 2\Delta_{11} + 4\Delta_{12} + 2\Delta_{22} - 4 & 2\Delta_{12} + 2\Delta_{13} + 2\Delta_{22} + 2\Delta_{23} - 4 & 2\Delta_{13} + 2\Delta_{14} + 2\Delta_{23} + 2\Delta_{24} - 4 \\ 2\Delta_{12} + 2\Delta_{13} + 2\Delta_{22} + 2\Delta_{23} - 4 & 2\Delta_{22} + 4\Delta_{23} + 2\Delta_{33} - 4 & 2\Delta_{23} + 2\Delta_{24} + 2\Delta_{33} + 2\Delta_{34} - 4 \\ 2\Delta_{13} + 2\Delta_{14} + 2\Delta_{23} + 2\Delta_{24} - 4 & 2\Delta_{23} + 2\Delta_{24} + 2\Delta_{33} + 2\Delta_{34} - 4 & 2\Delta_{33} + 4\Delta_{34} + 2\Delta_{44} - 4 \end{pmatrix}. \quad (35)$$

Let us consider the multistate $\Psi : [4] \rightarrow \mathcal{D}(\mathbb{C}^2)$ given by $\Psi(1) = |0\rangle\langle 0|$, $\Psi(2) = |+\rangle\langle +|$, $\Psi(3) = |1\rangle\langle 1|$, and $\Psi(4) = |-\rangle\langle -|$. This has an associated real-valued Bargmann invariant,

$$\begin{aligned} \Delta(\Psi) &= \text{Tr}(\Psi(1)\Psi(2)\Psi(3)\Psi(4)) \\ &= \langle 0|+\rangle\langle +|1\rangle\langle 1|-\rangle\langle -|0\rangle = -\frac{1}{4}. \end{aligned}$$

In this case, it is not difficult to see that $\Delta_{12}(\Psi) = \Delta_{14}(\Psi) = \Delta_{23}(\Psi) = \Delta_{34}(\Psi) = 1/2$ and $\Delta_{13}(\Psi) = \Delta_{24}(\Psi) = 0$, which implies that

$$P_4(\Delta(\Psi)) = \frac{1}{2} \left(\frac{1}{4} + \frac{1}{4} - 1 \right) = -\frac{1}{4}. \quad (36)$$

Since the determinant evaluates to zero in this case (as a straightforward but tedious calculations shows), we end up with

$$Q_4(\Delta(\Psi)) = \frac{1}{16} = P_4(\Delta(\Psi))^2. \quad (37)$$

that ϱ and $\Theta \varrho \Theta^\dagger$ have equal overlap tuples and therefore

$$C(\Delta(\varrho)) = C(\Delta(\Theta \varrho \Theta^\dagger)) \quad (29)$$

but opposite sign of the imaginary part of $\text{Tr}(\rho_1 \cdots \rho_n)$, thus implying that Eq. (27) cannot hold.

To conclude, we can see concrete examples of Theorem V.1. We start with the multistate $\Psi : [3] \rightarrow \mathcal{D}(\mathbb{C}^2)$ introduced by Bargmann given by Eq. (4). We see that for this case, the third-order Bargmann invariant satisfy that $\Delta(\Psi) = i/6$. The two-state overlaps are

$$\Delta_{12}(\Psi) = \frac{1}{2}, \quad \Delta_{13}(\Psi) = \frac{1}{3}, \quad \Delta_{23}(\Psi) = \frac{1}{6}. \quad (30)$$

In this case we have that the polynomial P_3 yields

$$P_3(\Delta(\Psi)) = \frac{1}{2} \left(\frac{1}{2} + \frac{1}{3} + \frac{1}{6} - 1 \right) = \frac{1}{2} \cdot 0 = 0, \quad (31)$$

and the polynomial Q_3 yields

$$\begin{aligned} Q_3(\Delta(\Psi)) &= \frac{1}{16} \det \begin{pmatrix} 1 & 0 & -\frac{1}{3} \\ 0 & 1 & -\frac{2}{3} \\ -\frac{1}{3} & -\frac{2}{3} & 1 \end{pmatrix} \\ &= \frac{1}{16} \cdot \frac{4}{9} = \frac{1}{36}. \end{aligned} \quad (32)$$

The theorem implies then that $\Delta(\Psi)^2 + Q_3(\Delta(\Psi)) = \Delta(\Psi)^2 + 1/36 = 0$ from which we conclude that $\Delta(\Psi) = \pm i/6$.

Let us now proceed to work an example with $n = 4$. In this case, we have that

$$P_4(\Delta) = \frac{1}{2}(\Delta_{12}\Delta_{34} + \Delta_{14}\Delta_{23} - \Delta_{13}\Delta_{24} \quad (33)$$

$$+ \Delta_{13} + \Delta_{24} - 1) \quad (34)$$

and

Finally, this leads to the equation

$$\begin{aligned} \Delta(\Psi)^2 - 2P_4(\Delta(\Psi))\Delta(\Psi) + P_4(\Delta(\Psi))^2 \\ = (\Delta(\Psi) - P_4(\Delta(\Psi)))^2 = 0 \Rightarrow \\ \Delta(\Psi) = P_4(\Delta(\Psi)) = -\frac{1}{4} \end{aligned} \quad (38)$$

as we wanted.

VI. CHARACTERIZATION OF SINGLE-QUBIT MULTISTATE COHERENCE

A. Rank-based criteria

It is trivial—but merits to be mentioned for completeness of our discussion—to show an analog of Theorem III.3 for the case of quantum coherence:

Theorem VI.1. A single-qubit multistate $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^2)$ has coherence, i.e., $\varrho \notin \mathcal{I}_n(\mathbb{C}^2)$, iff $\text{rank}(G_{\mathbf{r}_\varrho}) \geq 2$.

Proof. Clearly, ϱ has no coherence iff the elements in $\varrho([n])$ are mutually commutative. It suffices to prove that $\rho_i, \rho_j \in \varrho([n])$ commute for all i, j iff $\text{rank}(G_{\mathbf{r}_e}) \leq 1$. If all elements in $\varrho([n])$ are mutually commutative, then there exists some unitary $U \in \text{U}(2)$ such that $U\rho_k U^\dagger$ are all in diagonal form. Equivalently, $\Phi_U \mathbf{r}_k \propto (0, 0, 1)^T$ which also implies that $\mathbf{r}_k \propto \Phi_U^{-1}(0, 0, 1)^T$. Therefore, the rank of $G_{\mathbf{r}_e}$ is no larger than 1. On the other hand, if $\text{rank}(G_{\mathbf{r}_e}) \leq 1$, without loss of generality, then we assume that $\mathbf{r}_k = a_k \mathbf{r}_1$ for some real number a_k . As $\mathbf{r}_k \times \mathbf{r}_l = \mathbf{0}$, we have

$$\begin{aligned} (\mathbf{r}_k \sigma)(\mathbf{r}_l \sigma) &= \langle \mathbf{r}_k, \mathbf{r}_l \rangle \mathbb{1} + i(\mathbf{r}_k \times \mathbf{r}_l) \sigma \\ &= \langle \mathbf{r}_k, \mathbf{r}_l \rangle \mathbb{1} = (\mathbf{r}_l \sigma)(\mathbf{r}_k \sigma), \end{aligned}$$

which implies the commutative of ρ_k and ρ_l . $\blacksquare$

For the case of quantum coherence we have an even simpler situation than the geometric one provided by Fig. 2. A set of two single-qubit states is coherent iff their Bloch vectors all lie in a rotated axis of the Bloch sphere.

It is relevant to mention that multistates $\varrho : \{1, 2\} \rightarrow \mathcal{D}(\mathcal{H})$ can be coherent (contrasting Lemma III.5 which applies to the specific case of imaginarity) as we will shortly see, but this cannot be witnessed by a single two-state overlap alone, unless one assumes that the states are *pure*.

B. A simple remark beyond single-qubit states

We can state a necessary requirement for generic high-dimensional multistates $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^d)$ to be incoherent, similarly to Proposition III.4.

Proposition VI.2. If $\varrho : [n] \rightarrow \mathcal{D}(\mathbb{C}^d)$ is an incoherent multistate, i.e., $\varrho \in \mathcal{I}_n(\mathbb{C}^d)$, then $\text{rank}(G_{\mathbf{r}_e}) \leq d - 1$, where $\mathbf{r}_e$ are generalized Bloch vectors given with respect to the Gell-Mann basis.

Proof. If ϱ is incoherent, then its image is described by a set of pairwise commuting states. Therefore, there exists a basis $\mathbb{A}$ for which the associated density matrices are all diagonal in this basis. The traceless diagonal Gell-Mann matrices required to write such matrices span a $d - 1$ space, which implies that the associated Gram matrix $G_{\mathbf{r}_{\varrho U^\dagger}}$ has rank at most $d - 1$. From unitary invariance, $G_{\mathbf{r}_e}$ has also at most rank $d - 1$.

It is simple to write down a counterexample. Take $d = 3$ and the Gell-Mann matrices $\{\lambda_i\}_{i=1}^8$. Consider the two states given by

$$\rho_1 = \frac{1}{3}(\mathbb{1}_3 + \frac{1}{2}\lambda_1), \quad (39)$$

$$\rho_2 = \frac{1}{3}(\mathbb{1}_3 + \frac{1}{2}\lambda_3). \quad (40)$$

This pair $\{\rho_1, \rho_2\}$ is set coherent since $[\rho_1, \rho_2] \neq 0$ (which follows from the fact that $[\lambda_1, \lambda_3] \neq 0$). However, $\text{rank}(G_{\mathbf{r}_e}) = 2 = 3 - 1$.

We can leverage the system independence of Bargmann invariants mentioned in Sec. II to describe a simple necessary criteria for multistate coherence, which can be viewed as a generalization of a remark made in Ref. [90]. There, the authors comment that its possible to use the imaginary part of Bargmann invariants to witness multistate imaginarity since one has the implication

$$\text{Im}[\text{Tr}(\rho_1 \rho_2 \rho_3)] \neq 0 \Rightarrow (\rho_1, \rho_2, \rho_3) \notin \mathcal{R}_3(\mathcal{H}), \quad (41)$$

which holds for every space $\mathcal{H}$, regardless of the purity of the quantum states.

We can note that the condition $\text{Im}[\text{Tr}(\rho_1 \rho_2 \rho_3)] \neq 0$ can be viewed as the violation of an *equality constraint*, which follows from the fact that

$$\text{Tr}(\rho_1 \rho_2 \rho_3) \neq \text{Tr}(\rho_1 \rho_3 \rho_2). \quad (42)$$

When the equality is satisfied this has previously been called the *weak commutativity* [17] condition, mostly in the context of multiparameter estimation in quantum metrology [112].

We can consider the following simple witnesses of set coherence valid for all Hilbert spaces $\mathcal{H}$: Let $\varrho : [n] \rightarrow \mathcal{D}(\mathcal{H})$ be any multistate, $i_1, \dots, i_m \in [n]$ any finite sequence of labels, and P any permutation of m indexes. We have that

$$\text{Tr}(\rho_{i_1} \cdots \rho_{i_m}) \neq \text{Tr}(\rho_{P^{-1}(i_1)} \cdots \rho_{P^{-1}(i_m)}) \Rightarrow \varrho \notin \mathcal{I}_n(\mathcal{H}). \quad (43)$$

We can illustrate this with a simple example (borrowing from the two multistates considered by Designolle *et al.* [16] to show that $\mathcal{I}_n(\mathcal{H})$ is not convex). Let $\varrho, \varsigma : \{1, 2\} \rightarrow \mathcal{D}(\mathbb{C}^2)$ given by

$$\varrho(1) = |0\rangle\langle 0|, \quad \varrho(2) = \frac{1}{3}|0\rangle\langle 0| + \frac{2}{3}|1\rangle\langle 1| \quad (44)$$

and

$$\varsigma(1) = |+\rangle\langle +|, \quad \varsigma(2) = \frac{1}{4}|+\rangle\langle +| + \frac{3}{4}|-\rangle\langle -|. \quad (45)$$

We have that both $\varrho, \varsigma \in \mathcal{I}_2(\mathbb{C}^2)$. It is easy to see that for every $\omega \in (0, 1)$ the multistate $\xi := \omega\varrho + (1 - \omega)\varsigma \notin \mathcal{I}_2(\mathbb{C}^2)$ since

$$\text{Tr}(\xi_1 \xi_1 \xi_2 \xi_2) = \frac{1}{144}(9 + 18\omega + 94\omega^2 - 54\omega^3 + 13\omega^4)$$

$$\text{Tr}(\xi_1 \xi_2 \xi_1 \xi_2) = \frac{1}{144}(9 + 18\omega + 90\omega^2 - 46\omega^3 + 9\omega^4)$$

from which we conclude that

$$\text{Tr}(\xi_1 \xi_1 \xi_2 \xi_2) - \text{Tr}(\xi_1 \xi_2 \xi_1 \xi_2) = \frac{1}{36}\omega^2(1 - \omega)^2 \neq 0. \quad (46)$$

Therefore, using this simple equality-based witness one can infer the coherence of a multistate ξ .

VII. BOUNDING QUANTIFIERS OF MULTISTATE COHERENCE

Proceeding similarly as in the case of multistate imaginarity, we can provide explicit forms and precise bounds on the quantifier $\mathbf{C}_{R_1} : \mathcal{D}(\mathcal{H})^n \rightarrow \mathbb{R}_{\geq 0}$ for multistate coherence (proposed by Designolle *et al.* [16]), which is defined as

$$\mathbf{C}_{R_1}(\varrho) := \min_U \frac{1}{n} \sum_{j=1}^n \mathbf{C}_R(U \rho_j U^\dagger),$$

where, for single qubits, $\mathbf{C}_R$ denotes the generalized robustness of quantum coherence

$$\mathbf{C}_R(\rho) := \min_{\tau \in \mathcal{D}(\mathbb{C}^2)} \{s \geq 0 \mid \frac{\rho + s\tau}{s + 1} \in \mathcal{I}(\mathbb{C}^2, \mathbb{A}_{\text{st}})\}.$$

Using the Bloch vector decomposition of a state $\rho(\mathbf{r}) = \frac{\mathbb{1}_2 + \mathbf{r} \cdot \boldsymbol{\sigma}}{2}$, where $\mathbf{r} = (r_x, r_y, r_z)$ we have that for the single-qubit case the robustness of coherence relative to the standard basis becomes simply

$$\mathbf{C}_R(\rho) = |r_x + i r_y| = \sqrt{r_x^2 + r_y^2} \geq \text{Im}_R(\rho). \quad (47)$$

As before when focusing on $\text{Im}_{R_1}(\varrho)$, the minimization in the definition of $\mathbf{C}_{R_1}(\varrho)$ is taken over all unitaries $U \in \text{U}(2)$ for the case of single-qubit multistates.

By definition [and Eq. (47)], for every multistate ϱ the following inequality holds:

$$\text{Im}_{R_1}(\varrho) \leq \mathbf{C}_{R_1}(\varrho).$$

Moreover, in the case of single-qubit multistates we have that $\mathbf{C}_{R_1}(\varrho)$ takes the form

$$\mathbf{C}_{R_1}(\varrho) = \min_{\mathbf{p} \in \mathbb{S}^2} \frac{1}{n} \sum_{j=1}^n \|\mathbf{r}_j\| \cdot |\sin(\mathbf{r}_j, \mathbf{p})|, \quad (48)$$

where $(\mathbf{r}_j, \mathbf{p})$ represents the angle between the Bloch vector $\mathbf{r}_j$ of $\rho_j \in \varrho$ and a unit vector $\mathbf{p}$.

Equation (48) is taken from Ref. [16] and it is obtained as follows: Let $\rho(\mathbf{r}) = \frac{\mathbb{1} + \mathbf{r} \cdot \boldsymbol{\sigma}}{2}$, where $\mathbf{r} = (r_x, r_y, r_z)$. Then the Bloch vector of $U\rho U^\dagger$ is $\Phi_U \mathbf{r}$, where $\Phi_U \in \text{SO}(3)$. Since

$$\mathbf{C}_R(\rho) = \sqrt{r_x^2 + r_y^2} = \|\mathbf{r}\| \cdot |\sin(\mathbf{r}, \mathbf{e}_z)|,$$

where $\mathbf{e}_z = (0, 0, 1)$, which follows from $|\sin(\mathbf{r}, \mathbf{e}_z)| = \sqrt{1 - \cos^2(\mathbf{r}, \mathbf{e}_z)} = \frac{\sqrt{\|\mathbf{r}\|^2 - (\mathbf{r} \cdot \mathbf{e}_z)^2}}{\|\mathbf{r}\|} = \frac{\sqrt{r_x^2 + r_y^2}}{\|\mathbf{r}\|}$, we find that

$$\mathbf{C}_R(U\rho U^\dagger) = \|\Phi_U \mathbf{r}\| \cdot |\sin(\Phi_U \mathbf{r}, \mathbf{e}_z)| = \|\mathbf{r}\| \cdot |\sin(\mathbf{r}, \Phi_U^T \mathbf{e}_z)|.$$

Above, we have used the fact that unitaries preserve purity as viewed from the homomorphism Φ , i.e., that $\|\Phi_U \mathbf{r}\| = \|\mathbf{r}\|$. Moreover, we have also used that $(\Phi_U \mathbf{r}, \mathbf{e}_z) = (\mathbf{r}, \Phi_U^T \mathbf{e}_z)$. When optimizing U over all unitaries, Φ_U^T ranges over all elements in $\text{SO}(3)$, so defining $\mathbf{p} := \Phi_U^T \mathbf{e}_z$ makes the optimization to be equivalent to one ranging over all unit vectors in $\mathbb{S}^2$.

Using that $|\sin(\mathbf{r}_j, \mathbf{p})| = \sqrt{1 - (\frac{\mathbf{r}_j \cdot \mathbf{p}}{\|\mathbf{r}_j\|})^2}$ we can rewrite $\mathbf{C}_{R_1}(\varrho)$ as

$$\begin{aligned} \mathbf{C}_{R_1}(\varrho) &= \min_{\mathbf{p} \in \mathbb{S}^2} \frac{1}{n} \sum_{j=1}^n \sqrt{\|\mathbf{r}_j\|^2 - \langle \mathbf{r}_j, \mathbf{p} \rangle^2} \\ &= \min_{\psi \in \mathcal{P}_1(\mathbb{C}^2)} \frac{1}{n} \sum_{j=1}^n \sqrt{(2\text{Tr}(\rho_j^2) - 1) - (2\text{Tr}(\rho_j \psi) - 1)^2}, \end{aligned}$$

which is now fully expressed in terms of two-state overlaps. Since the expression is nonlinear it is unclear whether there is a trick to transform the problem above into an SDP.

For pure states, we know that the leading diagonal of $G_{\mathbf{r}_e}$ has all entries equal to 1 in which case we have that its trace, which equals the sum of all eigenvalues, is equal to

$$\lambda_1(G_{\mathbf{r}_e}) + \lambda_2(G_{\mathbf{r}_e}) + \lambda_3(G_{\mathbf{r}_e}) = n.$$

It is not difficult to show, following the same strategy as the one used in Theorem IV.1, that:

Theorem VII.1. Fix any $n \geq 2$, and any n -tuple of states $\varrho = (\rho_1, \rho_2, \dots, \rho_n) \in \mathcal{D}(\mathbb{C}^2)^n$. Then

$$\frac{\lambda_2(G_{\mathbf{r}_e}) + \lambda_3(G_{\mathbf{r}_e})}{n} \leq \mathbf{C}_{R_1}(\varrho) \leq \sqrt{\frac{\lambda_2(G_{\mathbf{r}_e}) + \lambda_3(G_{\mathbf{r}_e})}{n}},$$

where $\lambda_1(G_{\mathbf{r}_e}) \geq \lambda_2(G_{\mathbf{r}_e}) \geq \lambda_3(G_{\mathbf{r}_e}) \geq \dots \geq \lambda_n(G_{\mathbf{r}_e})$ denote the eigenvalues of $G_{\mathbf{r}_e}$ in decreasing order. Moreover,

$\mathbf{C}_{R_1}(\varrho) \leq \sqrt{\frac{2}{3}}$ for all $\varrho \in \mathcal{D}(\mathbb{C}^2)^n$.

Proof. Using the Cauchy-Schwarz inequality,

$$\begin{aligned} \sum_{j=1}^n \sqrt{\|\mathbf{r}_j\|^2 - \langle \mathbf{r}_j, \mathbf{p} \rangle^2} &\leq \sqrt{n \sum_{j=1}^n (\|\mathbf{r}_j\|^2 - \langle \mathbf{r}_j, \mathbf{p} \rangle^2)} \\ &= \sqrt{n \left(\text{Tr}[G_{\mathbf{r}_e}] - \langle \mathbf{p} | \sum_{j=1}^n |\mathbf{r}_j\rangle \langle \mathbf{r}_j| | \mathbf{p} \rangle \right)}. \end{aligned}$$

Above, we have used that $\sum_j \|\mathbf{r}_j\|^2 = \sum_j \langle \mathbf{r}_j, \mathbf{r}_j \rangle = \text{Tr}(G_{\mathbf{r}_e})$.

Let us denote A the $3 \times n$ matrix of column vectors $A = [\mathbf{r}_1; \dots; \mathbf{r}_n]$ such that $AA^\dagger = \sum_{j=1}^n |\mathbf{r}_j\rangle \langle \mathbf{r}_j|$. Dividing by n and minimizing over all possible $\mathbf{p} \in \mathbb{S}^2$ we obtain

$$\begin{aligned} \mathbf{C}_{R_1}(\varrho) &\leq \min_{\mathbf{p} \in \mathbb{S}^2} \sqrt{\frac{\sum_{j=1}^n \lambda_j(G_{\mathbf{r}_e}) - \langle \mathbf{p} | AA^\dagger | \mathbf{p} \rangle}{n}} \\ &= \sqrt{\frac{\sum_{j=1}^n \lambda_j(G_{\mathbf{r}_e}) - \max_{\mathbf{p} \in \mathbb{S}^2} \langle \mathbf{p} | AA^\dagger | \mathbf{p} \rangle}{n}} \\ &= \sqrt{\frac{\sum_{j=1}^n \lambda_j(G_{\mathbf{r}_e}) - \lambda_1(G_{\mathbf{r}_e})}{n}} \\ &= \sqrt{\frac{\lambda_2(G_{\mathbf{r}_e}) + \lambda_3(G_{\mathbf{r}_e})}{n}}. \end{aligned}$$

Above, we have used that

$$\max_{\mathbf{p} \in \mathbb{S}^2} \langle \mathbf{p} | AA^\dagger | \mathbf{p} \rangle = \lambda_1(AA^\dagger) = \lambda_1(G_{\mathbf{r}_e}),$$

since their spectrum is equal (up to zeros), i.e.,

$$\text{spec}(AA^\dagger) \setminus \{0\} = \text{spec}(G_{\mathbf{r}_e}) \setminus \{0\}.$$

Using $\sum_j \sqrt{a_j} \geq \sum_j a_j$ which holds whenever $0 \leq a_j \leq 1$ for all j we have that

$$\sum_{j=1}^n \sqrt{\|\mathbf{r}_j\|^2 - \langle \mathbf{r}_j, \mathbf{p} \rangle^2} \geq \sum_{j=1}^n (\|\mathbf{r}_j\|^2 - \langle \mathbf{r}_j, \mathbf{p} \rangle^2). \quad (49)$$

Therefore

$$\begin{aligned} \mathbf{C}_{R_1}(\varrho) &\geq \min_{\mathbf{p} \in \mathbb{S}^2} \frac{1}{n} \sum_{j=1}^n (\|\mathbf{r}_j\|^2 - \langle \mathbf{r}_j, \mathbf{p} \rangle^2) \\ &= \frac{1}{n} \sum_{j=1}^n (\|\mathbf{r}_j\|^2 - \max_{\mathbf{p} \in \mathbb{S}^2} \langle \mathbf{r}_j, \mathbf{p} \rangle^2) \\ &= \frac{1}{n} (\lambda_2(G_{\mathbf{r}_e}) + \lambda_3(G_{\mathbf{r}_e})). \end{aligned}$$

To conclude, again we note that $\lambda_1 + \lambda_2 + \lambda_3 = n$ which implies that $\lambda_1 \geq n/3$. Therefore,

$$\lambda_2 + \lambda_3 = n - \lambda_1 \leq n - \frac{n}{3} = \frac{2n}{3},$$

and we obtain our universal upper bound,

$$\mathcal{C}_{R_1}(\varrho) \leq \sqrt{\frac{2n/3}{n}} = \sqrt{\frac{2}{3}}. \quad (50)$$

■

VIII. PHYSICAL IMPLICATIONS AND APPLICATIONS

A. On the relationship between spin chirality and multistate imaginarity

Corollary III.7 has a physical interpretation related to the concept of *scalar spin chirality* following the results from Ref. [113]. Given a totally separable tripartite pure spin state

$$|\psi\rangle = |\mathbf{n}_1\rangle \otimes |\mathbf{n}_2\rangle \otimes |\mathbf{n}_3\rangle,$$

the (separable) scalar spin chirality is defined as

$$\chi_{1,2,3} = S^3 \langle \mathbf{n}_1, \mathbf{n}_2 \times \mathbf{n}_3 \rangle = S^3 \det([\mathbf{n}_1; \mathbf{n}_2; \mathbf{n}_3]),$$

where S is a constant. We can extend this notion of chirality to mixed states, allowing for the associated states to be mixed. Therefore, three (possibly mixed) single-qubit spin-1/2 states are chiral *iff* the associated single-qubit multistate has imaginarity.

For a simple intuitive example, we might consider the spin states given by

$$\mathbf{n}_1 = (1, 0, 0), \quad \mathbf{n}_2 = (0, 1, 0), \quad \mathbf{n}_3 = (0, 0, 1), \quad (51)$$

the three unit vectors defining axes in $\mathbb{R}^3$. Alternatively, in the Bloch sphere these correspond to the quantum states $|\mathbf{n}_1\rangle = |+\rangle$, $|\mathbf{n}_2\rangle = |+\rangle$, and $|\mathbf{n}_3\rangle = |0\rangle$. These define a positive (right-handed) chirality with $\chi_{1,2,3} = S^3$. The negative (left-handed) chirality would be obtained by letting $\mathbf{n}_2 = (0, 1, 0) \rightarrow \mathbf{n}'_2 = (0, -1, 0)$ in which case $|\mathbf{n}'_2\rangle = |-\rangle$ and we obtain $\chi_{1,2,3} = -S^3$. As mentioned, chirality happens *iff* the multistate defined by $\Psi(i) = |\mathbf{n}_i\rangle\langle\mathbf{n}_i|$ for $i = 1, 2$, and 3 has imaginarity. If instead $\chi_{1,2,3} = 0$, then the system presents no chirality (for example, if two of the spins are aligned, $\mathbf{n}_2 = \mathbf{n}_3$).

In chiral magnets, chirality gives rise to a phenomenon known as the *topological Hall effect* [114], which is known to be a nontrivial manifestation of the *Berry phase* [115,116]. Corollary III.7 shows that this (separable) chirality happens *iff* there are triplets of spin states having imaginarity in this basis-independent sense. As a matter of fact, our Theorem V.1 shows, furthermore, that for single-qubit spin-1/2 states the only information provided by the Berry phase—which is equal in module to the phase of a Bargmann invariant [117]—not encoded already in the two-state overlaps is the information of whether the path in the Bloch sphere formed by the associated triplet of Bloch vectors takes is clockwise (say, $\rho_1\rho_2\rho_3$) or counterclockwise ($\rho_3\rho_2\rho_1$).

B. Operational advantage for discrimination quantified by the robustness of multistate imaginarity

In abstract treatments of resource theories (focusing on a single state) robustness-based quantifiers are known to have an associated operational interpretation via instances of discrimination tasks [16,20,40,118–125].

For example, it is straightforward to translate the operational advantage in subchannel discrimination discussed by Designolle *et al.* [16] quantified there by the robustness of set coherence to the case of the robustness of set imaginarity since the only truly relevant aspect for the proof in Ref. [16] stems from the form of the quantifier and the convexity of the sets $\mathcal{I}(\mathcal{H}, \mathbb{A})$.

In the task of subchannel discrimination, one is given a quantum instrument $\mathcal{T} = \{\mathcal{T}_a\}_a$ and a measurement $M = \{E_a\}_a$, and the goal of the task is to correctly guess which map $\mathcal{T}_a$ was applied on a state ρ that can be prepared at will.

The probability of successfully guessing $\mathcal{T}_a$ provided the state ρ was prepared and a measurement M was performed is given by

$$p_{\text{succ}}(\rho, \mathcal{T}, M) = \sum_a \text{Tr}[\mathcal{T}_a(\rho)E_a]. \quad (52)$$

We remark that the task above can also be made probabilistic assuming that a map $\mathcal{T}_a$ is applied with probability p_a . As mentioned also by Kang-Da Wu *et al.* [40], it holds that

$$\sup_{\mathcal{T}, M} \frac{p_{\text{succ}}(\rho, \mathcal{T}, M)}{\max_{\sigma \in \mathcal{R}(\mathcal{H}, \mathbb{A}_{\text{st}})} p_{\text{succ}}(\sigma, \mathcal{T}, M)} = 1 + \text{Im}_R(\rho).$$

Provided with that intuition, we can extend this to the case where we have a set of subchannel discrimination tasks, as opposed to a single one. In this case, we are given lists of instruments $\mathcal{T} = (\mathcal{T}^{(1)}, \dots, \mathcal{T}^{(n)})$ and measurements $M = (M^{(1)}, \dots, M^{(n)})$. Our full protocol is then to implement a subchannel discrimination task for each label $i = 1, \dots, n$, and our goal is to guess the instruments $\mathcal{T}_a^{(i)}$ for each i given that we have prepared an initial state $\varrho(i)$ and performed measurement $M^{(i)}$.

Summing over all instances of the above where we let ρ be in the image of some multistate, and then maximizing over all possible unitaries (which amounts to maximizing over all possible choices of reference basis $\mathbb{A}$) we end up with

$$\begin{aligned} & \frac{1}{n} \min_U \sum_{i=1}^n \sup_{\mathcal{T}, M} \frac{p_{\text{succ}}(\rho_i, \mathcal{T}^{(i)}, M^{(i)})}{\max_{\sigma_i \in \mathcal{R}(\mathcal{H}, U \mathbb{A}_{\text{st}})} p_{\text{succ}}(\sigma_i, \mathcal{T}^{(i)}, M^{(i)})} \\ & = 1 + \text{Im}_{R_1}(\varrho). \end{aligned}$$

The interpretation of the above is then as the one provided by Ref. [16] for the case of set coherence: Regardless of one's choice of reference basis $\mathbb{A}$ there exists a collection of subchannel discrimination tasks in which the multistate having nonzero imaginarity ϱ outperforms any imaginarity-free multistate.

C. On the relevance of multistate coherence and imaginarity to multiphoton indistinguishability

As shown by Refs. [4,5], the output statistics of photon-resolving measurements in linear-optical interferometers depend *solely* on the Bargmann invariants of the single-photon internal states and on the unitary modeling the interferometer. Numerous experiments have since confirmed this prediction [6,7,60,75].

In practice, calibrating a linear photonic device often includes characterizing how indistinguishable the incoming photons are—a key figure of merit for, e.g., photon bunching

and Boson Sampling validation [79]. When photons are not perfectly identical, pairwise overlaps capture only part of the story: Higher-order Bargmann invariants can provide a more complete, and sometimes counter-intuitive [77], picture.

Indeed, Ref. [7] recently showed that three-photon indistinguishability—when the only distinguishing degree of freedom is, say, polarization—requires a three-state Bargmann invariant. They contrast an “incoherent partial distinguishability” regime, in which all three polarization Bloch vectors lie on a line (our notion of multistate incoherence), with a “coherent partial distinguishability” regime, where the three vectors span a nonzero volume in Bloch space (our notion of multistate imaginarity). By performing a tritter experiment, they directly accessed the imaginary part of the third-order Bargmann invariant—which is proportional to that volume—and thereby distinguished these two regimes even when the photons themselves were mixed.

Our analysis shows that, in two-dimensional Hilbert spaces, one can in principle infer this same volume from the determinant of the Gram matrix $G_{\mathbf{r}_e}$, i.e., from pairwise overlaps *alone*.

However, the output statistics of such experiments is better described as agnostic to the underlying Hilbert space dimensionality such that only unitary-invariant information truly matters: dimension upper-bounds and purity assumptions rarely hold exactly. Moreover, our counterexamples demonstrate that a single third-order invariant can fail to witness multistate imaginarity without these assumptions. Accordingly, the most robust experimental strategy is to measure the higher-order Bargmann invariants directly—just as in Ref. [7]—rather than rely solely on two-state overlaps or purity-and-dimension assumptions [126]. This gives a more fine-grained calibration of photon indistinguishability in realistic, imperfect sources. In this case, one can then use our witnesses based on equality constraints on Bargmann invariants of the form of Eq. (43).

IX. DISCUSSION AND OUTLOOK

We have provided a complete characterization of multistate imaginarity and coherence in qubit systems using Bargmann invariants and Gram matrix methods. We show that a single-qubit multistate has imaginarity if and only if the Gram matrix of its Bloch vectors has rank 3, while it exhibits coherence if and only if this Gram matrix has rank at least 2. Geometrically, this reveals that imaginarity-free states lie within a common plane of the Bloch sphere, while incoherent states are constrained to a single axis.

Beyond this geometric characterization of multistate coherence and imaginarity, we have also showed that (for single-qubit systems) *all* higher-order Bargmann invariants are completely determined by two-state overlaps *up to complex conjugation*, with the sign of the imaginary part being the only independent unitary-invariant information not encoded in pairwise overlaps. In particular, this also provides a characterization of the form of Bargmann invariants and on the information content provided by two-state overlaps of single-qubit states.

We have furthermore extended some of our results to provide necessary conditions—which can be viewed as coher-

ence witnesses—for arbitrary Hilbert space dimensions using the values of higher-order Bargmann invariants, generalizing one of the insights from Ref. [90] for multistate imaginarity to the more general case of multistate coherence.

Future work could approach our results from a formal resource-theoretic perspective. In particular, it would be interesting to analyze notions of free transformations associated with these two multistate resources, as well as the induced pre-order governing resource conversion. Such an analysis could shed new light on potential applications of the physical situations discussed here, as well as on the connection initially drawn in Ref. [17] between multistate imaginarity and multiparameter state estimation in quantum metrology. Furthermore, it would be worthwhile to explore how our techniques extend to the case of nonstabilizerness [91], which represents a distinguished form of coherence relevant to magic-state injection schemes in fault-tolerant quantum computation.

ACKNOWLEDGMENTS

R.W. thanks Filipa C. R. Peres, Ernesto Galvão, and Felix Ahnfeld for discussions on coherence and imaginarity, and David Schmid and Yujie Zhang for discussions on multistates. M.-S.L. acknowledges support from National Natural Science Foundation of China under Grant No. 12371458, the Guangdong Basic and Applied Basic Research Foundation under Grants No. 2024A1515010380 and No. 2023A1515012074. R.W. acknowledges support from the European Research Council (ERC) under the European Union’s Horizon 2020 research and innovation programme (Grant No. 856432, HyperQ). L.Z. is supported by Zhejiang Provincial Natural Science Foundation of China under Grants No. LZ23A010005.

DATA AVAILABILITY

No data were created or analyzed in this study.

APPENDIX: PROOF OF THEOREM V.1

Proof. We proceed similarly to Appendix B from Ref. [95]. For any single-qubit state $\rho \in \mathcal{D}(\mathbb{C}^2)$ we write $\rho = \rho(\mathbf{r}) = \frac{1}{2}(\mathbb{1}_2 + \mathbf{r} \cdot \boldsymbol{\sigma})$ using the Bloch representation. Define

$$\mathbf{Prod}_n = \rho_1 \rho_2 \cdots \rho_n = 2^{-n}(p_0^{(n)}\mathbb{1}_2 + \mathbf{p}^{(n)}\boldsymbol{\sigma}),$$

where we set $p_0^{(1)} = 1$ and $\mathbf{p}^{(1)} = \mathbf{r}_1$ the Bloch vector of state ρ_1 . Recursively, $\mathbf{Prod}_{n+1} = \mathbf{Prod}_n \rho_{n+1}$, which implies the following update rules:

$$\begin{aligned} p_0^{(n+1)} &= p_0^{(n)} + \langle \mathbf{p}^{(n)}, \mathbf{r}_{n+1} \rangle, \\ \mathbf{p}^{(n+1)} &= p_0^{(n)} \mathbf{r}_{n+1} + \mathbf{p}^{(n)} + i\mathbf{p}^{(n)} \times \mathbf{r}_{n+1}. \end{aligned}$$

If we write $p_0^{(n)} = a_0^{(n)} + ib_0^{(n)}$ and $\mathbf{p}^{(n)} = \mathbf{a}^{(n)} + i\mathbf{b}^{(n)}$, then we have the following recursive relations:

$$\begin{aligned} a_0^{(n+1)} &= a_0^{(n)} + \langle \mathbf{a}^{(n)}, \mathbf{r}_{n+1} \rangle, \\ b_0^{(n+1)} &= b_0^{(n)} + \langle \mathbf{b}^{(n)}, \mathbf{r}_{n+1} \rangle, \\ \mathbf{a}^{(n+1)} &= a_0^{(n)} \mathbf{r}_{n+1} + \mathbf{a}^{(n)} - \mathbf{b}^{(n)} \times \mathbf{r}_{n+1}, \\ \mathbf{b}^{(n+1)} &= b_0^{(n)} \mathbf{r}_{n+1} + \mathbf{b}^{(n)} + \mathbf{a}^{(n)} \times \mathbf{r}_{n+1}, \end{aligned} \quad (\text{A1})$$

with initial conditions $a_0^{(1)} = 1, b_0^{(1)} = 0, \mathbf{a}^{(1)} = \mathbf{r}_1, \mathbf{b}^{(1)} = \mathbf{0}$.

Let us now consider the following algebraic constructions:

$$\begin{aligned} R_n &:= \mathbb{Z}[\langle \mathbf{r}_i, \mathbf{r}_j \rangle, 1 \leq i, j \leq n], \\ S_n &:= \sum_{1 \leq i < j < k \leq n} R_n \det[\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k], \\ T_n &:= \sum_{k=1}^n R_n \mathbf{r}_k + \sum_{1 \leq i < j \leq n} S_n \mathbf{r}_i \times \mathbf{r}_j, \\ U_n &:= \sum_{k=1}^n S_n \mathbf{r}_k + \sum_{1 \leq i < j \leq n} R_n \mathbf{r}_i \times \mathbf{r}_j. \end{aligned} \quad (\text{A2})$$

Here R_n denotes the ring of polynomials over $\mathbb{Z}$ generated by the inner products $\langle \mathbf{r}_i, \mathbf{r}_j \rangle$ for $1 \leq i, j \leq n$, denoted as $\mathbb{Z}[\langle \mathbf{r}_i, \mathbf{r}_j \rangle, 1 \leq i, j \leq n]$. The space S_n is linearly generated by $\det[\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k]$ for $1 \leq i \leq j \leq k \leq n$, with coefficients in R_n . Similarly for T_n and U_n . In the following, we will prove by induction that for all $n \in \mathbb{N}$

$$a_0^{(n)} \in R_n, \quad b_0^{(n)} \in S_n, \quad \mathbf{a}^{(n)} \in T_n, \quad \mathbf{b}^{(n)} \in U_n.$$

Before the proof, we recall the following properties:

(A) The product $\det[\mathbf{r}_{i'}, \mathbf{r}_{j'}, \mathbf{r}_{k'}] \det[\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k]$ equals to

$$\begin{vmatrix} \langle \mathbf{r}_{i'}, \mathbf{r}_i \rangle & \langle \mathbf{r}_{i'}, \mathbf{r}_j \rangle & \langle \mathbf{r}_{i'}, \mathbf{r}_k \rangle \\ \langle \mathbf{r}_{j'}, \mathbf{r}_i \rangle & \langle \mathbf{r}_{j'}, \mathbf{r}_j \rangle & \langle \mathbf{r}_{j'}, \mathbf{r}_k \rangle \\ \langle \mathbf{r}_{k'}, \mathbf{r}_i \rangle & \langle \mathbf{r}_{k'}, \mathbf{r}_j \rangle & \langle \mathbf{r}_{k'}, \mathbf{r}_k \rangle \end{vmatrix}.$$

To show this, it suffices to use the simple properties of determinants $\det[A] = \det[A^T]$ and $\det[AB] = \det[A] \det[B]$.

(B) $\langle \mathbf{r}_i \times \mathbf{r}_j, \mathbf{r}_k \rangle = \det[\mathbf{r}_i, \mathbf{r}_j, \mathbf{r}_k]$.

(C) $(\mathbf{r}_i \times \mathbf{r}_j) \times \mathbf{r}_k = \langle \mathbf{r}_i, \mathbf{r}_k \rangle \mathbf{r}_j - \langle \mathbf{r}_j, \mathbf{r}_k \rangle \mathbf{r}_i$.

Clearly, $a_0^{(1)} \in R_1, b_0^{(1)} \in S_1, \mathbf{a}^{(1)} \in T_1, \mathbf{b}^{(1)} \in U_1$ holds (which provides our base step for $n = 1$). Assume this holds for $n = l$, now we need to prove it also holds for $n = l + 1$.

(1) (Inductive step for R_n) As $a_0^{(l+1)} = a_0^{(l)} + \langle \mathbf{a}^{(l)}, \mathbf{r}_{l+1} \rangle$, and $\mathbf{a}^{(l)} \in T_l$, so

$$\mathbf{a}^{(l)} = \sum_{k=1}^l r_k \mathbf{r}_k + \sum_{1 \leq i < j \leq l} s_{ij} \mathbf{r}_i \times \mathbf{r}_j.$$

Clearly, for each $1 \leq k \leq l$, $\langle \mathbf{r}_k, \mathbf{r}_{l+1} \rangle \in R_{l+1}$ and for each $s_{ij} = r_{i'j'k'} \det[\mathbf{r}_{i'}, \mathbf{r}_{j'}, \mathbf{r}_{k'}]$, where $1 \leq i' < j' < k' \leq l$ and $r_{i'j'k'} \in R_l$, by using properties (A) and (B), we can show that

$$\langle s_{ij} \mathbf{r}_i \times \mathbf{r}_j, \mathbf{r}_{l+1} \rangle \in R_{l+1}.$$

So we get $a_0^{(l+1)} \in R_{l+1}$.

(2) (Inductive step for S_n) As $b_0^{(l+1)} = b_0^{(l)} + \langle \mathbf{b}^{(l)}, \mathbf{r}_{l+1} \rangle$ and $\mathbf{b}^{(l)} \in T_l$, so

$$\mathbf{b}^{(l)} = \sum_{k=1}^l s_k \mathbf{r}_k + \sum_{1 \leq i < j \leq l} r_{ij} \mathbf{r}_i \times \mathbf{r}_j.$$

By definition $\langle s_k \mathbf{r}_k, \mathbf{r}_{l+1} \rangle = \langle \mathbf{r}_k, \mathbf{r}_{l+1} \rangle s_k \in S_{l+1}$. And the property (B) implies that

$$\langle r_{ij} \mathbf{r}_i \times \mathbf{r}_j, \mathbf{r}_{l+1} \rangle \in S_{l+1}.$$

Therefore, $b_0^{(l+1)} \in S_{l+1}$.

(3) (Inductive step for T_n) As $\mathbf{a}^{(l+1)} = a_0^{(l)} \mathbf{r}_{l+1} + \mathbf{a}^{(l)} - \mathbf{b}^{(l)} \times \mathbf{r}_{l+1}$, and $a_0^{(l)} \in R_l, \mathbf{a}^{(l)} \in T_l, \mathbf{b}^{(l)} \in U_l$, we have $a_0^{(l)} \mathbf{r}_{l+1} + \mathbf{a}^{(l)} \in T_{l+1}$ and

$$\mathbf{b}^{(l)} = \sum_{k=1}^l s_k \mathbf{r}_k + \sum_{1 \leq i < j \leq l} r_{ij} \mathbf{r}_i \times \mathbf{r}_j.$$

So by the definition of T_{l+1} and Property (C), we get

$$\mathbf{b}^{(l)} \times \mathbf{r}_{l+1} \in T_{l+1}.$$

Hence $\mathbf{a}^{(l+1)} \in T_{l+1}$.

(4) (Inductive step for U_n) As $\mathbf{b}^{(l+1)} = b_0^{(l)} \mathbf{r}_{l+1} + \mathbf{b}^{(l)} + \mathbf{a}^{(l)} \times \mathbf{r}_{l+1}$, and $b_0^{(l)} \in S_l, \mathbf{a}^{(l)} \in T_l, \mathbf{b}^{(l)} \in U_l$, we have $b_0^{(l)} \mathbf{r}_{l+1} + \mathbf{b}^{(l)} \in U_{l+1}$ and

$$\mathbf{a}^{(l)} = \sum_{k=1}^l r_k \mathbf{r}_k + \sum_{1 \leq i < j \leq l} s_{ij} \mathbf{r}_i \times \mathbf{r}_j.$$

So by the definition of U_{l+1} and Property (C), we get

$$\mathbf{a}^{(l)} \times \mathbf{r}_{l+1} \in U_{l+1}.$$

Hence $\mathbf{b}^{(l+1)} \in U_{l+1}$.

The Bargmann invariant for the tuple $\varrho = (\rho_1, \dots, \rho_n)$, where $\rho_k = \rho(\mathbf{r}_k)$, is thus given by $\Delta(\varrho) := \text{Tr}(\text{Prod}_n) = 2^{1-n} p_0^{(n)} = \frac{a_0^{(n)} + i b_0^{(n)}}{2^{n-1}}$. Note that

$$a_0^{(n)} \in R_n, \quad \text{and} \quad b_0^{(n)} \in S_n.$$

Using property (A), one obtains $S_n * S_n \in R_n$. In particular,

$$(a_0^{(n)})^2 + (b_0^{(n)})^2 \in R_n.$$

That is, the real part of $\text{Tr}[\rho_1 \cdots \rho_n]$ and the power of two of the imaginarity of $\text{Tr}[\rho_1 \cdots \rho_n]$ are determined by

$$\langle \mathbf{r}_i, \mathbf{r}_j \rangle = 2\text{Tr}[\rho_i \rho_j] - 1, \quad 1 \leq i, j \leq n.$$

The corresponding polynomial P_n can be obtained by replacing the $\langle \mathbf{r}_i, \mathbf{r}_j \rangle$ in $\frac{1}{2^{n-1}} a_0^{(n)}$ with $2\Delta_{ij} - 1$. The corresponding polynomial Q_n can be obtained by replacing the $\langle \mathbf{r}_i, \mathbf{r}_j \rangle$ in $\frac{(a_0^{(n)})^2 + (b_0^{(n)})^2}{2^{2n-2}}$ with $2\Delta_{ij} - 1$. ■

As a concrete example, the first three steps $n = 3, 4$, and 5 have been determined in Ref. [95] and are given by:

$$a_0^{(3)} = 1 + \sum_{1 \leq i < j \leq 3} \langle \mathbf{r}_i, \mathbf{r}_j \rangle,$$

$$b_0^{(3)} = \det(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3),$$

$$\begin{aligned} a_0^{(4)} &= (1 + \langle \mathbf{r}_1, \mathbf{r}_2 \rangle)(1 + \langle \mathbf{r}_3, \mathbf{r}_4 \rangle) \\ &\quad - (1 - \langle \mathbf{r}_1, \mathbf{r}_3 \rangle)(1 - \langle \mathbf{r}_2, \mathbf{r}_4 \rangle) \\ &\quad + (1 + \langle \mathbf{r}_1, \mathbf{r}_4 \rangle)(1 + \langle \mathbf{r}_2, \mathbf{r}_3 \rangle), \end{aligned}$$

$$b_0^{(4)} = \det(\mathbf{r}_1 + \mathbf{r}_2, \mathbf{r}_2 + \mathbf{r}_3, \mathbf{r}_3 + \mathbf{r}_4),$$

and

$$\begin{aligned}
 a_0^{(5)} &= 1 + \sum_{1 \leq i < j \leq 5} \langle \mathbf{r}_i, \mathbf{r}_j \rangle + \langle \mathbf{r}_1, \mathbf{r}_2 \rangle \langle \mathbf{r}_3, \mathbf{r}_4 \rangle - \langle \mathbf{r}_1, \mathbf{r}_3 \rangle \langle \mathbf{r}_2, \mathbf{r}_4 \rangle + \langle \mathbf{r}_1, \mathbf{r}_4 \rangle \langle \mathbf{r}_2, \mathbf{r}_3 \rangle + (\langle \mathbf{r}_2, \mathbf{r}_3 \rangle + \langle \mathbf{r}_2, \mathbf{r}_4 \rangle \\
 &\quad + \langle \mathbf{r}_3, \mathbf{r}_4 \rangle) \langle \mathbf{r}_1, \mathbf{r}_5 \rangle + (-\langle \mathbf{r}_1, \mathbf{r}_3 \rangle - \langle \mathbf{r}_1, \mathbf{r}_4 \rangle + \langle \mathbf{r}_3, \mathbf{r}_4 \rangle) \langle \mathbf{r}_2, \mathbf{r}_5 \rangle + (\langle \mathbf{r}_1, \mathbf{r}_2 \rangle - \langle \mathbf{r}_1, \mathbf{r}_4 \rangle \\
 &\quad - \langle \mathbf{r}_2, \mathbf{r}_4 \rangle) \langle \mathbf{r}_3, \mathbf{r}_5 \rangle + (\langle \mathbf{r}_1, \mathbf{r}_2 \rangle + \langle \mathbf{r}_1, \mathbf{r}_3 \rangle + \langle \mathbf{r}_2, \mathbf{r}_3 \rangle) \langle \mathbf{r}_4, \mathbf{r}_5 \rangle, \\
 b_0^{(5)} &= \sum_{1 \leq i < j < k \leq 5} \langle \mathbf{r}_i \times \mathbf{r}_j, \mathbf{r}_k \rangle + \langle \mathbf{r}_2, \mathbf{r}_3 \rangle \langle \mathbf{r}_1 \times \mathbf{r}_4, \mathbf{r}_5 \rangle - \langle \mathbf{r}_1, \mathbf{r}_3 \rangle \langle \mathbf{r}_2 \times \mathbf{r}_4, \mathbf{r}_5 \rangle + \langle \mathbf{r}_1, \mathbf{r}_2 \rangle \langle \mathbf{r}_3 \times \mathbf{r}_4, \mathbf{r}_5 \rangle + \langle \mathbf{r}_4, \mathbf{r}_5 \rangle \langle \mathbf{r}_1 \times \mathbf{r}_2, \mathbf{r}_3 \rangle.
 \end{aligned}$$

-
- [1] E. Chitambar and G. Gour, Quantum resource theories, *Rev. Mod. Phys.* **91**, 025001 (2019).
- [2] G. Gour, Resources of the quantum world, [arXiv:2402.05474](#).
- [3] B. Coecke, T. Fritz, and R. W. Spekkens, A mathematical theory of resources, *Inf. Comput.* **250**, 59 (2016).
- [4] V. S. Shchesnovich, Partial indistinguishability theory for multiphoton experiments in multiport devices, *Phys. Rev. A* **91**, 013844 (2015).
- [5] V. S. Shchesnovich and M. E. O. Bezerra, Collective phases of identical particles interfering on linear multiports, *Phys. Rev. A* **98**, 033805 (2018).
- [6] A. E. Jones, A. J. Menssen, H. M. Chrzanowski, T. A. W. Wolterink, V. S. Shchesnovich, and I. A. Walmsley, Multiparticle interference of pairwise distinguishable photons, *Phys. Rev. Lett.* **125**, 123603 (2020).
- [7] A. E. Jones, S. Kumar, S. D'Aurelio, M. Bayerbach, A. J. Menssen, and S. Barz, Distinguishability and mixedness in quantum interference, *Phys. Rev. A* **108**, 053701 (2023).
- [8] Z. Ji, Y.-K. Liu, and F. Song, Pseudorandom quantum states, in *Advances in Cryptology CRYPTO 2018* (Springer International, Cham, 2018), p. 126.
- [9] W. Kretschmer, Quantum pseudorandomness and classical complexity, in *16th Conference on the Theory of Quantum Computation, Communication and Cryptography (TQC 2021)* (Schloss Dagstuhl Leibniz-Zentrum für Informatik, Wadern, 2021).
- [10] N. Bansal, W.-K. Mok, K. Bharti, D. E. Koh, and T. Haug, Pseudorandom density matrices, *PRX Quantum* **6**, 020322 (2025).
- [11] A. Gu, L. Leone, S. Ghosh, J. Eisert, S. F. Yelin, and Y. Quek, Pseudomagic quantum states, *Phys. Rev. Lett.* **132**, 210602 (2024).
- [12] T. Haug, K. Bharti, and D. E. Koh, Pseudorandom unitaries are neither real nor sparse nor noise-robust, *Quantum* **9**, 1759 (2025).
- [13] A. Tanggara, M. Gu, and K. Bharti, Near-term pseudorandom and pseudoresource quantum states, [arXiv:2504.17650](#).
- [14] S. Aaronson, A. Bouland, B. Fefferman, S. Ghosh, U. Vazirani, C. Zhang, and Z. Zhou, Quantum pseudoentanglement, [arXiv:2211.00747](#).
- [15] A. Rivas, S. F. Huelga, and M. B. Plenio, Quantum non-Markovianity: Characterization, quantification and detection, *Rep. Prog. Phys.* **77**, 094001 (2014).
- [16] S. Designolle, R. Uola, K. Luoma, and N. Brunner, Set coherence: Basis-independent quantification of quantum coherence, *Phys. Rev. Lett.* **126**, 220404 (2021).
- [17] J. Miyazaki and K. Matsumoto, Imaginarity-free quantum multiparameter estimation, *Quantum* **6**, 665 (2022).
- [18] R. Salazar, J. Czartowski, and A. de Oliveira Junior, Resource theory of absolute negativity, [arXiv:2205.13480](#).
- [19] F. Buscemi, E. Chitambar, and W. Zhou, Complete resource theory of quantum incompatibility as quantum programmability, *Phys. Rev. Lett.* **124**, 120401 (2020).
- [20] R. Uola, T. Kraft, J. Shang, X.-D. Yu, and O. Gühne, Quantifying quantum resources with conic programming, *Phys. Rev. Lett.* **122**, 130404 (2019).
- [21] E. Martins, M. F. Savi, and R. M. Angelo, Quantum incompatibility of a physical context, *Phys. Rev. A* **102**, 050201(R) (2020).
- [22] A. F. Ducuara, P. Lipka-Bartosik, and P. Skrzypczyk, Multiobject operational tasks for convex quantum resource theories of state-measurement pairs, *Phys. Rev. Res.* **2**, 033374 (2020).
- [23] J. H. Selby, D. Schmid, E. Wolfe, A. B. Sainz, R. Kunjwal, and R. W. Spekkens, Contextuality without incompatibility, *Phys. Rev. Lett.* **130**, 230201 (2023).
- [24] R. Wagner, R. S. Barbosa, and E. F. Galvão, Inequalities witnessing coherence, nonlocality, and contextuality, *Phys. Rev. A* **109**, 032220 (2024).
- [25] E. F. Galvão and D. J. Brod, Quantum and classical bounds for two-state overlaps, *Phys. Rev. A* **101**, 062110 (2020).
- [26] Y. Zhang, Y. Yīng, and D. Schmid, Quantifiers and witnesses for the nonclassicality of measurements and of states, [arXiv:2504.02944](#).
- [27] Y. Zhang, D. Schmid, Y. Yīng, and R. W. Spekkens, Reassessing the boundary between classical and nonclassical for individual quantum processes, [arXiv:2503.05884](#).
- [28] G. Gour, T. Heinosaari, and R. Spekkens, *The Resource Theory of Incompatibility*, presented at the APS March Meeting 2018, Volume 63, Number 1 (APS, New York, 2018).
- [29] M. Horodecki, A. Sen(De), and U. Sen, Quantification of quantum correlation of ensembles of states, *Phys. Rev. A* **75**, 062329 (2007).
- [30] M. Piani, V. Narasimhachar, and J. Calsamiglia, Quantumness of correlations, quantumness of ensembles and quantum data hiding, *New J. Phys.* **16**, 113001 (2014).
- [31] C. A. Fuchs and M. Sasaki, Squeezing quantum information through a classical channel: Measuring the “quantumness” of a set of quantum states, *Quantum Info. Comput.* **3**, 377 (2003).
- [32] M. Horodecki, P. Horodecki, R. Horodecki, and M. Piani, Quantumness of ensembles from the no-broadcasting principle, *Int. J. Quantum Inf.* **04**, 105 (2006).
- [33] T. Baumgratz, M. Cramer, and M. B. Plenio, Quantifying coherence, *Phys. Rev. Lett.* **113**, 140401 (2014).
- [34] A. Streltsov, G. Adesso, and M. B. Plenio, Colloquium: Quantum coherence as a resource, *Rev. Mod. Phys.* **89**, 041003 (2017).

- [35] F. Ahnefeld, T. Theurer, D. Egloff, J. M. Matera, and M. B. Plenio, Coherence as a resource for Shor's algorithm, *Phys. Rev. Lett.* **129**, 120501 (2022).
- [36] M. Naseri, T. V. Kondra, S. Goswami, M. Fellous-Asiani, and A. Streltsov, Entanglement and coherence in the Bernstein-Vazirani algorithm, *Phys. Rev. A* **106**, 062429 (2022).
- [37] F. Ahnefeld, T. Theurer, and M. B. Plenio, Coherence as a resource for phase estimation, [arXiv:2505.18544](https://arxiv.org/abs/2505.18544).
- [38] G. Gour, Quantum resource theories in the single-shot regime, *Phys. Rev. A* **95**, 062314 (2017).
- [39] A. Hickey and G. Gour, Quantifying the imaginarity of quantum mechanics, *J. Phys. A: Math. Theor.* **51**, 414009 (2018).
- [40] K.-D. Wu, T. V. Kondra, S. Rana, C. M. Scandolo, G.-Y. Xiang, C.-F. Li, G.-C. Guo, and A. Streltsov, Operational resource theory of imaginarity, *Phys. Rev. Lett.* **126**, 090401 (2021).
- [41] K.-D. Wu, T. V. Kondra, S. Rana, C. M. Scandolo, G.-Y. Xiang, C.-F. Li, G.-C. Guo, and A. Streltsov, Resource theory of imaginarity: Quantification and state conversion, *Phys. Rev. A* **103**, 032401 (2021).
- [42] K.-D. Wu, T. V. Kondra, C. M. Scandolo, S. Rana, G.-Y. Xiang, C.-F. Li, G.-C. Guo, and A. Streltsov, Resource theory of imaginarity in distributed scenarios, *Commun. Phys.* **7**, 171 (2024).
- [43] T. J. Elliott, Strict advantage of complex quantum theory in a communication task, *Phys. Rev. A* **111**, 062401 (2025).
- [44] H. Zhu, Hiding and masking quantum information in complex and real quantum mechanics, *Phys. Rev. Res.* **3**, 033176 (2021).
- [45] Y. Kedem, Using technical noise to increase the signal-to-noise ratio of measurements via imaginary weak values, *Phys. Rev. A* **85**, 060102(R) (2012).
- [46] P. B. Dixon, D. J. Starling, A. N. Jordan, and J. C. Howell, Ultrasensitive beam deflection measurement via interferometric weak value amplification, *Phys. Rev. Lett.* **102**, 173601 (2009).
- [47] O. Hosten and P. Kwiat, Observation of the spin Hall effect of light via weak measurements, *Science* **319**, 787 (2008).
- [48] N. Brunner and C. Simon, Measuring small longitudinal phase shifts: Weak measurements or standard interferometry? *Phys. Rev. Lett.* **105**, 010405 (2010).
- [49] S. Gherardini and G. De Chiara, Quasiprobabilities in quantum thermodynamics and many-body systems, *PRX Quantum* **5**, 030201 (2024).
- [50] S. Hernández-Gómez, T. Isogawa, A. Belenchia, A. Levy, N. Fabbri, S. Gherardini, and P. Cappelaro, Interferometry of quantum correlation functions to access quasiprobability distribution of work, *npj Quantum Inf.* **10**, 115 (2024).
- [51] M. Sajjan, V. Singh, R. Selvarajan, and S. Kais, Imaginary components of out-of-time-order correlator and information scrambling for navigating the learning landscape of a quantum machine learning model, *Phys. Rev. Res.* **5**, 013146 (2023).
- [52] A. Wigderson, *Mathematics and Computation* (Princeton University Press, Princeton, NJ, 2019).
- [53] G. Popescu, *Unitary Invariants in Multivariable Operator Theory* (American Mathematical Society, Providence, RI, 2009), p. 91.
- [54] T.-Y. Chien and S. Waldron, A characterization of projective unitary equivalence of finite frames and applications, *SIAM J. Discr. Math.* **30**, 976 (2016).
- [55] M. Oszmaniec, D. J. Brod, and E. F. Galvão, Measuring relational information between quantum states, and applications, *New J. Phys.* **26**, 013053 (2024).
- [56] V. Bargmann, Note on Wigner's theorem on symmetry operations, *J. Math. Phys.* **5**, 862 (1964).
- [57] R. Wagner, Z. Schwartzman-Nowik, I. L. Paiva, A. Te'eni, A. Ruiz-Molero, R. S. Barbosa, E. Cohen, and E. F. Galvão, Quantum circuits for measuring weak values, Kirkwood–Dirac quasiprobability distributions, and state spectra, *Quantum Sci. Technol.* **9**, 015030 (2024).
- [58] N. Yunger Halpern, B. Swingle, and J. Dressel, Quasiprobability behind the out-of-time-ordered correlator, *Phys. Rev. A* **97**, 042105 (2018).
- [59] Y. Quek, E. Kaur, and M. M. Wilde, Multivariate trace estimation in constant quantum depth, *Quantum* **8**, 1220 (2024).
- [60] M. Pont, R. Albiero, S. E. Thomas, N. Spagnolo, F. Ceccarelli, G. Corielli, A. Briussel, N. Somaschi, H. Huet, A. Harouri, A. Lemaître, I. Sagnes, N. Belabas, F. Sciarrino, R. Osellame, P. Senellart, and A. Crespi, Quantifying n -photon indistinguishability with a cyclic integrated interferometer, *Phys. Rev. X* **12**, 031033 (2022).
- [61] K. Simonov, R. Wagner, and E. F. Galvão, Estimation of multivariate traces of states given partial classical information, *Phys. Rev. A* **112**, 062435 (2025).
- [62] J. G. Kirkwood, Quantum statistics of almost classical assemblies, *Phys. Rev.* **44**, 31 (1933).
- [63] P. A. M. Dirac, On the analogy between classical and quantum mechanics, *Rev. Mod. Phys.* **17**, 195 (1945).
- [64] D. R. M. Arvidsson-Shukur, W. F. Braasch Jr, S. De Bièvre, J. Dressel, A. N. Jordan, C. Langrenze, M. Lostaglio, J. S. Lundeen, and N. Y. Halpern, Properties and applications of the Kirkwood–Dirac distribution, *New J. Phys.* **26**, 121201 (2024).
- [65] D. Schmid, R. D. Baldijão, Y. Yīng, R. Wagner, and J. H. Selby, Kirkwood–Dirac representations beyond quantum states and their relation to noncontextuality, *Phys. Rev. A* **110**, 052206 (2024).
- [66] L. Liu and S. Cheng, The boundary of Kirkwood–Dirac quasiprobability, [arXiv:2504.09238](https://arxiv.org/abs/2504.09238).
- [67] J. R. González Alonso, N. Yunger Halpern, and J. Dressel, Out-of-time-ordered-correlator quasiprobabilities robustly witness scrambling, *Phys. Rev. Lett.* **122**, 040404 (2019).
- [68] R. Wagner and E. F. Galvão, Simple proof that anomalous weak values require coherence, *Phys. Rev. A* **108**, L040202 (2023).
- [69] H. F. Hofmann, Complex joint probabilities as expressions of reversible transformations in quantum mechanics, *New J. Phys.* **14**, 043031 (2012).
- [70] S. Silva Pratapsi, S. Deffner, and S. Gherardini, Quantum speed limit for Kirkwood–Dirac quasiprobabilities, *Quantum Sci. Technol.* **10**, 035019 (2025).
- [71] N. Mukunda, Arvind, S. Chaturvedi, and R. Simon, Bargmann invariants and off-diagonal geometric phases for multilevel quantum systems: A unitary-group approach, *Phys. Rev. A* **65**, 012102 (2001).
- [72] N. Mukunda, Arvind, E. Ercolessi, G. Marmo, G. Morandi, and R. Simon, Bargmann invariants, null phase curves, and a theory of the geometric phase, *Phys. Rev. A* **67**, 042114 (2003).

- [73] N. Mukunda, P. K. Aravind, and R. Simon, Wigner rotations, Bargmann invariants and geometric phases, *J. Phys. A: Math. Gen.* **36**, 2347 (2003).
- [74] A. Avdoshkin and F. K. Popov, Extrinsic geometry of quantum states, *Phys. Rev. B* **107**, 245136 (2023).
- [75] A. J. Menssen, A. E. Jones, B. J. Metcalf, M. C. Tichy, S. Barz, W. S. Kolthammer, and I. A. Walmsley, Distinguishability and many-particle interference, *Phys. Rev. Lett.* **118**, 153603 (2017).
- [76] A. M. Minke, A. Buchleitner, and C. Dittel, Characterizing four-body indistinguishability via symmetries, *New J. Phys.* **23**, 073028 (2021).
- [77] G. Rodari, C. Fernandes, E. Caruccio, A. Suprano, F. Hoch, T. Giordani, G. Carvacho, R. Albiero, N. D. Giano, G. Corrielli, F. Ceccarelli, R. Osellame, D. J. Brod, L. Novo, N. Spagnolo, E. F. Galvão, and F. Sciarrino, Experimental observation of counter-intuitive features of photonic bunching, [arXiv:2410.15883](https://arxiv.org/abs/2410.15883).
- [78] G. Rodari, L. Novo, R. Albiero, A. Suprano, C. T. Tavares, E. Caruccio, F. Hoch, T. Giordani, G. Carvacho, M. Gardina, N. Di Giano, S. Di Giorgio, G. Corrielli, F. Ceccarelli, R. Osellame, N. Spagnolo, E. F. Galvão, and F. Sciarrino, Semi-device-independent characterization of multiphoton indistinguishability, *PRX Quantum* **6**, 020340 (2025).
- [79] B. Seron, L. Novo, and N. J. Cerf, Boson bunching is not maximized by indistinguishable particles, *Nat. Photon.* **17**, 702 (2023).
- [80] T. Giordani, C. Esposito, F. Hoch, G. Carvacho, D. J. Brod, E. F. Galvão, N. Spagnolo, and F. Sciarrino, Witnesses of coherence and dimension from multiphoton indistinguishability tests, *Phys. Rev. Res.* **3**, 023031 (2021).
- [81] T. Giordani, D. J. Brod, C. Esposito, N. Viggianiello, M. Romano, F. Flamini, G. Carvacho, N. Spagnolo, E. F. Galvão, and F. Sciarrino, Experimental quantification of four-photon indistinguishability, *New J. Phys.* **22**, 043001 (2020).
- [82] D. J. Brod, E. F. Galvão, N. Viggianiello, F. Flamini, N. Spagnolo, and F. Sciarrino, Witnessing genuine multiphoton indistinguishability, *Phys. Rev. Lett.* **122**, 063602 (2019).
- [83] E. Annoni and S. C. Wein, Incoherent behavior of partially distinguishable photons, [arXiv:2502.05047](https://arxiv.org/abs/2502.05047).
- [84] K.-W. Bong, N. Tischler, R. B. Patel, S. Wollmann, G. J. Pryde, and M. J. W. Hall, Strong unitary and overlap uncertainty relations: Theory and experiment, *Phys. Rev. Lett.* **120**, 230402 (2018).
- [85] M. Lostaglio, A. Belenchia, A. Levy, S. Hernández-Gómez, N. Fabbri, and S. Gherardini, Kirkwood-Dirac quasiprobability approach to the statistics of incompatible observables, *Quantum* **7**, 1128 (2023).
- [86] A. Levy and M. Lostaglio, Quasiprobability distribution for heat fluctuations in the quantum regime, *PRX Quantum* **1**, 010309 (2020).
- [87] S. Hernández-Gómez, S. Gherardini, A. Belenchia, M. Lostaglio, A. Levy, and N. Fabbri, Projective measurements can probe nonclassical work extraction and time correlations, *Phys. Rev. Res.* **6**, 023280 (2024).
- [88] A. Santini, A. Solfanelli, S. Gherardini, and M. Collura, Work statistics, quantum signatures, and enhanced work extraction in quadratic fermionic models, *Phys. Rev. B* **108**, 104308 (2023).
- [89] L. Donati, F. S. Cataliotti, and S. Gherardini, Energetics and quantumness of fano coherence generation, *Sci. Rep.* **14**, 20145 (2024).
- [90] C. Fernandes, R. Wagner, L. Novo, and E. F. Galvão, Unitary-invariant witnesses of quantum imaginarity, *Phys. Rev. Lett.* **133**, 190201 (2024).
- [91] R. Wagner, F. C. R. Peres, E. Zambrini Cruzeiro, and E. F. Galvão, Unitary-invariant method for witnessing nonstabilizerness in quantum processors, *J. Phys. A: Math. Theor.* **58**, 285302 (2025).
- [92] R. Wagner, A. Camillini, and E. F. Galvão, Coherence and contextuality in a Mach-Zehnder interferometer, *Quantum* **8**, 1240 (2024).
- [93] L. Zhang, B. Xie, and Y. Tao, Bargmann-invariant framework for local unitary equivalence and entanglement, *Phys. Rev. A* **112**, 052426 (2025).
- [94] T. Giordani, R. Wagner, C. Esposito, A. Camillini, F. Hoch, G. Carvacho, C. Pentangelo, F. Ceccarelli, S. Piacentini, A. Crespi, N. Spagnolo, R. Osellame, E. F. Galvão, and F. Sciarrino, Experimental certification of contextuality, coherence, and dimension in a programmable universal photonic processor, *Sci. Adv.* **9**, eadj4249 (2023).
- [95] L. Zhang, B. Xie, and B. Li, Geometry of sets of Bargmann invariants, *Phys. Rev. A* **111**, 042417 (2025).
- [96] J. H. Selby, D. Schmid, E. Wolfe, A. B. Sainz, R. Kunjwal, and R. W. Spekkens, Accessible fragments of generalized probabilistic theories, cone equivalence, and applications to witnessing nonclassicality, *Phys. Rev. A* **107**, 062203 (2023).
- [97] S. Zamora, R. A. Macêdo, T. S. Sarubi, M. Alves, D. Poderini, and R. Chaves, Semi-device-independent nonstabilizerness certification in the prepare-and-measure scenario, *Phys. Rev. A* **112**, 042410 (2025).
- [98] T. C. Fraser, An estimation theoretic approach to quantum realizability problems, [arXiv:2402.10902](https://arxiv.org/abs/2402.10902).
- [99] R. Wagner, Coherence and contextuality as quantum resources, Ph.D. thesis, University of Minho, [arXiv:2511.16785](https://arxiv.org/abs/2511.16785).
- [100] J. Xu, Numerical ranges of Bargmann invariants, *Phys. Lett. A* **565**, 131091 (2026).
- [101] M.-S. Li and Y.-X. Tan, Bargmann invariants for quantum imaginarity, *Phys. Rev. A* **111**, 022409 (2025).
- [102] S. S. Pratapsi, J. a. Gouveia, L. Novo, and E. F. Galvão, Elementary characterization of Bargmann invariants, *Phys. Rev. A* **112**, 042421 (2025).
- [103] C. Budroni, A. Cabello, O. Gühne, M. Kleinmann, and J.-Å. Larsson, Kochen-specker contextuality, *Rev. Mod. Phys.* **94**, 045007 (2022).
- [104] G. Kimura, The Bloch vector for n -level systems, *Phys. Lett. A* **314**, 339 (2003).
- [105] R. A. Bertlmann and P. Krammer, Bloch vectors for qudits, *J. Phys. A: Math. Theor.* **41**, 235303 (2008).
- [106] Y. Kosmann-Schwarzbach, *Groups and Symmetries from Finite Groups to Lie Groups*, 2nd ed. (Springer Cham, 2022).
- [107] M. Gell-Mann, Symmetries of baryons and mesons, *Phys. Rev.* **125**, 1067 (1962).
- [108] We remark here that the matrices λ_i are different from the matrices U_i [$\langle \lambda_i, \lambda_j \rangle = 2\delta_{ij}$, but in general $\langle U_i, U_j \rangle = d\delta_{ij}$, where $d = 3$ for generators in $SU(3)$] considered in order to make $(\mathbf{r}_i, \mathbf{r}_j) = d\text{Tr}(\rho_i \rho_j) - 1$ back in Eq. (11).

- [109] A. Tavakoli, A. Pozas-Kerstjens, P. Brown, and M. Araújo, Semidefinite programming relaxations for quantum correlations, *Rev. Mod. Phys.* **96**, 045006 (2024).
- [110] In fact, we can even allow for C to be a function of any tuple of Bargmann invariants which are symmetric under word inversion as discussed above.
- [111] A. Uhlmann, Anti- (conjugate) linearity, *Sci. Chin. Phys. Mech. Astron.* **59**, 630301 (2016).
- [112] K. Matsumoto, A new approach to the Cramér-Rao-type bound of the pure-state model, *J. Phys. A: Math. Gen.* **35**, 3111 (2002).
- [113] L. I. Reascos, B. Murta, E. F. Galvão, and J. Fernández-Rossier, Quantum circuits to measure scalar spin chirality, *Phys. Rev. Res.* **5**, 043087 (2023).
- [114] G. Kimbell, C. Kim, W. Wu, M. Cuoco, and J. W. A. Robinson, Challenges in identifying chiral spin textures via the topological Hall effect, *Commun. Mater.* **3**, 19 (2022).
- [115] M. V. Berry, Quantal phase factors accompanying adiabatic changes, *Proc. R. Soc. Lond. A* **392**, 45 (1984).
- [116] J. Ye, Y. B. Kim, A. J. Millis, B. I. Shraiman, P. Majumdar, and Z. Tešanović, Berry phase theory of the anomalous Hall effect: Application to colossal magnetoresistance manganites, *Phys. Rev. Lett.* **83**, 3737 (1999).
- [117] R. Simon and N. Mukunda, Bargmann invariant and the geometry of the Güoy effect, *Phys. Rev. Lett.* **70**, 880 (1993).
- [118] K. Kuroiwa, R. Takagi, G. Adesso, and H. Yamasaki, Every quantum helps: Operational advantage of quantum resources beyond convexity, *Phys. Rev. Lett.* **132**, 150201 (2024).
- [119] K. Kuroiwa, R. Takagi, G. Adesso, and H. Yamasaki, Robustness- and weight-based resource measures without convexity restriction: Multicopy witness and operational advantage in static and dynamical quantum resource theories, *Phys. Rev. A* **109**, 042403 (2024).
- [120] R. Takagi, B. Regula, K. Bu, Z.-W. Liu, and G. Adesso, Operational advantage of quantum resources in subchannel discrimination, *Phys. Rev. Lett.* **122**, 140402 (2019).
- [121] C. Napoli, T. R. Bromley, M. Cianciaruso, M. Piani, N. Johnston, and G. Adesso, Robustness of coherence: An operational and observable measure of quantum coherence, *Phys. Rev. Lett.* **116**, 150502 (2016).
- [122] M. Piani, M. Cianciaruso, T. R. Bromley, C. Napoli, N. Johnston, and G. Adesso, Robustness of asymmetry and coherence of quantum states, *Phys. Rev. A* **93**, 042107 (2016).
- [123] P. Skrzypczyk, I. Šupić, and D. Cavalcanti, All sets of incompatible measurements give an advantage in quantum state discrimination, *Phys. Rev. Lett.* **122**, 130403 (2019).
- [124] M. Ozmaniec and T. Biswas, Operational relevance of resource theories of quantum measurements, *Quantum* **3**, 133 (2019).
- [125] R. Takagi and B. Regula, General resource theories in quantum mechanics and beyond: Operational characterization via discrimination tasks, *Phys. Rev. X* **9**, 031053 (2019).
- [126] For a comprehensive discussion of experimental measurements of Bargmann invariants across various platforms and how they compare, see Ref. [57], Sec. 4.5] and also Refs. [6,7,60,77,99,127–129] and references therein. For quantum-circuit implementations, see Refs. [55,59,61,113] and references therein.
- [127] P. C. Azado, R. Wagner, R. S. Barbosa, and E. F. Galvão, Measuring unitary invariants with the quantum switch, [arXiv:2508.02345](https://arxiv.org/abs/2508.02345).
- [128] G. Chiribella, K. Simonov, and X. Zhao, Dimension-independent weak value estimation via controlled swap operations, *Phys. Rev. Res.* **6**, 043043 (2024).
- [129] N. Gao, D. Li, A. Mishra, J. Yan, K. Simonov, and G. Chiribella, Measuring incompatibility and clustering quantum observables with a quantum switch, *Phys. Rev. Lett.* **130**, 170201 (2023).