Clifford covariance of Wigner functions, positive representation of Pauli measurement, and cohomology

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Abstract

The scheme of quantum computation with magic states, and in particular the role of the Wigner function as an indicator of quantumness, motivate the question of when Clifford-covariant Wigner functions exist, and when Wigner functions exist that represent Pauli measurements positively. This question has been settled affirmatively for all odd dimensions. Here, we discuss the case of even dimension, for Wigner functions obtained from operator bases. We find that such Clifford-covariant Wigner functions do not exist in any even dimension, and furthermore, Pauli measurement cannot be positively represented by them in any even dimension whenever the number of qudits is $n \geq 2$.

1 Introduction

The Wigner function [1] is the closest quantum mechanical counterpart to the classical concept of probability distributions over phase space. The difference is that Wigner functions can take negative values, making them quasiprobability distributions. Wigner functions have many applications in physics, specifically quantum optics, and also relate to foundations of quantum mechanics. In certain settings, negativity in a Wigner function is an indicator of quantumness [2–4].

Wigner functions have been adapted to finite-dimensional Hilbert spaces [5–7], and thereby reached the field of quantum computation. Recently, Gross' Wigner function [6] has been established as an indicator of potential for speedup in quantum computation [9]. Namely, within the model of quantum computation with magic states (QCM) [24], a quantum speedup can occur only if the Wigner function of the initial state takes negative values. This result has first been derived for the case of odd local Hilbert space dimension [9]. Since then, various works have tackled the harder case of even dimension, in particular the multi-qubit case [11–13, 21, 33, 40].

The overall picture for the case of odd-dimensional qudits is conceptually satisfying. The negativity of a Wigner function is a physics concept, which has already been suggested as an indicator of quantumness in other contexts. Furthermore, for QCM, the justification for Wigner function negativity as indicator of quantumness is computational: absence of negativity implies efficient classical simulation, hence precludes quantum speedup. Finally, negativity in the Wigner function of a given quantum state is equivalent to the inviability of a non-contextual hidden variable model describing that state w.r.t. Pauli measurements [14]. Thus, irrespective of whether one looks at quantum computation with magic states from a physics, computer science or foundations of quantum mechanics perspective, the boundary between the classical and the quantum domain is located in the same place. The three a priori distinct perspectives reinforce each other.

However, for this picture to not be merely accidental, it needs to hold in all dimensions; so what about even dimensions? The existing generalizations of the initial result [9] to even dimensions exhibit structural differences compared to the odd-dimensional case. They group into two approaches, namely (I) the set of operations in quantum computation with magic states is reduced, without compromising quantum computational universality; and (II) the uniqueness of quasiprobability distribution is dispensed with.

An example for Approach I is the rebit construction [11]. Therein, the Clifford group is shrunk to the CSS-ness preserving subgroup, and the set of measurable observables is shrunk to Pauli observables of CSS type. Examples for Approach II invoke quasiprobability functions over the set of stabilizer states [21], so-called cnc-sets [13] (also see [39]), and probability functions over the vertices of the Λ-polytopes [40] (also see [41]). Denote by Ω_{stab}, Ω_{cnc} and Ω_Λ the sets of quantum states which, respectively, can be represented positively in those schemes. These sets are related via $\Omega_{\text{stab}} \subsetneq \Omega_{\text{cnc}} \subsetneq \Omega_\Lambda$. Furthermore, Ω_Λ is the set of *all* quantum states [40].

The above two approaches to even dimension may be criticized as follows. Approach I shies away from the full problem, and solves simpler problems instead. In Approach II, according to the Stratonovich-Weyl criteria for what constitutes a Wigner function [37,38], the nonunique quasiprobability functions invoked are not Wigner functions anymore.

And so the question arises of whether one can get closer. Specifically, *Is it possible to define multiqudit Wigner functions in even dimension, for which negativity is a precondition for quantum speedup, exactly as in the odd-dimensional case?*—This is the question we address in the present paper, for Wigner functions constructed from operator bases (as in odd dimension). For that setting, our answer is negative. In even dimensions, such Wigner functions do not exist.

The link between Wigner function negativity and quantum speedup rests on two structural properties of the Wigner function employed, namely (i) its covariance under Clifford gates, and (ii) positive representation of Pauli measurement. In odd local dimension, the Wigner function described by Gross has these properties. Regarding even dimension, for $d = 2$ it is known that Clifford-covariant Wigner functions constructed from operator bases do not exist [17], and for a subset of such Wigner functions it is known that they cannot represent Pauli measurement positively whenever the number of qubits is $n \geq 2$ [12].

The contribution of this paper is two-fold: First, we extend the scope of the no-go results to all even dimensions. Namely, we show that, in all even dimensions, Wigner functions constructed from operator bases (i) cannot be Clifford-covariant, and (ii) cannot represent Pauli measurement positively. Second, we formalize the obstructions to the existence of Wigner functions with the above "nice" properties. These obstructions are cohomological in nature. Our main results are stated as Theorems 4 – 7, in Sections 4 and 5.

The remainder of this paper is organized as follows. In Section 2 we provide the necessary background on the Pauli and Clifford groups, quantum computation with magic states, Wigner functions, cohomology, and contextuality. In Section 3 we define the Wigner functions of present interest, which are constructed from operator bases. Section 4 is on the possibility of Clifford covariance of such Wigner functions. Theorem 4 identifies a necessary and sufficient cohohomological condition for the existence of Clifford covariant Wigner functions, and Theorem 5 applies this condition to the case of even dimension. Section 5 discusses positive representation of Pauli measurement by the considered Wigner functions. Theorem 6 provides a necessary and sufficient cohomological criterion for when Wigner functions representing Pauli measurement positively exist, and Theorem 7 applies this criterion to even dimension. Section 6 is the discussion.

2 Background

In this section we review the necessary background material, namely the Pauli and the Clifford group, quantum compuation with magic states, Wigner functions and the Stratonovich-Weyl criteria, and cohomology. We also review two types of proofs for the contextuality of quantum mechanics, namely parity-based and symmetry-based contextuality proofs. The latter are not necessary to understand our main results, Theorems 4–7; but they are based on the same cohomological structures, and thus connect the present discussion to a broader picture.

2.1 The Pauli group and the Clifford group

Pauli observables and Clifford unitaries are of central importance for this paper. Here we provide the definitions for reference.

2.1.1 The Pauli group

Definition. Let $d \geq 2$ be a natural number. The 1-qudit Pauli group is defined using the usual shift X and the phase Z operators acting on $\mathbb{C}^d$:

$$X|k\rangle = |k+1\rangle, \quad Z|k\rangle = \omega^k |k\rangle \tag{1}$$

where $k \in \mathbb{Z}_d$ and $\omega = e^{2\pi i/d}$. Tensor products of these operators are used to construct the n-qudit Pauli group. There is a distinction between the odd and the even cases: Let $\mu = \omega$ and $Z_\mu = \mathbb{Z}_d$ ($\mu = \sqrt{\omega}$ and $Z_\mu = \mathbb{Z}_{2d}$) if d is odd (even). Pauli operators are defined by

$$T_a = \mu^{\gamma(a)} Z(a_z) X(a_x) \tag{2}$$

where $a = (a_Z, a_X) \in \mathbb{Z}_d^n \times \mathbb{Z}_d^n =: E$, $Z(a_Z) := \bigotimes_{k=1}^n Z^{a_Z[k]}$, $X(a_X) := \bigotimes_{k=1}^n X^{a_X[k]}$, and $\gamma : E \to Z_\mu$ is a function chosen such that all operators T_a satisfy $(T_a)^d = I$. For even d, the requirement that $(T_a)^d = I$ restricts γ to $\gamma(a) \mod 2 = (a_z)^T a_x \mod 2$.

The n-qudit Pauli group P_n is generated by the operators T_a where $a \in E$, yielding $P_n = \{\mu^\lambda T_a : \lambda \in Z_\mu, a \in E\}$. The commutation relation among Pauli operators can be expressed in terms of a symplectic form, $T_a T_b = \omega^{[a,b]} T_b T_a$, with

$$[a,b] := (a_Z)^T b_X - (a_X)^T b_Z \mod d. \tag{3}$$

Thus, T_a and T_b commute if and only if $[a,b] = 0$. Of interest to us is the multiplication table of Pauli observables, especially among commuting ones,

$$T_a T_b = \omega^{\beta(a,b)} T_{a+b}, \ \ [a,b] = 0. \tag{4}$$

This relation defines the function β with values in $\mathbb{Z}_d$.

Structural properties. We have the following structural results about the multiplication table of Eq. (4).

Observation 1 ([6]) *If the dimension d is odd, then for any number n of qudits the phases $\gamma(a)$ in Eq. (2) can be chosen such that $\beta \equiv 0$.*

The proof of Observation 1 is constructive; choose

$$\gamma(a) = -2^{-1}(a_Z)^T a_X. \tag{5}$$

Among the phenomenological implications of Observation 1 are (i) the fact that there is no parity-based contextuality proof on Pauli observables [10,12] (i.e., no counterpart to Mermin's square and star) when d is odd; and (ii) the multi-qudit Wigner function defined in [6] is positivity-preserving under all Pauli measurements. Both properties are important for identifying Wigner function negativity and state-dependent contextuality as preconditions for quantum speedup in quantum computation with magic states, see [9], [14].

The even-dimensional counterpart of Observation 1 will be discussed in Section 5.3. For the special case of $d = 2$ the following is known.

Observation 2 ([15]) *If $d = 2$ then for all $n \geq 2$ and any choice of the function γ in Eq. (2) it holds that $\beta \not\equiv 0$.*

The Proof of Observation 2 is provided by Mermin's square [15].

2.1.2 Clifford group

The n-qudit Clifford group Cl_n is the normalizer of the Pauli group P_n, with the phases modded out,

$$\mathrm{Cl}_n = N(P_n)/U(1). \tag{6}$$

Of central interest to us is how the Clifford group acts on Pauli observables by conjugation,

$$g(T_a) := gT_a g^\dagger = \omega^{\tilde{\Phi}_g(a)} T_{S_g a}, \;\; \forall g \in \mathrm{Cl}_n, \, \forall a \in E. \tag{7}$$

where S_g is a symplectic transformation acting on E, i.e. an element of $\mathrm{Sp}(E)$ (also denoted by $\mathrm{Sp}_{2n}(\mathbb{Z}_d)$). Here we are using two observations: (1) S_g is a group homomorphism $E \to E$ since g respects products of Pauli operators, i.e. $g(T_a T_b) = g(T_a)g(T_b)$, and (2) S_g is symplectic since g respects commutators in the sense that $[g(T_a), g(T_b)] = g([T_a, T_b])$. The Pauli group with the phases modded out, $\mathcal{P}_n := P_n/(U(1) \cap P_n) \cong \mathbb{Z}_d^n \times \mathbb{Z}_d^n$, is a normal subgroup of Cl_n, and it holds that $\mathrm{Sp}(E) \cong \mathrm{Cl}_n/\mathcal{P}_n$.

The phase function $\tilde{\Phi}$ plays an important role in the subsequent discussion. $U(1)$-phases in $N(P_n)$ do not affect $\tilde{\Phi}$ in Eq. (7), which is why we may mod out those phases to begin with, cf. the definition of Cl_n in Eq. (6).

2.2 Quantum computation with magic states

Quantum computation with magic states (QCM) [24] is a scheme for universal quantum computation. It is closely related to the circuit model, but there is an important difference: the set of realizable quantum gates is restricted to the Clifford gates, hence not universal. Quantum computational universality is restored by the inclusion of so-called magic states.

2.2.1 Operations in QCM

There are two types of operations in quantum computation with magic states, the "free" operations and the resources. The free operations are (i) preparation of all stabilizer states, (ii) all Clifford unitaries, and (iii) measurement of all Pauli observables.

The resource are arbitrarily many copies of the state

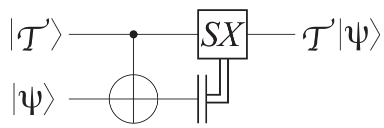
$$|\mathcal{T}\rangle = \frac{|0\rangle + e^{i\pi/4}|1\rangle}{\sqrt{2}}. \tag{8}$$

The state $|\mathcal{T}\rangle$ is called a "magic state", because of its capability to restore universality, given Clifford gates and Pauli measurements.

The distinction between free operations and resources in QCM is motivated by the Gottesman-Knill theorem. Namely, the free operations alone are not universal for quantum computation, and, in fact, can be efficiently classically simulated.

2.2.2 Computational universality

For the case of qubits, $d = 2$, it is well known [28] that the gates $\{\mathrm{CNOT}_{ij}, H_i, \mathcal{T}_i;\ 1 \leq i,j \leq n, i \neq j\}$ form a universal set, i.e., enable universal quantum computation. Therein, the only non-Clifford element is $\mathcal{T}_i = \exp\left(-i\frac{\pi}{8}Z_i\right)$. This gate can be simulated by the use of a single magic state $|\mathcal{T}\rangle$ in a circuit of Clifford gates and Pauli measurements (circuit reproduced from Fig. 10.25 of [27]),



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The lower qubit is measured in the Z-basis, and S is the Clifford gate $S_i = \exp\left(-i\frac{\pi}{4}Z_i\right)$. Thus, the magic states Eq. (8) boost the free operations to quantum computational universality.

2.2.3 A variant of QCM

We observe that in quantum computation with magic states, the Clifford unitaries can be eliminated without loss of computational power. Given the magic states, the computational power rests with the Pauli measurements.

This can be seen as follows. Consider the most general QCM, consisting of a sequence of Clifford gates interspersed with Pauli measurements, both potentially conditional on the outcomes of prior Pauli measurements. Now, starting with the last and ending with the first, the Clifford unitaries may be propagated forward in time, past the last Pauli measurement. Since the computation ends with the last measurement (all measurement outcomes have been gathered), after propagation the unitaries may be dropped without loss.

The only effect of the Clifford unitaries is that, in propagation, they change the measured observables by conjugation. But, by the very definition of the Clifford group, Pauli measurements remain Pauli measurements under conjugation by Clifford unitaries. Thus, for every QCM circuit consisting of Clifford unitaries and Pauli measurements, there is a computationally equivalent circuit that consists of Pauli measurements only.

This observation impacts the interpretation of the results of this paper. Theorems 4 and 5 below deal with the question of when Clifford covariant Wigner functions exist, and Theorems 6 and 7 with the question of when Wigner functions exist that represent Pauli measurements positively. With the observation just made, the latter two are more important for quantum computation with magic states. However, we still address Clifford covariance, as it has traditionally been invoked in the discussion of QCM [9], and as it is of general interest.

2.3 Wigner functions

The Wigner function [29] forms the basis of an alternative formulation of quantum mechanics in which states are represented by a quasiprobability function over the position-momentum phase space. The Wigner function behaves much like a probability distribution over phase space, the basis of classical statistical mechanics. The essential difference is that the Wigner function can take negative values. This property allows the Wigner function to represent quantum mechanics, and as a result, negativity in the Wigner functions of states has been proposed as a measure that distinguishes classically behaving subsystems of quantum mechanics from those which are genuinely quantum [4].

Many other quasiprobability representations of quantum mechanics have also been defined. They are related through the Stratonovich-Weyl (SW) correspondence—a set of criteria that reasonable quasiprobability representations over generalized phase spaces should satisfy [37] (also see [38]). Quasiprobability functions in the SW class have the form $W_A : \mathcal{V} \to \mathbb{C}$ where W_A is the quasiprobability function representing the linear operator A defined over phase space $\mathcal{V}$. The SW criteria are as follows:

(sw0) (Linearity): the map $A \rightarrowtail W_A$ is one-to-one and linear,

(sw1) (Reality):
$$W_{A^\dagger}(x) = (W_A(x))^* \quad \forall x \in \mathcal{V},$$

(sw2) (Standardization):
$$\int_{\mathcal{V}} d\mu(x) W_A(x) = \mathrm{Tr}(A),$$

(sw3) (Covariance):
$$W_{g\cdot A}(g \cdot x) = W_A(x) \quad \forall x \in \mathcal{V}\; \forall g \in G$$
where G is a symmetry group of the phase space.

(sw4) (Traciality):
$$\int_{\mathcal{V}} d\mu(x) W_A(x) \Theta_B(x) = \mathrm{Tr}(AB)$$
where Θ is a quasiprobability function dual to W.

Interpreting negativity in quasiprobability functions as an indicator of genuine quantumness, with many applications in quantum information processing, has also been proposed for discrete Wigner functions—quasiprobability functions used for describing finite-dimensional quantum mechanics. For a system of n qudits, each with local Hilbert space dimension d, the discrete Wigner function is usually defined over the finite phase space $\mathbb{F}_d^{2n}$ [5] or $\mathbb{Z}_d^{2n}$ [6,31]. When $d = p$ is prime, $\mathbb{F}_d \cong \mathbb{Z}_d$, and so the two choices for the phase space are equivalent. The scope of the former choice is limited to the case where the local Hilbert space dimension $d = p^N$ is a power of a prime since a finite field with d elements exists if and only if d is a power of a prime. In this case, there is a map $\iota : \mathbb{F}_{p^N}^2 \to \mathbb{F}_p^{2N}$ which preserves the structure of the phase space, and so Wigner functions defined over $\mathbb{F}_{p^N}^{2n}$ coincide with Wigner functions defined over $\mathbb{Z}_p^{2nN}$ up to relabeling of phase space points [31]. Therefore, choosing the phase space defined over $\mathbb{F}_{p^N}$ is equivalent to representing each $d = p^N$-dimensional qudit as a system of N independent p-dimensional qudits with the overall phase space $\mathbb{Z}_p^{2nN}$. Many other phase spaces for finite-dimensional systems have also been proposed, see [32] for a review. For the purposes of the present paper we are interested in Wigner functions defined over the phase space $V := \mathbb{Z}_d^{2n}$.

One particularly useful example of a discrete Wigner function that satisfies the SW criteria is Gross' Wigner function for systems of odd-dimensional qudits [6]. This is a Wigner function defined over the phase space $V = \mathbb{Z}_d^{2n}$ where d is odd. To start we choose the phase convention of the Pauli operators in Eq. (2) as in Eq. (5). Then points in phase space are associated with phase-space point operators defined as

$$A_u = \frac{1}{d^n} \sum_{v \in V} \omega^{-[u,v]} T_v^\dagger, \quad \forall u \in V.$$

These operators form an orthonormal basis for the space of Hermitian operators on d^n-dimensional Hilbert space. Therefore, for any density matrix ρ representing a quantum state, there is a decomposition in phase point operators of the form

$$\rho = \sum_{u \in V} W_\rho(u) A_u. \tag{9}$$

The coefficients in this expansion define the Wigner function $W_\rho : V \to \mathbb{R}$ of the state ρ. Equivalently, by orthogonality, the Wigner function can be defined as

$$W_\rho(u) = \frac{1}{d^n} \operatorname{Tr}(A_u \rho).$$

This Wigner function has several properties which make it useful for describing quantum computation with magic states. First, it is covariant with respect to all Clifford group operations. That is, for any linear operator Y and for all $g \in \mathrm{Cl}_n$ it holds that

$$W_{g(Y)}(S_g v + a_g) = W_Y(v). \tag{10}$$

Therein, S_g is the symplectic matrix introduced in Eq. (7) and a_g is a translation vector, both dependent on g. This follows from the fact that phase point operators map to phase point operators under conjugation by Clifford group elements:

$$g(A_u) = A_{S_g u + a_g} \quad \forall u \in V \; \forall g \in \mathrm{Cl}_n.$$

The Wigner function also satisfies the condition of positivity preservation of the Wigner function under Pauli measurements. That is, if a state ρ has a non-negative Wigner function and a Pauli measurement is performed, the resulting postmeasurement state also has a non-negative Wigner function. This follows from the fact that under Pauli measurements phase point operators map to probabilistic combinations of phase point operators.

In fact, the update of the phase point operators under Clifford unitaries and Pauli measurements can be computed efficiently classically. This leads to an efficient classical simulation algorithm for quantum computation with magic states based on sampling from the Wigner probability distribution of the input state that applies whenever the Wigner function of the input state is non-negative. This can be formalized in the following theorem.

Theorem 1 ([9], adapted) *Consider quantum computation with magic states on n qudits of odd prime dimension d. If the initial magic state $\rho = \rho(1)_1 \otimes \rho(2)_2 \otimes .. \otimes \rho(n)_n$ satisfies $W_\rho \geq 0$, then any quantum computation in the magic state model starting with ρ can be efficiently classically simulated.*

We have rephrased this Theorem here to make the statement self-contained, for the original formulation, see Theorem 1 in [9]. This result can be extended to apply to quantum computation with magic states on qudits of any odd dimension [52]. When the discrete Wigner function of the input state takes negative values classical simulation is still possible [36], but it is inefficient in general.

Many no-go results have provided obstructions to a similar result for systems of even-dimensional qudits. For example, it has been shown that no Wigner function in the SW class for systems of multiple qubits can be Clifford covariant [17]. Quasiprobability representations for systems of even-dimensional qudits have been defined for the purpose of describing quantum computation with magic states, e.g. [13, 21, 33–35], but these generally require relaxing some of the constraints provided by the SW criteria. In this paper we explore the underlying reasons for the difference between Wigner functions in the SW class of even- and odd-dimensional qudits in terms of Clifford covariance and positivity preservation under Pauli measurements.

2.4 Cohomology

The purpose of the section is to explain that the function β defined in Eq. (4) and the phase function $\tilde{\Phi}$ defined in Eq. (7) are cohomological objects. As it will turn out, β governs the existence of Wigner functions that represent Pauli measurement positively, and $\tilde{\Phi}$ governs the existence of Wigner functions that are Clifford covariant. Thus, Clifford covariance of Wigner functions and positive representation of Pauli measurement by Wigner functions are cohomological properties of the Clifford and Pauli groups.

2.4.1 Motivation

Here we lay out a short path to recognizing β and $\tilde{\Phi}$ as cohomological objects. A problem gets us started. The Pauli operators contain in their definition an arbitrary phase γ, cf. Eq. (2), with no physical significance. Respecting the constraint on γ imposed by the condition $(T_a)^d = I$, $\forall a \in E$, the phases γ can be changed as

$$\begin{array}{rcll} \gamma & \longrightarrow & \gamma+\nu, & \text{if } d \text{ is odd,} \\ \gamma & \longrightarrow & \gamma+2\nu, & \text{if } d \text{ is even.} \end{array} \tag{11}$$

The corresponding effect on β is, irrespective of whether d is even or odd,

$$\beta(a,b) \longrightarrow \beta(a,b) + \nu(a) + \nu(b) - \nu(a+b) \mod d. \tag{12}$$

An object can be of physical significance only if it is invariant under the gauge transformations of Eq. (11). Can we construct such objects out of the function β?

The prepared eye recognizes Eq. (12) as a cohomological equivalence transformation $\beta \longrightarrow \beta + d\nu$ and this gives a clue. Namely, the cohomology classes $[\beta]$ are invariant objects!

Indeed, as we demonstrate in Section 5, those cohomology classes determine the existence of Wigner functions that represent Pauli measurement positively. To provide the foundation for the cohomological formulation, in Section 2.4.2 we describe the chain complex where β lives.

The motivation for the cohomological description of $\tilde{\Phi}$ is analogous. With Eq. (7), the effect of the equivalence transformation Eq. (11) on $\tilde{\Phi}$ is

$$\tilde{\Phi}_g(a) \longrightarrow \tilde{\Phi}_g(a) + \nu(a) - \nu(S_g a) \mod d. \tag{13}$$

Again, this looks like an equivalence transformation in group cohomology, $\tilde{\Phi} \longrightarrow \tilde{\Phi} - d^h\nu$. Therein, d^h is the coboundary operator in group cohomology. The bi-complex where $\tilde{\Phi}$ lives is introduced in Section 2.4.3. As we demonstrate in Section 4, the existence of Clifford covariant Wigner functions hinges on a cohomological invariant extracted from $\tilde{\Phi}$.

2.4.2 β is a cocycle

Let $\mathcal{C}_* = (C_0, C_1, C_2, C_3)$ denote the chain complex for which C_k is defined to be the free $\mathbb{Z}_d$-module with basis $[v_1|v_2|\cdots|v_k]$, where $v_i \in E$ and

$$[v_i, v_j] = 0,\ \forall i, j = 1, \cdots, k. \tag{14}$$

Note that $C_0 = \mathbb{Z}_d$. The boundary map ∂ is given by the formula

$$\partial[v_1|v_2|\cdots|v_k] = [v_2|\cdots|v_k] + \left(\sum_{i=1}^{k-1}(-1)^i[v_1|\cdots|v_i + v_{i+1}|\cdots|v_k]\right) + (-1)^k[v_1|\cdots|v_{k-1}]. \tag{15}$$

There is also an associated cochain complex $\mathcal{C}^*$ whose k-cochains C^k are given by $\mathbb{Z}_d$-module maps (i.e. $\mathbb{Z}_d$-linear functions) $f : C_k \to \mathbb{Z}_d$. The coboundary map δ is defined by the formula $\delta f(-) = f(\partial -)$.

With the identification $\beta([a|b]) := \beta(a, b)$, the above definitions make β a 2-cochain in $\mathcal{C}^*$, i.e. $\beta \in C^2$. But we can say more; β is in fact a cocycle, $d\beta = 0$. Namely, associativity of operator multiplication, $T_a(T_bT_c) = (T_aT_b)T_c$, implies, for all $a, b, c \in E$ such that $[a, b] = [a, c] = [b, c] = 0$,

$$\beta(b, c) - \beta(a + b, c) + \beta(a, b + c) - \beta(a, b) = 0.$$

The surface $F := [b|c] - [a+b|c] + [a|b+c] - [a|b]$ is the boundary of the volume $V = [a|b|c]$, $F = \partial V$. Thus, $0 = \beta(\partial V) = d\beta(V)$, for all volumes V. Hence,

$$d\beta = 0, \tag{16}$$

as claimed. The equivalence class of β is now defined by

$$[\beta] := \{\beta + d\nu, \nu \in C^1\}. \tag{17}$$

The equivalence classes of 2-cocycles form the second cohomology group $H^2(\mathcal{C}, \mathbb{Z}_d)$. They are independent of the choice of phase γ in Eq. (2).

To provide a first application of the cohomological formulation, recall that in Section 2.1.1 we discussed whether the phase factors in the Pauli operator multiplication table of Eq. (4) can be eliminated by a clever choice of the phase convention γ. We now find that this is a topological question. Namely, with Eqs. (11) and (17), the phase factor ω^β can be removed if and only if $[\beta] = 0$. Observations 1 and 2 may thus be reformulated in a cohomological fashion as (i) If d is odd then for any n it holds that $[\beta] = 0$, and (ii) If $d = 2$ then for any $n \geq 2$ it holds that $[\beta] \neq 0$.

2.4.3 The group cocycles $\tilde{\Phi}$ and Φ_{cov}

In this section we will regard $\tilde{\Phi}$, introduced in Eq. (7), as a cocycle and relate its cohomology class to certain properties of Wigner functions. For this we need to introduce a chain complex which is slightly different than the one used above. The main difference is that we remove the commutativity constraint imposed on tuples constituting the basis of the chain complexes. We define a chain complex $\tilde{\mathcal{C}}_* = (\tilde{C}_0, \tilde{C}_1, \tilde{C}_2, \tilde{C}_3)$. Here $\tilde{C}_k$ is the free $\mathbb{Z}_d$-module with basis consisting of the tuples $[v_1|v_2|\cdots|v_k]$ where $v_i \in E$. The boundary map is the same as in Eq. (15). The associated cochain complex is denoted by $\tilde{\mathcal{C}}^* = (\tilde{C}^0, \tilde{C}^1, \tilde{C}^2, \tilde{C}^3)$ and the coboundary map $\delta : \tilde{C}^k \to \tilde{C}^{k+1}$ is induced by the boundary map as before. Note that by definition $\tilde{C}_1 = C_1$ and $\tilde{C}^1 = C^1$, thus in this case we remove the extra decoration for simplicity of notation. We also note that the (co)chain complex defined here is the standard complex (which is called the bar construction) that computes the group (co)homology of the abelian group E.

For a symmetry group specified by a subgroup $G \subset \mathrm{Cl}_n$, we consider the bicomplex $C^p(G, \tilde{C}^q)$; see also [16, Section 5.2]. The bicomplex $C^p(G, \tilde{C}^q)$ comes with two types of coboundaries: group cohomological $d^h : C^p(G, \tilde{C}^q) \to C^{p+1}(G, \tilde{C}^q)$, and $d^v : C^p(G, \tilde{C}^q) \to C^p(G, \tilde{C}^{q+1})$ induced by δ.

The phase function $\tilde{\Phi} : G \to C^1$ is per definition a 1-cochain in group cohomology. Its coboundary, a 2-cochain, is

$$(d^h\tilde{\Phi})_{g,h}(a) := \tilde{\Phi}_h(a) - \tilde{\Phi}_{gh}(a) + \tilde{\Phi}_g(S_h a). \tag{18}$$

In fact, $\tilde{\Phi}$ is not only a 1-cochain but a 1-cocycle, i.e., $d^h\tilde{\Phi} = 0$. Namely, with the associativity of matrix multiplication, it holds that $(gh)(T_a) = g(h(T_a))$, $\forall g, h \in \mathrm{Cl}_n$, $\forall a \in E$. Evaluating both sides using Eq. (7) yields $\tilde{\Phi}_{gh}(a) = \tilde{\Phi}_h(a) + \tilde{\Phi}_g(S_h a)$, $\forall g, h \in \mathrm{Cl}_n$, $\forall a \in E$. Thus, with Eq. (18), $(d\tilde{\Phi})_{g,h}(a) = 0$, for all $g, h \in \mathrm{Cl}_n$ and all $a \in E$. $\tilde{\Phi}$ is indeed a group cocycle.

This group cocycle may be trivial or nontrivial. Consider a 0-cochain ν in group cohomology. Its coboundary, a 1-cocycle, is

$$(d^h\nu)_g(a) := \nu(S_g a) - \nu(a). \tag{19}$$

We define the group cohomology classes

$$[\tilde{\Phi}] = \{\tilde{\Phi} + d^h\nu,\ \forall \nu \in C^1\}.$$

A cocycle $\tilde{\Phi}$ is trivial iff it can be written in the form $\tilde{\Phi} = d^h\nu$, for some $\nu \in C^1$. A class $[\tilde{\Phi}]$ is trivial, $[\tilde{\Phi}] = 0$, if and only if it contains $\tilde{\Phi} \equiv 0$.

The cocycle $\tilde{\Phi}$ may not only be evaluated on edges $a \in E$ but on all 1-chains. By definition it is linear in this second argument; i.e., it holds that $\tilde{\Phi}_g(c + c') = \tilde{\Phi}_g(c) + \tilde{\Phi}_g(c')$, for all $c, c' \in C_1$. Subsequently, we will have occasion to evaluate $\tilde{\Phi}$ on boundaries ∂f, for $f \in C_2$. It is easily verified that, for boundaries ∂f,

$$\tilde{\Phi}_g(\partial f) = \tilde{\Phi}_{[g]}(\partial f),\ \forall g \in \mathrm{Cl}_n,$$

where $[g] \in \mathrm{Cl}_n/\mathcal{P}_n$. That is, when $\tilde{\Phi}$ is evaluated on a boundary, it depends on its first argument g only through the equivalence class $[g]$.

To formalize this property, let $N \subset G$ denote the subgroup of symmetries g such that S_g is the identity transformation. The quotient group $Q = G/N$ is the essential part of the symmetries acting on the complex. Let $\tilde{B}_1$ denote the image of the boundary map $\partial : \tilde{C}_2 \to C_1$. We write U_{cov} for the set of $\mathbb{Z}_d$-module maps $\tilde{B}_1 \to \mathbb{Z}_d$. We choose a set-theoretic section $\theta : Q \to G$ of the quotient map $\pi : G \to Q$. Then $\Phi_{\mathrm{cov}} \in C^1(Q, U_{\mathrm{cov}})$ is defined to be the composite

$$\Phi_{\mathrm{cov}} : Q \xrightarrow{\theta} G \xrightarrow{\tilde{\Phi}} C^1 \xrightarrow{d^v} U_{\mathrm{cov}} \tag{20}$$

where the last map can also be thought of as the restriction of a $\mathbb{Z}_d$-module map $C_1 \to \mathbb{Z}_d$ to the boundaries $\tilde{B}_1$. More explicitly we have

$$\Phi_{\mathrm{cov}}(q, \partial f) = d^v\tilde{\Phi}_{\theta(q)}(f) = \tilde{\Phi}_{\theta(q)}(\partial f)$$

for any $q \in Q$ and $f \in \tilde{C}_2$. Although $\tilde{C}^1 = C^1$, the object U_{cov} is different from its counterpart U introduced in [16, Eq. (39)] as part of the symmetry discussion in contextuality. See also Theorem 3 below.

Like $\tilde{\Phi}$, Φ_{cov} is also a group cocycle, $d^h\Phi_{\mathrm{cov}} = 0$. The cocycle class of Φ_{cov} is given by

$$[\Phi_{\mathrm{cov}}] = \{\Phi_{\mathrm{cov}} + d^h\nu,\ \nu \in U_{\mathrm{cov}}\}.$$

$[\Phi_{\text{cov}}]$ is the object of interest for Wigner function covariance.

As a first application of the group cohomological formalism, recall Theorem 37 from [6], on the structure of the Clifford group in odd dimension. Items (i) and (iii) of that theorem read: (i) For any symplectic S, there is a unitary operator $\theta(S)$ such that $\theta(S)T_a\theta(S)^\dagger = T_{Sa}$; (iii) Up to a phase, any Clifford operation is of the form $U = T_b\,\theta(S)$, for a suitable $b \in E$ and symplectic transformation S.

Comparing the relation in item (i) with the general relation Eq. (7), we find that $\tilde{\Phi}_{\theta(S)} = 0$ for all symplectic S, w.r.t. the phase convention γ chosen in [6]. Thus, in particular, $\tilde{\Phi}_{\theta(S)}(\partial f) = 0$ for all $f \in \tilde{C}_2$. Since Pauli flips don't change $\tilde{\Phi}$ on boundaries, $\tilde{\Phi}_{T_b\,\theta(S)}(\partial f) = 0$ for all $f \in \tilde{C}_2$ and all $b \in E$. But with item (iii) this covers the entire Clifford group. I.e., there is a phase convention γ such that $\Phi_{\text{cov}} \equiv 0$. The phase-convention independent version of this statement is

Observation 3 *For the Clifford group Cl_n in any odd dimension d it holds that $[\Phi_{\text{cov}}] = 0$.*

2.5 Contextuality

Unlike the previous parts of this background section, the material on contextuality discussed here is not necessary to understand the main results of this paper, Theorems 4 – 7. However, it is helpful for connecting to the broader picture. Namely, two previously established theorems on state-independent contextuality [16], restated below as Theorems 2 and 3, are structurally akin to Theorems 4 and 6, on the existence of Wigner functions with "nice" properties. They invoke the same cohomological conditions. This background portion prepares for the discussion in Section 6.

Contextuality is a foundational property that distinguishes quantum mechanics from classical physics. A priori, one may attempt to describe quantum phenomena by so-called hidden variable models (HVMs) in which all observables have predetermined outcomes that are merely revealed upon measurement. A probability distribution over such predetermined outcomes is then intended to mimic the randomness of quantum measurement. An additional constraint on HVMs is the assumption of noncontextuality: the value assigned to any given observable just depends on that particular observable, and not on any compatible observable that may be measured in conjunction. The Kochen-Specker theorem says that, in Hilbert spaces of dimension greater than two, no noncontextual hidden variable model can reproduce the predictions of quantum mechanics. Since noncontextual hidden variable models fail in this realm, quantum mechanics is called "contextual".

The original proof of the Kochen-Specker theorem is intricate. However, when sacrificing a modest amount of generality, namely the case of Hilbert space dimension 3, a very simple proof can be given—Mermin's square [15]. Here we review two types of proofs of the Kochen-Specker theorem, the parity-based proofs (Mermin's square is the simplest example), and the symmetry-based proofs.

Parity-based proofs. The main examples of parity-based proofs are the well-known Mermin's square in dimension 4 and Mermin's star in dimension 8 [15]. In those examples, the proof is based on a cleverly chosen set of Pauli observables. However, for parity proofs to work, the observables don't need to be of Pauli type; it suffices that all their eigenvalues are kth roots of unity for some fixed $k \in \mathbb{N}$.

Parity proofs have a cohomological formulation. With the cocycle β and corresponding cohomology class $[\beta]$ in $H^2(\mathcal{C})$ defined as in Section 2.4, but this time for a set $\mathcal{O}$ of observables whose eigenvalues are all powers of ω (not necessarily, but possibly, Pauli observables), we have the following result.

Theorem 2 ([16]) *For a set of observables $\mathcal{O}$ with all eigenvalues of form $e^{i2\pi m/k}$, for $m, k \in \mathbb{N}$ and k fixed, a parity-based contextuality proof exists if and only if $[\beta] \neq 0$.*

Symmetry-based proofs. Proofs of the Kochen-Specker theorem may also be based on the transformation behavior of a set $\mathcal{O}$ of observables under a symmetry group G [16]. To be a symmetry group, G (i) needs to map the set $\mathcal{O}$ to itself up to phases that preserve the constraint on the eigenvalue spectrum, and (ii) needs to preserve algebraic relations among the transformed observables. Again, the symmetry-based contextuality proofs have a cohomological formulation.

Theorem 3 ([16]) *For a given set $\mathcal{O}$ of observables as above, and a corresponding symmetry group G, if $[\Phi] \neq 0 \in H^1(Q, U)$ then $\mathcal{O}$ exhibits state-independent contextuality.*

There is a small difference between Φ in Theorem 3 and Φ_{cov} from Section 2.4.3. Both phase functions are defined only on boundaries ∂f where $f = [a|b]$. However, for Φ all f are constraint to $[a, b] = 0$, whereas for Φ_{cov} as defined in Section 2.4.3 this extra condition is not imposed.

3 Wigner functions from operator bases

In this section we define the Wigner functions we are concerned with in this paper, namely Wigner functions based on operator bases, and derive elementary properties of them. This lays the groundwork for Sections 4 and 5, where we discuss Clifford covariance of Wigner functions and positive representation of Pauli measurement, respectively.

Our results refer to the following, more specific formulations of the SW criteria:

(OB) For any quantum state ρ, a corresponding Wigner function W_ρ satisfies

$$\rho = \sum_{v \in V} W_\rho(v) A_v, \tag{21}$$

where the operators $\{A_v,\, v \in V\}$ form an operator basis and the phase space is $V = \mathbb{Z}_d^n \times \mathbb{Z}_d^n$.

(SW1) (Reality):

$$W_{A^\dagger}(u) = (W_A(u))^* \quad \forall u \in V,$$

(SW2) (Standardization):

$$\sum_{u \in V} W_A(u) = \mathrm{Tr}(A),$$

(SW3) (Pauli covariance):

$$W_{T_a(A)}(u + a) = W_A(u) \quad \forall u \in V\ \forall a \in E$$

,

(SW4) (Traciality):

$$\sum_{u \in V} W_A(u) \Theta_B(u) = \mathrm{Tr}(AB)$$

where Θ is a quasiprobability function dual to W.

Condition (OB) implies (SW0) but is not implied by it. (SW2) and (SW4) are obtained from (sw2) and (sw4) by choosing a natural measure μ. As opposed to (sw3), (SW3) refers to a specific symmetry group G—the Pauli group—and a particular action of the symmetry group on the phase space.

Among the Wigner functions permitted by the constraints (OB) and (SW1)–(SW4) we are interested in those that transform covariantly under all Clifford gates and represent Pauli measurement positively.

To prepare for the subsequent discussion, we parametrize the phase point operators. Pauli covariance (SW3) holds if and only if

$$A_v = \frac{1}{d^n} \sum_b \omega^{-[v,b]} c_b T_b^\dagger, \ \forall v \in V, \tag{22}$$

where $c_b \in \mathbb{C}$ for all b, $V = \mathbb{Z}_d^n \times \mathbb{Z}_d^n$.

Additionally imposing Standardization (SW2) and the fact that the operators A_v span an operator basis (OB) is equivalent to the following conditions on the coefficients c_b appearing on the r.h.s. of Eq (22):

$$c_0 = \mu^{\gamma(0)}, \tag{23a}$$
$$c_b \neq 0, \ \forall b. \tag{23b}$$

With these properties established, we are now ready to address the questions of Clifford covariance and positive representation of Pauli measurement.

4 Clifford covariance

We start out from the following

Definition 1 *A Wigner function W is called Clifford covariant if*

$$W_{g(Y)}(S_g u + a_g) = W_Y(u) \quad \forall u \in \mathcal{V}\ \forall g \in \mathcal{C}l_n \tag{24}$$

where S_g is the symplectic transformation defined in Eq. (7).

It is useful to restate the covariance condition Eq. (24) in terms of phase point operators. With Eq. (21) it holds that $W_{A_w} = \delta_w(v)$. Now, for any Clifford gate g we have

$$\begin{array}{rcl} g(A_w) & = & \sum_v W_{g(A_w)}(v) A_v \\ & = & \sum_v W_{g(A_w)}(S_g v + a_g) A_{S_g v + a_g} \\ & = & \sum_v W_{A_w}(v) A_{S_g v + a_g} \\ & = & \sum_v \delta_w(v) A_{S_g v + a_g} \\ & = & A_{S_g w + a_g} \end{array} \tag{25}$$

Therein, in the second line we have relabeled the summation index, and in the third line we have used the covariance condition Eq. (24). Thus, Eq. (24) implies Eq. (25).

Now we show the reverse. Assuming Eq. (25), the operator $g(Y)$ can be expanded in two ways

$$g(Y) = \sum_v W_Y(v) g(A_v) = \sum_v W_Y(v) A_{S_g v + a_g},$$

and

$$g(Y) = \sum_v W_{g(Y)}(v) A_v = \sum_v W_{g(Y)}(S_g v + a_g) A_{S_g v + a_g}$$

Comparing the r.h.s.-es, and noting that by (OB) the expansions are unique, Eq. (24) follows.

Both arguments combined show that a Wigner function W satisfying (OB) is Clifford covariant if and only if

$$g(A_v) = A_{S_g v + a_g}, \;\; \forall v \in V, \; \forall g \in \mathrm{Cl}_n. \tag{26}$$

4.1 Existence of Clifford covariant Wigner functions

Given a particular Wigner function in terms of phase point operators, Clifford covariance may be verified using the criterion Eq. (26). Now we are concerned with the question of whether for a system of n qudits of d levels a Clifford covariant Wigner function *exists*. The result of this section is a cohomological criterion for the existence of a Clifford covariant Wigner function.

Theorem 4 *For any given n,d, a Clifford-covariant Wigner function according to (OB) exists if and only if* $[\Phi_\mathrm{cov}] = 0 \in H^1(Q, U_\mathrm{cov})$.

Proof of Theorem 4. "Only if": Suppose W is Clifford covariant. Then, with Eq. (26), $T_a(A_v) = A_{v+y(a)}$ $\forall a \in E$, where for readability we write $y(a)$ instead of a_g with $g = T_a$. First, we want to show that $y : \mathbb{Z}_d^{2n} \to \mathbb{Z}_d^{2n}$ is invertible. $T_a T_b(A_v) = T_{a+b}(A_v)$ implies that y is linear. Therefore, y is invertible if and only if its kernel is trivial, $\mathrm{Ker}(y) = \{0\}$. We expand $A_v = \sum_b c_b(v) T_b^\dagger$. Note that, in contrast to Ansatz (22), this expansion does not restrict A_v. Now assume that $\mathrm{Ker}(y) \ni a \neq 0$. Then $\sum_b c_b(v) T_b^\dagger = A_v = T_a(A_v) = \sum_b c_b(v) \omega^{[b,a]} T_b^\dagger$ $\forall v$ or, equivalently,

$$c_b(v) = 0 \;\; \forall b \in E : [b,a] \neq 0, \; \forall v \in V. \tag{27}$$

For any $a \neq 0$ there is a b such that $[b,a] \neq 0$. Thus, there is a $b \in E$ such that $c_b(v) = 0$ $\forall v$. Since this contradicts (OB), y must be invertible.

Because of Clifford covariance, for any $g \in \mathrm{Cl}_n$ it holds that $g(A_0^\dagger) = A_{a_g}^\dagger$. Therein, we have $g(A_0^\dagger) = \sum_b c_b^*(0)\, g(T_b) = \sum_b c_b^*(0) \omega^{\tilde{\Phi}_g(b)}\, T_{S_g b}$, and $A_{a_g}^\dagger = \sum_b \omega^{[y^{-1}(a_g), b]} c_b^*(0)\, T_b$. For any $g \in \mathrm{Cl}_n$ and any pair $b, S_g b \in E$ it follows that

$$c_{S_g b}(0) = c_b(0)\, \omega^{[y^{-1}(a_g), S_g b] - \tilde{\Phi}_g(b)}.$$

This implies that there is a function $\nu : E \longrightarrow \mathbb{Z}_d$ such that $c_b(0) = c_{\langle b \rangle}\, \omega^{\nu(b)}$ $\forall b \in E$, where $c_{\langle b \rangle} \in \mathbb{C}$ only depends on the Clifford orbit $\langle b \rangle$ of b. The phase function $\tilde{\Phi}$ and the function ν are mutually constrained by the relation

$$\nu(S_g b) - \nu(b) = [y^{-1}(a_g), S_g b] - \tilde{\Phi}_g(b), \;\; \forall b \in E, \; \forall g \in \mathrm{Cl}_n.$$

Now consider a face $f \in C_2(\tilde{\mathcal{C}})$ with boundary $\partial f = [a] + [b] - [a+b]$, and add up the above relations for the edges in the boundary. Because of its linearity, the commutator term then vanishes, and we obtain

$$\nu(g\partial f) - \nu(\partial f) = -\tilde{\Phi}_g(\partial f) = -\Phi_\mathrm{cov}([g], \partial f), \; \forall f \in C_2(\mathcal{C}'), \; \forall g \in \mathrm{Cl}_n,$$

where $g\partial f := [S_g a] + [S_g b] - [S_g(a+b)]$. Thus, $\Phi_\mathrm{cov} = d^h(-\nu)$, i.e., $[\Phi_\mathrm{cov}] = 0$.

"If": Assume that $[\Phi_\mathrm{cov}] = 0$. Thus, there is a phase convention γ such that $\tilde{\Phi}^{(\gamma)}|_{\tilde{B}_1} \equiv 0$. But this means that $\tilde{\Phi}_g^{(\gamma)}(\cdot)$ is a linear function for any $g \in \mathrm{Cl}_n$, and we may write it as

$$\tilde{\Phi}_g^{(\gamma)}(a) = [x_g, a],$$

for suitable x_g, $g \in \mathrm{Cl}_n$. Let $W^{(\gamma)}$ be the Wigner function defined by the phase point operators $A_v^{(\gamma)} = \frac{1}{d^n}\sum_a \omega^{-[v,b]}\left(T_b^{(\gamma)}\right)^\dagger$. Since the $A_v^{(\gamma)}$ constitute a special case of Ansatz (22) with Conditions (23a) and (23b), we already know that they span an operator basis (OB). Moreover, $W^{(\gamma)}$ is Clifford covariant. Namely,

$$\begin{aligned} g\left(A_v^{(\gamma)}\right) &= \tfrac{1}{d^n}\textstyle\sum_b \omega^{-[v,b]}\, g\left[\left(T_b^{(\gamma)}\right)^\dagger\right] \\ &= \tfrac{1}{d^n}\textstyle\sum_b \omega^{-[v,b]-\tilde{\Phi}_g^{(\gamma)}(b)}\, \left(T_{S_g b}^{(\gamma)}\right)^\dagger \\ &= \tfrac{1}{d^n}\textstyle\sum_b \omega^{-[v+x_g,b]}\, \left(T_{S_g b}^{(\gamma)}\right)^\dagger \\ &= \tfrac{1}{d^n}\textstyle\sum_b \omega^{-[S_g v+S_g x_g,b]}\, \left(T_b^{(\gamma)}\right)^\dagger \\ &= A_{S_g v+S_g x_g}^{(\gamma)} \end{aligned}$$

This is Eq. (26) with $a_g = S_g x_g$. $\square$

Remark: Folklore has it that Wigner function covariance hinges on the splitting of the covariance group, e.g., for Clifford covariance on whether $\mathrm{Cl}_n = Q \ltimes P_n$ for a given number n of qudits of dimension d. Splitting is also a notion of group cohomology, living at the second level.

However, there is no one-to-one correspondence between covariance and splitting. This is illustrated with the following 1-qubit example: We consider the covariance group $\mathbb{Z}_2$ generated by the Hadamard gate H. It splits trivially, i.e., there is no non-trivial subgroup of P_1 to mod out. However, $[\Phi_{\text{cov}}] \neq 0$. Namely, consider the Pauli operators $T_{a_Y} = X$, $T_{a_Y} = Y$, $T_{a_Z} = Z$. Then, $\tilde{\Phi}_H(a_X) = \tilde{\Phi}_H(a_Z) = 0$, and $\tilde{\Phi}_H(a_Y) = 1$. Thus, $\Phi_{\text{cov}}(H, \partial[a_X|a_Z]) = \tilde{\Phi}_H(\partial[a_X|a_Z]) = 1$ and $H\partial[a_X|a_Z] = \partial[a_X|a_Z]$. These relations imply that $[\Phi_{\text{cov}}] \neq 0$ (see the proof of Lemma 1). Thus, with the proof of Theorem 4, no covariant Wigner function satisfying (OB), (SW1)-(SW4) exists.

4.2 Even vs. odd dimension

For odd dimension d, and all numbers n of qudits, a Clifford-covariant Wigner function satisfying the conditions (OB), (SW1)–(SW4) has been explicitly constructed in [6]. In the present formalism, the existence of a Clifford-covariant Wigner function satisfying (OB) follows by Observation 3 and Theorem 4.

In even dimension we have the following result.

Theorem 5 *If the local dimension d is even, then for any number n of local systems, a Clifford-covariant Wigner function satisfying (OB) does not exist.*

To prove the above theorem, we first establish the following statement.

Lemma 1 *For all even local dimensions d and all qudit numbers n, it holds that $[\Phi_{\text{cov}}] \neq 0$.*

Proof of Lemma 1. The basic proof strategy is to identify a group element $g \in \mathrm{Cl}_n$ and a 2-chain $f \in C_2$ such that

$$g\partial f = \partial f, \text{ and } \tilde{\Phi}_g(\partial f) \neq 0. \tag{28}$$

Assume Eq. (28) holds and $[\Phi_{\text{cov}}] = 0$. From the latter, $\tilde{\Phi}_g(\partial f) = \Phi_{\text{cov}}([g], \partial f) = \nu(\partial f) - \nu(g\partial f)$, for some $\nu \in C^0(G, U_{\text{cov}})$. Therein, with Eq. (28), $0 \neq 0$—Contradiction. Thus, the existence of a pair g, f satisfying Eq. (28) implies that $[\Phi_{\text{cov}}] \neq 0$.

In the following, we show that g, f can be chosen in accordance with Eq. (28), for all even d. We focus on $n=1$; replacing g by $g\otimes I^{\otimes n-1}$ and all $a_z, a_x \in \mathbb{Z}_d$ by $(a_z,0,\dots,0),(a_x,0,\dots,0)\in\mathbb{Z}_d^n$ immediately generalizes the proof to all $n\in\mathbb{N}$. For concreteness, we set $\gamma(a)=a_za_x$, but our final statement is independent of the phase convention γ.

For $d=4m+2$, $m\in\mathbb{N}_0$, we consider the Fourier transform $g=\frac{1}{\sqrt{d}}\sum_{k,l=0}^{d-1}\omega^{kl}|k\rangle\langle l|$, which is a Clifford unitary that acts by conjugation as

$$g\,\cdot\,g^\dagger: X\longrightarrow Z\longrightarrow X^{-1}\longrightarrow Z^{-1}\longrightarrow X. \tag{29}$$

Further, $f:=[u|v]$, with $u=(u_z,u_x)$ and $v=(v_z,v_x)$ by $u_x=v_z=0$ and $u_z=v_x=2m+1$. Then

$$\begin{aligned} T_u &= Z^{2m+1}, & T_v &= X^{2m+1} & T_{u+v} &= \sqrt{\omega}^{(2m+1)^2}Z^{2m+1}X^{2m+1}, \\ gT_ug^\dagger &= T_v, & gT_vg^\dagger &= T_u, & gT_{u+v}g^\dagger &= \omega^{-(2m+1)}T_{u+v}. \end{aligned} \tag{30}$$

Hence, $g\partial[u|v]=\partial[u|v]$ but $\tilde{\Phi}_g(\partial[u|v])=0+0+(2m+1)=d/2\neq 0\in\mathbb{Z}_d$. Thus, Eq. (28) applies.

For $d=4m$, $m\in\mathbb{N}$, we introduce the unitary $g=\frac{1}{d}\sum_{k,l=0}^{d-1}\omega^{mk^2}\left(\sum_{j=0}^{d-1}\omega^{mj^2+(k-l)j}\right)|k\rangle\langle l|$, which is in the Clifford group since

$$gZg^\dagger=\sqrt{\omega}^{2m}ZX^{2m},\quad gXg^\dagger=\sqrt{\omega}^{\,-2m}Z^{2m}X. \tag{31}$$

Choosing $f:=[u|v]$, with $u_z=v_z=1$, $u_x=0$, and $v_x=2m$ yields

$$\begin{aligned} T_u &= Z, & T_v &= \sqrt{\omega}^{2m}ZX^{2m} & T_{u+v} &= \sqrt{\omega}^{d}Z^2X^{2m}, \\ gT_ug^\dagger &= T_v, & gT_vg^\dagger &= \omega^{2m}T_u, & gT_{u+v}g^\dagger &= T_{u+v}. \end{aligned} \tag{32}$$

Again, $\partial f=g\partial f$, and $\tilde{\Phi}_g(\partial[u|v])=0+2m-0=d/2\neq 0\in\mathbb{Z}_d$. Eq. (28) thus applies. □

Proof of Theorem 5. The statement is the combined conclusion of Lemma 1 and Theorem 4. □

5 Positive representation of Pauli measurement

In this section we first define "positive representation of Pauli measurement", and then establish a necessary and sufficient condition for it, applicable to all Wigner functions that satisfy (OB), (SW1)–(SW4). Finally, we apply this result to even and odd dimensions, making use of the respective structure theorems for Pauli observables.

5.1 When are Pauli measurements positively represented?

Denote by $\Pi_{a,s}$ the projector associated with the outcome $s\in\mathbb{Z}_d$ in the measurement of the Pauli observable T_a, i.e., $\Pi_{a,s}$ is the projector onto the eigenspace of T_a with eigenvalue ω^s. Further, denote by $p_a(s|\rho)$ the probability of obtaining s in the measurement of T_a on the state ρ; $p_a(s|\rho)=\mathrm{Tr}(\Pi_{a,s}\rho)$. We then have the following definition of "positive representation of Pauli measurement":

Definition 2 *A Wigner function W represents Pauli measurements positively if the following two properties hold.*

(a) For all Pauli measurements, the Born rule is represented by

$$\mathrm{Tr}(\Pi_{a,s}\rho)=\sum_{v\in V}\Theta_{\Pi_{a,s}}(v)W_\rho(v) \tag{33}$$

with $\Theta_{\Pi a,s} : V \longrightarrow \mathbb{R}$ *and*

$$0 \leq \Theta_{\Pi_{a,s}}(v) \leq 1, \ \forall v \in V, \forall a, s. \tag{34}$$

(b) For all Pauli measurements, the non-negativity of the Wigner function is preserved under measurement, i.e.,

$$W_\rho \geq 0 \Longrightarrow W_{\Pi_{a,s}\rho\Pi_{a,s}} \geq 0, \forall a, s. \tag{35}$$

The above definition of "positive representation of Pauli measurement" is intuitive. Condition (a) says that the effects $\Theta_{\Pi_{a,s}}$ associated with all Pauli measurements are non-negative, and if the Wigner function W_ρ is non-negative as well, then the outcome probabilities for Pauli measurements can be obtained by sampling from the phase space V. Condition (b) says that if a state ρ is represented by a non-negative Wigner function, then for any Pauli measurement with any outcome, the post-measurement state is also represented by a non-negative Wigner function.

5.2 Cohomological condition for positive representation

Here we show the following.

Theorem 6 *For any system of n qudits with d levels, $n, d \in \mathbb{N}$, a Wigner function satisfying (OB), (SW1)–(SW4) that represents Pauli measurement positively exists if and only if $[\beta] = 0$.*

The proof of Theorem 6 proceeds in several steps. To begin, we note that $(T_b)^k \sim T_{bk}$, and define phases $\varphi_b : \mathbb{Z}_d \longrightarrow \mathbb{Z}_d$, for all b, such that

$$(T_b)^k = \omega^{\varphi_b(k)} T_{bk}, \ \ \forall b, \ \forall k. \tag{36}$$

Imposed by Reality (SW1), in Ansatz (22) we have $c_b^* T_b = c_{-b} T_{-b}^\dagger$, and hence

$$c_b^* = \omega^{\varphi_{-b}(-1)} c_{-b}. \tag{37}$$

To prepare for subsequent applications, we establish two further properties of the phases φ_b. (i) applying Eq. (37) to $-b$ instead of b gives $c_{-b}^* = \omega^{\varphi_b(-1)} c_b$. Combining this with Eq. (37) yields $|c_b|^2 \omega^{\varphi_b(-1)} = |c_{-b}|^2 \omega^{\varphi_{-b}(-1)}$, and hence

$$\varphi_b(-1) = \varphi_{-b}(-1), \ \ \forall b. \tag{38}$$

(ii) We observe that $(T_b)^{kl} = \left((T_b)^k\right)^l$, for all $k, l \in \mathbb{Z}_d$ and all b. For the phases φ_b defined in Eq. (36) this implies

$$\varphi_b(kl) = \varphi_{kb}(l) + l\varphi_b(k).$$

We will later make use of this relation for the special case of $l = -1 \mod d$,

$$\varphi_b(-k) = \varphi_{kb}(-1) - \varphi_b(k). \tag{39}$$

As the next step towards proving Theorem 6, we have the following two results.

Lemma 2 *For all Wigner functions satisfying (OB), (SW3), the functions $\Theta_{\Pi_{a,s}}(\cdot)$ are, for all a, s, of the form*

$$\Theta_{\Pi_{a,s}}(v) = \frac{1}{d} \sum_k \omega^{-ks'} c_a(k) \tag{40}$$

with $s' := s + [v, a]$, $c_a(k) := \omega^{\varphi_a(k)} c_{ka}$, and

$$c_a(k)^* = c_a(-k). \tag{41}$$

In particular, all $\Theta_{\Pi_{a,s}}(\cdot)$ are real-valued.

Further,

Lemma 3 *For any system of n qudits with d levels, $n, d \in \mathbb{N}$, a Wigner function satisfying (OB), (SW1)–(SW4) can represent measurement positively only if $|c_b| = 1$, $\forall b$.*

Proof of Lemma 2. For any a, the projector $\Pi_{a,s}$ can be represented as

$$\Pi_{a,s} = \frac{1}{d}\sum_{i=0}^{d-1} \omega^{-si}(T_a)^i.$$

Starting from the definition Eq. (33), by direct computation we obtain

$$\Theta_{\Pi_{a,s}}(v) = \frac{1}{d}\sum_{k=0}^{d-1} \omega^{-k(s+[v,a])+\varphi_a(k)} c_{ka}. \tag{42}$$

We have thus established all $\Theta_{\Pi_{a,s}}$ as functions from V to $\mathbb{C}$. We still need to show that all $\Theta_{\Pi_{a,s}}(v)$ are real-valued. To this end, we use the above definitions $s' = s + [v, a]$ and $c_a(k) = \omega^{\varphi_a(k)} c_{ka}$, which simplify $\Theta_{\Pi_{a,s}}(v)$ to Eq. (40).

The $\Theta_{\Pi_{a,s}}(v)$ are thus real-valued if $c_a(k)^* = c_a(-k)$, for all a and all k. This property we now demonstrate.

$$\begin{array}{rcl} c_a(k)^* &=& c_{ka}^*\, \omega^{-\varphi_a(k)} \\ &=& c_{-ka}\, \omega^{\varphi_{-ka}(-1)-\varphi_a(k)} \\ &=& c_{-ka}\, \omega^{\varphi_{ka}(-1)-\varphi_a(k)} \\ &=& c_a(-k)\, \omega^{-\varphi_a(-k)+\varphi_{ka}(-1)-\varphi_a(k)} \\ &=& c_a(-k) \end{array}$$

Therein, the first and fourth line follow by the definition of $c_a(\cdot)$, the second line by Eq. (37), and the third line by Eq. (38). Finally, using Eq. (39) in the last relation, we obtain Eq. (41). □

The proof of Lemma 3 relies on a discrete version of Bochner's theorem.

Lemma 4 *(Variation on Bochner's theorem) For a given function $f : \mathbb{Z}_d \longrightarrow \mathbb{C}$ the Fourier transform $\hat{f}$ of f is non-negative if and only if the matrix M with coefficients*

$$M^x_y = f(x-y),\ \ \forall x, y \in \mathbb{Z}_d, \tag{43}$$

is positive semidefinite.

The proof of Lemma 4 is the same as in [6] (Theorem 44 therein). To explicitly demonstrate that it applies in both odd and even dimensions, we restate it in Appendix A.

Proof of Lemma 3. Consider the expectation value $\langle T_a\rangle_\rho$. With Eqs. (21) and (22),

$$\langle T_a\rangle_\rho = \sum_{v\in V} W_\rho(v)\omega^{-[v,a]} c_a.$$

Now assume that $|c_a| < 1$, and consider quantum states ρ that are positively represented by W, i.e., $W_\rho \geq 0$. Then,

$$\begin{array}{rcl} |\langle T_a\rangle_\rho| &\leq& \sum_{v\in V} |W_\rho(v)||c_a| \\ &<& \sum_{v\in V} |W_\rho(v)| \\ &=& \sum_{v\in V} W_\rho(v) \\ &=& 1. \end{array}$$

Therein, the first line holds by the triangle inequality, the second line invokes the assumption $|c_a| < 1$, the third line invokes the other assumption $W_\rho \geq 0$, and the fourth line follows from the Standardization condition (SW2).

Given the assumption $|c_a| < 1$ for any $a \in E$, consider any eigenstate $\rho(a,s)$ of the Pauli observable T_a, with an eigenvalue ω^s. Further assuming that $W_{\rho(a,s)} \geq 0$ in the above, we are led to $1 > 1$. Contradiction. Thus, $|c_a| < 1$ implies that $W_{\rho(a,s)} < 0$, for all $s \in \mathbb{Z}_d$.

Now, with Eqs. (21), (22), we observe that the completely mixed state I/d^n has a positive Wigner function. However, the post-measurement states resulting from measuring T_a on I/d^n are of the type $\rho(a,s)$. Thus, if $|c_a| < 1$ then W is not positivity preserving under measurement of the Pauli observable T_a. That is, a Wigner function represents Pauli measurement positively only if

$$|c_a| \geq 1, \quad \forall a. \tag{44}$$

Now we need to exclude the possibility of $|c_a| > 1$ for any a, which is where Bochner's theorem comes in. We assume that the given Wigner function represents Pauli measurement positively; hence $\Theta_{\Pi_{a,s}} \geq 0$ for all a, s (cf. Def. 2).

We now return to Eq. (40) and observe that the r.h.s only depends on s'. Thus, we may regard $\Theta_{\Pi_{a,s}}$ as a function of s' rather than v. The dependence on v is still implicitly included through the relation $s' = s + [v, a]$.

We then further observe that $\Theta_{\Pi_{a,s}}(s')$ is the Fourier transform of $c_a(k)$. Since $\Theta_{\Pi_{a,s}}(\cdot) \geq 0$ by assumption, with Bochner's theorem it follows that the matrices $M(a)$ with entries

$$M(a)^x_y = c_a(x - y) \tag{45}$$

are all positive semidefinite. Therefore, for any subset J of rows and the corresponding columns, the submatrices $M(a)|_{J\times J}$ are also positive semidefinite, and hence must have a non-negative determinant. Picking $J = \{1, 2\}$, and also using the previously established relation $c_a(1)^* = c_a(-1)$, this yields the constraint $|c_a(0)|^2 - |c_a(1)|^2 \geq 0$, $\forall a \in E$. Further, by Eq. (23a) and $|c_a(1)| = |c_a|$, we arrive at

$$|c_a| \leq 1, \quad \forall a. \tag{46}$$

Now, combining Eqs. (44) and (46) leaves $|c_a| = 1$ as the only option, for all a. $\Box$

Next we need to constrain the phases of the coefficients $c_a(k)$, cf. Lemma 2. This will complete the proof of Theorem 6.

Proof of Theorem 6. "Only if": We assume that a given Wigner function W represents Pauli measurement positively. Our first goal is to show that the coefficients $c_a(k)$ may then be expressed in the form

$$c_a(k) = (\omega^{r_a})^k, \text{ with } r_a \in \mathbb{Z}_d, \ \forall a. \tag{47}$$

The set $\{r_a, \forall a\}$ characterizes the phase point operators $\{A_v\}$.

With Lemma 3, we can express the coefficients $c_a(k)$ as $c_a(k) = e^{i\chi_a(k)}$, $\chi_a(k) \in \mathbb{R}$. We furthermore observe that, with Eqs. (23a) and (36), it holds that $c_a(0) = 1$, $\chi_a(0) = 0$, for all $a \in E$. If $d = 2$, then Eq. (47) follows directly from Eq. (41); namely the $c_a(k)$ are all real.

For $d > 2$, we consider the submatrix $M(a)|_{J\times J}$ for the set of rows (and columns) $J = \{1, 2, k+1\}$, which, using Eq. (41), reads

$$M(a)|_{J\times J} = \begin{pmatrix} 1 & e^{i\chi_a(1)} & e^{i\chi_a(k)} \\ e^{-i\chi_a(1)} & 1 & e^{i\chi_a(k-1)} \\ e^{-i\chi_a(k)} & e^{-i\chi_a(k-1)} & 1 \end{pmatrix}.$$

By Lemma 4, we require the determinant of this matrix to be non-negative, which leads to the constraint

$$e^{i(\chi_a(1)+\chi_a(k-1)-\chi_a(k))} + \text{c.c.} \geq 2.$$

The only solution of that constraint is $\chi_a(k) = \chi_a(k-1) + \chi_a(1)$, which we may use as a recursion relation for computing the angles $\chi_a(k)$, for all k. With $\chi_a(0) = 0$,

$$\chi_a(k) = k\,\chi_a(1).$$

With the relation $c_a(k)^* = c_a(-k \mod d)$ we further find

$$d\chi_a(1) = 0 \mod 2\pi, \;\; \forall a.$$

Eq. (47) follows from the last two relations, where $\omega^{r_a} = e^{i\chi_a(1)}$. With Eq. (40) this implies

$$\Theta_{\Pi_{a,s}}(v) = \delta_{r_a, s+[v,a]}. \tag{48}$$

Consider the simultaneous measurement of the commuting observables T_a, T_b and T_{a+b}, with outcomes $s(a)$, $s(b)$ and $s(a+b)$, respectively. Given the phase point v, the above form of the Θ-function implies

$$\begin{array}{rcl} s(a) & = & r_a - [v,a], \\ s(b) & = & r_b - [v,b], \\ s(a+b) & = & r_{a+b} - [v,a+b]. \end{array}$$

Further, the quantum mechanical measurement record must satisfy

$$s(a) + s(b) - s(a+b) = \beta(a,b).$$

Combining the last two equations, we obtain

$$r_a + r_b - r_{a+b} = \beta(a,b);\;\; \forall a,b \text{ with } [a,b]=0. \tag{49}$$

Eq. (49) has a solution only if $[\beta] = 0$.

"If": Assume that $[\beta] = 0$ holds. Then we can choose a gauge such that $\beta \equiv 0$. In this gauge it holds that $\varphi_a \equiv 0$ for all a, cf. Eq. (36). We assert

$$c_a = \omega^{[a,x]}, \tag{50}$$

and for this choice verify the conditions Eq. (34) and (35) of Def. 2.

(i) *Condition Eq. (34).* With Eq. (50), we obtain $\Theta_{\Pi_{a,s}} = \delta_{s,[a,x+v]}$. Eq. (34) is thus satisfied.

(ii) *Condition Eq. (35).* It suffices to show that $\Pi_{a,s} A_v \Pi_{a,s} = \sum_{w \in V} q_v(w) A_w$, with all $q_v(w)$

real and non-negative. We have

$$\begin{aligned}
\Pi_{a,s}A_v\Pi_{a,s} &= \Pi_{a,s}\sum_{b|\,[a,b]=0}\frac{1}{d^n}\omega^{[b,x]+[b,v]}T_b^\dagger \\
&= \left(\frac{1}{d}\sum_{k=0}^{d-1}\omega^{-ks}(T_a)^k\right)\left(\sum_{b|\,[a,b]=0}\frac{1}{d^n}\omega^{[b,v+x]}T_b^\dagger\right) \\
&= \frac{1}{d^{n+1}}\sum_{k=0}^{d-1}\omega^{-ks}\sum_{b|[a,b]=0}\omega^{[b,v+x]}T_{b-ka}^\dagger \\
&= \frac{1}{d^{n+1}}\sum_{k=0}^{d-1}\omega^{k([a,v+x]-s)}\sum_{b|[a,b]=0}\omega^{[b,v+x]}T_b^\dagger \\
&= \frac{\delta_{s,[a,v+x]}}{d^n}\sum_b\delta_{[a,b],0}\,\omega^{[b,v+x]}T_b^\dagger \\
&= \frac{\delta_{s,[a,v+x]}}{d^{n+1}}\sum_{k=0}^{d-1}\sum_b\omega^{[b,v+x]+k[b,a]}T_b^\dagger \\
&= \delta_{s,[a,v+x]}\frac{1}{d}\sum_{k=0}^{d-1}A_{v+ka}
\end{aligned} \tag{51}$$

Therein, in the first line we have used the ansatz Eq. (50). To remove the non-commuting elements ($[a,b]\neq 0$), we have used the following argument: $\Pi_{a,s}T_a = T_a\Pi_{a,s} = \omega^s\Pi_{a,s}$, and hence $\Pi_{a,s}T_b\Pi_{a,s} = \omega^{-s}\Pi_{a,s}T_aT_b\Pi_{a,s} = \omega^{-s+[a,b]}\Pi_{a,s}T_bT_a\Pi_{a,s} = \omega^{[a,b]}\Pi_{a,s}T_b\Pi_{a,s}$. Thus, if $[a,b]\neq 0$ then $\Pi_{a,s}T_b\Pi_{a,s}=0$. On the other hand, if $[a,b]=0$ then $\Pi_{a,s}T_b\Pi_{a,s} = \Pi_{a,s}\Pi_{a,s}T_b = \Pi_{a,s}T_b$. In the third line we have used the phase convention that yields $\beta\equiv 0$, and in the fourth line we re-organized the sum over b. Thus, all non-zero coefficients in the expansion of $\Pi_{a,s}A_v\Pi_{a,s}$ are positive, as required.

We now address the Stratonovich-Weyl criteria (SW1)–(SW4).

(OB), (SW2), and (SW3) are ensured since we use Ansatz (22) and fulfill Conditions (23a) and (23b).

(SW1)–Reality. For any $a\in E$, we consider the face $f=[a,-a]$. Recall that we work in the gauge $\beta\equiv 0$, hence $\beta(a,-a)=0$. Thus, with Eq. (4), $T_aT_{-a}=I$, or, equivalently,

$$T_{-a} = T_a^\dagger,\ \forall a\in E.$$

Now, with the ansatz of Eq. (50) and Eq. (22),

$$\begin{aligned}
A_v^\dagger &= \left(\frac{1}{d^n}\sum_{a\in E}\omega^{-[a,x-v]}T_a^\dagger\right)^\dagger \\
&= \frac{1}{d^n}\sum_{a\in E}\omega^{[a,x-v]}T_a \\
&= \frac{1}{d^n}\sum_{a\in E}\omega^{[a,x-v]}T_{-a}^\dagger \\
&= \frac{1}{d^n}\sum_{a\in E}\omega^{-[a,x-v]}T_a^\dagger.
\end{aligned}$$

Hence $A_v^\dagger = A_v$, for all $v\in V$. Therefore, with Eq. (21), for all linear operators O it holds that $W_{O^\dagger}(v) = W_O(v)^*$, $\forall v\in V$.

$T_a = Z^{-1} \otimes I$	$\times$	$T_b = I \otimes Z$	$\times$	$T_{a+b}^{-1} = Z \otimes Z^{-1}$	$= I \Rightarrow$	$\beta(a,b) = 0$
$\times$		$\times$		$\times$		
$T_c = I \otimes \tilde{X}$	$\times$	$T_d = \tilde{X}^{-1} \otimes I$	$\times$	$T_{c+d}^{-1} = \tilde{X} \otimes \tilde{X}^{-1}$	$= I \Rightarrow$	$\beta(c,d) = 0$
$\times$		$\times$		$\times$		
$T_{a+c}^{-1} = Z \otimes \tilde{X}^{-1}$	$\times$	$T_{b+d}^{-1} = \tilde{X} \otimes Z^{-1}$	$\times$	$T_{a+b+c+d} = \tilde{Y}^{-1} \otimes \tilde{Y}$	$= I \Rightarrow$	$\beta(a+c, b+d) = 0$
$\Vert$		$\Vert$		$\Vert$		
I		I		$-I$		
$\Downarrow$		$\Downarrow$		$\Downarrow$		
$\beta(a,c) = 0$		$\beta(b,d) = 0$		$\beta(a+b, c+d) = d/2$		

Table 1: Mermin's square (shaded cells) generalized to arbitrary even dimension for the proof of Lemma 5. In each row and column of Mermin's square, the Pauli observables commute and imply a value of β as stated. For the definition of $\tilde{X}$ and $\tilde{Y}$ see text.

(SW4)–Traciality. Lemma 2 ensures that traciality holds for all products of a density matrix with a Pauli projector, $\mathrm{Tr}(\rho\Pi_{a,s}) = \sum_{v\in V} W_\rho(v)\Theta_{\Pi_{a,s}}(v)$. Linearity of Tr and W in ρ implies $\mathrm{Tr}(A\Pi_{a,s}) = \sum_{v\in V} W_A(v)\Theta_{\Pi_{a,s}}(v)$ for any linear operator A. Furthermore any linear operator B can be decomposed into $\Pi_{a,s}$, $B = \sum_{a,s} b_{a,s}\Pi_{a,s}$, by first expanding B in T_a and then T_a in $\Pi_{a,s}$. Hence, with $\Theta_B := \sum_{a,s} b_{a,s}\Theta_{\Pi_{a,s}}$ we obtain $\mathrm{Tr}(AB) = \sum_{v\in V} W_A(v)\Theta_B(v)$ for any A, B. $\Box$

5.3 Even vs. odd dimension

For odd local dimension, a Wigner function which represents Pauli measurement positively has been explicitly constructed [6]. In the framework established here, the existence of such a Wigner function follows by Observation 1 and Theorem 6.

For even local dimension, we have the following result.

Theorem 7 *For any system of $n \geq 2$ qudits with an even number d of levels, a Wigner function satisfying (OB), (SW1)–(SW4) that represents all Pauli measurements positively does not exist.*

To prove this theorem, we first establish the following fact.

Lemma 5 *If the dimension d is even, then for any number $n \geq 2$ of local systems it holds that $[\beta] \neq 0$.*

Proof of Lemma 5. The proof proceeds by a construction generalizing Mermin's square to arbitrary even dimension. For any even d, define

$$\tilde{X} = X^{d/2}, \tilde{Y} = \sqrt{\omega}^{d/2} X^{d/2} Z.$$

Now consider the generalized Mermin square shown in Tab. 1 and its equivalent topological reformulation depicted in Fig. 1. The overall strategy of the proof is to identify a 2-cycle F in the chain complex corresponding to Fig. 1 such that $\partial F = 0$ but $\beta(F) \neq 0$. Any such surface F implies that $[\beta] \neq 0$. Namely, assume $[\beta] = 0$, i.e., $\beta = d\gamma$ for some $\gamma \in C^1$. Then, for the above surface F, $\beta(F) = d\gamma(F) = \gamma(\partial F) = \gamma(0) = 0$, which contradicts the assumption $\beta(F) \neq 0$.

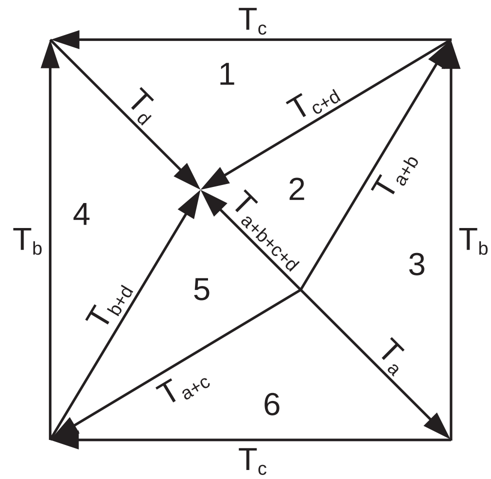

Figure 1: Topological reformulation of Mermin's square: each row and column of Mermin's square corresponds to the boundary of an elementary face f_j with $j \in \{1, \ldots, 6\}$ as indicated. The exterior edges are identified as shown. The arrows give an orientation to the edges. For the explicit expressions for the Pauli observables appearing in this figure, see Table 1.

The overall surface $F \in C_2$ of the torus in Fig. 1 has the required properties. More precisely, orienting F such that all boundaries point counterclockwise and labeling the elementary faces f_j as in Fig. 1, we observe that $F = \sum_{j=1}^{6} f_j$ with $f_1 = [c|d]$, $f_2 = [a+b|c+d]$, $f_3 = [a|b]$, $f_4 = -[b|d]$, $f_5 = -[a+c|b+d]$, and $f_6 = -[a|c]$, and $\partial F = 0$. It remains to be shown that $\beta(F) \neq 0$. First, the top row of the square in Tab. 1 reads $T_a T_b T_{a+b}^{-1} = I$; or equivalently, in the form matching Eq. (4), $T_a T_b = \omega^0\, T_{a+b}$, such that $\beta(f_3) = 0$. Now we turn to the rightmost column of Tab. 1, which is $T_{a+b}^{-1} T_{c+d}^{-1} T_{a+b+c+d} = -I$. Again we transform this into the normal form of Eq. (4), which yields $\omega^{d/2} T_{a+b+c+d} = T_{a+b} T_{c+d}$ and $\beta(f_2) = d/2$. In the same fashion, we find $\beta(f_1) = \beta(f_4) = \beta(f_5) = \beta(f_6) = 0$. Indeed, $\partial F = 0$ and $\beta(F) \mod d = d/2$. Hence $[\beta] \neq 0$. $\square$

Proof of Theorem 7. The statement is the combined conclusion of Lemma 5 and Theorem 6. $\square$

6 Discussion

In this paper, we have addressed the questions of when—that is, as a function of the number of particles n and the local Hilbert space dimension d—Wigner functions constructed from operator bases can be Clifford covariant and represent Pauli measurement positively. These questions are motivated by the scheme of quantum computation with magic states, and specifically the connection between Wigner functions and quantum speedup that arises therein [9].

These questions are fully resolved in odd dimension. Gross' Wigner function [6], for any n, is Clifford covariant and represents Pauli measurement positively. Regarding even dimension, for $d = 2$ Clifford-covariant Wigner functions from operator bases do not exist [17].

The contribution of this paper is two-fold: First, we have extended the scope of the no-go results to all even dimensions. Namely, we have shown that, in all even dimensions, Clifford-covariant Wigner functions from operator bases do not exist, and—whenever $n \geq 2$—Wigner functions from operator bases cannot represent Pauli measurement positively. This is the content of Theorems 5 and 7. Second, we have formalized the obstructions to the existence of Wigner functions with the above "nice" properties. These obstructions are cohomological in nature; see Theorems 4 and 6.

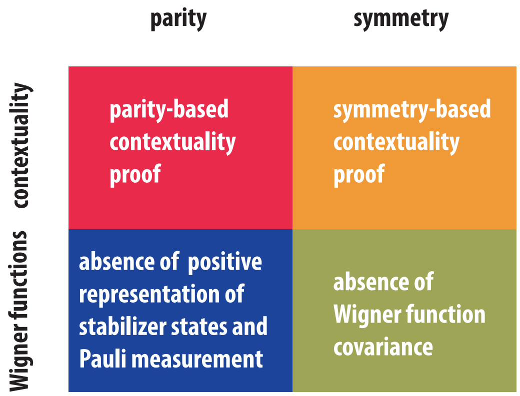

Figure 2: The combined phenomonolgy of the present paper and [16].

One question remains in this regard. From the perspective of replicating the odd-dimensional picture [9] in even dimension, we observe that for the quasiprobability function of [13] almost all Stratonovich-Weyl criteria are satisfied, but one is not. The one criterion those quasiprobability functions don't satisfy is uniqueness. We are thus led to ask: Is there a physical reason for requiring uniqueness of quasiprobability functions? We remark that other branches of physics are accustomed to non-uniqueness of representation. The vector potential in electromagnetism is an example.

Now broadening our view, we observe that cohomology arises as an organizing principle for the interrelated subjects of Kochen-Specker contextuality, Wigner functions on finite state spaces, and quantum computation. Regarding the former two, we observe that Theorem 6 on the existence of Wigner functions which represent Pauli measurement positively has an exact counterpart on the contextuality side [16], restated here as Theorem 2. Both theorems invoke the cohomological condition $[\beta] \neq 0$. Furthermore, our Theorem 5 has a very close counterpart in symmetry-based proofs of contextuality [16], restated here as Theorem 3. In both cases, the non-triviality of $[\Phi_{\text{cov}}]$ / $[\Phi]$ is invoked. The situation is illustrated graphically in Fig. 2.

In addition, we point out that precisely the same cohomomological constructs, $[\beta]$ and $[\Phi]$, were also found to bear on measurement-based quantum computation [42], so far at least in the case of flat temporal order. The case of proper temporal order remains to be understood.

To generalize even further, group cohomology classifies symmetry-protected (SPT) phases of quantum matter, and the subject of SPT order has a connection to measurement-based quantum computation (MBQC) by way of *computational phases of quantum matter* [43–50]. The question thus arises whether the SPT-MBQC phenemonolgy can be related to contextuality, with group cohomology as the linking element. The work [51] is a step in this direction.

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A Proof of Lemma 4

Lemma 4 is a restatement of Theorem 44 in [6]. The entire chapter in [6] to which Theorem 44 belongs is written under the assumption that d is odd. We restate the proof here, to clarify that for this particular lemma the assumption of odd d is not needed.

Proof of Lemma 4. Denote by ν_k, $k \in \mathbb{Z}_d$, a character of $\mathbb{Z}_d$, $\nu_k(x) = \omega^{kx}$, for all $x \in \mathbb{Z}_d$; and by the same symbol the vector $\nu_k = (1, \omega^k, \omega^{2k}, .., \omega^{(d-1)k})^T$. For any $d \times d$ matrix M defined in Eq. (43) it holds that

$$\begin{array}{rcl}[M\nu_k]_y &=& \sum_x f(x-y)\omega^{kx}\\ &=& \sum_x f(x)\omega^{kx}\omega^{ky}\\ &=& d\,\hat{f}(k)\,\omega^{ky},\end{array}$$

and hence ν_k is an eigenvector of M with eigenvalue $d\,\hat{f}(k)$. Since there are d characters ν_k, the matrix M is diagonal in their basis. All its eigenvalues are non-negative if and only if $\hat{f}$ is non-negative. □

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