All noncontextuality inequalities for the n-cycle scenario

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The problem of separating classical from quantum correlations is, in general, intractable and has been solved explicitly only in a few cases. In particular, known methods cannot provide general solutions for an arbitrary number of settings. We provide the complete characterization of the classical correlations and the corresponding maximal quantum violations for the case of $n \geqslant 4$ observables $X_0, \ldots, X_{n-1}$, where each consecutive pair $\{X_i, X_{i+1}\}$, sum mod n, is jointly measurable. This generalizes both the Clauser-Horne-Shimony-Holt and the Klyachko-Can-Binicioğlu-Shumovsky scenarios, which are the simplest ones for locality and noncontextuality, respectively. In addition, we provide explicit quantum states and settings with maximal quantum violation and minimal quantum dimension.

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I. INTRODUCTION

Quantum correlations among the results of jointly measurable observables go beyond the limits of classical correlations and provide a whole new set of resources for physics [1], computation [2], and communication [3,4]. Yet, surprisingly, necessary and sufficient conditions for classicality—all the noncontextuality (or Bell) inequalities—are known only for a few scenarios, the most famous being the Clauser-Horne-Shimony-Holt (CHSH) scenario [5], completely characterized in Ref. [6], and the Klyachko-Can-Binicioğlu-Shumovsky (KCBS) scenario [7,8]. In both cases, quantum correlations go beyond the classical ones [8,9].

Unlike the CHSH scenario, the KCBS scenario cannot be associated with correlations among the results of measurements on different subsystems but rather with the results of measurements on a single system [10–13]. In this case, the existence of quantum correlations outside the classical set shows the impossibility of noncontextual hidden variable (NCHV) theories [14–17]. Quantum contextuality is a natural generalization of quantum nonlocality that neither privileges spacelike-separated observables (among other jointly measurable observables), composite systems (among other physical systems), nor entangled states (among other quantum states), and provides advantage versus classical (noncontextual) resources even in scenarios with no spacelike separation [18–20].

Both the CHSH and the KCBS scenarios can be understood as particular cases of a much larger family: The scenario of n dichotomic observables X_i such that the pairs $\{X_i, X_{i+1}\}$, mod n, are jointly measurable. If we represent observables as nodes of a graph and link them with edges when they are jointly measurable, the resulting graph is the n-cycle (see Fig. 1). Besides the CHSH and KCBS scenarios, i.e., $n = 4,5$, other cases have also been completely characterized: The cases $n = 2$ [21,22] and $n = 3$ [14,23,24] and a partial characterization have been given in Refs. [24,25] (for odd n) and in Refs. [26–28] (in terms of entropic inequalities, necessary but not sufficient conditions for any n), and the case $n = 6$ has been discussed in Ref. [13] in relation to the test of the KCBS inequality.

The main difficulty in the characterization of correlations resides in the fact that the existing general approaches for obtaining classical [23] and quantum [29,30] bounds involve the use of algorithms that must be applied to specific cases and that require an amount of resources for computation rapidly growing with the number of settings. In fact, the only known case in which a complete characterization of classical bounds and the corresponding quantum violation has been given for any number n of settings is the bipartite Bell scenario in which Alice can choose between two dichotomic observables and Bob can choose among n [31,32].

In this paper, we provide the complete set of noncontextuality inequalities, i.e., necessary and sufficient conditions for noncontextuality, and the corresponding quantum violations for the n-cycle. Moreover, we exhibit quantum states and measurements which maximally violate the noncontextuality inequalities for each n with minimum dimension of the corresponding Hilbert space.

II. PRELIMINARY NOTIONS

The simplest way to introduce the notion of noncontextuality is by analogy with the well-known notion of locality (e.g., Refs. [27,33,34]). Here we will follow Ref. [27]. The difference between the two resides in the definition of joint measurability: One no longer considers only joint measurements of spacelike-separated observables but also admits the joint measurement of a collection of mutually compatible observables—a *context*. Consequently, the assumption of context independence for outcomes replaces the assumption of locality, i.e., independence between spacelike-separated measurements. We recall that an operational definition of

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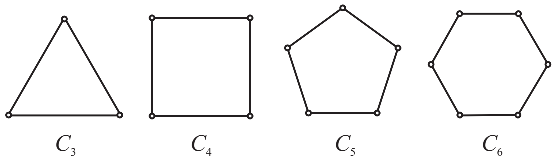

FIG. 1. Graphs associated with the compatibility relations among the observables X_i for $n = 3,\ldots,6$. C_4 corresponds to the CHSH case with the labeling of nodes A_1, B_1, A_2, B_2, in the usual notation for Alice and Bob observables, and C_5 corresponds to the KCBS case with the labeling $X_0,\ldots,X_4$.

compatibility can be given independently of quantum formalism, i.e., without referring to commutativity [35,36].

More precisely, given a set of observables $\{X_0,\ldots,X_{n-1}\}$, a context $\mathfrak{c}$ is a set of indices such that X_i is compatible with X_j whenever $i,j \in \mathfrak{c}$. Notice that all subsets of $\mathfrak{c}$, including one-element sets, must be admissible contexts. A contextuality scenario is, therefore, given by a set of observables $\{X_i\}$ together with the set of admissible contexts $\mathcal{C} = \{\mathfrak{c}_k\}$ or simply the maximal ones. For each context, one will, then, measure joint statistics for its observables, and the set of all these statistics for some given contextuality scenario is known simply as correlations.

Analogous with the study of locality, here we will consider three kinds of correlations: no-disturbance, quantum, and noncontextual. The no-disturbance condition here is a simple generalization of the well-known no-signaling condition, that applies not only to observables that act on separate subsystems, but also to any set of observables that is in a context [37]. As the set of no-signaling correlations, the set of correlations that respect no disturbance is also a polytope, the *no-disturbance* polytope.

If our correlations respect no-disturbance and come from dichotomic observables (as will always be the case in this paper), then they can always be represented as a vector $\mathbf{v} = (v_{\mathfrak{c}} | \mathfrak{c} \in \mathcal{C})$, where $v_{\mathfrak{c}}$ is the expectation value of the product of the observables in context $\mathfrak{c}$ [38]. Deterministic noncontextual classical models assign a definite outcome $x = (x_0,\ldots,x_{n-1}) \in \{-1,1\}^n$ to the observables $X_0,\ldots,X_{n-1}$, and the assignments for the correlations within each context are, thus, given by $v_{\mathfrak{c}} = \prod_{i\in\mathfrak{c}} x_i$ in a context-independent way.

As a consequence, the set of correlations consistent with a noncontextual model is given by the convex hull of the deterministic assignments for the correlation vector $\mathbf{v}$—the noncontextual polytope. Tight noncontextuality inequalities are, therefore, affine bounds defined as the facets of the noncontextuality polytope, namely $(p-1)$-dimensional faces of a p-dimensional polytope. In this sense, tight inequalities are the minimal set of necessary and sufficient conditions for classicality of correlations.

The n-cycle contextuality scenario is given by n observables $X_0,\ldots,X_{n-1}$ and the set of maximal contexts,

$$\mathcal{C}_n = \{\{X_0,X_1\},\ldots,\{X_{n-2},X_{n-1}\},\{X_{n-1},X_0\}\}. \tag{1}$$

It can be depicted as a graph where nodes represent observables and edges represent joint measurability (see Fig. 1). All correlations are then given by the $2n$-dimensional vector,

$$(\langle X_0\rangle,\ldots,\langle X_{n-1}\rangle,\langle X_0X_1\rangle,\ldots,\langle X_{n-1}X_0\rangle). \tag{2}$$

The no-disturbance polytope for this scenario is easy to characterize. Since representing the correlations via expectation values already implies no disturbance and normalization of the probabilities, the only condition left to enforce is their positivity. This condition, written in terms of elements of the vector (2), gives us

$$4p(++|X_iX_{i+1}) = 1 + \langle X_i\rangle + \langle X_{i+1}\rangle + \langle X_iX_{i+1}\rangle \geqslant 0, \tag{3a}$$

$$4p(+-|X_iX_{i+1}) = 1 + \langle X_i\rangle - \langle X_{i+1}\rangle - \langle X_iX_{i+1}\rangle \geqslant 0, \tag{3b}$$

$$4p(-+|X_iX_{i+1}) = 1 - \langle X_i\rangle + \langle X_{i+1}\rangle - \langle X_iX_{i+1}\rangle \geqslant 0, \tag{3c}$$

$$4p(--|X_iX_{i+1}) = 1 - \langle X_i\rangle - \langle X_{i+1}\rangle + \langle X_iX_{i+1}\rangle \geqslant 0, \tag{3d}$$

which are the facets of the no-disturbance polytope.

III. MAIN RESULT

In the remainder of the paper, we will always take $n \geqslant 3$. For the 2-cycle, the only facets of the noncontextual polytope are the four positivity conditions (3), i.e., the noncontextual polytope coincides with the no-disturbance polytope.

Theorem 1. All 2^{n-1} tight noncontextuality inequalities for the n-cycle noncontextual polytope are

$$\Omega = \sum_{i=0}^{n-1} \gamma_i \langle X_iX_{i+1}\rangle \overset{\text{NCHV}}{\leqslant} n-2, \tag{4}$$

where $\gamma_i \in \{-1,1\}$ such that the number of $\gamma_i = -1$ is odd.

Proof. We apply the method based on the results of Ref. [38] and presented in Ref. [39], namely, that the existence of a classical model for a set of observables is equivalent to the existence of classical models for particular subsets coinciding on their intersection. In our proof, we use that the existence of a classical probability model for the observables $\{X_0,\ldots,X_{n-1}\}$ is equivalent to the existence of classical models for $\{X_0,\ldots,X_{n-2}\}$ and $\{X_0,X_{n-1},X_{n-2}\}$, coinciding on their intersection $\{X_0,X_{n-2}\}$ (see Fig. 2). Such a consistency condition for the intersection is written in terms of the "unmeasurable correlation" $\langle X_0X_{n-2}\rangle$, i.e., a correlation between observables that are not in a context and, therefore, cannot be jointly measured but, nevertheless, have a well-defined correlation in every classical model [40]. The final set of inequalities must not contain the variable $\langle X_0X_{n-2}\rangle$,

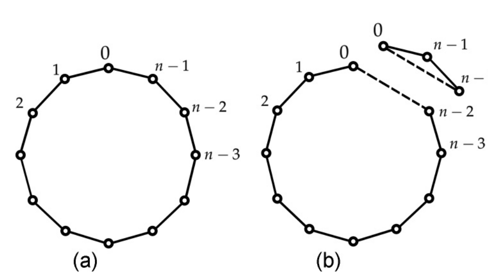

FIG. 2. (a) n-cycle scenario. (b) Subsets of observables that can be associated with the $(n-1)$-cycle and 3-cycle scenarios by considering the unmeasurable correlation $\langle X_0X_{n-2}\rangle$ (dashed line).

which must be removed by applying Fourier-Motzkin (FM) elimination [41], i.e., by summing inequalities where it appears with the minus sign with those where it appears with the plus sign. This step of the proof is a simple application of the techniques from Ref. [39]. For the convenience of the reader, details are presented in Appendix A.

We can now proceed by induction on n. The case $n = 3$ is known. For the inductive step, following the above argument, we calculate the n-cycle inequalities by combining the $(n-1)$-cycle inequalities for the subset $\{X_0,\dots,X_{n-2}\}$ with the 3-cycle inequalities for $\{X_0,X_{n-1},X_{n-2}\}$. We apply FM elimination on the variable $\langle X_0X_{n-2}\rangle$ from the whole set of inequalities. All inequalities in (4) are obtained by combining one inequality for the $(n-1)$-cycle with one for the 3-cycle and are in the right number. Combining two inequalities for the $(n-1)$-cycle, or two for the 3-cycle, gives a redundant inequality as happens for the combination of positivity conditions (3) with inequalities of the form (4), the latter being obtainable as a sum of $n-1$ (or three) positivity conditions. There are no other inequalities. The proof of their tightness is presented in Appendix B. ■

The reader, familiar with Fine's proof for the 4-cycle [6], obtained by combining two 3-cycles, may have noticed that the above is a straightforward generalization.

We can also characterize the vertices of the no-disturbance polytope.

Theorem 2. The vertices of the no-disturbance polytope are the 2^n noncontextual deterministic correlation vectors,

$$(\langle X_0\rangle,\dots,\langle X_{n-1}\rangle,\langle X_0\rangle\langle X_1\rangle,\dots,\langle X_{n-1}\rangle\langle X_0\rangle), \tag{5}$$

where $\langle X_i\rangle = \pm 1$ together with the 2^{n-1} contextual correlation vectors of the form

$$(0,\dots,0,\langle X_0X_1\rangle,\dots,\langle X_{n-1}X_0\rangle), \tag{6}$$

where $\langle X_iX_{i+1}\rangle = \pm 1$ such that the number of negative components is odd.

Proof. By definition, the vertices of the polytope are given by the intersection of $2n$ independent hyperplanes, i.e., as a unique solution for a set of $2n$ independent linear equations chosen among the $4n$ equations saturating (3). The above vertices are obtained by choosing two equations among (3a)–(3d) for each index i. In particular, contextual vertices are obtained by choosing Eqs. (3a) and (3d) for an odd number of indices i and Eqs. (3b) and (3c) for the remaining indices. It is straightforward to check that all other possible strategies for obtaining a vertex, i.e., involving the choice of one, two, or three equations for each index i, give the same set of vertices. ■

To summarize our results: The no-disturbance polytope, defined by the $4n$ positivity conditions (3), has $2^n + 2^{n-1}$ vertices of which 2^n are noncontextual and 2^{n-1} are contextual. The noncontextuality polytope, defined by the 2^n noncontextual vertices (5), has $4n + 2^{n-1}$ facets [it is trivial to check that inequalities (3) are tight for the noncontextuality polytope]. Also note that, for each vertex in (6), there exists an inequality in (4) such that $\langle X_iX_{i+1}\rangle = \gamma_i$, i.e., contextual vertices and noncontextuality inequalities are in a one-to-one correspondence.

IV. QUANTUM VIOLATIONS

Here we address the problems of whether quantum mechanics (QM) violates the inequalities (4), which is the maximum quantum violation—the Tsirelson bound—and how to achieve it.

Theorem 3. Quantum mechanics violates the noncontextuality inequalities (4) for any $n \geqslant 4$. The Tsirelson bound is

$$\Omega_{\rm QM} = \begin{cases} \frac{3n\cos(\frac{\pi}{n})-n}{1+\cos(\frac{\pi}{n})} & \text{for odd } n, \\ n\cos(\frac{\pi}{n}) & \text{for even } n. \end{cases} \tag{7}$$

Proof. Without loss of generality, we can restrict our discussion to the inequalities in which, for odd n, $\gamma_i = -1$ for all i and, for even n, $\gamma_i = -1$ for all i except $\gamma_{n-1} = 1$. Using that

$$\pm\langle X_iX_{i+1}\rangle = 2[p(+\pm|X_i,X_{i+1}) + p(-\mp|X_i,X_{i+1})] - 1, \tag{8}$$

we can rewrite Ω as $2\Sigma - n$, where Σ is a sum of probabilities.

Any sum of probabilities is upperbounded in quantum mechanics by the Lovász ϑ function $\vartheta(G)$ of the graph G in which nodes are the arguments of the probabilities and edges link exclusive events [e.g., $(++|X_0,X_1)$ and $(--|X_1,X_2)$] [25].

If n is odd, the graph G associated with Σ is the prism graph of order n, Y_n (see Fig. 3). Its ϑ function is

$$\vartheta(Y_n) = \frac{2n\cos(\frac{\pi}{n})}{1+\cos(\frac{\pi}{n})}, \tag{9}$$

therefore, if n is odd, the Tsirelson bound $\Omega_{\rm QM}$ is upperbounded by $2\vartheta(Y_n) - n$. The following quantum state and observables saturate this bound [24]: $|\psi\rangle = (1,0,0)$ and $X_j = 2|v_j\rangle\langle v_j| - \mathbb{1}$, where $|v_j\rangle = (\cos\theta, \sin\theta\cos[j\pi(n-1)/n], \sin\theta\sin[j\pi(n-1)/n])$ and $\cos^2\theta = \cos(\pi/n)/[1+\cos(\pi/n)]$.

For even n, the proof can be obtained simply by noting that our inequalities are closely related to the Braunstein-Caves inequalities [42], whose Tsirelson bound was found in Ref. [43]. A small modification of the proof in Ref. [43] then suffices. The following quantum state and observables saturate this bound: $|\psi\rangle = (0,1/\sqrt{2},-1/\sqrt{2},0)$ and $X_j = \tilde{X}_j \otimes \mathbb{1}$ for even j and $X_j = \mathbb{1}\otimes\tilde{X}_j$ for odd j, where $\tilde{X}_j = \cos(j\pi/n)\sigma_x + \sin(j\pi/n)\sigma_z$ and σ_x,σ_z are Pauli matrices.

The calculations for $\vartheta(Y_n)$ and the proof for even n are presented in Appendix C. ■

It is also interesting to examine the even case with the same technique we used for the odd case. If n is even, the graph G associated with Σ is the Möbius ladder of order $2n$, M_{2n} (see

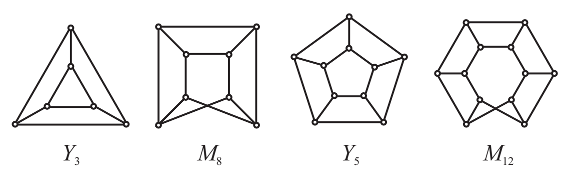

FIG. 3. Graphs associated with the sum of probabilities Σ in the tight noncontextuality inequalities for $n = 3,\dots,6$.

Fig. 3). We conjecture its ϑ function to be

$$\vartheta(M_{2n}) = \frac{n}{2}\left(1 + \cos\frac{\pi}{n}\right) \tag{10}$$

for which we present evidence in Appendix D.

It can also be proved that these choices of state and observables saturating the quantum bounds are optimal in the sense that such bounds cannot be reached in a Hilbert space of lower dimension. In fact, for odd n, there is nothing left to prove since, according to our definition of contextuality, there is no contextual behavior in a two-dimensional Hilbert space. For even n, it can be proved (see Appendix E) that, in a three-dimensional Hilbert space,

$$\Omega^n_{\text{QM3D}} = \Omega^{n-1}_{\text{QM}} + 1. \tag{11}$$

This fact can be used as a dimension witness [44].

V. OBSERVATIONS

The quantum bounds for odd n were found first in Refs. [24,25] and for even n in Ref. [43] in relation with Braunstein-Caves inequalities [42]. However, we do think it is enlightening to show how graph theory provides a simple and unified approach to the problem.

Another observation is that, although Braunstein-Caves inequalities are not tight Bell inequalities [32,45], our inequalities (4) are tight noncontextuality inequalities. This is possible because the locality and contextuality scenarios are different: In the case of Bell inequalities, we demand every X_i with even i to be measurable together with every X_j with odd j, and so the graph that represents these relations is the complete bipartite graph $K_{n/2,n/2}$, which is not isomorphic to the n-cycle (except for $n = 4$, the CHSH case).

VI. CONCLUSIONS

The n-cycle contextuality scenario is the natural generalization of CHSH [5,6] and KCBS [8] scenarios, the most fundamental scenarios for locality and noncontextuality, and has recently attracted increasing attention [24–28]. We have provided the complete characterization of the associated set of classical correlations for an arbitrary number n of settings, the only other example of this kind being the Bell bipartite scenario with two observables for Alice and n for Bob [31,32]. We have explicitly obtained the maximum quantum violation of all these inequalities with the minimal quantum dimension. We also completely characterized the associated no-disturbance correlations by finding the vertices of the corresponding polytope.

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APPENDIX A: DETAILED PROOF OF THEOREM 1

Here we present the details missing in the proof of Theorem 1, namely, the proof that the existence of a classical probability model for the observables $\{X_0,\dots,X_{n-1}\}$ is equivalent to the existence of classical models for $\{X_0,\dots,X_{n-2}\}$ and $\{X_0,X_{n-1},X_{n-2}\}$, coinciding on their intersection $\{X_0,X_{n-2}\}$.

The first step is to extend the definition of graph representation given in Figs. 1 and 2 (graphs in Fig. 3 have a different interpretation). We said that nodes represent dichotomic observables and edges represent compatibility relations, which means that, if two nodes are connected by an edge, the corresponding pair of observables admits a classical probability model. Such a definition can be generalized as follows:

(i) a node represents a subset of observables,

(ii) if two nodes are connected by an edge, then the corresponding subset of observables, i.e., the union of the two subsets, admits a classical probability model.

Such classical models are, in general, extensions to broader subsets of the classical probability models associated with subsets of commuting observables by QM (i.e., spectral theorem). We can now recall the following result [38]:

Lemma 1. A set of probability assignments associated with a tree graph always admits a classical probability model.

Our strategy for the proof is then depicted in Fig. 4: If the two subsets of observables in Fig. 4(b), $(n-1)$-cycle and 3-cycle, admit a classical representation, i.e., all the corresponding inequalities are satisfied, then the set of probabilities can be extended, following (i) and (ii) as in Fig. 4(c), i.e., two classical models for $\{0,1,\dots,n-3,n-2\}$ and for $\{0,n-1,n-2\}$ coinciding on their intersection $\{0,n-2\}$. By Lemma 1, such a set already admits a classical representation.

By the above procedure, we obtain a set of conditions that includes the unmeasurable correlation $\langle X_0X_{n-2}\rangle$, which plays a fundamental role since it constrains the two models on their intersection, but it is not actually measurable in the n-cycle scenario [see Fig. 4(a)]. Such a variable must be, therefore, eliminated from the final set of conditions by means of FM elimination [39]. We recall that FM elimination of a variable from a system of linear inequalities consists of summing each

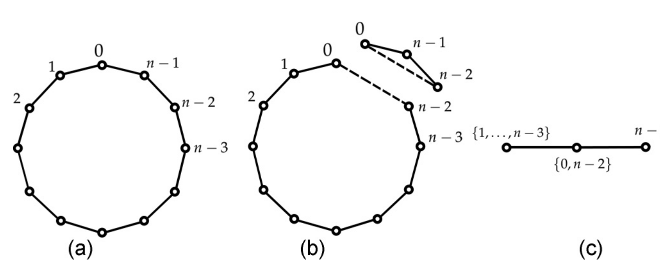

FIG. 4. (a) n-cycle scenario. (b) Subsets of observables that can be associated with the $(n-1)$-cycle and 3-cycle scenarios by considering the unmeasurable correlation $\langle X_0X_{n-2}\rangle$ (dashed line). (c) Extended classical model that can be obtained if the two subsets admit a classical representation coinciding on their intersection. Such a model is automatically classical as it can be depicted as a tree graph.

pair of inequalities where such a variable appears, respectively, with $+1$ and -1 coefficients (after a proper normalization of the inequalities) and keeping the inequalities where it does not appear [41]. As a result, the final system of inequalities admits a solution if and only if the initial system of inequalities does.

To summarize: If a set of probability assignments for the n-cycle scenario satisfies the set of inequalities obtained as FM elimination of the variable $\langle X_0 X_{n-2}\rangle$ from the set of inequalities for the $(n-1)$-cycle (for $\{0,\ldots,n-2\}$) and the 3-cycle (for $\{0,n-2,n-1\}$), then both subsets of observables admit a classical representation with consistent assignments for $\langle X_0 X_{n-2}\rangle$, i.e., such representations coincide on their intersection as depicted in Fig. 4(c). By Lemma 1, these conditions are already sufficient for the existence of a classical model for the whole set of observables $\{0,1,\ldots,n-2,n-1\}$.

APPENDIX B: PROOF OF TIGHTNESS OF THE INEQUALITIES

Tightness can be proved by showing that inequalities (4) correspond to facets of the $2n$-dimensional correlation polytope, i.e., they are saturated by $2n$ noncontextual vertices which generate an affine subspace of dimension $2n-1$. First, focus on the inequality of the odd n-cycle for which all $\gamma_i = -1$. It is saturated by $2n$ vertices which can be written as $(\pm v_i, w_i)$, for $i = 0,\ldots,n-1$, where w_i is a n-dimensional vector given by a cyclic permutation of the components of $w_0 = (+1,-1,-1,\ldots,-1)$ and v_i is the vector with ith component equal to $+1$ that satisfies relation (2). Then it holds that $v_i + v_{i+1} = 2e_{i+1}$, where $\{e_0,\ldots,e_{n-1}\}$ is the canonical basis of $\mathbb{R}^n$, and $w_i + (1,1,\ldots,1) = 2e_i$. As a consequence, $\{(\pm v_i, w_i)\}_{i=1,\ldots,2n}$ is a basis for $\mathbb{R}^{2n}$, showing independence. Since all the other vertices and inequalities are obtained from this one via the mapping $X_i \mapsto -X_i$, this proves the odd n case. The proof for even n is analogous.

APPENDIX C: DETAILED PROOF OF THEOREM 3

An orthonormal representation (OR) for a graph $G = (V,E)$ is a set of unit vectors $\{v_i\}$ associated with vertices $V = \{i\}$ such that two vectors are orthogonal if the corresponding vertices are adjacent, i.e., $(i,j) \in E$. The Lovász ϑ function is defined as the maximum, over all OR, of the norm of the operator given by sum of the unidimensional projectors associated with vectors [46,47]. Notice that different vertices can be mapped onto the same vector, but then, the corresponding projector appears in the sum once for each vertex associated with it.

For the prism graph Y_n, in general, it holds that $\vartheta(Y_n) \leqslant 2\vartheta(C_n) = \frac{2n\cos(\frac{\pi}{n})}{1+\cos(\frac{\pi}{n})}$ since a graph consisting of two copies of C_n, let us denote it as G, can be obtained from Y_n by removing the edges connecting vertices of the outer cycle with those of the inner cycle.

Consider an OR for C_n, say $v_0,\ldots,v_{n-1}$, which gives the maximum value for the norm of the corresponding sum of projectors, i.e., $\vartheta(C_n)$. Clearly, the $2n$ vectors v_i, v_i' with $v_i' = v_i$ for $i = 0,\ldots,n-1$ form an OR for G, giving $\vartheta(G) = 2\vartheta(C_n)$. To show that $\vartheta(Y_n) = \vartheta(G) = 2\vartheta(C_n)$, it is sufficient to notice that the above vectors also are an OR for Y_n. Such an OR is obtained by associating the vector v_i with the ith vertex of the outer cycle and the vector v_{i+1}' with sum mod n with the ith vertex of the inner cycle, this completes the discussion for the case of odd n.

For the case of even n, the proof is based on positive semidefiniteness conditions analogous to those discussed in Refs. [29,30,43]. Via them, we can show that Eq. (10) is an upper bound to the Tsirelson bound, and the proof is completed by noting that we already provided quantum observables and states saturating it.

Let us consider a quantum state ρ and n dichotomic observables $X_0,\ldots,X_{n-1}$ with even n. Then the complex matrix $\Gamma_{ij} = \mathrm{tr}(\rho X_i X_j)$ must be positive semidefinite. In fact, given a complex vector v, we have

$$\begin{aligned} v^\dagger \Gamma v &= \sum_{ij} v_i^* \Gamma_{ij} v_j = \mathrm{tr}\left(\rho \sum_{ij} v_i^* v_j X_i X_j\right) \\ &= \mathrm{tr}\left(\rho \sum_i v_i^* X_i \sum_j v_j X_j\right) = \mathrm{tr}(\rho O^\dagger O) \geqslant 0, \end{aligned} \tag{C1}$$

with $O \equiv \sum_i v_i X_i$. An upper bound for the quantum violation of the expression,

$$\sum_{i=0}^{n-1} \gamma_i \langle X_i X_{i+1}\rangle, \tag{C2}$$

with $\gamma_{n-1} = -1$ and all other coefficients $+1$ can be, therefore, obtained as the semidefinite program (SDP),

$$\begin{aligned} &\text{maximize:} \quad \tfrac{1}{2}\mathrm{tr}(\beta\Gamma), \\ &\text{subject to:} \quad \Gamma \succeq 0, \quad \Gamma_{ii} = 1, \end{aligned} \tag{C3}$$

where β is a symmetric real matrix such that $\frac{1}{2}\mathrm{tr}(\beta\Gamma) = \sum_{i=0}^{n-1} \gamma_i \Gamma_{i,i+1}$. The optimality of the solution $n\cos(\frac{\pi}{n})$ for the above SDP, up to a reordering of the coordinates, has been proved by Wehner [43]. Together with the explicit state and observables presented in the main text, this concludes our proof.

APPENDIX D: EVIDENCE FOR THE CONJECTURED LOVÁSZ ϑ FUNCTION FOR MÖBIUS LADDER GRAPHS

In Eq. (10), we conjectured an expression for $\vartheta(M_{2n})$. The evidence we have for it is both numerical and mathematical: We explicitly calculated the value for $\vartheta(M_{2n})$ for even n up to $n = 64$, i.e., $\vartheta(M_{128})$, and it coincides with the expression given in Eq. (10) with very high precision. Moreover, since M_{2n} is a regular graph (each vertex has the same number of neighbors), $\vartheta(M_{2n})$ can be upperbounded by the expression [46],

$$\vartheta(M_{2n}) \leqslant \frac{-n\lambda_{2n}}{\lambda_1 - \lambda_{2n}}, \tag{D1}$$

where $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{2n}$ are the eigenvalues for the adjacency matrix A for M_{2n}. Since A is a circulant matrix, they can be explicitly computed [48], and with them, we obtain

$$\vartheta(M_{2n}) \leqslant \frac{n\left[2\cos\left(\frac{\pi}{n}\right)+1\right]}{2+\cos\left(\frac{\pi}{n}\right)}. \tag{D2}$$

Comparing (D2) with our conjecture for $\vartheta(M_{2n})$ in the asymptotic limit $n \to \infty$, we obtain

$$\frac{n\left[2\cos\left(\frac{\pi}{n}\right)+1\right]}{2+\cos\left(\frac{\pi}{n}\right)} - \frac{n}{2}\left(1+\cos\frac{\pi}{n}\right) \approx \frac{\pi^2}{12n}. \tag{D3}$$

APPENDIX E: QUANTUM BOUNDS FOR EVEN n IN DIMENSION THREE

Consider the inequalities,

$$\Omega = \sum_{i=0}^{n-1} \gamma_i \langle X_i X_{i+1}\rangle \overset{\text{NCHV}}{\leqslant} n-2, \tag{E1}$$

where $\gamma_i \in \{-1,1\}$ such that the number of $\gamma_i = -1$ is odd and n is even. By the symmetry of the problem, namely, the fact that each inequality is obtained via the substitution $X_i \to -X_i$ for some indices i, the quantum bound for (E1) must be the same for all possible choices of γ.

Let us start with n general three-dimensional observables X_i and a vector γ giving the left-hand side of Eq. (E1). Since we are in three dimensions, for each i, either X_i or $-X_i$ is given by a one-dimensional projector P_i as $\pm X_i = 2P_i - 1$. The substitution $X_i \to -X_i$ simply amounts to a new definition of the vector γ. We have, therefore, a new expression (E1) where all the X_i's are given by one-dimensional projectors. For such observables, it holds

$$[X_i, X_{i+1}] = 0 \Longleftrightarrow P_i P_{i+1} = 0 \quad \text{or} \quad P_i = P_{i+1}. \tag{E2}$$

Let us assume, for the moment, that the condition $P_i P_{i+1} = 0$ holds for all $i = 0, \ldots, n-1$, we will discuss the other cases later. We want to calculate the maximum of the left-hand side of (E1) over all γ, namely,

$$\max_{\gamma, P_i, \rho} \sum_{i=0}^{n-1} \gamma_i \langle (2P_i - 1)(2P_{i+1} - 1)\rangle, \tag{E3}$$

which can be rewritten as

$$\max_{\gamma, P_i, \rho} \sum_{i=0}^{n-1} \gamma_i [1 - 2\langle P_i + P_{i+1}\rangle]$$
$$= \max_{\gamma, P_i, \rho} \frac{1}{2} \sum_{i=0}^{n-1} [-(\gamma_i + \gamma_{i-1})](4\langle P_i\rangle - 1). \tag{E4}$$

Since the number of $\gamma_i = -1$ must be odd and n is even, at least two terms $(\gamma_i + \gamma_{i-1})$ and $(\gamma_{i+1} + \gamma_i)$ must be zero. Without loss of generality, we can assume it holds for $i = n-2$. We have, therefore,

$$\max_{\gamma, P_i, \rho} \frac{1}{2} \sum_{i=0}^{n-1} [-(\gamma_i + \gamma_{i-1})](4\langle P_i\rangle - 1)$$
$$\leqslant \max_{P_i, \rho} 4 \sum_{i=0}^{n-3} \langle P_i\rangle - (n-2)$$
$$= 2(n-2) - (n-2) = n-2, \tag{E5}$$

where we used the fact that the maximum of $\sum_{i=0}^{n-3} \langle P_i\rangle$ is bounded by $\frac{n-2}{2}$. In fact, $\langle P_i + P_{i+1}\rangle \leqslant 1$ since their sum is still a projector.

We must now consider the other possibilities given by (E2). If for a given index, say $i = 0$, $P_i = P_{i+1}$, we simply have that $X_0 = X_1$, therefore, Eq. (E1) reduces to

$$\sum_{i=0}^{n-1} \gamma_i \langle X_i X_{i+1}\rangle = \gamma_0 + \sum_{i=1}^{n-1} \gamma_i \langle X_i X_{i+1}\rangle \leqslant \Omega_{\text{QM}}^{n-1} + 1, \tag{E6}$$

since $\langle X_0 X_{n-1}\rangle = \langle X_1 X_{n-1}\rangle$.

If for two indices i,j, $P_i = P_{i+1}$ and $P_j = P_{j+1}$, the problem is reduced to the case $n-2$, and so on for all the other cases.

We have, therefore, proved that the *optimal bound* for n-cycle inequalities in three dimensions is given by

$$\Omega_{\text{QM3D}}^{n} = \Omega_{\text{QM}}^{n-1} + 1 \quad \text{for even } n. \tag{E7}$$

Remember that $\Omega_{\text{QM3D}}^{n} \geqslant n-2$ since $\Omega_{\text{QM}}^{n-1} \geqslant n-3$ and that the bound in (E6) can always be achieved with one-dimensional projectors.

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