# Irreducible Magic Sets for $n$-Qubit Systems

Stefan Trandafir,[1,*] Petr Lisoněk,[1,†] and Adán Cabello[2,3,‡]
[1]Department of Mathematics, Simon Fraser University, Burnaby, British Columbia V5A 1S6, Canada
[2]Departamento de Física Aplicada II, Universidad de Sevilla, E-41012 Sevilla, Spain
[3]Instituto Carlos I de Física Teórica y Computacional, Universidad de Sevilla, E-41012 Sevilla, Spain

(Received 15 March 2022; revised 30 July 2022; accepted 16 September 2022; published 7 November 2022)

Magic sets of observables are minimal structures that capture quantum state-independent advantage for systems of $n \geq 2$ qubits and are, therefore, fundamental tools for investigating the interface between classical and quantum physics. A theorem by Arkhipov (arXiv:1209.3819) states that $n$-qubit magic sets in which each observable is in exactly two subsets of compatible observables can be reduced either to the two-qubit magic square or the three-qubit magic pentagram [N. D. Mermin, Phys. Rev. Lett. **65**, 3373 (1990)]. An open question is whether there are magic sets that cannot be reduced to the square or the pentagram. If they exist, a second key question is whether they require $n > 3$ qubits, since, if this is the case, these magic sets would capture minimal state-independent quantum advantage that is specific for $n$-qubit systems with specific values of $n$. Here, we answer both questions affirmatively. We identify magic sets that cannot be reduced to the square or the pentagram and require $n = 3$, 4, 5, or 6 qubits. In addition, we prove a generalized version of Arkhipov's theorem providing an efficient algorithm for, given a hypergraph, deciding whether or not it can accommodate a magic set, and solve another open problem, namely, given a magic set, obtaining the tight bound of its associated noncontextuality inequality.

DOI: 10.1103/PhysRevLett.129.200401

*Introduction.*—A magic set for a system of $n \geq 2$ qubits [1–5] is a set of Pauli observables (i.e., those represented by $n$-fold tensor products of single-qubit Pauli operators $I$, $X$, $Y$, and $Z$) and contexts (subsets of compatible observables represented by commuting operators and such that their product is the identity—in the case of "positive" contexts—or minus the identity—in the case of "negative" contexts—) with the following properties: (i) each observable is in an even number of contexts. (ii) The number of negative contexts is odd. (iii) The set is minimal: properties (i) and (ii) do not hold if any observable is removed. As a simple parity argument shows, properties (i) and (ii) make it impossible to assign a predetermined outcome, either 1 or $-1$, to each observable while satisfying that the product of the outcomes for the observables of a positive (negative) context is 1 ($-1$), as predicted by quantum mechanics (QM). Consequently, any magic set provides a simple state-independent proof of the impossibility of simulating QM with noncontextual hidden variable (NCHV) models [1–6].

In addition, the most famous magic sets have a fourth property: (iv) their hypergraph of compatibility (i.e., the one in which each vertex represents an observable and each hyperedge a context) is vertex-transitive (i.e., its automorphism group acts transitively on its vertices). A hypergraph $H = (V, E)$ is a finite set $V$ of vertices and a finite set $E$ of hyperedges, where each hyperedge is a multiset of vertices. Besides symmetry and elegance, vertex transitivity is helpful for experimental purposes.

There are two famous magic sets. One is the "magic square," "Peres-Mermin table," or "Mermin square" for $n = 2$ qubits found [7] by Peres [1–3] and Mermin [4,5] and shown in Fig. 1(a). The other is the "magic pentagram" or "Mermin's star" for $n = 3$ qubits found by Mermin [4,5] and shown in Fig. 1(b). Both sets were introduced as simplified proofs of the Kochen-Specker theorem [8]. The adjective "magic" was first used in [9].

Magic sets have multiple applications (for details, see Ref. [10]), including Greenberger-Horne-Zeilinger-like proofs with two observers [13], bipartite Bell inequalities with maximal quantum violation saturating the

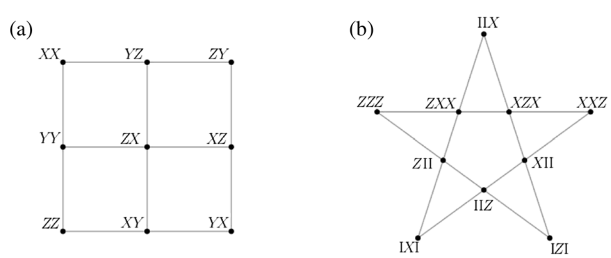


FIG. 1. (a) The magic square. (b) The magic pentagram. Each dot represents a Pauli observable. $XZ$ denotes the observable represented by $\sigma_x \otimes \sigma_z$. $IXI$ denotes the observable represented by $\mathbb{1} \otimes \sigma_x \otimes \mathbb{1}$, where $\mathbb{1}$ is the $2 \times 2$ identity matrix. Observables in the same straight line are mutually compatible and the product of their operators is the identity, except for the three vertical lines in (a) and the horizontal line in (b), where it is minus the identity.

 

nonsignaling bound [13,15,16,31,32], obtaining Kochen-Specker sets of rays [2,34], nonlocal games [9,17,21], state-independent noncontextuality inequalities [6,22–25], measurement-based quantum computation [36–39], nonlocality based on local contextuality [41–43], device-independent quantum key distribution [44,45], memory cost of classically simulating sequences of quantum measurements [57–59], state-independent quantum dimension witnessing [46], entropic inequalities [60], device-independent self-testing [47–50], and quantum gravity [51].

In a nutshell, the importance of magic sets lies in the fact that they are minimal structures that capture quantum state-independent advantage for an $n$-qubit system and thus are fundamental tools for investigating the interface between classical and quantum physics [10].

Magic sets are useful to capture the quantum advantage. But the quantum advantage grows with $n$. Therefore, an interesting question is whether there are magic sets for $n > 3$ and how they are related to those for smaller values of $n$. A theorem by Arkhipov [53] (see also Ref. [61]) suggests that the cases $n = 2$ and $n = 3$ are special. Arkhipov's theorem states that the intersection graph of the contexts of any magic set in which each observable is in exactly two contexts must contain either the intersection graph of the contexts of the magic square or the magic pentagram. The intersection graph of a family of sets is a graph in which each set is represented by a vertex and edges connect intersecting sets. A consequence of Arkhipov's theorem is that "the magic square and magic pentagram are 'universal' for magic games" in which each observable is in exactly two contexts [53]. A second consequence is that the magic sets with $n > 3$ qubits described in the literature [62–68] derive from the square and the pentagram. However, Arkhipov's theorem leaves open some key questions. (1) For $n = 2$ qubits, each Pauli observable can be only in three contexts. Therefore, for $n = 2$, the only even number that can be used to define magic sets following condition (i) is two. But this is not true for $n \geq 3$ qubits. Does the conclusion of Arkhipov's theorem hold if the requirement of each observable being in exactly two contexts is replaced by the requirement of each observable being in an even number $m$ of contexts? Are there, in this more general case, magic sets that cannot be reduced to the square and the pentagram? (2) If the answer to the second question in (1) is affirmative, are there magic sets that cannot be reduced to any magic set with $n = 2$ or $n = 3$ qubits and thus are genuine to systems of $n > 3$ qubits? This is important as it would identify fundamental structures that are genuine for a specific number of qubits and thus can be used to certify whether a system has at least $n$ qubits. (3) If the answer to (2) is affirmative, how does one identify those magic sets? Is it possible to generalize Arkhipov's theorem (which is essentially an efficient algorithm to check whether or not a hypergraph can accommodate a magic set under the assumption that each observable is in exactly two contexts), while removing the extra assumption?

All these questions seem to be important and, collectively, can be rephrased as follows: are there simple tools to detect and quantify quantum computational advantage for $n$-qubit systems that are specific for each value of $n$ and have gone unnoticed? In this Letter, we answer all these questions in the affirmative.

Any magic set provides a logical contradiction between QM and NCHV models. However, translating that contradiction to an experiment requires deriving a noncontextuality inequality [6] that is violated (for any initial state) measuring the elements of the magic set. There exists a general method for, given a magic set, obtaining a contextuality witness [41]. Calculating the quantum value of that witness is immediate. Calculating its maximum for NCHV models is straightforward if the magic set is small. However, an open problem is obtaining the bound for NCHV models in general. In this Letter, we also solve this problem.

*Methodology.*—Finding all magic sets for any $n > 3$ is intractable. There are $4^n - 1$ Pauli observables, each of them is in $\prod_{j=1}^{n-1}(1 + 2^j)$ positive or negative contexts of $2^n - 1$ elements. These contexts of maximal size contain subsets whose product is the identity or minus the identity (e.g., $\{IIX, IXI, XII, XXX, IXX, XIX, XXI\}$ contains two subsets whose product is the identity: $\{IIX, IXI, XII, XXX\}$ and $\{IXX, XIX, XXI\}$). Unlike the case $n = 2$, where $m$ can only be 2 (since, each observable is in exactly 3 contexts of maximal size), the possible values for $m$ grow with $n$.

However, since our main motivation is answering whether or not there are magic sets not covered by Arkhipov's theorem, we restrict our computational search to magic sets in which each observable is in four contexts (the simplest case not covered by Arkhipov's theorem) and assume that contexts have four or five observables. The theoretical results presented in this Letter do not require these assumptions.

In addition, we use the following observation. Given a magic set $S$, each Pauli observable $o \in S$ can be represented by a vertex $v \in V$ and each context by an hyperedge $e \in E$ of its hypergraph of compatibility $H = (V, E)$. For example, Figs. 1(a) and 1(b) show $H$ for the magic square and pentagram, respectively (representing vertices by dots and hyperedges by straight lines connecting several dots). For a fixed $n$, there are different sets of Pauli observables whose relations of compatibility are represented by the same $H$. We say that two magic sets belong to the same class if they have the same $H$. For example, for $n = 2$ qubits, there are 10 magic sets sharing the hypergraph $H$ shown in Fig. 1(a). Our strategy for finding magic sets is thus based on identifying hypergraphs $H$ that can represent magic sets. Specifically, we use the following algorithm. (a) We fix the number of observables, say $N$, in the putative

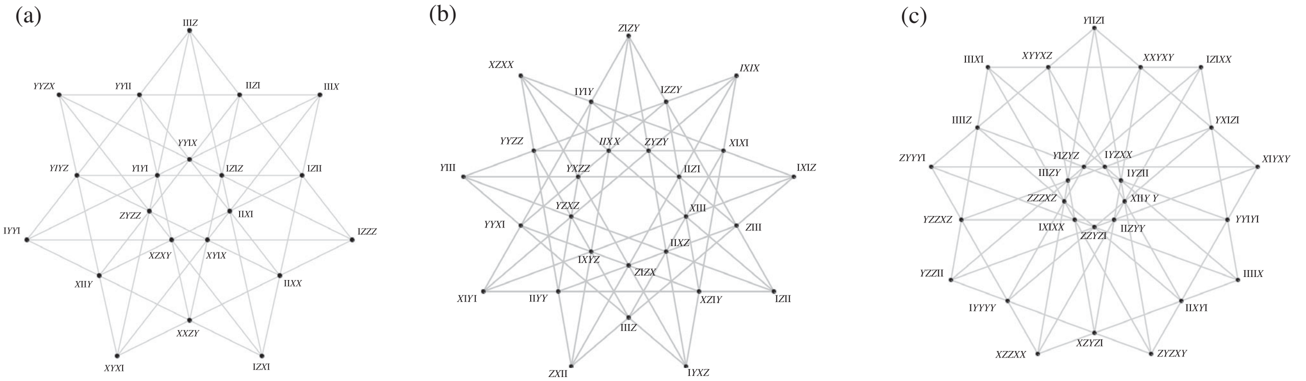


FIG. 2. The three magic sets with vertex-transitive graphs of compatibility with straight line representations in the Euclidean plane that cannot be reduced to the square or pentagram that we have found in this Letter. The notation is the same as that used in Fig. 1. (a) MS4-21 requires $n = 4$ qubits and has 21 observables and 21 contexts. In the example shown, 3 of the contexts are negative. (b) MS4-27 requires $n = 4$ qubits and has 27 observables and 27 contexts. In the example shown, 5 of them are negative. (c) MS5-27 requires $n = 5$ qubits and has 27 observables and 27 contexts. In the example shown, 13 of them are negative.

magic set. We then use the list of groups acting transitively on $N$ points provided by computer algebra systems such as GAP [69] or MAGMA [70]. For each group $G$, we generate the orbits of $G$ acting on the subsets of $\{1, \ldots, N\}$ of size $s$, where $s \in \{4, 5\}$. If any such orbit contains exactly $4N/s$ sets, then, by a simple counting argument, these sets are the hyperedges of a vertex-transitive hypergraph $H$ in which each vertex is in four edges. (b) We then use a theorem (Theorem 7 in [10]) to determine whether $H$ admits a magic assignment of its vertices by $n$-qubit Pauli operators for some $n$ (i.e., an $n$-qubit magic set). If it does, then we also determine the smallest such $n$. We can also iterate through all such assignments. (c) Whenever we find structures that are not minimal [i.e., which do not satisfy (iii)], we can find new structures that are minimal by a method detailed in [10], which also contains further details on the whole algorithm. We can also compute the minimum number of qubits needed and assignments in this case. The examples we find from this procedure need not be vertex-transitive and may have contexts of larger size and observables in a larger number of contexts.

*Results.*—With the assumptions made above, it can be seen that $H$ must have $N \geq 13$ vertices. By exhaustive computer search, we have found that there are no magic sets with fewer than 19 vertices (Pauli observables), even if we drop the requirement that the hypergraph is vertex-transitive. We have also found that there are no magic sets with fewer than 20 vertices that have at least one nontrivial automorphism.

We have found four classes of irreducible magic sets that have a vertex-transitive hypergraph of compatibility [i.e., that also satisfy property (iv)] like the square and pentagram. Their hypergraphs and a magic assignment for each of them are presented in Figs. 2(a)–2(c), and 3.

The one with the smallest number of observables is the class shown in Fig. 2(a), which requires $n = 4$ qubits and has 21 observables and 21 contexts. Its $H$ is the so-called Grünbaum-Rigby configuration [71] already described by Klein [72].

Each of the other three classes has 27 observables and 27 contexts. The class in Fig. 3 requires $n = 3$ qubits. The class in Fig. 2(b) requires $n = 4$ qubits. Its $H$ is the 3-astral 4-configuration in [73] [Fig. 3.7.2(b)]. The class in Fig. 2(c) requires $n = 5$ qubits. Its $H$ is the smallest known weakly flag-transitive configuration [74].

The automorphism groups of the classes in Figs. 2(a)–2(c) allow for straight line representations in the Euclidean plane (the ones shown in Fig. 2). However, such a representation is not possible for the class in Fig. 3. Instead, we can visualize its hypergraph by describing its automorphism group, as shown in Fig. 3.

We have also found irreducible magic sets not satisfying property (iv) (vertex-transitivity). They include one with $n = 6$ qubits. See Ref. [10] for details.

These sets by themselves answer question (1): there are magic sets that cannot be reduced to the square and the pentagram, including some that also satisfy property (iv). They also answer question (2): there are magic sets that are genuine (irreducible to any magic set with a smaller number of qubits) to systems of $n = 4$ [Figs. 2(a) and 2(b)], $n = 5$ qubits [Fig. 2(c)], and $n = 6$ qubits [10].

*Extending Arkhipov's theorem.*—Here, we address question (3). Arkhipov's theorem provides an efficient algorithm to check whether or not an hypergraph yields a Pauli-based magic assignment satisfying that each observable is in exactly two contexts and the number of negative contexts is odd. The question is whether there is an efficient algorithm to check whether or not a hypergraph admits a Pauli-based magic assignment [i.e., can accommodate Pauli observables satisfying properties (i), (ii), and (iii)].

Steps (b) to (c) of our algorithm provide an efficient algorithm to check whether or not a hypergraph admits a Pauli-based magic assignment satisfying (i) and (ii). Therefore, in a sense, they answer question (3). Additionally,

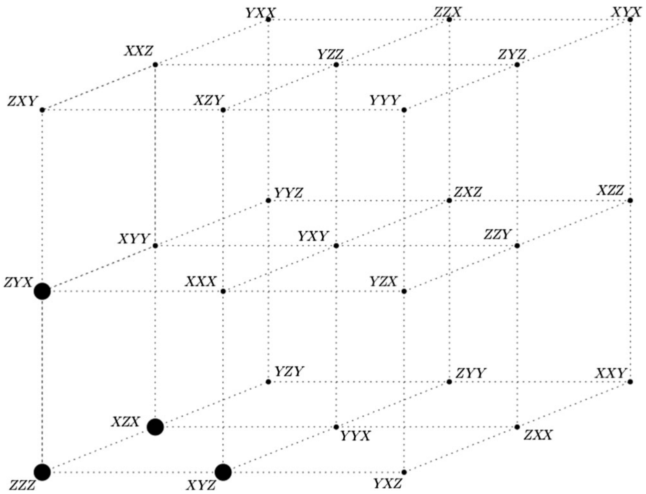


FIG. 3. The fourth magic set with vertex-transitive graph of compatibility that cannot be reduced to the square or pentagram that we have found, MS3-27, requires $n = 3$ qubits and has 27 observables and 27 contexts. It does not admit a straight line representation in the Euclidean plane. Here, observables are given by coordinate points $(x, y, z) \in \mathbb{Z}_3^3$ (the $x$ axis is horizontal, the $y$ axis goes into the page, and the $z$ axis is vertical) and all contexts can be obtained by applying translations to a starter context. A possible starter context $\beta$ given by the observables corresponding to the coordinates (0,0,0),(1,0,0),(0,1,0),(0,0,1) is depicted by the four larger dots. All 27 contexts can be generated by applying the translations $T_{a,b,c}: \mathbb{Z}_3^3 \to \mathbb{Z}_3^3$, $0 \leq a, b, c \leq 2$ given by $(x, y, z) \to (x + a, y + b, z + c)$ to each of the observables of the starter context. For example, one obtains the context $\{ZYY, XXY, ZXZ, XYZ\}$ by applying the translation $T_{1,2,0}$ to the observables of $\beta$. In the example shown, all the contexts are negative. The dotted edges appear only as a visual aid to make clear the correspondence of the vertices to the coordinates. Like the magic square [see Fig. 1(a)], MS3-27 can be implemented using all $3^n$ $n$-qubit Pauli observables not containing $I$.

step (c) allows us to generate and iterate through magic assignments of minimal structures. The main result we exploit is the following theorem.

**Theorem 1:** Let $H$ be a proper Eulerian hypergraph with valid Gram space $\mathcal{V}$. Let $\mathcal{B}$ be any basis for $\mathcal{V}$. Then, (1) $H$ has a magic assignment with Pauli observables if and only if there is a magic Gram matrix in $\mathcal{B}$; and (2) $H$ has a magic assignment with Pauli observables for a system of $k$ qubits satisfying (i) and (ii) if and only if there is a magic Gram matrix of binary rank at most $2k$ in $\mathcal{V}$.

A proper Eulerian hypergraph is a hypergraph with each vertex in an even number of distinct hyperedges. The valid Gram space is the set of $|V| \times |V|$ matrices $M$ whose entries satisfy the following linear equations: (a) $M_{i,j} = 0$ whenever vertices $v_i$, $v_j$ occur in the same hyperedge; and (b) $\sum_{v_i \in e} M_{i,j} = 0$, for all $1 \leq j \leq |E|$ for all hyperedges $e \in E$. A magic assignment $\alpha: V \to GL(\mathcal{H})$, where $\mathcal{H}$ is a Hilbert space, is an assignment such that: (A) $\alpha(v)^2 = I$ and $\alpha(v)$ is Hermitian for all $v \in V$. (B) $\alpha(v)\alpha(w) = \alpha(w)\alpha(v)$ whenever $v$, $w$ are in a common hyperedge $e \in E$. (C) $\prod_{v \in e} \alpha(v) = \pm I$ for each hyperedge $e \in E$. (D) $\prod_{v \in e} \alpha(v) = -I$ for an odd number of hyperedges $e \in E$.

Using Arkhipov's result, our methodology yields a novel algorithm for checking graph planarity ([10], Corollary 12). Additionally, in the case that the graph $G$ is nonplanar, this algorithm also produces a magic Gram matrix encoding a copy of $K_{3,3}$ or $K_5$ appearing as a topological minor of $G$.

*Noncontextuality inequalities.*—Given a set of Pauli observables satisfying (i) and (ii) (i.e., not necessarily minimal), let us call $C_p$ its set of positive contexts and $C_n$ its set of negative contexts. Then, as shown for the square and the pentagram in [6], and for more general cases in [41], the following inequality must be satisfied by any NCHV model:

$$\sum_{\mathcal{C}_i \in C_p} \langle \mathcal{C}_i \rangle - \sum_{\mathcal{C}_j \in C_n} \langle \mathcal{C}_j \rangle \leq b, \tag{1}$$

where $\langle \mathcal{C}_i \rangle$ denotes the mean value of the products of all the observables in context $\mathcal{C}_i$. QM makes a prediction for each context (that the product is either $-1$ or 1). The limit for NCHV models is $b = 2s - |C_p| - |C_n|$, where $s$ is the maximum number of quantum predictions that can be simultaneously satisfied by a NCHV model [41]. An open problem [41] is, given a hypergraph $H$ corresponding to a magic set, what is $b$? Here, we solve this problem in two senses. On the one hand, we give a method for computing $b$ by using results from coding theory (see Ref. [10] for details). Computing $b$ is important for, e.g., computing the resistance to noise of the quantum advantage of any magic set [41]. On the other hand, we prove a more general result.

**Theorem 2:** Let $H = (V, E)$ be a magic Eulerian hypergraph with incidence matrix $M$. Let $\alpha$ be a magic assignment of $H$, and let $w_{\min}$ be the minimum of Hamming weights of elements of the affine space $c(\alpha) + \mathrm{row}(M)$. Then, the noncontextual bound for $\alpha$ is $b = |E| - 2w_{\min}$.

Given a hypergraph $H = (V, E)$ with vertices $v_1, \ldots, v_m$ and edges $e_1, \ldots, e_n$, the incidence matrix of $H$ is the $m \times n$ binary matrix $M$ for which $M_{i,j} = 1$ whenever $v_i \in e_j$. By $\mathrm{row}(M)$ we denote the row space of the matrix $M$. The Hamming weight of a binary vector $w$ is the number of nonzero coordinates of $w$. Given a magic assignment $\alpha$ of $H$, we define $c(\alpha) \in GF(2)^n$ to be the vector for which $c(\alpha)_i = 0$ whenever $\prod_{v \in e_i} \alpha(v) = 1$ and $c(\alpha)_i = 1$ otherwise.

*Conclusions.*—Minimal vertex-transitive magic sets are fascinating objects used in a wide variety of areas as they capture minimal quantum state-independent advantage for $n$-qubit systems and are thus fundamental tools for investigating the interface between classical and quantum physics. While Arkhipov's theorem might have been taken as an indication that there are only two classes of irreducible vertex-transitive magic sets, one requiring two and the other requiring three qubits, and that all magic sets derive from them, in this Letter, we have shown that the landscape of magic sets is quite different from the one suggested by Arkhipov's theorem as there are, at least, four more classes: one requiring three qubits, here called MS3-27, that cannot be drawn in a plane (see Fig. 3); two requiring four qubits, here called MS4-21 [see Fig. 2(a)] and MS4-27 [see Fig. 2(b)]; and one requiring five qubits, MS5-27 [see Fig. 2(c)]. We have also found other irreducible magic sets requiring from three to six qubits (but not vertex-transitive ones).

In the light of these results, it seems that each $n$ has its own set of irreducible vertex-transitive magic sets. Finding them and especially finding the ones with minimum number of observables (so far, the magic square for $n = 2$, the magic pentagram for $n = 3$, MS4-21 for $n = 4$, and MS5-27 for $n = 5$) is an interesting challenge for the reasons that have motivated this Letter (namely, identifying minimal structures providing state-independent quantum advantage and requiring a specific number of qubits). One possible way to obtain these sets would be by generalizing to a higher number of qubits the geometrical structure of the sequence pentagram, MS4-21, and MS5-27, as well as the sequence square and MS3-27.

In addition, we have proven a general expression for the classical (noncontextual) bound of the inequality associated to any magic state (minimal or not), which is useful for many purposes as it allows us, e.g., to compute the robustness to noise in the implementation of the Pauli observables (or, in general, versus any type of experimental limitation) for any given magic set [10]. We hope these results stimulate further research on magic sets and their applications.

We thank T. Pisanski for pointing out that the hypergraphs in Figs. 2(b) and 2(c) appeared in Refs. [73,74], respectively. This work was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC, Project No. RGPIN-2015-06250 and RGPIN-2022-04526), Project Qdisc (Project No. US-15097, Universidad e Sevilla), with FEDER funds, QuantERA grant SECRET, by MINECO (Project No. PCI2019-111885-2), and MICINN (Project No. PID2020–113738 GB-I00).

*Appendix A: Sketch of the proof of Theorem 1.*—Theorem 1 describes an algorithm that, given a proper Eulerian hypergraph $H = (V, E)$, either proves that $H$ has no magic assignment using Pauli observables, or determines the minimal number of qubits needed for a magic assignment of $H$ using Pauli observables. One can also generate such assignments if they exist.

Given an assignment of the vertices of $H$ with Pauli observables, the commutativity relations between all pairs of observables yield enough information to determine whether the Pauli observables constitute a magic set. We encode the commutativity information via a binary matrix called a Gram matrix. The set of Gram matrices encoding magic sets associated to $H$ forms an affine subspace of the valid Gram space of $H$. Therefore, if a basis for the valid Gram space of $H$ contains a Gram matrix whose associated assignments are magic sets, then $H$ admits Pauli-based proofs. Otherwise it does not.

To determine the number of qubits, we use a result on symplectic graphs [ [52], Theorem 8.11.1], which, translated to our problem, states the following: for a Gram matrix $M$ in the valid Gram space of $H$ and binary rank $2k$, $k$ is the minimum number of qubits for which a Pauli-based assignment of $H$ can respect all commutativity conditions of $M$.

*Appendix B: Sketch of the proofs of Theorem 2.*—To compute the bound of the noncontextuality inequality associated to a given magic set, one can search over all possible $2^{|V|}$ assignments of 1 or $-1$ to the vertices of $H$. We take a different approach. Given a magic set, we produce another magic set that has the same noncontextual bound, but for which the NCHV assignment using all 1's is optimal.

If two magic sets have the same set of negative contexts, then they must also have the same noncontextual bound. Thus, for magic sets represented as magic assignments of $H$, $\alpha$, and $\alpha'$, we see that if $c(\alpha) = c(\alpha')$, then $b_\alpha(H) = b_{\alpha'}(H)$.

If a magic set is obtained from another by negating observables [e.g., replacing $XX$ by $-XX$ in Fig. 1(a)], then they must have the same noncontextual bound. This can be expressed using linear algebra via the incidence matrix of $H$: if $c(\alpha) - c(\alpha') \in \mathrm{row}(M)$, then $b_\alpha(H) = b_{\alpha'}(H)$. Moreover, the set of negative contexts for each of the possible $2^{|V|}$ magic sets obtained by negations of observables is the affine space $c(\alpha) + \mathrm{row}(M)$. The number of negative contexts of $\alpha$ is exactly the Hamming weight of $c(\alpha)$ [by definition, since each negative context of $\alpha$ corresponds to a 1 in $c(\alpha)$]. Thus, the magic assignment $\alpha'$ with the fewest negative contexts obtainable from $\alpha$ by observable negations has the property that $c(\alpha')$ is a minimum Hamming weight element of $c(\alpha) + \mathrm{row}(M)$. This minimum Hamming weight is $w_{\min}$ in Theorem 2.

For $\alpha'$, the assignment using all 1's yields the noncontextual bound, since flipping a 1 to a $-1$ produces the same result as negating the corresponding observable. The noncontextual bound $b_\alpha(H)$ is thus $|E| - 2w_{\min}$.

[*]Corresponding author.
stefan_trandafir@sfu.ca
[†]Corresponding author.
plisonek@sfu.ca
[‡]Corresponding author.
adan@us.es

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[10] See Supplemental Material, which includes Refs. [11–57], at http://link.aps.org/supplemental/10.1103/PhysRevLett.129.200401 for further details on applications of magic sets (Appendix A), the methodology followed in this Letter (Appendix B), noncontextuality inequalities (Appendix C), and more magic sets (Appendix D).

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