An abstract structure determines the contextuality degree of observable-based Kochen-Specker proofs*

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Abstract

This article delves into the concept of quantum contextuality, specifically focusing on proofs of the Kochen-Specker theorem obtained by assigning Pauli observables to hypergraph vertices satisfying a given commutation relation. The abstract structure composed of this hypergraph and the graph of anticommutations is named a hypergram. Its labelings with Pauli observables generalize the well-known magic sets. A first result is that all these correct quantum labelings of a given hypergram inherently possess the same degree of contextuality. Then we provide a necessary and sufficient condition for the existence of such quantum labelings and an efficient algorithm to find one of them. We finally attach to each assignable hypergram an abstract notion of contextuality degree. By presenting the study of observable-based Kochen-Specker proofs from the perspectives of graphs and matrices, this abstraction opens the way to new methods to search for original contextual configurations.

1 Introduction

In classical physical theories, the measured value of a physical quantity does not depend on that of other quantities simultaneously measured, called its *context*. This independence no longer holds in quantum theory, where Kochen-Specker theorem predicts the existence of experiments whose measurement outcomes necessarily depend on measurements that are simultaneously measurable in principle. This phenomenon is called *quantum contextuality* (see, e. g., [Bud+22] for a recent comprehensive review of this topic). It is a core aspect of quantum mechanics, especially for quantum computation.

Several approaches have been proposed to study quantum contextuality, such as binary [CM14] and linear [CLS17] constraint systems, which are generalizations of the Boolean case [FOC25], and graph-based [CSW14] and hypergraph-based [Ací+15] approaches, where vertices are events and edges are mutually exclusive events. Note that those hypergraphs are not the same as the hypergraphs we introduce in this work, whose vertices represent observables and whose hyperedges represent contexts. There is also a homotopical approach [OR20] that describes topological criteria for the commutation relations of quantum observables, and a study of contextuality in the framework of Lie algebras [Agu+24].

This work is about (observable-based) *contextuality proofs*, whose measurements are multiqubit Pauli observables. These proofs are *state-independent*, because their measurements reveal quantum contextuality when applied to any initial quantum state. When the number of qubits of the Pauli observables is small enough, they are *testable*, in the sense that they can be turned

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into experimental tests of contextuality on existing quantum computers (see, e.g., [Kir+09] or [Hol21]).

Structurally, these contextuality proofs are described by hypergraphs whose vertices are multiqubit Pauli observables and whose hyperedges, also called *contexts*, group together compatible, that is, commuting observables whose product is either the identity matrix (*positive* hyperedge or context) or its opposite (*negative* hyperedge or context). How much a proof is contextual can be quantified by an integer called its *contextuality degree* [de +22], which is the minimal number of context signs which cannot be satisfied by any assignment of all its observables/vertices by one of their measurement values (see Section 2.6 for a detailed mathematical definition).

A widely studied subfamily of contextuality proofs is that of *contextual configurations* [HS17], aka. *magic sets*, whose observables belong to an even number of contexts (*parity condition*), whose number of negative contexts is odd (*oddness condition*), and which are incidence geometries, meaning that two observables share at most one context (*incidence condition*). The contextuality of a magic set is an immediate logical consequence of these conditions [HS17]. Typical examples are the Mermin-Peres squares [Mer93; Per90], composed of nine two-qubit observables and six contexts of three observables, with one or three negative contexts among them.

Previous works inspired by finite geometry [San+21; Mul+22; Mul+24] exhibit contextuality proofs which do not satisfy the first two conditions of magic sets. For example, multi-qubit doilies [Mul+22] comprise three contexts per observable, thus do not satisfy the parity condition. Moreover, three-qubit doilies with four negative lines do not satisfy the oddness condition, but also provide contextuality proofs. Actually, whatever their number of qubits and configuration of negative contexts, all doilies have been proved to be contextual and to admit the same contextuality degree, whose value is 3 [Mul+22, Proposition 1]. Independently, the non-contextual bound of magic sets – linearly related to their contextuality degree, as detailed in Section 2.6 – has recently been shown not to depend on their number of qubits [TLC22b, Theorem 2].

At first glance, according to its definition, the degree of a contextuality proof depends on the distribution of positive and negative contexts in it, itself arising from the Pauli observables which label their vertices. The main objective of this work is to clarify this dependence. We achieve this by introducing the notion of hypergram (Definition 1), which is an observable-free graph- and hypergraph-based structure admitting a definition of contextuality degree. It is *abstract* because it is defined independently of a number of qubits and more generally without recourse to any quantum-related concept.

In this paper, we first define hypergrams and related notions (Section 2). Then, we demonstrate that the contextuality degree of its labelings by Pauli observables (hereafter called "Pauli assignments") does not depend on their number of qubits (Section 3). Then we derive from [TLC22a] (which provides supplemental material for [TLC22b]) a necessary and sufficient condition for a hypergram to admit a Pauli assignment and we propose an efficient algorithm to find such an assignment when this condition holds (Section 4). An immediate consequence is that only one adequate labeling of vertices with Pauli observables is sufficient to compute the degree. In Section 5 we present several examples of hypergrams, labeled with minimal numbers of qubits and negative contexts. A comparison with related work is provided in Section 6.

2 Definitions and notations

After Sections 2.1 and 2.2 providing minimal essential background about the Pauli group and its relation with symplectic polar spaces, Section 2.3 introduces a new abstract structure, composed of a hypergraph and a graph, which will later be shown to admit a notion of contextuality degree, inherited from the contextuality degree common to all the labelings of its vertices by Pauli observables. The remainder of the section brings together definitions from independent previous work, mainly [TLC22a] and [de +22; Mul+24], and exhibits correspondences between these definitions, when it is useful, for example between the notions of "Pauli assignment" and "quantum configuration" in Section 2.4, and between the notions of "contextuality degree" and "noncontextual bound" in Section 2.6.

2.1 Multi-qubit Pauli group

Let

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$
, $Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ and $Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

be the Pauli matrices, I the 2×2 identity matrix, ' \otimes ' denote the tensor product of matrices and $I^{\otimes n}$ denote the n-fold tensor $I \otimes I \otimes \ldots \otimes I$ of the identity. A local n-qubit (Pauli) observable is a tensor product $G_1 \otimes G_2 \otimes \cdots \otimes G_n$ with $G_i \in \{I, X, Y, Z\}$, usually denoted $G_1 G_2 \cdots G_n$, by omitting the symbol \otimes for the tensor product. Let '' denote the matrix product and M^2 denote $M \cdot M$. It is easy to check that $X^2 = Y^2 = Z^2 = I$, $X \cdot Y = iZ = -Y \cdot X$, $Y \cdot Z = iX = -Z \cdot Y$, and $Z \cdot X = iY = -X \cdot Z$. The n-qubit observables with the multiplicative factors ± 1 and $\pm i$, called phase, form the (generalized) (n-qubit) Pauli group $\mathcal{P}^{\otimes n} = (\{1, -1, i, -i\} \times \{I, X, Y, Z\}^{\otimes n}, \cdot)$.

2.2 Connection with symplectic polar spaces

Let a and b be two elements of the two-element field $\mathbb{F}_2 = \{0, 1\}$. Their sum, denoted a + b, and their product, denoted ab, respectively correspond to the logical operations of exclusive disjunction and conjunction, when 0 encodes "false" and 1 encodes "true".

The 2n-dimensional vector space \mathbb{F}_2^{2n} over \mathbb{F}_2 has vector subspaces for each dimension $0 \le k \le 2n$. A subspace is *totally isotropic* if any two vectors x and y in it are mutually orthogonal $(\langle x \mid y \rangle = 0)$, for the symplectic form $\langle . \mid . \rangle$ defined by

$$\langle x \mid y \rangle = x_1 y_2 + x_2 y_1 + x_3 y_4 + x_4 y_3 + \dots + x_{2n-1} y_{2n} + x_{2n} y_{2n-1}.$$
 (1)

The totally isotropic subspaces of \mathbb{F}_2^{2n} , without their zero vector, form the *symplectic* (*polar*) *space* W(2n-1,2) of projective dimension 2n-1. This name, in which 2 is the order of the field \mathbb{F}_2 , is hereafter shortened as W_n . In other words, a (totally isotropic) subspace of W_n of (projective) dimension k, with $1 \le k \le n-1$, is a totally isotropic vector subspace of \mathbb{F}_2^{2n} of dimension k+1 without its 0.

The 4^n-1 phase-free n-qubit observables $G_1\cdots G_j\cdots G_n$ in $\mathcal{P}^{\otimes n}$ other than the identity $I^{\otimes n}$ are bijectively identified with the 4^n-1 vectors $(x_1,x_2,\ldots,x_{2j-1},x_{2j},\ldots,x_{2n-1},x_{2n})$ which are the points of W_n , by the extension $\psi:\{I,X,Y,Z\}^{\otimes n}\to\mathbb{F}_2^{2n}$ of the encoding bijection $\psi:\{I,X,Y,Z\}\to\mathbb{F}_2^{2n}$ defined by

$$\psi(I) = (0,0), \ \psi(X) = (0,1), \ \psi(Y) = (1,1) \text{ and } \psi(Z) = (1,0).$$
 (2)

This extension is defined by $\psi(G_1 \cdots G_j \cdots G_n) = (x_1, x_2, \dots, x_{2j-1}, x_{2j}, \dots, x_{2n-1}, x_{2n})$ with $\psi(G_j) = (x_{2j-1}, x_{2j})$ for $1 \le j \le n$.

With the symplectic form defined by (1), two commuting observables are represented by two orthogonal vectors.

2.3 Abstract structure

A simple graph is an undirected graph without multiple edges and loops, i. e., edges $\{v,v\}$ for some vertex v. A hypergraph $\mathcal{H}=(V,H)$ is a finite set V of vertices and a (finite) set H of hyperedges, which are (distinct) subsets of vertices in V. Two vertices are adjacent (in \mathcal{H}) if they are in the same hyperedge of H. The complement graph of the hypergraph $\mathcal{H}=(V,H)$ is the (simple) graph $\mathrm{cplt}(\mathcal{H})=(V,\mathrm{cplt}(H))$ with the same vertices as \mathcal{H} and whose (undirected and non-loop) edges are the sets of two distinct non-adjacent vertices in \mathcal{H} . Formally, $\{v,v'\}\in\mathrm{cplt}(H)\Leftrightarrow v\neq v'\land \nexists h\in H$. $\{v,v'\}\subseteq h$. Following [GR01], a graph is said to be reduced if it has no isolated vertex and no pair of vertices with the same neighborhood, which is their set of adjacent vertices.

With these definitions in mind, we can now introduce the hypergram that we propose as the abstract structure underlying operator-based contextuality proofs and determining their degree of contextuality.

Definition 1. A *hypergram* is a triple (V, H, G) where V is a non-empty finite set of *vertices*, (V, H) is a hypergraph (called *context hypergraph*) without isolated vertices (outside any hyperedge) and empty hyperedges and (V, G) is a simple reduced graph (called *anticommutation graph*) such that $G \subseteq \text{cplt}(H)$. We say that two vertices i and j *commute* if $\{i, j\} \notin G$.

By definition, each vertex commutes with itself. The inclusion $G \subseteq \operatorname{cplt}(H)$ means that all pairs of adjacent vertices in H commute.

The following definition introduces two classical finite point-line geometries which will serve as examples of hypergrams.

Definition 2. The *doily* is the triangle-free self-dual finite incidence geometry composed of 15 points and 15 lines, with three points on a line and, dually, three lines through a point. In Figure 1 the doily is represented by all the lines, either dashed or plain. A *two-spread* is a point-line geometry obtained from the doily by removing a *spread*, i. e., a set of hyperedges covering every vertex exactly once. In Figure 1 the removed spread is represented by the dashed lines, and the two-spread by the plain lines.

When G = cplt(H), the hypergram (V, H, G) is identified with its hypergraph (V, H), as in Example 1. Under the more restrictive conditions of magic sets, these hypergraphs (V, H) are considered in [TLC22b].

Example 1 (Doily). As a hypergram, the doily is $S_d = (\{1, ..., 15\}, H_d, G_d) = (\{1, ..., 15\}, H_d)$ with $H_d = \{\{1, 2, 3\}, \{1, 8, 9\}, \{1, 10, 11\}, \{2, 4, 6\}, \{2, 5, 7\}, \{3, 12, 15\}, \{3, 13, 14\}, \{4, 8, 12\}, \{4, 10, 14\}, \{5, 8, 13\}, \{5, 10, 15\}, \{6, 9, 15\}, \{6, 11, 13\}, \{7, 9, 14\}, \{7, 11, 12\} \}$ and $G_d = \text{cplt}(H_d)$.

The anticommutation graph G added in our definition extends the framework to a wider range of cases, when $G \subseteq \text{cplt}(H)$, as illustrated by Example 2 and detailed in Section 5.

Example 2 (Running example). As running example, let us consider the hypergram $S_{2s} = (V_{2s}, H_{2s}, G_{2s})$, called *two-spread hypergram*, with the set of 15 vertices $V_{2s} = \{1, ..., 15\}$, the set of ten hyperedges $H_{2s} = \{\{1, 2, 3\}, \{1, 10, 11\}, \{2, 4, 6\}, \{3, 13, 14\}, \{4, 8, 12\}, \{5, 8, 13\}, \{5, 10, 15\}, \{6, 9, 15\}, \{7, 9, 14\}, \{7, 11, 12\}\}$ and the set of anticommutations $G_{2s} = \{\{1, 4\}, \{1, 5\}, \{1, 6\}, \{1, 7\}, \{1, 12\}, \{1, 13\}, \{1, 14\}, \{1, 15\}, \{2, 8\}, \{2, 9\}, \{2, 10\}, \{2, 11\}, \{2, 12\}, \{2, 13\}, \{2, 14\}, \{2, 15\}, \{3, 4\}, \{3, 5\}, \{3, 6\}, \{3, 7\}, \{3, 8\}, \{3, 9\}, \{3, 10\}, \{3, 11\}, \{4, 5\}, \{4, 7\}, \{4, 9\}, \{4, 11\}, \{4, 13\}, \{4, 15\}, \{5, 6\}, \{5, 9\}, \{5, 11\}, \{5, 12\}, \{5, 14\}, \{6, 7\}, \{6, 8\}, \{6, 10\}, \{6, 12\}, \{6, 14\}, \{7, 8\}, \{7, 10\}, \{7, 13\}, \{7, 15\}, \{8, 10\}, \{8, 11\}, \{8, 14\}, \{8, 15\}, \{9, 10\}, \{9, 11\}, \{9, 12\}, \{9, 13\}, \{10, 12\}, \{10, 13\}, \{11, 14\}, \{11, 15\}, \{12, 13\}, \{12, 14\}, \{13, 15\}, \{14, 15\}\}$. For instance, the edge $\{1, 8\}$ is in cplt(H_{2s}) but not in G_{2s} , so $G_{2s} \subseteq \text{cplt}(H_{2s})$ in this case.

2.4 Assignments and quantum configurations

A (*n*-qubit) Pauli assignment of a hypergram (V, H, G) is an injective function α from V to {I, X, Y, Z}^{$\otimes n$} - { $I^{\otimes n}$ } that assigns a distinct n-qubit Pauli observable (different from identity) to all its vertices, such that two distinct Pauli observables $\alpha(v_1)$ and $\alpha(v_2)$ anticommute if and only if { v_1, v_2 } $\in G$ (*commutation condition*), and the product of all assignments of vertices in any hyperedge $h \in H$ is the identity matrix or its opposite (formally, $\prod_{v \in h} \alpha(v) = \pm I^{\otimes n}$) (*product condition*).

Example 2 (continued). An example of 2-qubit Pauli assignment of the two-spread hypergram S_{2s} is the function $\alpha_{2s}: V_{2s} \to \{I, X, Y, Z\}^{\otimes 2} - \{I^{\otimes 2}\}$ defined by $\alpha_{2s}(1) = IX$, $\alpha_{2s}(2) = XI$, $\alpha_{2s}(3) = XX$, $\alpha_{2s}(4) = IZ$, $\alpha_{2s}(5) = IY$, $\alpha_{2s}(6) = XZ$, $\alpha_{2s}(7) = XY$, $\alpha_{2s}(8) = ZI$, $\alpha_{2s}(9) = ZX$, $\alpha_{2s}(10) = YI$, $\alpha_{2s}(11) = YX$, $\alpha_{2s}(12) = ZZ$, $\alpha_{2s}(13) = ZY$, $\alpha_{2s}(14) = YZ$, and $\alpha_{2s}(15) = YY$. This assignment is illustrated by a labeling in Figure 1.

A Pauli assignment corresponds to a "quantum satisfying assignment" of a binary constraint system [CM14] and to a "finite dimensional operator solution" to a binary linear system [CLS17], whose matrix is the incidence matrix of the hypergraph *H*. It also corresponds to a generalization of a "quantum realization of a signed arrangement" [Ark12], without the condition that each

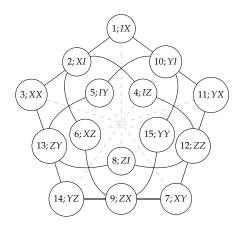


Figure 1: Illustration of the two-spread hypergram S_{2s} defined in Example 2. Each circled node is labeled by a vertex i in V_{2s} , a semi-colon, and the Pauli observable $\alpha_{2s}(i)$ assigned to the vertex i by the 2-qubit Pauli assignment α_{2s} presented in Section 2.4. Each hyperedge is represented by a single or double continuous line, either straight or curved. It is composed of three vertices. The negative context is represented by a double line. The set G_{2s} of anticommutation edges is composed of all pairs of vertices not belonging to a common continuous or dashed line, either simple or double.

vertex is included in exactly two hyperedges of the hypergraph that depicts the contexts. Other works [CSW14; Ací+15] consider graphs and hypergraphs whose vertices represent measurement outcomes, while we consider hypergraphs whose vertices are labeled by Pauli observables. A correspondence between these approaches can be found in [Ací+15, Appendix D]. This notion is also close to that of a Pauli-based assignment [TLC22a] (see Section 6 for details) and to the following one, coming from our previous work.

A quantum configuration [Mul+24] (called quantum geometry in [de +22]) is a pair (O, C) where O is a non-empty finite set of observables $(2^n$ -dimensional Hermitian operators) and C is a finite set of non-empty subsets of O, called *contexts*, such that (i) each observable $a \in O$ satisfies $a^2 = I^{\otimes n}$ (so, its eigenvalues are in $\{-1,1\}$); (ii) any two observables a and b in the same context commute, i. e., $a \cdot b = b \cdot a$; (iii) the product of all observables in each context is either $I^{\otimes n}$ (positive context) or $-I^{\otimes n}$ (negative context). In all that follows, these observables are always phase-free Pauli observables.

Example 2 (continued). Figure 1 also shows a two-spread as a quantum configuration, with only one negative context, represented by a double line. The product of the 3 observables in this line is equal to -II, as opposed to +II for all the other lines.

A pair composed of a hypergram (V, H, G) and an n-qubit Pauli assignment α of it can be associated to any quantum configuration (O, C) with |O| n-qubit phase-free Pauli observables, as follows. Let $V = \{1, 2, \ldots, |O|\}$. Let α be a bijection from V to O. With a small abuse of notation, let us also denote by α the extension of α to subsets of V, and the extension of the latter to subsets of subsets of V. Let V be the inverse image of V by this last extension V. In other words, V is the set of subsets V of V such that V and V' are in V if and only if V and V are in the same context in V. Let V be defined by V, V, V is a hypergram and V is a hypergram and V is an V-qubit Pauli assignment on it. An important part of the article establishes conditions under which the quantum notion of degree of contextuality, initially defined on a quantum configuration (as detailed in Section 2.6) becomes an abstract notion on the corresponding hypergram, as summarized in Section 4.4.

Conversely, the *quantum configuration associated to* a Pauli assignment α of a hypergram (V, H, G) is the pair (O, C) such that $O = \alpha(V)$ and $C = \alpha(H)$. In all that follows, most of the notions associated with a hypergram have their counterpart for the corresponding quantum configuration through this correspondence.

Note that a consequence of the commutation condition and the inclusion condition $G \subseteq \operatorname{cplt}(H)$ for any hypergram (V, H, G) is that all elements of a context (image of a hyperedge by a Pauli assignment α) mutually commute. This is why this condition is not in our definition of a Pauli assignment.

2.5 Sign functions

For any subset *S* of the Pauli group whose elements mutually commute, commutativity enables us to define Π_S as the generalized product $\Pi_{S \in S}$ of all the elements of *S*.

Let α be an n-qubit Pauli assignment of a hypergram (V,H,G), and h a hyperedge in H. Since all elements in any context $\alpha(h)$ mutually commute, the product $\Pi_{\alpha(h)}$ is well-defined. The sign (or valuation) (function) of α is the function $sgn_{\alpha}: H \to \{-1,1\}$ such that $\Pi_{\alpha(h)} = sgn_{\alpha}(h) I^{\otimes n}$ for all hyperedges h in H. Similarly, the sign function for a quantum configuration (O,C) of n-qubit observables is the function $s: C \to \{-1,1\}$ defined by $\Pi_c = s(c) I^{\otimes n}$ for each context $c \in C$.

A classical assignment $a: V \to \{-1, +1\}$ assigns a value ± 1 to each vertex of a hypergram (V, H, G). The sign (function) of the classical assignment a is the function $\operatorname{sgn}_a: H \to \{-1, 1\}$ defined by $\operatorname{sgn}_a(h) = \Pi_{a(h)} = \Pi_{v \in h} a(v)$ for all hyperedges h in H.

The hyperedge h in H is said to be *satisfied* (resp., *unsatisfied*) when the signs $\operatorname{sgn}_{\alpha}(h)$ and $\operatorname{sgn}_{a}(h)$ of its Pauli and classical assignments are the same (resp., differ, and thus are opposite). These definitions also apply to contexts and lines.

Example 3. In Figures 2a to 2c, the classical assignment is represented by the numbers below the observables in each node. The dashed lines are the unsatisfied lines on which the signs of the Pauli and classical assignments differ.

In the above-mentioned approach of constraint/linear systems [CM14; CLS17], the second member of these systems is composed of the values of a given sign function. Similarly, by definition, a quantum realization of a signed arrangement [Ark12] should also satisfy a given sign function. A significant difference in [TLC22b] and in the present work is that we address a potentially simpler problem, namely finding a Pauli assignment without targeting any given sign function. We precisely show in Section 3 that satisfying a given sign function is a too strong constraint for the objective we pursue of finding remarkable state-independent Kochen-Specker proofs.

2.6 Contextuality degree and noncontextual bound

With the former definitions, the contextuality of a Pauli assignment can be defined and quantified by a natural number, such as the "degree of contextuality" [Mul+24] or the "noncontextual bound" [Cab10], with the following definitions and relation between them.

Definition 3. A Pauli assignment α of a hypergram (V, H, G) is *contextual* if there is no classical assignment a with the same sign function as α (over H). The *contextuality degree* [de +22] d of the Pauli assignment α for the hypergram (V, H, G) is the minimal Hamming distance (i. e., number of different values) between its sign function $\operatorname{sgn}_{\alpha}$ and the sign function sgn_{a} of any classical assignment $a: V \to \{-1, +1\}$.

In other words, the degree of contextuality is the minimal number of different hyperedge products between this Pauli assignment and any classical assignment. For instance, we shall see (Proposition 15) that the contextuality degree of all two-spreads is 1, meaning that at least one product will always be different between any classical and Pauli assignments of a two-spread.

For any quantum configuration (O, C), let

$$\chi = \sum_{c \in C} s(c) \langle c \rangle \tag{3}$$

be the sum of the expectation values $\langle c \rangle$ of all contexts c, multiplied by their sign. A *Non-Contextual Hidden-Variable theory* is a theory in which the values of the physical observables are the same irrespectively of the experimental context which they belong to (NCHV hypothesis). Without this NCHV hypothesis, all the sign constraints can be satisfied, with the expectation value +1 for positive contexts and -1 for negative ones, so the upper bound for χ is the number |C| of contexts of (O,C). However, under the NCHV hypothesis, at least d sign constraints cannot be satisfied. The expectation value of each unsatisfied context being the opposite of its sign, the upper bound of χ under this hypothesis is reduced by 2d. This *noncontextual bound* [Cab10; TLC22b] b is thus related to d by

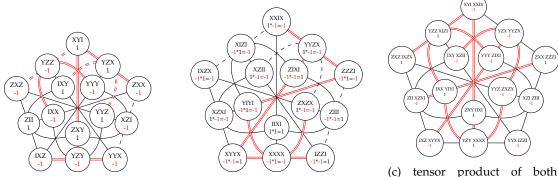
$$b = |C| - 2d. \tag{4}$$

A quantum configuration (O, C) can be transformed into an experimental observable-based test to witness state-independent contextuality (see, e. g., [KH25]). It is successful if the measurement errors are small enough to measure a value of χ above its upper bound (|C|-2d) under the NCHV hypothesis. Furthermore, a quantum configuration (O,C) can be turned into a non-local game, providing a proof of nonlocality of quantum physics, as detailed in [CM14; CLS17], since it can be associated with a binary constraint system.

3 All Pauli assignments have the same contextuality degree

This section shows how to transfer a classical assignment between two Pauli assignments of the same hypergram (Lemma 4) and proves that all these Pauli assignments have the same contextuality degree (Theorem 5), a generalization of [TLC22a, Proposition 14] to all hypergrams.

Let the *tensor product of two Pauli assignments* α_1 and α_2 of the same hypergram (V, H, G) be the Pauli assignment $\alpha_{1\otimes 2}$ defined by $\alpha_{1\otimes 2}(v) = \alpha_1(v) \otimes \alpha_2(v)$ for all vertices v in V. Figure 2 presents an example of tensor product of two Pauli assignments of the doily structure. It will serve to illustrate the proof arguments for Lemma 4 and Theorem 5.



(a) 3-qubit doily with a known classical assignment

(b) 4-qubit doily with a computed classical assignment

(c) tensor product of both doilies, with a classical assignment satisfying all its contexts

Figure 2: Illustration of the classical assignment transfer process, between two Pauli assignments of the same structure, here the doily. The dashed lines are the unsatisfied ones.

Lemma 4. Let α_1 and α_2 be two Pauli assignments of the same hypergram (V, H, G). Let a_1 be a classical assignment of V and S the subset of hyperedges in H satisfied by a_1 for α_1 . Then there exists a classical assignment a_2 whose set of hyperedges satisfied for α_2 is also S.

Proof. For any two vertices v_1 and v_2 in V, either the two pairs $(\alpha_1(v_1), \alpha_1(v_2))$ and $(\alpha_2(v_1), \alpha_2(v_2))$ of their images by α_1 and α_2 anticommute (if $\{v_1, v_2\} \in G$), or they both commute. By elementary

algebraic computations, with $s = \pm 1$,

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\begin{split} \alpha_{1\otimes 2}(v_1) \cdot \alpha_{1\otimes 2}(v_2) &= (\alpha_1(v_1) \otimes \alpha_2(v_1)) \cdot (\alpha_1(v_2) \otimes \alpha_2(v_2)) = (\alpha_1(v_1) \cdot \alpha_1(v_2)) \otimes (\alpha_2(v_1) \cdot \alpha_2(v_2)) \\ &= (s \ \alpha_1(v_2) \cdot \alpha_1(v_1)) \otimes (s \ \alpha_2(v_2) \cdot \alpha_2(v_1)) \\ &= s^2 \ (\alpha_1(v_2) \cdot \alpha_1(v_1)) \otimes (\alpha_2(v_2) \cdot \alpha_2(v_1)) \\ &= (\pm 1)^2 \ (\alpha_1(v_2) \otimes \alpha_2(v_2)) \cdot (\alpha_1(v_1) \otimes \alpha_2(v_1)) \\ &= \alpha_{1\otimes 2}(v_2) \cdot \alpha_{1\otimes 2}(v_1). \end{split}
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This means that all observables in the image $O \equiv \alpha_{1 \otimes 2}(V)$ of $\alpha_{1 \otimes 2}$ pairwise commute.

With $C = \alpha_{1\otimes 2}(H)$, the quantum configuration (O, C) is therefore commutative. By [Ark12, Proposition 8], it is non-contextual. Let $a_{1\otimes 2}$ be a classical assignment satisfying all sign constraints of (O, C), and let a_2 be the classical assignment of V defined by $a_2(v) = a_{1\otimes 2}(v)a_1(v)$.

Then, by the fact that for all hyperedges $h \in H$, $\prod_{v \in h} a_2(v) = \prod_{v \in h} (a_{1 \otimes 2}(v)a_1(v))$, we obtain that the classical assignment a_2 satisfies for α_2 exactly the same hyperedges as a_1 for α_1 .

Figure 2 illustrates the operational aspect of Lemma 4 and its proof, as a way to transfer a classical assignment from a given Pauli assignment to another one with the same structure. Assume we already know a classical assignment a_1 reaching the contextuality degree in the 3-qubit doily in Figure 2a. Figure 2c shows the tensor product of the first two doilies, for which a non-contextual solution $a_{1\otimes 2}$ is easily computed. Finally, the product of the classical assignment a_1 of Figure 2a and the solution $a_{1\otimes 2}$ of Figure 2c provides an optimal classical assignment a_2 for the 4-qubit doily in Figure 2b, with the same subset of satisfied hyperedges, so the same contextuality degree, as generalized in the following theorem.

Theorem 5. Let (V, H, G) be a hypergram. Then all Pauli assignments of (V, H, G) have the same contextuality degree and noncontextual bound.

Proof. When (V, H, G) admits no Pauli assignment, the theorem trivially holds. Otherwise, let α_1 be any Pauli assignment of (V, H, G), with the contextuality degree d_1 , and let a_1 be a classical assignment of α_1 for this contextuality degree d_1 , i. e., at the minimal Hamming distance d_1 from α_1 . Let α_2 be another Pauli assignment whose contextuality degree d_2 is unknown. By Lemma 4, we know that there is a classical assignment a_2 with the same set of unsatisfied hyperedges for α_2 as a_1 for α_1 , and thus at the same Hamming distance d_1 from α_2 , which means that the contextuality degree d_2 of α_2 is at most d_1 . The same reasoning with α_1 and α_2 exchanged entails that d_1 is at most d_2 , so $d_1 = d_2$.

The noncontextual bound b being related to d by the linear relation (4), α_1 and α_2 also have the same noncontextual bound.

4 Assignability

By Theorem 5 all Pauli assignments α of a hypergram have the same contextuality degree. However, a given hypergram (V, H, G) does not necessarily admit a Pauli assignment. If it does, it is said to be (*Pauli-)assignable*. After providing a counterexample and introducing some definitions and notations, we establish in Theorems 8 and 9 a necessary and sufficient condition on H and G for the assignability of (V, H, G). When this *assignability condition* is satisfied, the algorithm presented in Section 4.1 efficiently computes such a Pauli assignment α , used in Section 4.2 to complete the proof of Theorem 8. The algorithmic complexity of this algorithm is discussed in Section 4.3. Finally, Section 4.4 proposes a definition of contextuality degree for any assignable hypergram.

From here, we superimpose to the (hyper)graph point of view of the previous sections the algebraic point of view promoted by algebraic graph theory [GR01], through the following definitions and identifications. For this purpose, the hyperedges in the set H of a context hypergraph (V, H) are assumed to be numbered from 1 to |H| in a arbitrary but fixed order.

Definition 6. The *context matrix* $C(H) \in \mathbb{F}_2^{|H| \times |V|}$ of the context hypergraph (V, H) is its incidence matrix, defined by $C(H)_{k,v} = 1$ if the vertex $v \in V = \{1, \dots, |V|\}$ is in the k-th hyperedge $(1 \le k \le |H|)$, and 0 otherwise. The *anticommutation matrix* $A(G) \in \mathbb{F}_2^{|V| \times |V|}$ of the anticommutation graph (V, G) is its adjacency matrix, defined as the symmetric matrix such that $A(G)_{i,j} = 1$ if $\{i, j\} \in G$, and 0 otherwise.

Since the anticommutation graph (V, G) is loopless, all the diagonal entries of A(G) are equal to zero.

To lighten the notations (for instance in Example 4 and Theorem 8) and without risk of confusion, we adopt the following identification conventions: we also designate by H the context matrix C(H) and by G the anticommutation matrix A(G), whenever it is clear from the context whether we are talking about a matrix or a set.

Example 4. Consider the hypergram S = (V, H, G) with $V = \{v_1, v_2, v_3, v_4, v_5\}$, $H = \{\{v_1, v_2, v_3\}, \{v_1, v_4, v_5\}\}$ and $G = \{\{v_3, v_5\}\}$. Its context matrix is the incidence matrix

$$H = \begin{pmatrix} 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 & 1 \end{pmatrix}$$

and its anticommutation matrix is the adjacency matrix

The two 1s in **bold** come from the anticommutation between v_3 and v_5 in the set G.

The following lemma from [TLC22a] is a key argument in the proof of Theorem 8. It is reproduced here (with a slight adaptation to our notations) in order to make the paper self-contained. The *Gram matrix* of the sequence of vectors $s_1, \ldots, s_m \in \mathbb{F}_2^{2n}$ with respect to the symplectic form $\langle . | . \rangle$ is the $m \times m$ matrix whose (i, j) entry $G_{i,j}$ is $\langle s_i | s_j \rangle$.

Lemma 7 ([TLC22a, Lemma 3]). Let $s_1, \ldots, s_m \in \mathbb{F}_2^{2n}$ for some positive integer n, and let G be their Gram matrix with respect to the symplectic form $\langle . | . \rangle$, with rows r_1, \ldots, r_m . If a subset $\{r_{i_1}, \ldots, r_{i_j}\}$ of the rows is linearly independent, then the corresponding set of vectors $\{s_{i_1}, \ldots, s_{i_j}\}$ is also linearly independent.

Theorem 8. A hypergram (V, H, G) admits a Pauli assignment if and only if

$$H \cdot G = 0. \tag{5}$$

In Equation (5), called the (matricial) assignability condition, the dot is the matrix product and its right-hand side 0 is the $|H| \times |V|$ zero matrix. In other words, the condition is that each column of the matrix G is in the null space $\ker(H)$ of the matrix H.

Example 4 (continued). The fifth column of *G* in our example is the vector $(0\ 0\ 1\ 0\ 0)^T$. Since $H \cdot (0\ 0\ 1\ 0\ 0)^T \neq (0\ 0)^T$, the hypergram *S* is not assignable.

Proof. First, we show that each Pauli assignment for (V, H, G) satisfies the assignability condition (5).

Let α be an n-qubit Pauli assignment of (V, H, G), with V assumed to be $\{1, 2, \ldots, |V|\}$ here. The commutation condition $G_{i,j} = \langle \psi(\alpha(i)) \mid \psi(\alpha(j)) \rangle$ for α is equivalent to the fact that G is the Gram matrix of $\psi \circ \alpha$, by definition of a Gram matrix. On the other hand, the commutation and product conditions for α entail that $\psi \circ \alpha : V \to \mathbb{F}_2^{2n}$ and G satisfy the hypotheses of Lemma 7, which provides the consequence that G is a valid Gram matrix for the hypergraph (V, H), as defined

in [TLC22a, page 8]. In particular, the following second condition for a valid Gram matrix holds, for all hyperedges h in H and all vertices $1 \le v \le |V|$:

$$\sum_{i \in h} G_{i,v} = 0. \tag{6}$$

In matricial form this system of linear equations is Equation (5).

Conversely, the fact that Equation (5) implies the existence of a Pauli assignment is justified after presenting the algorithm in Section 4.1, which constructs such a Pauli assignment α of (V, H, G) from the anticommutation matrix G.

It is sometimes more convenient and more pictorial to express the assignability condition by using the language of graphs, as in the following theorem.

Theorem 9. A hypergram (V, H, G) admits a Pauli assignment if and only if, for each vertex $v \in V$, each hyperedge $h \in H$ contains an even number of vertices which are adjacent to v in the graph (V, G).

In other words, this *graphical assignability condition* requires that each vertex anticommutes with an even number of vertices of each hyperedge. Since all the vertices in a hyperedge mutually commute, it is sufficient to consider the vertices not belonging to the hyperedge.

Proof. Equation (5) is an algebraic form of the graphical assignability condition. Indeed, consider the entry $(H \cdot G)_{h,v}$ at row h and column v in the product of the matrices H and G. Each 1 in this sum is the product of a 1 entry in the matrix H, meaning that some vertex i is in the hyperedge h, and a 1 entry in the matrix G, meaning that this vertex i anticommutes with v. The sum of these 1s as natural numbers would be the number of such vertices i in h anticommuting with v. The sum being computed over \mathbb{F}_2 , it is zero as required in Equation (6) if and only if this number is even.

Example 4 (continued). In our example where $G = \{\{v_3, v_5\}\}$ the vertex v_5 anticommutes with v_3 and commutes with v_1 and v_2 , so it anticommutes only with one vertex in the first hyperedge $\{v_1, v_2, v_3\}$. By Theorem 9, the hypergram S is not assignable.

Corollary 10. For all assignable hypergrams (V, H, G),

$$|V| \le 2^{rk(ker(H))} - 1. \tag{7}$$

Proof. Direct consequence of the assignability condition and the fact that (V, G) is a reduced graph: G has no line of zeros and no duplicated columns. So, each column of G is a distinct vector in the null space of G. The lhs of the inequality (7) is the number of columns of G. Its rhs is the number of non-null vectors in the kernel space of G.

4.1 Pauli-labeling Algorithm

Let (V, H, G) be a hypergram whose set of vertices $V = \{1, ..., |V|\}$ is totally ordered by <. From V and the anticommutation matrix G, Algorithm 1 modifies a copy B of the input matrix G until reaching the null matrix, as in the algorithm left implicit in the proof of Lemma 8.9.3 in [GR01]. Moreover, Algorithm 1 computes and returns a function $\alpha: V \to \{I, X, Y, Z\}^{\otimes n}$ that labels all the vertices in V with n-qubit observables. It also returns the number n of qubits in these labels.

Algorithm 1 Pauli Assignment from an Anticommutation Matrix *G* on the Set of Vertices *V*

```
1: function PauliAssignmentFromAnticommutations(V, G)
          n \leftarrow 0
 2:
          B \leftarrow G
 3:
 4:
          while i, j \leftarrow \text{FindOverdiagonalOne}(B) do
 5:
               n \leftarrow n + 1
               for k \in V do
 6:
                    \alpha(k)_n \leftarrow \psi^{-1}\left(B_{k,i}, B_{k,j}\right)
 7:
 8:
               B \leftarrow B + B \cdot e_i \cdot (B \cdot e_i)^T + B \cdot e_i \cdot (B \cdot e_i)^T
 9:
          end while
10:
          return \alpha, n
11:
12: end function
```

Calling the function FindOverdiagonalOne on Line 4 either returns vertices i and j such that i < j and $B_{i,j} = 1$, or false when no such pair of vertices exists, which ends the loop. For any vertex $k \in V$ and $1 \le s \le t \le n$, let $\alpha(k)_s$ denote the s-th qubit of $\alpha(k)$ and $\alpha(k)_{s..t}$ denote its sequence of qubits from the s-th one to the t-th one included. For $n \ge 1$ the assignment on Line 7 computes at the n-th iteration of Algorithm 1 the n-th Pauli matrix $\alpha(k)_n$ of the label $\alpha(k)$ of all vertices $k \in V$, by using the inverse ψ^{-1} of the encoding function ψ defined by (2).

For $m \in V$, let e_m denote the m-th standard basis vector. Then $B \cdot e_m$ is the m-th column of B and $e_l^T \cdot B \cdot e_m = B_{l,m}$ is its entry at row l in this column. On Line 9 the i-th and j-th columns of the matrix B are used to add zeros in B, as detailed in Section 4.2.1.

4.2 Justification

When Equation (5) holds, the present section shows that the labeling α returned by PauliAssignmentFromAnticommutations(V,G) is a Pauli assignment of the hypergram (V,H,G), thus completing the proof of Theorem 8. More precisely, Section 4.2.1 justifies the commutation condition, Section 4.2.3 justifies that the labels according to α are pairwise distinct and different from the identity and Section 4.2.4 justifies the product condition under a condition on the rank of G proved in Section 4.2.2.

In all that follows, when there is no risk of confusion, the function ψ is often omitted, for instance when writing $\langle \alpha(l) \mid \alpha(m) \rangle$ instead of $\langle \psi(\alpha(l)) \mid \psi(\alpha(m)) \rangle$ in Equation (8).

4.2.1 Commutation condition

The following lemma provides a key argument for the commutation condition. A loop invariant is a property which is true before the loop and is preserved by each iteration of the loop. Consequently, it also holds after the loop.

Lemma 11. *The formula*

$$\forall l, m \in V. B_{l,m} = G_{l,m} + \langle \alpha(l) \mid \alpha(m) \rangle \tag{8}$$

is an invariant for the loop of Algorithm 1.

Proof. For $n \ge 1$, let $B^{(n-1)}$ denote the value of the matrix B at the beginning of the n-th iteration of Algorithm 1, just before Line 5. Consequently, $B^{(n)}$ denotes the value of B at the end of the n-th iteration, just after Line 9. In particular, $B^{(0)} = G$.

The notation $\alpha(l)$ in (8) stands for $\alpha(l)_{1..n}$ at Line 9. Its value when n=0 can be chosen constant, so that $\langle \alpha(l) \mid \alpha(m) \rangle = 0$ before the loop. Thus (8) is initially true, because B=G before the loop. It remains to prove that (8) is preserved by the assignment on Line 9, under the assumption

$$\alpha(k)_n = \psi^{-1} \left(B_{k,i}^{(n-1)}, B_{k,j}^{(n-1)} \right)$$
(9)

coming from Line 7, equivalent to

$$\psi(\alpha(k))_{2n-1} = B_{k,i}^{(n-1)}$$
 and $\psi(\alpha(k))_{2n} = B_{k,j}^{(n-1)}$ (10)

for all vertices *k*. This preservation is justified by the following sequence of equalities:

$$\begin{split} B_{l,m}^{(n)} &= B_{l,m}^{(n-1)} + \left(B^{(n-1)} \cdot e_i \cdot (B^{(n-1)} \cdot e_j)^T + B^{(n-1)} \cdot e_j \cdot (B^{(n-1)} \cdot e_i)^T \right)_{l,m} \\ &= B_{l,m}^{(n-1)} + \left(B^{(n-1)} \cdot e_i \cdot (B^{(n-1)} \cdot e_j)^T \right)_{l,m} + \left(B^{(n-1)} \cdot e_j \cdot (B^{(n-1)} \cdot e_i)^T \right)_{l,m} \\ &= B_{l,m}^{(n-1)} + B_{l,i}^{(n-1)} B_{m,j}^{(n-1)} + B_{l,j}^{(n-1)} B_{m,i}^{(n-1)} \\ &= B_{l,m}^{(n-1)} + \psi(\alpha(l))_{2n-1} \psi(\alpha(m))_{2n} + \psi(\alpha(l))_{2n} \psi(\alpha(m))_{2n-1} \end{aligned} \qquad \text{by (10)}$$

$$= B_{l,m}^{(n-1)} + \left\langle \psi(\alpha(l)_n) \mid \psi(\alpha(m)_n) \right\rangle \qquad \text{by (1)}$$

$$= B_{l,m}^{(0)} + \left\langle \psi(\alpha(l)_1) \mid \psi(\alpha(m)_1) \right\rangle + \dots + \left\langle \psi(\alpha(l)_n) \mid \psi(\alpha(m)_n) \right\rangle \qquad \text{by induction on } n$$

$$= G_{l,m} + \left\langle \psi(\alpha(l)_{1..n}) \mid \psi(\alpha(m)_{1..n}) \right\rangle,$$

so (8) is an invariant of the loop.

It is easy to check similarly that the symmetry of B and its diagonal of zeros are two other loop invariants. All these invariants still hold after the loop, together with the negation of the loop condition. So, at the end of the algorithm, B is the null matrix and thus $G_{l,m} = \langle \alpha(l) \mid \alpha(m) \rangle$ for all vertices l and m, meaning that the returned labeling $\alpha: V \to \{I, X, Y, Z\}^{\otimes n}$ satisfies the commutation condition.

4.2.2 Rank and number of qubits

The following lemma establishes the relation r = 2n between the rank r of G and the number n of qubits of the labeling generated by the algorithm. It could be justified in one sentence saying that it is the first conclusion of Theorem 8.10.1 in [GR01], but, in order to make the paper self-contained, we prefer to provide a proof of it, with our notations and more details. This proof is strongly inspired by that of Lemma 8.9.3 in the same reference [GR01].

Lemma 12. The rank of the matrix G is twice the number n of iterations returned by the application PauliAssignmentFromAnticommutations(V, G) of Algorithm 1 to V and G.

Proof. It is sufficient to show that each execution of Line 9 reduces the rank rk(*B*) of *B* by two, since the rank of the final null matrix *B* is zero.

Let A be B just before Line 9, $y = A \cdot e_i$ and $z = A \cdot e_j$ be the i-th and j-th columns of A and $C = y \cdot z^T + z \cdot y^T$ be the matrix subtracted to A to update B on Line 9. Since $A_{i,j} = 1$ and $A_{i,i} = A_{j,j} = 0$, the i-th column of C is the i-th column of A, the $A_{i,i} = A_{i,j} = 0$ and the other columns of $A_{i,i} = A_{i,j} = 0$ and the other columns of $A_{i,i} = A_{i,j} = 0$ and the other columns of $A_{i,i} = A_{i,j} = 0$ and the other columns of $A_{i,i} = A_{i,j} = 0$ and the other columns of $A_{i,i} = A_{i,j} = 0$ and the other columns of $A_{i,i} = A_{i,j} = 0$ and the other columns of $A_{i,i} = A_{i,j} = 0$ and the other columns of $A_{i,i} = A_{i,j} = 0$ and the other columns of $A_{i,i} = A_{i,j} = 0$ and $A_{i,i} = A_{i,i} = A_{i,i} = 0$ and $A_{i,i} = A_{i,i} = A_{i,i}$

Since A = B + C after Line 9, the m-th column of A is a linear combination of the m-th column of B and the i-th and j-th columns y and z of A. So, the column space of A is spanned by the union of the columns of B with the vectors y and z, so $\operatorname{rk}(A) \le \operatorname{rk}(B) + 2$.

Altogether, rk(B) = rk(A) - 2, which ends the proof.

4.2.3 Image conditions

The anticommutation matrix G is the Gram matrix of the function $\psi \circ \alpha$. If α is not injective, then there are two distinct vertices v and v' such that $\psi(\alpha(v)) = \psi(\alpha(v'))$ and the corresponding rows in G are equal. Similarly, if $\alpha(v) = I^{\otimes n}$ for some vertex v, then $\psi(\alpha(v)) = 0 \in \mathbb{F}_2^{2n}$ and the corresponding row in G is a row of zeros. Since the anticommutation graph (V, G) is reduced (by definition of a hypergram), its adjacency matrix G has no duplicated rows and no row of zeros, so α is injective and its image is included in $\{I, X, Y, Z\}^{\otimes n} - \{I^{\otimes n}\}$.

4.2.4 Product condition

Finally, the product condition is also respected, since α satisfies all the hypotheses of the following lemma.

Lemma 13. Let (V, H, G) be an assignable hypergram with $V = \{1, ..., |V|\}$. Let r be the rank of G and n = r/2. Let $\alpha : V \to \{I, X, Y, Z\}^{\otimes n}$ be a vertex labeling with n-qubit observables satisfying the commutation condition $\langle \alpha(i) | \alpha(j) \rangle = G_{i,j}$ for all vertices $1 \le i, j \le |V|$. Then α satisfies the product condition $\prod_{v \in h} \alpha(v) = \pm I^{\otimes n}$ for all hyperedges $h \in H$.

Proof. By the correspondence with symplectic polar spaces (Section 2.2) it is equivalent to prove that $\sum_{v \in h} \alpha(v) = 0$ for the null vector 0 in \mathbb{F}_2^{2n} . As already mentioned in the proof of Theorem 8, the commutation condition for α entails that G is the Gram matrix of α . Let $b = (c_1, \ldots, c_r)$ be composed of r columns of G and forming a basis of the vector space span(G) spanned by the columns of G. By Lemma 7 applied to the tuple of vectors $(\alpha(v))_{v \in V}$, to their Gram matrix G and to the subset of vectors in B, the corresponding vectors $\alpha(v_1), \ldots, \alpha(v_r)$ are linearly independent vectors in \mathbb{F}_2^{2n} . By Lemma 12, $r = 2n = \dim(\mathbb{F}_2^{2n})$, so these vectors form a basis of \mathbb{F}_2^{2n} .

For $1 \le \overline{j} \le r$, we have on the one hand

$$\sum_{v \in h} G_{v,v_j} = \sum_{v \in h} \left\langle \psi(\alpha(v)) \mid \psi(\alpha(v_j)) \right\rangle \qquad \text{(by the commutation condition)}$$

$$= \left\langle \sum_{v \in h} \psi(\alpha(v)) \mid \psi(\alpha(v_j)) \right\rangle \qquad \text{(by linearity of the symplectic product)}.$$

On the other hand, $\sum_{v \in h} G_{v,v_i} = 0$ by the assignability condition (6). So

$$\left\langle \sum_{v \in h} \alpha(v) \mid \alpha(v_j) \right\rangle = 0 \tag{11}$$

for all the vectors of the basis $(\alpha(v_i))_{1 \le j \le r}$, which is possible only if $\sum_{v \in h} \alpha(v) = 0$.

4.3 Algorithmic complexity

Multiple methods in [TLC22a, Theorem 8] are suggested for generating labelings, including searching subgraphs of the graph of the whole symplectic space, or using backtracking techniques. None of them is polynomial. However, a recent work [ZPL24, Theorem 2] describes a polynomial algorithm for finding such a labeling, but at the cost of not guaranteeing that the resulting labeling has the smallest possible number of qubits, since it is equal to the number of anticommuting pairs in an independent set of vectors of the Gram matrix. For example, an independent set of the doily being a set of five vectors, the algorithm will return a labeling with at least five qubits, while our algorithm returns a labeling with only two qubits.

The algorithm presented in Section 4.1 is polynomial, with a complexity in $O(|V|^3)$, and provides a labeling with the minimal number of qubits. This is first because the number of iterations of the loop in Algorithm 1 is at most |V|/2 for a G of full rank. Then, inside this loop, the assignment of the matrix B on Line 9 is more costly than the inner loop on Line 6, because the matrix assignment is done in $O(|V|^2)$, while the inner loop is done in O(|V|).

4.4 Contextuality degree of an assignable hypergram

By Theorem 8 all assignable hypergrams admit a Pauli assignment. By Theorem 5 all these assignments have the same degree of contextuality. Putting everything together we propose the following notion of degree for any assignable hypergram.

Definition 14 (Contextuality degree of an assignable hypergram). Let (V, H, G) be an assignable hypergram, n = rk(G)/2 be half the rank of G (known to be even) and α be the vertex labeling from V to $\{I, X, Y, Z\}^{\otimes n} - \{I^{\otimes n}\}$ computed by the algorithm PauliAssignmentFromAnticommutations(V, G). Let $\text{sgn}_{\alpha}: H \to \{-1, 1\}$ be its sign function, defined by $\Pi_{v \in h} \alpha(v) = \text{sgn}_{\alpha}(h) I^{\otimes n}$ for all hyperedges h in H. The (contextuality) degree of an assignable hypergram (V, H, G) is the minimal Hamming distance between the sign function sgn_{α} and the sign function sgn_{α} of any classical assignment $a: V \to \{-1, +1\}$ of its vertices, defined by $\text{sgn}_{a}(h) = \Pi_{v \in h} a(v)$ for all hyperedges h in H

5 Generalization of former results

When the contextuality degree of some n-qubit Pauli assignment of some hypergram is known, the contextuality degree of all N-qubit Pauli assignments of the same hypergram is also known for all the numbers of qubits $N \ge n$, because Theorem 5 asserts that all these degrees have the same value. So, all contextuality degree results established in former work (e.g., [Mul+24; Mul+25]) only for $n \le N \le n'$ for some small number of qubits n', indeed hold by Theorem 5 without limit for all $N \ge n$. Moreover, instead of being obtained as in [Mul+24; Mul+25] after long computations considering all possible Pauli assignments for all the values of N in this interval [n,n'], they can now be obtained much more efficiently, by considering only one Pauli assignment of the hypergram they share in common, with the smallest number of qubits n. This section revisits with this larger point of view several former results about the contextuality degree of multi-qubit quantum configurations.

Moreover, as announced in Section 2.3, we illustrate here with examples how the anticommutation relation G added in our framework of hypergrams (V, H, G) to the hypergraph (V, H) of usual quantum configurations opens the door to a much wider range of cases. To clarify this widening, we classify the quantum configurations studied in former works [TLC22a; de +22; Mul+24] into two families. The first family is composed of all the structures whose hypergram (V, H, G) satisfies $G = \operatorname{cplt}(H)$, where $\operatorname{cplt}(H)$ is the anticommutation graph of the hypergraph H. In other words, in this case, two observables are in the same context if and only if they commute. The second family is composed of all the other structures, where $G \subseteq \operatorname{cplt}(H)$. In other words, in this case, some commuting pairs of observables are absent in all contexts.

Each following subsection is devoted to a particular category of quantum configurations.

5.1 1-spaces

This section is about quantum configurations whose contexts are totally isotropic subspaces with the projective dimension 1, also called 1-spaces or lines. Their underlying hypergram belongs to the first family.

For each number of qubits $n \ge 2$, let L_n be the quantum configuration whose contexts are **all** the lines of W_n . For instance, L_2 is the 2-qubit doily. The number of observables in L_n is $2^{2n} - 1$. Its number of contexts is

$$\frac{(4^n - 1)(4^{n-1} - 1)}{3}. (12)$$

Its number of negative contexts [Cab10] is

$$\frac{1}{6} \sum_{c=0}^{n-2} \sum_{a,b} 3^{2n-a-b-2c} \binom{n}{c} \binom{n-c}{a} \binom{n-c-a}{b}. \tag{13}$$

For $n \le 7$, these numbers are respectively given in this order in the second, third and four column of Table 1. Its last two columns gathers the results from Tables 1 and 3 in [Mul+25], up to seven qubits. We present here neither better bounds for the contextuality degree d nor a speedup for the computation time of its upper bounds (displayed in the last column), obtained by the heuristic method presented in [Mul+25], run on a machine with a 5.4 GHz P-cores and 4.3 GHz E-cores Intel Core i9-13900K processor. These computations use less than 1.3 Gb out of 64 Gb of RAM. What is new here is the **interpretation** of these data, detailed in the following paragraph.

п	# obs.	# contexts	# neg. contexts	Value or bounds for <i>d</i>	Duration
2	15	15	3	3	0.01 s
3	63	315	90	63	0.1 s
4	255	5 355	1908	$1071 \le d \le 1575$	0.1 s
5	1 023	86 955	35 400	$17391 \le d \le 31479$	1 s
6	4 095	1 396 395	615 888	$279279 \le d \le 553140$	2 mn
7	16 383	22 362 795	10 352 160	$4472559 \le d \le 9405663$	1 h 34 mn

Table 1: Dimensions, exact values (for n = 2,3) or bounds (for $n \ge 4$) for the contextuality degree d of quantum configurations in W_N (for all $N \ge n$) isomorphic to the quantum configuration L_n whose contexts are all the lines of W_n .

Each row in Table 1 not only concerns L_n , but also all the quantum configurations isomorphic to L_n whose contexts are distinct lines of a symplectic space W_N for some $N \ge n$. Of course, when N > n, these quantum configurations do not contain **all** the lines of W_N , and their numbers of negative contexts can differ from that of L_n . However, Theorem 5 guarantees that all of them have the same contextuality degree, whose value is either exactly given or bounded in the fifth column of Table 1, for $2 \le n \le 7$.

It was already known that the contextuality degree of all n-qubit doilies is 3, for $n \ge 2$. This was formerly proved by computing this degree for the 12 possible configurations of their negative lines [Mul+22]. A direct consequence of Theorem 5 is a much simpler proof, which does not rely on such an enumeration, but justifies only that the contextuality degree of the 2-qubit doily is 3.

In the same way, it is known that the contextuality degree of L_3 (all the 3-qubit lines) is 63 and that there is a minimal subset of unsatisfied hyperedges isomorphic to the split Cayley hexagon of order two [Mul+24]. By Theorem 5 the contextuality degree of all quantum configurations isomorphic to L_3 (i. e., having the same underlying hypergram as it) labeled by N-qubit observables with $N \ge 3$ is also 63. Moreover, by Lemma 4, all these configurations share the same subset of unsatisfied hyperedges. So, we now know that one of the minimal subsets of unsatisfied hyperedges in any Pauli assignment of L_3 by N-qubit observables with $N \ge 3$ is isomorphic to the split Cayley hexagon of order two.

5.2 Two-spreads

The case of two-spreads is of interest because all the two-spreads considered up to now in relation with contextuality [Mul+24] are small magic sets whose underlying hypergram S_{2s} belongs to the second family, as detailed in Example 2.

For $n \ge 2$, it is known that all n-qubit two-spreads are contextual, and that their contextuality degree is 1 [Mul+24, Proposition 7]. The proof of this proposition in [Mul+24] relies on the fact that two-spreads feature an odd number of negative contexts. The latter fact relies on a careful inspection of $72 = 6 \cdot 12$ possible configurations of their negative lines, obtainable by removing one of its 6 spreads of lines from one of the 12 possible configurations of negative lines in an n-qubit doily. Thanks to Theorem 5, we provide here the following much simpler proof of a similar proposition about two-spreads, more precise by expliciting its underlying hypergram.

Proposition 15. The contextuality degree of all n-qubit labelings of the two-spread hypergram S_{2s} is 1.

Proof. As a point-line geometry, disregarding line signs, any n-qubit two-spread is isomorphic to the two-spread of the 2-qubit doily presented in Example 2 and represented in Figure 1. The latter contains only one negative line, so its contextuality degree d is at most 1. Moreover, it is a magic set, which implies that it is contextual [HS17], so $d \ge 1$. Consequently, d = 1, and by isomorphism and Theorem 5, the contextuality degree of all n-qubit two-spreads whose underlying hypergram is S_{2s} is also 1. □

In order to illustrate the impact of the anticommutation graph on contextuality, the following example presents a non-contextual two-spread embeddable in W_3 .

Example 5. Let us consider the hypergram $S' = (V_{2s}, H_{2s}, G')$, variant of the two-spread hypergram $S_{2s} = (V_{2s}, H_{2s}, G_{2s})$, with the same underlying hypergraph (V_{2s}, H_{2s}) but the anticommutation graph $G' = \{\{1,5\}, \{1,7\}, \{1,8\}, \{1,9\}, \{1,12\}, \{1,15\}, \{2,5\}, \{2,8\}, \{2,10\}, \{2,11\}, \{2,12\}, \{3,7\}, \{3,9\}, \{3,10\}, \{3,11\}, \{3,15\}, \{4,5\}, \{4,7\}, \{4,10\}, \{4,11\}, \{4,13\}, \{4,14\}, \{5,11\}, \{5,12\}, \{6,7\}, \{6,8\}, \{6,12\}, \{6,13\}, \{6,14\}, \{7,8\}, \{7,10\}, \{7,13\}, \{7,15\}, \{8,9\}, \{8,11\}, \{9,11\}, \{9,12\}, \{9,13\}, \{10,12\}, \{10,14\}, \{11,14\}, \{11,15\}, \{12,13\}, \{12,14\}, \{14,15\}$ different from G_{2s} . Whereas S_{2s} is contextual, with degree 1, this variant S' is not contextual. This hypergram S' and its 3-qubit labeling produced by Algorithm 1 are presented in Figure 3. This two-spread labeling is a genuine three-qubit two-spread, which lives in W_3 but can be found neither in W_2 nor in a doily of W_3 .

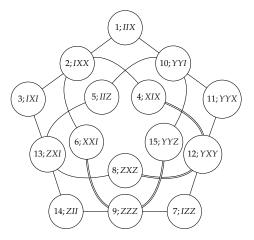


Figure 3: Illustration of the non-contextual hypergram $S' = (V_{2s}, H_{2s}, G')$ sharing the same underlying hypergraph (V_{2s}, H_{2s}) as the two-spread hypergram S_{2s} , but with a different anticommutation graph G'. The vertices are represented by the numbers from 1 to 15. The hyperedges are represented by the lines. The two negative lines are represented by the double lines. The anticommutation graph G' is not shown here to keep the figure readable.

5.3 Other quantum configurations

Other quantum configurations studied in former work include k-spaces for $k \ge 2$, Mermin-Peres squares and quadrics. They all belong to the first family. As for the elliptic and hyperbolic quadrics, they belong to the first family by definition, because their lines contain all the lines passing through the corresponding points satisfying their corresponding quadratic form.

Using an optimization algorithm, Saniga, Holweck, Kelleher and we [Mul+25] have found upper bounds for the degree of contextuality of all hyperbolic and elliptic quadrics of W_n , for $4 \le n \le 7$. For n = 4, this upper bound is 315 and is the same for hyperbolic and elliptic quadrics. For n = 5, the bounds for elliptic and hyperbolic quadrics respectively are 7 087 and 6975. For n = 6, they respectively are 131 700 and 132 391. For n = 7, they respectively are

2294580 and 2331191. While there are numerous different hyperbolic and elliptic quadrics in W_n , all hyperbolic (resp. elliptic) quadrics with the same number n of qubits share the same hypergram. So, by Theorem 5, they all have the same degree, and it is sufficient to estimate it for one of them. This property has been exploited in our former work [Mul+25] to dramatically reduce the computation effort.

6 Related work

This section details in what sense our results can be considered as extensions or improvements of results from [TLC22a], with an emphasis on the algorithmic point of view.

We start by recalling some definitions from [TLC22a]. An Eulerian hypergraph $\mathcal{H}=(V,H)$ is a hypergraph whose vertices are in an even number of distinct hyperedges. A Pauli-based assignment is defined in [TLC22a] as a **magic** assignment $\alpha:V\to \mathcal{P}^{\otimes n}$ whose values are in the n-qubit Pauli group. A magic assignment satisfies the condition $\prod_{v\in h}\alpha(v)=-I$ for an odd number of hyperedges $h\in H$, hereafter called the *oddness condition*.

Our Theorem 5 and its proof are similar to Proposition 14 of [TLC22a] and its proof, but it holds for all Pauli assignments, our more general notion than Pauli-based assignments in [TLC22a], free of its unnecessary oddness condition (odd number of negative hyperedges). It also holds under one less assumption on the hypergraph, that we do not assume to be Eulerian, i. e., it is not necessarily for each vertex to be in an even number of distinct hyperedges. With three lines incident to each vertex the doily is a significant example without this property. Pauli assignments admit two restrictions not present in [TLC22a]: they are injective and assign only Pauli observables with phase 1. However these restrictions can be considered as technical details that do not significantly weaken the results: duplicating labels would have no interest, there are already plenty of interesting phase-free assignments to study and all examples in [TLC22a] and other work only consider vertices labeled by phase-free Pauli observables.

Finally, our claim that the labeling α returned by PauliAssignment From Anticommutations (V, G) is a Pauli assignment and its justification (in Section 4.2) are a generalization of Proposition 5 in [TLC22a] and its proof, because here the hypergraph (V, H) is again not assumed to be Eulerian. Moreover, from the algorithmic point of view, our polynomial Algorithm 1 is more efficient than the two approaches mentioned in [TLC22a], the first one being a search for subgraphs of the graph of the whole symplectic space, and the second one using backtracking techniques. Both of them have an exponential complexity: first in the number of vertices because of the nature of the algorithms used, and second in the number of qubits because of the exponentially growing size of the symplectic space W_n .

7 Conclusion

The notion of assignable hypergram proposed in this paper can not only be attached an abstract notion of contextuality degree, as detailed here, but characterizes an exploration space where original state-independent Kochen-Specker proofs can be looked for. Finding efficient ways to explore that space is the main perspective. A preliminary perspective is to add criteria to reduce the size of the space and orient the search.

The proposed framework includes the well-known magic sets, but is much wider. Magic sets are attractive notably because their contextuality can be proved by a simple human reasoning. However they have restrictions that we show here to be unnecessary for the existence of Pauli assignments, such as the oddness condition. When considering more general objects, we accept to loose the nice property of a simple proof of contextuality and to rely on software to decide contextuality and to compute bounds for the contextuality degree, as in [Mul+24].

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Author declarations

Conflict of Interest. The authors have no conflicts to disclose.

Author contributions. Axel Muller: Conceptualization; Software (main developer); Writing (50%). Alain Giorgetti: Methodology; Software (advice); Supervision; Writing (50%).

Data Availability Statement

The data that support the findings of this study are openly available in https://github.com/quantcert/quantcert.github.io/releases/tag/v1.2.0.

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