

# Entanglement and nonclassical properties of hypergraph states

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**Abstract.** Hypergraph states are multi-qubit states that form a subset of the locally maximally entangleable states and a generalization of the well-established notion of graph states. Mathematically, they can conveniently be described by a hypergraph that indicates a possible generation procedure of these states; alternatively, they can also be phrased in terms of a non-local stabilizer formalism. In this paper, we explore the entanglement properties and nonclassical features of hypergraph states. First, we identify the equivalence classes under local unitary transformations for up to four qubits, as well as important classes of five- and six-qubit states, and determine various entanglement properties of these classes. Second, we present general conditions under which the local unitary equivalence of hypergraph states can simply be decided by considering a finite set of transformations with a clear graph-theoretical interpretation. Finally, we consider the question whether hypergraph states and their correlations can be used to reveal contradictions with classical hidden variable theories. We demonstrate that various noncontextuality inequalities and Bell inequalities can be derived for hypergraph states.

## 1. Introduction

The study of multiparticle entanglement has attracted much attention in the last years. From the theoretical side, multiparticle entanglement may be a key element to improve various applications like quantum information processing or quantum metrology, or to understand and simulate physical systems, such as quantum spin chains undergoing a quantum phase transition. From the experimental side, the generation and certification of the various interesting multiparticle states poses tremendous challenges, but it offers the opportunity to demonstrate the advances in controlling and manipulating physical systems at the quantum level.

Since the dimension of the Hilbert space grows exponentially with the number of particles, it has turned out to be fruitful to identify families of multiparticle states which allow for a simple description with few parameters. Such a simple description may, for instance, originate from the symmetries of the states under scrutiny. In fact, many cases are known where various symmetries allow the solution of problems in quantum information theory that are not yet solved in the general case.

One interesting family of multi-qubit states that has attracted a lot of attention in the last ten years are the so-called graph states [1, 2]. These states are of importance in various applications of quantum information processing, such as measurement-based quantum computation and quantum error correction. Apart from their relevance for applications, they have a simple description in terms of graphs: Starting from an arbitrary graph (that is, a set of vertices with edges connecting them), one can generate the graph states from a product state by applying entangling quantum operations on the connected vertices. In addition, graph states can also be described as eigenstates of a set of commuting local observables, the so-called stabilizer. Due to their importance and their simple mathematical description, the entanglement properties of graph states have intensively been studied. For instance, different entanglement classes of graph states up to eight qubits have been identified [2, 3], their entanglement properties have been discussed [4–6] and purification protocols have been provided [7, 8]. The stabilizer formalism for graph states has turned out to be a very useful tool to develop Bell inequalities or Kochen-Specker arguments [9–11]. Interestingly, this was known already long before the mathematical formulation of graph states was given.

A possible generalization of graph states are the locally maximally entangleable (LME) states. Their notion goes back to the study for which multi-qubit states there is a local interaction with local auxiliary systems, so that after this operation all the auxiliary systems are maximally entangled with the initial qubits. States with this property are called LME states, and they have been characterized in Ref. [12]. It has turned out that they can be generated similarly to graph states from a product state with simple interactions (parameterized with a phase  $\varphi$ ), but in this case also interactions between three or more particles are needed. Mathematically, they are distinguished by the fact that they still can be described by a stabilizer of commuting hermitian observables. In contrast to the usual graph states, however, the stabilizer observables are non-local, and not simple tensor products of Pauli matrices. The usual graph states mentioned above belong to the family of LME states. For them, only two-qubit interactions with a phase  $\varphi = \pi$  are required. The states with multi-qubit interactions but still a restricted phase of  $\varphi = \pi$  are called  $\pi$ -LME states or hypergraph states. As noted in Refs. [13, 14] these states have a simple description in terms of more general objects than graphs, the so-called hypergraphs, which has motivated the name. In a hypergraph, one edge is allowed to connect any number of vertices, so there are also edges with three, four, or more vertices. Hypergraph states occur naturally in the analysis of quantum algorithms such as the Deutsch-Jozsa algorithm and the Grover algorithm [14, 15]. Despite their simple and elegant description, and in contrast to graph states, hypergraph states can be

complex in the sense of Kolmogorov complexity, so they could, for instance, be used for quantum fingerprinting protocols [16]. Moreover, entanglement purification protocols for these states have been developed [8]. All these facts support the conjecture that hypergraph states can be a good test-bed to explore the subtleties of multiparticle entanglement.

In this paper, we investigate the entanglement properties of hypergraph states. First, we ask for which cases different hypergraphs lead to locally equivalent hypergraph states. By locally equivalent we mean that the two states are connected with a local unitary transformation, that is a local change of the basis. Consequently, all their entanglement properties are the same. For graph states, it is already known that different graphs can lead to locally equivalent states, and a significant effort has been devoted to the characterization of the equivalence classes [1, 3–5]. We extend here this approach to hypergraph states. We first provide all entanglement classes for up to four qubits, as well as special classes for up to six qubits. Then, we derive some general conditions, under which the quest for local unitary equivalence can be simplified by considering local Pauli operations only. In the second part of the paper, we ask, whether the non-local stabilizer formalism of hypergraph states can be used to develop arguments that discriminate between quantum physics and classical hidden-variable theories. First, we show that a similar argument to the one by Greenberger, Horne and Zeilinger (GHZ) can be developed for the non-local stabilizer. Based on this, various novel noncontextuality inequalities and Bell inequalities can be developed. Finally, we conclude and discuss possible extensions of our research.

## 2. Hypergraph states

In this section we review the notions of hypergraphs, hypergraph states and recall some of their basic properties. We stress that essentially all of the facts presented in this section have been shown before [8, 12–14, 17, 18]. However, in order to be self-contained we recall these results here. Finally, it may be useful that some of our proofs are significantly shorter than some of the existing proofs in the literature.

### 2.1. Properties of the controlled phase gate

Before defining hypergraph states it is useful to explain some properties of the controlled phase gates, as they play a central role in the definition of the states.

We consider a system of  $N$  qubits. We denote by  $e = \{i_1, \dots, i_n\}$  a subset of  $n$  qubits. Then, the controlled phase gate on the set  $e$  is the unitary transformation given by the matrix

$$C_e = \mathbb{1} - 2|1\dots1\rangle\langle 1\dots1| \quad (1)$$

In other words,  $C_e$  is a diagonal  $2^n \times 2^n$  matrix in the standard basis with all entries equal to 1 except from the last one, which has the value  $-1$ . Clearly, this transformation is invariant under permutation of the qubits and it fulfills  $(C_e)^2 = \mathbb{1}$ . For a single qubit,

$C_{\{i\}} = \sigma_z$  equals a Pauli matrix. Furthermore, in order to formulate general formulae later, if  $e = \emptyset$  is an empty set we define  $C_\emptyset = -1$  as an overall negative sign. Finally, we will sometimes use the notation  $C_{ijk}$  instead of  $C_{\{i,j,k\}}$ .

For our purposes it is important to understand the relation of the controlled phase gate to the Pauli matrices. Here and in the following, we denote by  $X_k, Y_k, Z_k$  the Pauli matrices  $\sigma_x, \sigma_y, \sigma_z$  acting on the  $k$ -th qubit. The following Lemma presents two simple rules, which are relevant for many of the further calculations.

**Lemma 1.** *If  $k \in e$ , the following identities hold:*

$$X_k C_e X_k = C_e C_{e \setminus \{k\}} \quad (2)$$

$$C_e X_k C_e = X_k \otimes C_{e \setminus \{k\}} \quad (3)$$

In the following, we will refer to Eq. (2) as the *first rule* and to Eq. (3) as the *second rule*.

*Proof.* For Eq. (2) we can assume that  $e = \{1, 2, 3, \dots, n\}$  and  $k = 1$ . Then we have  $C_e = |0\rangle\langle 0| \otimes \mathbb{1} + |1\rangle\langle 1| \otimes C_{e \setminus \{k\}}$  and it follows that

$$\begin{aligned} X_k C_e X_k &= |1\rangle\langle 1| \otimes \mathbb{1} + |0\rangle\langle 0| \otimes C_{e \setminus \{k\}} = \mathbb{1} - 2|01 \cdots 1\rangle\langle 01 \cdots 1| \\ &= (\mathbb{1} - 2|11 \cdots 1\rangle\langle 11 \cdots 1|)(\mathbb{1} - 2|01 \cdots 1\rangle\langle 01 \cdots 1| - 2|11 \cdots 1\rangle\langle 11 \cdots 1|) \\ &= C_e (\mathbb{1} \otimes C_{e \setminus \{k\}}). \end{aligned} \quad (4)$$

For Eq. (3) we can apply the first rule to see that  $C_e X_k C_e = C_e X_k C_e X_k X_k = C_e C_e C_{e \setminus \{k\}} X_k = X_k \otimes C_{e \setminus \{k\}}$ .  $\square$

A more general commutation rule is the following:

**Lemma 2.** *Let  $e$  be a set of qubits,  $K \subseteq e$  a subset of  $e$ , and  $\mathcal{P}(K)$  the power set of  $K$  (that is, the set of all subsets of  $K$ , including the empty set). Then we have*

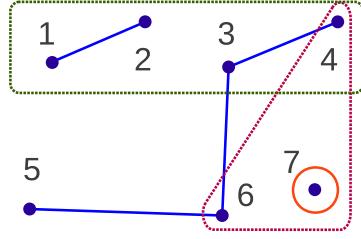
$$C_e \left( \bigotimes_{k \in K} X_k \right) = \left( \bigotimes_{k \in K} X_k \right) \left( \prod_{f \in \mathcal{P}(K)} C_{e \setminus f} \right) \quad (5)$$

Note that for  $K = e$  the operator  $C_{e \setminus K} = C_\emptyset = -1$  appears, so a sign occurs. Also, for  $K = e = \{k\}$  this is the usual commutator relation  $Z_k X_k = -X_k Z_k$ .

*Proof.* The proof works by induction in the number of elements in  $K$ . If  $K = \{k\}$  consists of only one element then Eq. (5) is nothing but a reformulation of Eq. (2). The induction step is straightforward.  $\square$

## 2.2. Hypergraphs and hypergraph states

Let us first explain the notion of hypergraphs. A hypergraph  $H = \{V, E\}$  consists of a set  $V = \{1, \dots, N\}$  of  $N$  vertices and a set  $E$  of edges connecting the vertices. In a usual graph, an edge connects only two vertices, that is, any  $e \in E$  is of the type  $e = \{i, j\}$  with  $i, j \in V$ . For hypergraphs, however, also edges connecting any number



**Figure 1.** Example of a hypergraph with seven vertices. The graph has one one-edge  $\{7\}$ , four two-edges  $\{1,2\}, \{3,4\}, \{3,6\}$ , and  $\{5,6\}$ , one three-edge  $\{4,6,7\}$ , and one four-edge  $\{1,2,3,4\}$ .

of vertices are allowed and a general edge is just a subset of  $V$ . Note that the set of all possible hypergraphs is significantly larger than the set of all graphs: for  $N$  vertices, there are  $2^{N(N-1)/2}$  standard graphs, but there are  $2^{2^N}$  hypergraphs. This implies that hypergraph states can be complex in the sense of Kolmogorov complexity. An example of a hypergraph is given in Fig. 1.

Some more terminology is in order here. The cardinality  $k$  of an edge is the number of vertices within this edge; we also speak of a  $k$ -edge. We call a hypergraph uniform of cardinality  $k$ , or  $k$ -uniform, if all edges are  $k$ -edges. Furthermore, the neighborhood of a vertex  $i$  consists of all vertices which are connected with  $i$  via some edge. Finally, we denote by  $E(i)$  the set of all edges  $e \in E$  with  $i \in e$ .

As for graph states, an  $N$ -qubit hypergraph state  $|H\rangle$  can be defined by association to a hypergraph of  $N$  vertices via the interaction history. Indeed, if one starts with a product state  $|\psi\rangle = |+\rangle^{\otimes N}$  (where  $|+\rangle = (|0\rangle + |1\rangle)/\sqrt{2}$  is the eigenstate of  $X$ ), and applies all the non-local unitaries  $C_e$  for all  $e \in E$ , one arrives at the hypergraph state,

$$|H\rangle = \prod_{e \in E} C_e |+\rangle^{\otimes N}. \quad (6)$$

That is, a hypergraph state is associated to a hypergraph, where each qubit corresponds to a vertex and each interaction  $C_e$  is present if the hyperedge  $e$  belongs to the associated hypergraph.

As in the case of graph states, a hypergraph state can also be defined via the stabilizer formalism. Starting from the stabilizer  $X_i$  of  $|+\rangle_i$ , and using that  $C_e^2 = \mathbb{1}$  and the rules in Lemma 1, one can define for each vertex  $i$  a stabilizing operator  $g_i$  as

$$g_i \equiv \left( \prod_{e \in E} C_e \right) X_i \left( \prod_{e \in E} C_e \right) = \left( \prod_{e \in E(i)} C_e \right) X_i \left( \prod_{e \in E(i)} C_e \right) = X_i \otimes \left( \prod_{e \in E(i)} C_{e \setminus \{i\}} \right) \quad (7)$$

From this definition one immediately sees that the stabilizers commute, since  $g_i g_j = (\prod_{e \in E} C_e) X_i X_j (\prod_{e \in E} C_e) = (\prod_{e \in E} C_e) X_j X_i (\prod_{e \in E} C_e) = g_j g_i$ . The  $g_i$  are traceless and form a maximal set of  $N$  commuting observables with eigenvalues  $\pm 1$ , hence there must be a common eigenbasis. More directly, the hypergraph state  $|H\rangle$  can be defined as the common eigenstate to all  $g_i$  with the eigenvalue  $+1$ ,

$$g_i |H\rangle = |H\rangle \quad \text{for all } i. \quad (8)$$

The other states in the eigenbasis can be defined by taking other possibilities as eigenvalues. The resulting  $2^N$  states are all orthogonal, and form the so-called hypergraph-state basis, which can be generated by successive application of Pauli  $Z$  transformations, that is  $|H_k\rangle \equiv |H_{k_1, \dots, k_N}\rangle = Z_1^{k_1} \otimes \cdots \otimes Z_N^{k_N}|H\rangle$ .

The definition of the stabilizing operators can be used to define the stabilizer as a group. Let us consider the set of  $2^N$  observables

$$\mathcal{S} = \{S_{\mathbf{x}}|S_{\mathbf{x}} = \prod_{i \in V} (g_i)^{x_i} \text{ with } \mathbf{x} \in \mathbb{Z}_2^N\}, \quad (9)$$

which consists of all products of the operators  $g_i$ .  $\mathcal{S}$  is an Abelian group with  $2^N$  elements, and for any element we have  $S_{\mathbf{x}}|H\rangle = |H\rangle$ . Furthermore, we can express the hypergraph state as

$$|H\rangle\langle H| = \frac{1}{2^N} \sum_{\mathbf{x} \in \mathbb{Z}_2^N} S_{\mathbf{x}} = \prod_{i=1}^N \frac{g_i + \mathbb{1}}{2}. \quad (10)$$

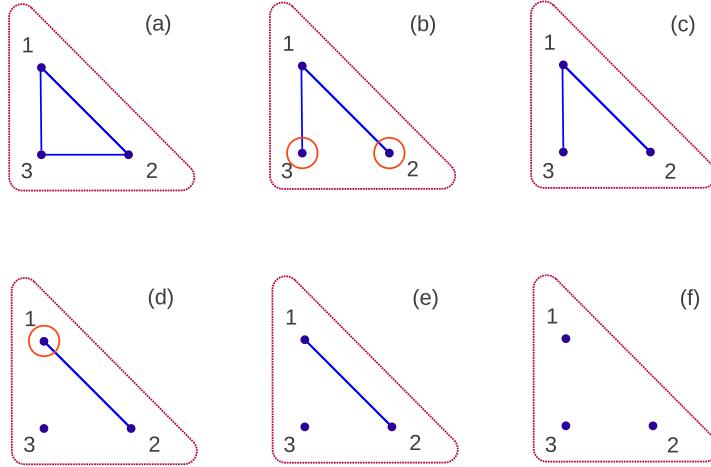
These formulas can directly be verified by using the fact that any product of the  $g_i$  is diagonal in the hypergraph-state basis. Such a result is, of course, well known for graph states. The only difference here is that for hypergraph states the stabilizer contains also nonlocal observables.

Before proceeding to a general discussion of the properties of hypergraph states it is useful to note that the set of edges  $E$  can also contain single vertex edges of the type  $e = \{k\}$ , but also the empty edge  $e = \emptyset$ . Such contributions will occur in the formulae in forthcoming discussion. These edges are, however, not relevant for the entanglement properties of the hypergraph state: An edge  $e = \{k\}$  corresponds to a local unitary transformation  $C_k = Z_k$  on the  $k$ -th qubit and the empty edge  $e = \emptyset$  induces a global sign shift on the state  $|H\rangle$ . Both transformations do not change any entanglement properties, so we will usually neglect the single-vertex edges and empty edge in the following.

As mentioned before, hypergraph states are a special case of the more general class of LME states. These states are defined by  $2^N$  real phases, and can be prepared by applying general phase operators  $\tilde{C}_e(\varphi) = \mathbb{1} - (1 - e^{i\varphi})|1 \cdots 1\rangle\langle 1 \cdots 1|$  to the state  $|+\rangle^{\otimes N}$ . As in the case of graph states, LME states can be associated to a weighted hypergraph, where the weight of each edge corresponds to the phase of its associated operator. Setting the phases to  $\pi$  results in the class hypergraph states or  $\pi$ -LME states.

### 2.3. Local Pauli transformations and graph transformations

In this section we will discuss the possible actions of Pauli matrices as local unitary transformations on a hypergraph state. First, we have mentioned already the action of the unitary transformation  $Z_k$  on some qubit  $k$ . It adds the edge  $e = \{k\}$  to the set  $E$  if this edge was not yet contained in  $E$ . If, however, the edge  $e = \{k\}$  was already in  $E$ , the transformation  $Z_k$  removes this edge again, since  $(C_k)^2 = \mathbb{1}$ .



**Figure 2.** Example of the different local Pauli operations and their action on the hypergraph. (a→b) The operation  $X_1$  on the first qubit. (b→c) The two one-edges are removed by  $Z$  operations on the qubits 2 and 3. (c→d) The operation  $X_2$  on the second qubit. (d→e) The one-edge is removed by a  $Z_1$  operation. (e→f) The operation  $X_3$  on the third qubit.

A more interesting transformation is the application of the unitary matrix  $X_k$ . We can directly calculate that

$$X_k|H\rangle = X_k \left( \prod_{e \in E} C_e \right) |+\rangle^{\otimes N} = \left( \prod_{e \in E} C_e \right) \left( \prod_{e \in E(k)} C_{e \setminus \{k\}} \right) |+\rangle^{\otimes N}. \quad (11)$$

This is again a hypergraph state. Its edges can be conveniently described, if one considers the symmetric difference of sets. Generally, the symmetric difference of two sets  $A$  and  $B$  is given by

$$A \Delta B = (A \cup B) \setminus (A \cap B), \quad (12)$$

that is, both sets are joined, but then the elements which are in both sets are removed. Let us define the set of edges

$$E^{(k)} = \{e \setminus \{k\} | e \in E(k)\}. \quad (13)$$

This set is formed by first taking all edges in  $E$  which contain  $k$ , and then removing  $k$  out of all these edges. The set of edges of the state  $X_k|H\rangle$  is then given by

$$E^{\text{new}} = E \Delta E^{(k)}. \quad (14)$$

The hypergraph of the state  $X_k|H\rangle$  can directly be determined graphically: One picks the vertex  $k$  and determines the set  $E^{(k)}$ . Then one removes or adds these edges to  $E$ , depending on whether they exist already in  $E$  or not. This is demonstrated in an example in Fig. 2. Finally, the unitary transformation  $Y_k$  can be implemented by first applying  $X_k$  and then  $Z_k$ .

In the following, we will investigate which hypergraph states are equivalent under local unitary transformations, especially local Pauli operations. We will show that under

certain constraints local unitary (LU) equivalence is the same as equivalence under local Pauli transformations. It can be seen already from the present discussion that some properties of the hypergraph remain invariant under local Pauli operators, so they can be used to distinguish equivalence classes. The main property concerns the edges with the highest cardinality, that is, the edges which connect the largest number of vertices. These remain invariant under  $X_k$  transformations, since the set  $E^{(k)}$  cannot contain edges with maximal cardinality. From this, it immediately follows that any  $k$ -uniform hypergraph state cannot be Pauli-equivalent to another  $k'$ -uniform hypergraph, unless they are identical. This fact was noted for the case  $k \neq k'$  before; the proof in Ref. [14] required, however, lengthy calculations. Moreover, if one has a  $k$ -edge  $e$  in a hypergraph, and a  $(k-1)$ -edge  $e'$  within this edge ( $e' \subset e$ ), then one can always remove  $e'$  with a local Pauli operation (but this may introduce new edges of cardinality  $k-1$  since there may be other  $k$ -edges apart from  $e$ ). For the special case that an  $N$ -qubit hypergraph state contains an  $N$ -edge, one can remove all the  $(N-1)$ -edges. This explains why the hypergraphs no. 17-27 in Fig. 3 do not contain any 3-edges.

### 3. Entanglement classes

In this section, we distinguish and investigate the different LU equivalence classes for hypergraph states. Two states are LU equivalent, and belong to the same class, if they are connected by local unitary transformations. That is, if there exist local unitary operators  $U_1, \dots, U_N$  such that

$$|\psi\rangle = U_1 \otimes \cdots \otimes U_N |\phi\rangle. \quad (15)$$

In this case we also write  $|\psi\rangle \simeq_{\text{LU}} |\phi\rangle$ . We stress that other equivalence transformations are worth to be considered, for instance stochastic local operations and classical communication (SLOCC) [19]. For the present paper, however, we focus on equivalence under local unitaries and local Pauli operations, as the latter have a clear graph-theoretical interpretation.

In our classification, we focus on hypergraph states which have at least one edge with three or more vertices. The reason is that the states with only two-edges are graph states and their entanglement classes have already been extensively discussed [1, 3–5].

#### 3.1. Three qubits

For three qubits, there is only one LU equivalence class of hypergraph states. It can be represented by the hypergraph in Fig. 2(f). This figure also shows that any other three-qubit hypergraph state with a three-edge can be transformed into this state by local Pauli transformations. Despite this fact has been noted before [13], we will discuss it in some detail, since this allows us to introduce the concepts and quantities that are also used for the general case.

This hypergraph state is given by

$$|\hat{H}_3\rangle = \frac{1}{\sqrt{8}}(|000\rangle + |001\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |110\rangle - |111\rangle), \quad (16)$$

but after a Hadamard transformation on the third qubit one arrives at the simpler form

$$|H_3\rangle = \frac{1}{2}(|000\rangle + |010\rangle + |100\rangle + |111\rangle). \quad (17)$$

The entanglement properties of this state are the following: The reduced single-qubit matrices have all the largest eigenvalue equal to 3/4 and, consequently, the second eigenvalue is 1/4. A possible entanglement witness detecting the entanglement in a general hypergraph state is of the type

$$\mathcal{W} = \alpha_S \mathbb{1} - |H\rangle\langle H|, \quad (18)$$

where  $\alpha_S$  is the maximal squared overlap between the state  $|H\rangle$  and any biseparable pure state, that is a state of the form  $|\phi\rangle = |\alpha\rangle_M |\beta\rangle_{\bar{M}}$  where  $M|\bar{M}$  is some bipartition of the  $N$  qubits. This overlap  $\alpha_S$  can be directly computed as the maximum of all eigenvalues of all reduced states, so we have for the three-qubit state  $\alpha_S = 3/4$ . In general, one can show that for  $N$ -qubit hypergraph states consisting of only a single  $N$ -edge, one has that  $\alpha_S = 1 - 2^{(1-N)}$  [15].

The entanglement in the state  $|H_3\rangle$  can be quantified by several entanglement monotones. First, the bipartite negativity, defined as the sum of the absolute values of all negative eigenvalues, is for the  $A|BC$  bipartition given by  $N_{A|BC}(\varrho) \equiv \sum_k |\lambda_k^-(\varrho^{TA})| = \sqrt{3}/4$ , for the other bipartitions it is the same. Second, we consider the geometric measure of entanglement, which is for pure states defined via

$$E_G(|\psi\rangle) = 1 - \max_{|\phi\rangle=|a\rangle|b\rangle|c\rangle} |\langle\phi|\psi\rangle|^2, \quad (19)$$

as one minus the maximal squared overlap with fully product states. For mixed states, this entanglement monotone can be extended using the convex roof. Since LU equivalent states have the same geometric measure, this quantity can be used to prove that two states are not LU equivalent. For the three-qubit hypergraph state we find by direct numerical optimization  $E_G(|H_3\rangle) = 0.32391$ .

A third measure which can be used to characterize genuine multipartite entanglement is the genuine multiparticle negativity, coming from the characterization of multiparticle entanglement using PPT mixtures [20,21]. This measure can for general mixed states be computed via semidefinite programming (SDP), but for pure states and using the normalization of Ref. [22] it is given by the minimal bipartite negativity, so in our case we have  $N_G(|H_3\rangle) = \sqrt{3}/4$ .

Finally, we can investigate the robustness of the entanglement under noise. For that we consider states of the form

$$\varrho(p) = (1-p)|H\rangle\langle H| + p\frac{\mathbb{1}}{2^N} \quad (20)$$

and ask for the maximal value  $p_{\max}$  for which the state is still genuine multiparticle entangled. Using the approach of PPT mixtures, a lower bound  $p_{\text{ppt}}$  on the maximal  $p_{\max}$  can directly be computed via SDP [21], and for the state  $|H_3\rangle$  we find  $p_{\text{ppt}} = 0.4952$ . Two comments are in order here: First,  $p_{\text{ppt}}$  is clearly invariant under local unitaries, so it can be used to distinguish different LU classes. It is better suited for this task than the geometrical measure  $E_G$ , since for  $p_{\text{ppt}}$  the SDP results in a certified solution, while the computation of  $E_G$  may, at least in principle, have the problem of not finding the global optimum. Second, since for  $|H_3\rangle$  the state  $\varrho(p)$  is locally equivalent to a permutationally invariant three-qubit state, the PPT mixture condition is a necessary and sufficient condition for separability [23]. So we have  $p_{\max} = p_{\text{ppt}}$  and states  $\varrho(p)$  with  $p > 0.4952$  are biseparable.

Finally, note that for the three-qubit fully entangled hypergraph states without three-edge, that is, the usual graph states, there is one further equivalence class. This is given by the fully connected graph with the edges  $E = \{\{1, 2\}, \{2, 3\}, \{1, 3\}\}$  and in a suitable basis the representing state is the three-qubit GHZ state  $|GHZ_3\rangle = \frac{1}{\sqrt{2}}(|000\rangle + |111\rangle)$ .

### 3.2. Four qubits

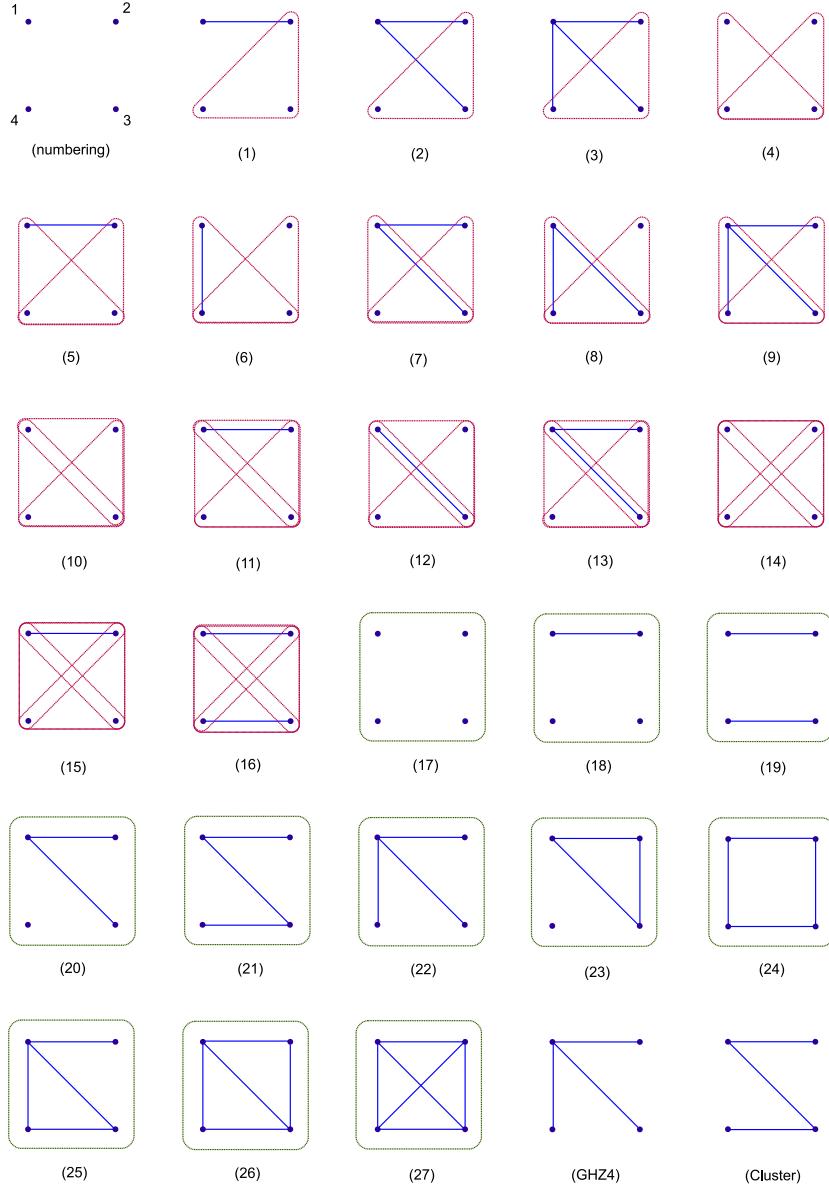
In order to characterize all the entanglement classes for four qubits we proceed as follows: We investigate all the  $2^{2^4} = 65536$  possible hypergraphs and test for equivalence under local Pauli operations as well as under permutation of the qubits. After that, we find 27 classes among all hypergraphs which contain at least one three-edge and where all vertices are connected. These hypergraphs are shown in Fig. 3.

In Table 1 we list the entanglement properties of the corresponding hypergraph states. From the properties of the reduced density matrices and the reported values of  $E_G$  and  $p_{\text{ppt}}$  one can directly conclude that these states are inequivalent under general local unitary transformations and not only under local Pauli transformations.

Three states among the 27 states are of special interest. These are the states no. 3, no. 9 and no. 14, as for these states the reduced single qubit matrices are maximally mixed. Therefore, they are all in the maximally entangled set [24], i.e. they cannot be reached by transformations consisting of local operations and classical communication from any other state with the same number of qubits. The state no. 3 can, after applying a Hadamard transformation on the first qubit, be written as:

$$\begin{aligned} |V_3\rangle &= \frac{1}{\sqrt{8}}[(|0011\rangle + |0101\rangle + |0110\rangle + |1001\rangle + |1010\rangle + |1100\rangle) + (|0000\rangle - |1111\rangle)] \\ &= \sqrt{\frac{3}{4}}|D_4\rangle + \frac{1}{2}|GHZ_4^-\rangle, \end{aligned} \quad (21)$$

where  $|GHZ_4^-\rangle = (|0000\rangle - |1111\rangle)/\sqrt{2}$  and  $|D_4\rangle = (|0011\rangle + |0101\rangle + |0110\rangle + |1001\rangle + |1010\rangle + |1100\rangle)/\sqrt{6}$ . That is, it is a superposition of the four-qubit Dicke state with two excitations with a four-qubit GHZ state. From this form it is clear that the state



**Figure 3.** Representatives of all the 27 equivalence classes under local unitary transformations for hypergraph states of four qubits. In addition, the usual graphs of the four-qubit GHZ state and the four-qubit cluster state are shown.

$|V_3\rangle$  belongs to the symmetric subspace. The state  $|V_3\rangle$  can be viewed as if first a GHZ state via two-body interactions is created, then, an additional controlled phase gate on the qubits  $\{2, 3, 4\}$  is applied. This still increases the entanglement, since the geometric measure as well as the robustness  $p_{\text{ppt}}$  is higher than for a GHZ state.

The second state, no. 9, can (after applying  $X_3$  and  $Z_1$  and further Hadamard transformations on qubits 3 and 4) be written as

$$|V_9\rangle = \frac{1}{\sqrt{2}}|GHZ_4^-\rangle + \frac{1}{2}|01\rangle|\gamma\rangle + \frac{1}{2}|10\rangle|\bar{\gamma}\rangle, \quad (22)$$

where  $|\gamma\rangle = (|00\rangle + |01\rangle - |10\rangle + |11\rangle)/2$  and  $|\bar{\gamma}\rangle = (|00\rangle - |01\rangle + |10\rangle + |11\rangle)/2$  are Bell-type states. From this form, a symmetry under simultaneous permutation of the qubits  $1 \leftrightarrow 2$  and  $3 \leftrightarrow 4$  becomes apparent.

The third state with the property that all single qubit reduced states are  $\mathbb{1}/2$  is the state no. 14. After a Hadamard and a  $Z$  transformation on the fourth qubit this is given by

$$\begin{aligned} |V_{14}\rangle &= \frac{1}{\sqrt{8}} [(|0011\rangle + |0101\rangle + |0110\rangle + |1001\rangle + |1010\rangle + |1100\rangle) + (|0001\rangle - |1110\rangle)] \\ &= \sqrt{\frac{3}{4}} |D_4\rangle + \frac{1}{2} |\overline{GHZ}_4^-\rangle, \end{aligned} \quad (23)$$

where  $|\overline{GHZ}_4^-\rangle = (|0001\rangle - |1110\rangle)/\sqrt{2}$ , so it is a superposition of a Dicke state with another GHZ state. Note that in a suitable basis this state belongs to the symmetric subspace again, as can be seen from the symmetry of the hypergraph.

Besides these highly entangled states, seven hypergraph states have a very simple form, if they are written in the appropriate basis. These are

$$\begin{aligned} |V_1\rangle &= \frac{1}{2} (|0000\rangle + |0001\rangle + |1100\rangle + |1111\rangle), \\ |V_2\rangle &= \frac{1}{2} (|0000\rangle + |0111\rangle + |1010\rangle + |1100\rangle), \\ |V_4\rangle &= \frac{1}{2} (|0000\rangle + |0001\rangle + |0010\rangle + |1111\rangle), \\ |V_6\rangle &= \frac{1}{2} (|0000\rangle + |0010\rangle + |0111\rangle + |1001\rangle), \\ |V_8\rangle &= \frac{1}{2} (|0000\rangle + |1001\rangle + |1010\rangle + |1111\rangle), \\ |V_{10}\rangle &= \frac{1}{\sqrt{8}} (2|0000\rangle + |0011\rangle + |0110\rangle + |1010\rangle - |1111\rangle), \\ |V_{12}\rangle &= \frac{1}{\sqrt{8}} (2|0000\rangle + |0010\rangle - |0111\rangle + |1011\rangle + |1110\rangle). \end{aligned} \quad (24)$$

In addition to the 27 classes, there are two LU equivalence classes for the usual graph states, the GHZ and the cluster state. The corresponding graphs are also shown in Fig. 3. Finally, it is worth mentioning that some other well-known states for four qubits [19], such as the W state  $|W_4\rangle$ , the four-qubit singlet state  $|\Psi_4\rangle$  or the  $\chi$ -state  $|\chi_4\rangle$  are not locally equivalent to any hypergraph state.

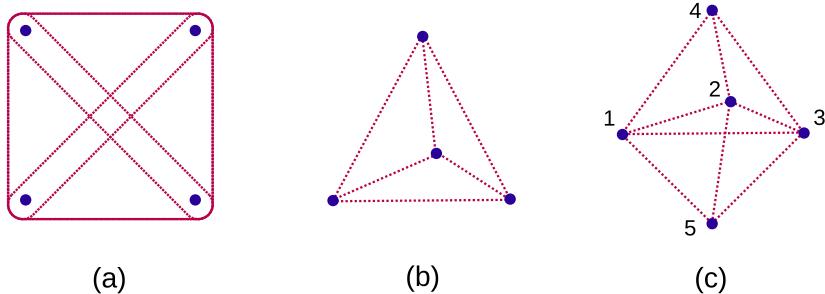
### 3.3. Five qubits

For five qubits, there are already  $2^{32}$  possible hypergraphs, which makes an exhaustive classification difficult. Moreover, it can be expected that the resulting number of classes is significantly larger than in the four-qubit case and therefore a complete classification is of limited use.

Class	$E_G$	$\varrho_A$	$\varrho_B$	$\varrho_C$	$\varrho_D$	$\varrho_{AB}$	$\varrho_{AC}$	$\varrho_{AD}$	$\alpha_{BS}$	$N_{\text{gen}}$	$p_{\text{ppt}}$
1	0.50000	1/2	1/2	3/4	3/4	3/4	1/2	1/2	3/4	$\sqrt{3}/4$	0.5430
2	0.65651	1/2	1/2	1/2	3/4	1/2	1/2	1/2	3/4	$\sqrt{3}/4$	0.5803
3	0.65277	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	0.5664
4	0.34549	3/4	3/4	3/4	3/4	3/4	$\Gamma_1$	$\Gamma_1$	3/4	$\sqrt{3}/4$	0.5286
5	0.57322	1/2	1/2	3/4	3/4	3/4	$\Gamma_2$	$\Gamma_2$	3/4	$\sqrt{3}/4$	0.5549
6	0.50000	3/4	3/4	3/4	1/2	1/2	$\Gamma_1$	$\Gamma_1$	3/4	$\sqrt{3}/4$	0.5466
7	0.62500	1/2	1/2	1/2	3/4	1/2	$\Gamma_2$	$\Gamma_2$	3/4	$\sqrt{3}/4$	0.5722
8	0.63572	3/4	3/4	1/2	1/2	1/2	$\Gamma_1$	$\Gamma_1$	3/4	$\sqrt{3}/4$	0.5409
9	0.63572	1/2	1/2	1/2	1/2	1/2	$\Gamma_2$	$\Gamma_2$	1/2	1/2	0.5848
10	0.50000	3/4	3/4	1/2	3/4	$\Gamma_1$	$\Gamma_1$	$\Gamma_1$	3/4	$\sqrt{3}/4$	0.5306
11	0.59872	1/2	1/2	1/2	3/4	$\Gamma_1$	$\Gamma_2$	$\Gamma_2$	3/4	$\sqrt{3}/4$	0.5700
12	0.37500	3/4	3/4	3/4	3/4	$\Gamma_1$	$\Gamma_1$	$\Gamma_1$	3/4	$\sqrt{3}/4$	0.5242
13	0.62500	1/2	1/2	3/4	3/4	$\Gamma_1$	$\Gamma_2$	$\Gamma_2$	3/4	$\sqrt{3}/4$	0.5523
14	0.57161	1/2	1/2	1/2	1/2	$\Gamma_1$	$\Gamma_1$	$\Gamma_1$	$\Gamma_1$	1/2	0.5346
15	0.58726	3/4	3/4	1/2	1/2	$\Gamma_1$	$\Gamma_2$	$\Gamma_2$	3/4	$\sqrt{3}/4$	0.5568
16	0.43750	3/4	3/4	3/4	3/4	$\Gamma_1$	$\Gamma_1$	$\Gamma_1$	3/4	$\sqrt{3}/4$	0.5157
17	0.19018	7/8	7/8	7/8	7/8	$\Gamma_3$	$\Gamma_3$	$\Gamma_3$	7/8	$\sqrt{7}/8$	0.4316
18	0.43187	5/8	5/8	7/8	7/8	$\Gamma_3$	$\Gamma_4$	$\Gamma_4$	7/8	$\sqrt{7}/8$	0.4806
19	0.64376	5/8	5/8	5/8	5/8	$\Gamma_3$	$\Gamma_2$	$\Gamma_2$	$\Gamma_3$	3/8	0.5411
20	0.46240	5/8	5/8	5/8	7/8	$\Gamma_4$	$\Gamma_4$	$\Gamma_4$	7/8	$\sqrt{7}/8$	0.5261
21	0.65277	5/8	5/8	5/8	5/8	$\Gamma_4$	$\Gamma_2$	$\Gamma_2$	5/8	$\sqrt{15}/8$	0.5736
22	0.46097	5/8	5/8	5/8	5/8	$\Gamma_4$	$\Gamma_4$	$\Gamma_4$	5/8	$\sqrt{15}/8$	0.5423
23	0.54497	5/8	5/8	5/8	7/8	$\Gamma_4$	$\Gamma_4$	$\Gamma_4$	7/8	$\sqrt{7}/8$	0.5193
24	0.55656	5/8	5/8	5/8	5/8	$\Gamma_2$	$\Gamma_4$	$\Gamma_2$	5/8	$\sqrt{15}/8$	0.5744
25	0.62926	5/8	5/8	5/8	5/8	$\Gamma_4$	$\Gamma_2$	$\Gamma_2$	5/8	$\sqrt{15}/8$	0.5728
26	0.53879	5/8	5/8	5/8	5/8	$\Gamma_2$	$\Gamma_4$	$\Gamma_2$	5/8	$\sqrt{15}/8$	0.5699
27	0.55637	5/8	5/8	5/8	5/8	$\Gamma_4$	$\Gamma_4$	$\Gamma_4$	5/8	$\sqrt{15}/8$	0.5229
GHZ	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	1/2	4/7
Cluster	3/4	1/2	1/2	1/2	1/2	1/2	1/4	1/2	1/2	1/2	8/13

**Table 1.** Entanglement properties of the 27 equivalence classes of four-qubit hypergraph states. The table shows the values of the geometric measure of entanglement  $E_G$ , the maximal eigenvalues of the single-qubit reduced states ( $\varrho_A, \varrho_B, \varrho_C, \varrho_D$ ), the maximal eigenvalues of the two-qubit reduced states ( $\varrho_{AB}, \varrho_{AC}, \varrho_{AD}$ ), the maximal overlap with biseparable states ( $\alpha_{BS}$ ), the genuine multiparticle negativity ( $N_{\text{gen}}$ ) and the noise robustness of multiparticle entanglement according to the PPT mixture approach ( $p_{\text{ppt}}$ ). The used constants are given by  $\Gamma_1 = (3 + \sqrt{5})/8 \approx 0.65450$ ,  $\Gamma_2 = (2 + \sqrt{2})/8 \approx 0.42677$ ,  $\Gamma_3 = (4 + \sqrt{7})/8 \approx 0.83071$ , and  $\Gamma_4 = (8 + 13/\sqrt[3]{z} + \sqrt[3]{z})/24 \approx 0.60170$  with  $z = 8 + i3\sqrt{237}$ .

For five and more qubits we focus therefore on  $k$ -uniform hypergraphs, since for them an exhaustive treatment is still possible. These type of states are arguably relevant



**Figure 4.** (a, b) The graph of the four-qubit hypergraph state No. 14 can also be depicted as a tetrahedron, where the triangles on the surface represent the three-edges. (c) The hypergraph of the only three-uniform five-qubit state with maximally mixed reduced states can be represented in a similar way. This hypergraph has 7 edges corresponding to the triangles. In fact, all possible three-edges apart from the ones that contain 4 and 5 are present.

for experiments, as their generation requires the same type of multiqubit interaction. As can be seen from the hypergraph transformation rule outlined in Section 2.3, any  $k$ -uniform hypergraph cannot be converted into a different  $k$ -uniform hypergraph by local Pauli operators. We focus our discussion only on the  $k$ -uniform hypergraphs where for the corresponding states the reduced single-particle states are maximally mixed. As mentioned before, these states are relevant because they are in the maximally entangled set [24], and, moreover, the condition of having the single-qubit reduced states maximally mixed is necessary for quantum error correction. Note that for two-uniform hypergraphs (i.e. corresponding to graph states), any state has the property that the reduced states are maximally mixed, and hence is also in the maximally entangled set.

For five qubits, one directly finds that there is exactly one further  $k$ -uniform hypergraph state with this property. The hypergraph is three-uniform and depicted in Fig. 4. The hypergraph state is symmetric on the first three qubits, and, after applying Hadamard transformations on all qubits, it can be written as

$$|F_1\rangle = \frac{1}{\sqrt{2}}|GHZ_5\rangle + \frac{1}{2}|\eta\rangle|00\rangle + \frac{1}{2}|\bar{\eta}\rangle|11\rangle, \quad (25)$$

where  $|GHZ_5\rangle = (|00000\rangle + |11111\rangle)/\sqrt{2}$  is the five-qubit GHZ state,  $|\eta\rangle = (|100\rangle + |010\rangle + |001\rangle - |111\rangle)/2$  is a three-qubit state unitarily equivalent to the three-qubit GHZ state, and  $|\bar{\eta}\rangle = X_1X_2X_3|\eta\rangle$  arises from  $|\eta\rangle$  when all qubits are flipped.

The geometric measure of entanglement for this state is  $E_G = 0.6000$ , and the genuine negativity is  $N_G = 1/2$ . The overlap with biseparable states is  $\alpha_S = (3 + \sqrt{5})/8 \approx 0.65450$ , and the noise robustness is given by  $p_{\text{ppt}} = 0.6070$ .

### 3.4. Six qubits

Also for six qubits, a full characterization of all  $k$ -uniform hypergraph states with maximally mixed reduced single-particle states is possible. Apart from the usual graph

states, one finds such states only for three-uniform hypergraphs. It turns out that there are 24 different classes, a detailed list is given in Table 2 in the Appendix. For these states one can say the following: All of them are LU inequivalent, as for all of them the geometric measure  $E_G$  is different. For none of these states, also all of the two-qubit reduced density matrices are maximally mixed.

Two states in this set may be of interest: First the state which has (after appropriate local unitary transformations) the simplest form in the standard basis is the representative of the first class,

$$\begin{aligned} |S_1\rangle = \frac{1}{8} [ &(|000000\rangle - |111111\rangle) + (|001\rangle + |010\rangle + |100\rangle) \otimes |000\rangle + \\ &+ (|110\rangle + |101\rangle + |011\rangle) \otimes |111\rangle ]. \end{aligned} \quad (26)$$

This state has a geometric measure  $E_G(|S_1\rangle) = 0.6$ . The state with the highest geometric measure of entanglement is the representative of the 21th class, and its measure is  $E_G(|S_{21}\rangle) = 0.817$ .

#### 4. General conditions on local unitary equivalence and local Pauli equivalence

As shown in the previous section, the finite set of local Pauli operations is sufficient to characterize the LU equivalence classes for hypergraph states of four qubits. So the question arises, under which conditions this is true in more general cases. We note that it cannot be true in general, since for the usual graph states not even the larger set of local Clifford operations is sufficient to characterize LU equivalence.

In this section we establish general conditions, under which local Pauli (LP) transformations are the only transformations that have to be checked in order to prove LU equivalence. We first review a necessary and sufficient condition for LU equivalence of general  $N$ -partite states presented in Refs. [25, 26], and then show that for many hypergraph states this can be reduced to equivalence under the action of LP operators, which transform the corresponding hypergraph in a simple way.

##### 4.1. Local unitary equivalence of multipartite states

First, we will use the notation  $\varrho_i = \text{tr}_{-i}(|\psi\rangle\langle\psi|)$  for the single-qubit reduced state of  $|\psi\rangle$ , and equivalently  $\sigma_i$  for  $|\phi\rangle$ . It has been shown that two generic states, where the single-qubit reduced states are not maximally mixed (that is,  $\varrho_i, \sigma_i \not\propto \mathbb{1}$  for all  $i$ ), are LU equivalent if and only if their corresponding so-called *unique standard form* coincides. Moreover, for non-generic states, there exists an algorithm that determines the local unitaries that transform  $|\phi\rangle$  to  $|\psi\rangle$  in case they exist [25, 26].

As we are concerned here with the LU equivalence of generic states, we briefly recall the criteria of LU equivalence in this case. The standard form  $|\psi^s\rangle$  of an  $N$ -partite state  $|\psi\rangle$  can be obtained in three steps [25]. First, the state is transformed to its *trace*

decomposition,

$$|\psi^t\rangle = U_1^t \otimes \cdots \otimes U_N^t |\psi\rangle, \quad (27)$$

where  $U_i^t$  are local unitaries such that the single-qubit reduced states are diagonal, i.e.  $\varrho_i^t = U_i^t \varrho_i(U_i^t)^\dagger = D_i \equiv \text{diag}(\mu_i^1, \mu_i^2)$  in the standard basis. Second, the *sorted trace decomposition*  $|\psi^{st}\rangle$  is the trace decomposition with  $\mu_i^1 \geq \mu_i^2$  for all  $i$ . This decomposition can be reached by applying local  $X$  operators to  $|\psi^t\rangle$  when necessary. The sorted trace decomposition is already unique, up to a global phase  $\alpha_0$  and local phase operators  $Z_i(\alpha_i) = \text{diag}(1, e^{i\alpha_i})$ . That is,  $e^{i\alpha_0} \bigotimes_i Z_i(\alpha_i) |\psi^{st}\rangle$  is also a sorted trace decomposition of  $|\psi\rangle$ . So finally, the sorted trace decomposition is made unique by imposing the following conditions on the phases. We write the sorted trace decomposition in the computational basis,  $|\psi^{st}\rangle = \sum_{\mathbf{i}} \lambda_{\mathbf{i}} |\mathbf{i}\rangle$ , with  $\mathbf{i} \in \mathbb{Z}_2^N$  being a binary vector of length  $N$ . Then, from the set  $\Lambda = \{\mathbf{i} : \lambda_{\mathbf{i}} \neq 0\}$ , we pick a maximal set of linearly independent vectors  $\mathbf{i}$  by going through the set  $\Lambda$  in the order given by the computational basis. These vectors then form the set  $\bar{\Lambda} \subseteq \Lambda$ . The global phase  $\alpha_0$  is set such that

$$\lambda_{\mathbf{0}} > 0 \quad \text{if } \lambda_{\mathbf{0}} \neq 0 \quad (28)$$

$$\lambda_{\mathbf{i}_0} > 0 \quad \text{if } \lambda_{\mathbf{0}} = 0, \quad (29)$$

where  $\mathbf{i}_0$  is the first linearly *dependent* vector in  $\Lambda$ . The other  $N$  phases  $\alpha_1, \dots, \alpha_N$  are set so that  $e^{i\alpha_0} \lambda_{\mathbf{i}} > 0$  for  $\mathbf{i} \in \bar{\Lambda}$ . Since the resulting *standard form*  $|\psi^s\rangle$  is unique, we have

$$|\psi\rangle \simeq_{LU} |\phi\rangle \text{ iff } |\psi^s\rangle = |\phi^s\rangle. \quad (30)$$

This necessary and sufficient condition can be rewritten in the following way [26]:

$$|\psi\rangle \simeq_{LU} |\phi\rangle \text{ if and only if:} \quad (31)$$

$$\text{there exist } \{\alpha_i\}_{i=0}^N, \mathbf{k}, \{U_i^t\}_{i=1}^N, \{V_i^t\}_{i=1}^N \text{ such that } \bigotimes_i U_i^t |\psi\rangle = e^{i\alpha_0} \bigotimes_i Z_i(\alpha_i) X_i^{k_i} V_i^t |\phi\rangle.$$

Here  $U_i^t$  and  $V_i^t$  are the local unitaries that transform  $|\psi\rangle$  and  $|\phi\rangle$  to their trace decompositions  $|\psi^t\rangle$  and  $|\phi^t\rangle$ , respectively, and  $\mathbf{k} \in \mathbb{Z}_2^N$  is a bit string such that the operators  $X_i^{k_i}$  make the order of the eigenvalues of the single qubit reduced states  $U_i^t \varrho_i(U_i^t)^\dagger$  and  $V_i^t \sigma_i(V_i^t)^\dagger$  coincide. Then, one only needs to check that a solution for the set  $\{\alpha_i\}_{i=0}^N$  exists. In this case, the unitaries of Eq. (15) that transform  $|\phi\rangle$  to  $|\psi\rangle$  (up to a global phase) are  $U_i = (U_i^t)^\dagger Z_i(\alpha_i) X_i^{k_i} V_i^t$ .

#### 4.2. LU equivalence of generic LME states

As shown in Ref. [12], a state is an LME state if and only if it is LU equivalent to

$$|\psi\rangle = \frac{1}{\sqrt{2^N}} \sum_{\mathbf{x} \in \mathbb{Z}_2^N} e^{i\alpha_{\mathbf{x}}} |\mathbf{x}\rangle, \quad (32)$$

with  $\alpha_{\mathbf{x}}$  being real phases. Such a general LME state with arbitrary phases is brought to the trace decomposition by local unitaries  $HZ(-\beta_i)$ , where  $\cot(\beta_i) = \frac{\langle X_i \rangle}{\langle Y_i \rangle}$  if  $\langle Y_i \rangle \neq 0$

and  $\beta_i = 0$  else [26]. We call the state  $\bigotimes_i Z_i(-\beta_i)|\psi\rangle$  an LME state in the  $Z$  basis. In the following, we consider an LME states to be always in this basis, unless otherwise stated. This means that for every qubit  $i$ , the single-qubit reduced state is of the form

$$\varrho_i \propto \begin{pmatrix} 1 & x \\ x & 1 \end{pmatrix} \quad (33)$$

with  $x \in \mathbb{R}$ . If the state is generic, then  $x \neq 0$  since the reduced states are not maximally mixed. In this basis, the state is brought to the trace decomposition by applying the Hadamard transformation  $H^{\otimes N}$ .

Hence, for  $|\psi\rangle$  and  $|\phi\rangle$  generic LME states in the  $Z$  basis, the LU equivalence condition (31) reads

$|\psi\rangle \simeq_{LU} |\phi\rangle$  if and only if:

$$\text{there exist } \{\alpha_i\}_{i=0}^N, \mathbf{k} \text{ such that } \bigotimes_i H_i |\psi\rangle = e^{i\alpha_0} \bigotimes_i Z_i(\alpha_i) X_i^{k_i} H_i |\phi\rangle, \quad (34)$$

and the unitaries (15) that transform  $|\phi\rangle$  to  $|\psi\rangle$  must be of the form

$$U_i = H_i Z_i(\alpha_i) X_i^{k_i} H_i = X_i(\alpha_i) Z_i^{k_i}, \quad (35)$$

up to a global phase. Here we defined  $X_i(\alpha_i) \equiv H_i Z_i(\alpha_i) H_i$ . As one can see, the allowed unitaries are already quite restricted, as all the unitaries bringing a generic LME state to its trace-decomposition are the same. That is, the difference from just Pauli operators comes from the freedom of local phase operators in the sorted trace decomposition.

In the following lemma we show that, for certain LME states, this freedom can be further reduced and it is enough to consider  $\alpha_i \in \{0, \pi\}$ , i.e. either the identity or  $X_i$ , which implies that in this basis, and up to a global phase,  $|\psi\rangle$  is LU equivalent to  $|\phi\rangle$  if and only if they are local Pauli (LP) equivalent. First, we define  $M_{|\phi^t\rangle}$  as the matrix whose rows are the first linearly independent vectors  $\mathbf{x}$  such that  $\langle \mathbf{x} | \phi^t \rangle \neq 0$ . That is,  $M_{|\phi^t\rangle}$  is analogous to the set  $\bar{\Lambda}$  but for the trace decomposition, and expressed in matrix form.

**Lemma 3.** *Let  $|\psi^t\rangle$  and  $|\phi^t\rangle$  be  $N$ -qubit LME states in the trace-decomposition that fulfill the following conditions:*

- (i) *They have real coefficients  $\langle \mathbf{x} | \psi^t \rangle, \langle \mathbf{x} | \phi^t \rangle \in \mathbb{R}$ .*
- (ii) *Coefficients  $\langle \mathbf{0} | \psi^t \rangle$  and  $\langle \mathbf{0} | \phi^t \rangle$  are different from 0.*
- (iii)  *$M_{|\phi^t\rangle}$  is square and invertible in  $\mathbb{Z}_2$ , i.e.—  $|M_{|\phi^t\rangle}| \equiv 1 \pmod{2}$ .*

*Then,  $|\phi^t\rangle$  can be converted to  $|\psi^t\rangle$  by local unitary phase operators if and only if  $|\phi^t\rangle$  can be converted to  $|\psi^t\rangle$  by local  $Z$  operators, i.e.*

$$\begin{aligned} &\text{There exist } \{\alpha_i\}_{i=0}^n \in \mathbb{R} \text{ such that } |\psi^t\rangle = e^{i\alpha_0} \bigotimes_{i=1}^n Z_i(\alpha_i) |\phi^t\rangle \text{ if and only if} \\ &\text{There exist } \tilde{\alpha}_0 \in \mathbb{R}, \text{ and } \mathbf{l} \in \mathbb{Z}_2^n \text{ such that } |\psi^t\rangle = e^{i\tilde{\alpha}_0} \bigotimes_{i=1}^n Z_i^{l_i} |\phi^t\rangle. \end{aligned} \quad (36)$$

Note that the lemma considers states  $|\psi^t\rangle$  and  $|\phi^t\rangle$  that are related by local phase operators, so their coefficients have the same absolute value, i.e.  $|\langle \mathbf{x} | \psi^t \rangle| = |\langle \mathbf{x} | \phi^t \rangle|$  for all  $\mathbf{x}$ . Moreover, since the coefficients are real they can only differ by a sign.

*Proof.* The sufficient condition is straightforward, as one can set  $\alpha_i = \pi l_i$  and  $\alpha_0 = \tilde{\alpha}_0$ . For the necessary condition, note that due to condition (i) we have that  $|\psi^*\rangle = |\psi\rangle$  and  $|\phi^*\rangle = |\phi\rangle$ , where  $|\psi^*\rangle$  denotes the complex conjugate of  $|\psi\rangle$  in the computational basis. Hence, we can impose the following condition on the phases:

$$|\phi^t\rangle = e^{i2\alpha_0} \bigotimes_i Z_i(2\alpha_i) |\phi^t\rangle. \quad (37)$$

Since  $\langle \mathbf{0} | \phi^t \rangle \neq 0$ , we can see that  $\alpha_0$  is fixed to either 0 or  $\pi$ . Since the coefficients of  $|\phi^t\rangle$  and  $|\psi^t\rangle$  can differ only by a sign, we have the more general condition

$$\alpha_0 + \mathbf{x}^\top \boldsymbol{\alpha} = \pi k_{\mathbf{x}} \quad \forall \mathbf{x} \in S_{\phi^t}, \quad (38)$$

where we defined  $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_n)^\top \in \mathbb{R}^n$ , and  $S_{\phi^t} = \{\mathbf{x} : \langle \mathbf{x} | \phi^t \rangle \neq 0\}$ . Note that  $S_{\phi^t}$  is analogous to the set  $\Lambda$  previously defined, but for the trace decomposition. Using the matrix  $M = M_{|\phi^t\rangle}$  and that  $\alpha_0 \in \{0, \pi\}$ , Eq. (38) can also be rewritten as

$$M\boldsymbol{\alpha} = \pi \mathbf{k}. \quad (39)$$

Here  $\mathbf{k} \in \mathbb{Z}_2^N$  is the vector whose entries are  $k_{\mathbf{x}} + \frac{\alpha_0}{\pi} \pmod{2}$ , with  $\mathbf{x}$  the vectors forming the matrix  $M$ .

As  $M$  is an integer matrix, so is the adjugate matrix  $A \equiv |M|M^{-1}$  (that is, the transpose of the cofactor matrix,  $A = C^\top$ , where each entry  $C_{ij}$  is the  $i, j$ -minor of  $M$ ). Using this, Eq. (39) can be written as

$$\frac{|M|\boldsymbol{\alpha}}{\pi} = A\mathbf{k} \pmod{2}. \quad (40)$$

As  $M$  is invertible in  $\mathbb{Z}_2$ ,  $|M| \equiv 1 \pmod{2}$ , so the vector  $\boldsymbol{\alpha} = \pi \mathbf{l}$ , with  $\mathbf{l} \equiv A\mathbf{k} \pmod{2} \in \mathbb{Z}_2^N$ , is a solution to the previous equation. This shows that the phases can always be chosen to be either 0 or  $\pi$ , and hence  $|\psi^t\rangle$  and  $|\phi^t\rangle$  are equivalent under the action of  $Z$  operators.  $\square$

Note that the conditions  $\langle \mathbf{0} | \psi^t \rangle \neq 0$  and  $\langle \mathbf{0} | \phi^t \rangle \neq 0$  can be relaxed, as long as there exists at least a linearly *dependent* vector  $\mathbf{x}$  such that the global phase can be fixed to 0 or  $\pi$ .

We are now going to use this lemma to derive a simple necessary and sufficient condition for LU equivalence of certain LME states. To this end, we redefine generic LME states by adding a second condition that excludes a set of zero measure. We call an LME state  $|\phi\rangle$  generic if it fulfills the following two conditions: (i) none of the single-qubit reduced states are completely mixed (i.e.  $\varrho_i \not\propto \mathbb{1} \forall i$ ); and (ii) let  $|\phi\rangle$  be in the  $Z$  basis, then there exists a  $\mathbf{k} \in \mathbb{Z}_2^n$  such that the state  $|\phi_{\mathbf{k}}\rangle = Z^{\mathbf{k}}|\phi\rangle$  fulfills that

$\langle \mathbf{0}|H^{\otimes n}|\phi_{\mathbf{k}}\rangle \neq 0$  and  $\langle \mathbf{x}|H^{\otimes n}|\phi_{\mathbf{k}}\rangle \neq 0$  for all  $\mathbf{x} \in \mathbb{Z}_2^n$  with  $|\mathbf{x}| = 1$ . ( $|\mathbf{x}\rangle$  is a state of the computational basis.) Nearly all LME states fulfill these two conditions. Note also that for our purposes condition (ii), which is equivalent to  $M_{H^{\otimes n}|\phi_{\mathbf{k}}\rangle} = \mathbb{1}$ , can be relaxed to  $|M_{H^{\otimes n}|\phi_{\mathbf{k}}\rangle}| \equiv 1 \pmod{2}$ .

As we mentioned before, the allowed unitaries that transform  $|\phi\rangle$  to  $|\psi\rangle$  can be different from Pauli operators due to the freedom of local phase operators in the sorted trace decomposition. A generic LME state  $|\phi\rangle$  always has a Pauli equivalent state  $|\phi_{\mathbf{k}}\rangle$  that fulfills conditions (ii) and (iii) of Lemma 3. This leads to the proof of the following theorem:

**Theorem 4.** *Let  $|\psi\rangle$  and  $|\phi\rangle$  be  $N$ -qubit generic LME states in the  $Z$  basis with real coefficients in the trace decomposition. Then  $|\psi\rangle \simeq_{LU} |\phi\rangle$  if and only if  $|\psi\rangle$  and  $|\phi\rangle$  are equivalent under the action of local Pauli operators (in the  $Z$  basis).*

*Proof.* The sufficient condition is straightforward. For the necessary condition, note that  $|\phi\rangle \equiv |\phi_0\rangle$  is equivalent under Pauli operators to  $|\phi_{\mathbf{k}}\rangle$  for all  $\mathbf{k}$ . Hence, proving the theorem for any  $|\psi_{\mathbf{k}'}\rangle$  and any  $|\phi_{\mathbf{k}}\rangle$  is enough. Recall that  $|\psi\rangle \simeq_{LU} |\phi_{\mathbf{k}}\rangle$  if and only if there exists a binary vector  $\mathbf{k}'$  and real phases  $\{\alpha_i\}_{i=0}^N$  such that (see also Eq. (35))

$$|\psi_{\mathbf{k}'}\rangle = \bigotimes_{i=1}^N Z_i^{k'_i} |\psi\rangle = e^{i\alpha_0} \bigotimes_{i=1}^N X_i(\alpha_i) |\phi_{\mathbf{k}}\rangle, \quad (41)$$

or equivalently if there exists such vector  $\mathbf{k}'$  and phases  $\{\alpha_i\}_{i=0}^N$ , and

$$|\psi_{\mathbf{k}'}^t\rangle = e^{i\alpha_0} \bigotimes_{i=1}^N Z_i(\alpha_i) |\phi_{\mathbf{k}}^t\rangle. \quad (42)$$

We choose  $|\phi_{\mathbf{k}}\rangle$  such that  $\langle \mathbf{0}|\phi_{\mathbf{k}}^t\rangle \neq 0$  and  $M_{|\phi_{\mathbf{k}}^t\rangle} = \mathbb{1}$ , which is always possible due to condition (ii) of generic states. Then, due to Lemma 3  $|\psi_{\mathbf{k}'}^t\rangle$  and  $|\phi_{\mathbf{k}}^t\rangle$  are equivalent under local  $Z$  operators, i.e.  $|\psi_{\mathbf{k}'}\rangle$  and  $|\phi_{\mathbf{k}}\rangle$  are equivalent under local  $X$  operators. Each of these states are equivalent to  $|\psi\rangle$  and  $|\phi\rangle$  under the actions of local  $Z$  operators, respectively, which concludes the proof.  $\square$

#### 4.3. LU equivalence of hypergraph states

Now we are able to show that in many cases, two hypergraph states are LU equivalent if and only if they are LP equivalent. That is, if and only if their associated hypergraphs are related by a sequence of the hypergraph transformations studied in Section 2.3. We identify some conditions that have to be fulfilled by two  $N$ -qubit hypergraph states so that they are LU equivalent if and only if they are LP equivalent.

A hypergraph state in the computational basis has only real coefficients,

$$|\psi\rangle = \frac{1}{\sqrt{2^N}} \sum_{\mathbf{x} \in \mathbb{Z}_2^N} (-1)^{f(\mathbf{x})} |\mathbf{x}\rangle, \quad (43)$$

where

$$f(\mathbf{x}) = \bigoplus_{e \in E} \prod_{i \in e} x_i \quad (44)$$

is a boolean function expressed as a sum of polynomials (modulo 2) that depends on the hypergraph structure (and we define  $\prod_{i \in \emptyset} x_i \equiv 1$  for the empty edge). The degree  $d$  of such a polynomial representation is defined as  $d = \max\{|e| : e \in E\}$ , where  $|e|$  stands for the cardinality of the edge  $e$ . Hence,  $d$  equals the cardinality of the largest edge that appears in the graph.

If  $|\psi\rangle$  is a generic LME state, then the unitaries bringing it to the trace decomposition are  $H^{\otimes N}$ . This leads to the following corollary:

**Corollary 5.** *Let  $|\psi\rangle$  and  $|\phi\rangle$  be  $N$ -qubit hypergraph states that belong to the family of generic LME states [see conditions (i) and (ii) of the definition]. Then  $|\psi\rangle \simeq_{LU} |\phi\rangle$  if and only if  $|\psi\rangle$  and  $|\phi\rangle$  are equivalent under the action of local Pauli operators.*

Note that by far not all hypergraph states fulfill the condition stated in the corollary. In fact, for the four-qubit hypergraphs in Fig. (3) only 14 of 27 fulfill the condition that none of the reduced density matrices is maximally mixed. Further notable exceptions to the first condition of generic states are the connected graph states (with  $\varrho_i \propto \mathbb{1}$  for all  $i$ ) and other  $k$ -uniform hypergraph states, such as the states from Table 2. Hence, the set of connected graph states, for which in general local Clifford operations are not sufficient to characterize LU equivalence, is excluded. The second condition allows us to ignore some problematic states, where the Lemma 3 cannot be applied.

We have explained above that two  $k$ - and  $k'$ -uniform hypergraph states are not equivalent under the action of local Pauli operators unless they are the same. So we obtain the following corollary:

**Corollary 6.** *Let  $|\psi\rangle$  and  $|\phi\rangle$  be two different uniform  $N$ -qubit hypergraph states that belong to the family of generic LME states. Then  $|\psi\rangle$  is not LU equivalent to  $|\phi\rangle$ .*

Finally, we are able to identify a large class of states where Corollary 5 can be applied. More precisely, we show that if two hypergraphs contain the maximal edge  $\{1, \dots, N\}$ , then the two corresponding hypergraph states are LU equivalent if and only if they are LP equivalent. In order to do so, consider again the boolean function  $f(\mathbf{x})$  defined in Eq. (44). The quantity  $(-1)^{f(\mathbf{x})}$ , that defines the amplitudes of the hypergraph state, can be conveniently rewritten as

$$(-1)^{f(\mathbf{x})} = 1 - 2f(\mathbf{x}) \equiv f_{\pm}(\mathbf{x}). \quad (45)$$

The Hadamard transform of  $f(\mathbf{x})$  is defined as

$$\hat{f}(\mathbf{w}) = \frac{1}{2^N} \sum_{\mathbf{x}} f(\mathbf{x})(-1)^{\mathbf{x}^\top \mathbf{w}}. \quad (46)$$

The Hadamard transform of  $f_{\pm}$ , denoted by  $\hat{f}_{\pm}$ , gives the coefficients of the hypergraph

state in the trace decomposition, i.e.

$$\begin{aligned}\hat{f}_\pm(\mathbf{w}) &= \frac{1}{2^N} \sum_{\mathbf{x}} (-1)^{f(\mathbf{x})} (-1)^{\mathbf{x}^\top \mathbf{w}} \\ &= \frac{1}{2^N} \sum_{\mathbf{x}} [1 - 2f(\mathbf{x})] (-1)^{\mathbf{x}^\top \mathbf{w}} \\ &= \delta_{\mathbf{w}, \mathbf{0}} - 2\hat{f}(\mathbf{w}),\end{aligned}\tag{47}$$

since the linear function  $\mathbf{x}^\top \mathbf{w}$  of  $\mathbf{x}$  is always balanced as long as  $\mathbf{w} \neq \mathbf{0}$ .

The cardinality of the support of  $\hat{f}$ , i.e. the number of strings  $\mathbf{w}$  such that  $\hat{f}(\mathbf{w}) \neq 0$ , is bounded from below as  $|\text{supp}(\hat{f})| \geq 2^d$  [27]. Thus, using Eq. (47), it follows that  $|\text{supp}(\hat{f}_\pm)| \geq 2^d - 1$ , as  $\hat{f}_\pm(\mathbf{w})$  is proportional to  $\hat{f}(\mathbf{w})$  whenever  $\mathbf{w} \neq \mathbf{0}$ . If the hypergraph contains the largest edge of cardinality  $N$ , then the associated boolean function  $f$  has degree  $d = N$ . Furthermore, the cardinality of  $\text{supp}(f)$ , that we denote by  $F \equiv |\text{supp}(f)|$ , is always an odd number [18]. This can easily seen by noting that every  $C_e$  different from the one acting on all qubits contains an even number of  $-1$ , and hence also the product of different  $C_e$  does. Multiplying this product with the operator  $C_V$  on all qubits leads then to an operator with an odd number of  $-1$ . As a consequence, the function  $f$  is never balanced. It is also easy to see that the off-diagonal term of the single-qubit reduced state  $\varrho_i$  is [18]

$$\begin{aligned}(\varrho_i)_{01} &= \frac{1}{2^N} \sum_{\mathbf{x} \in \mathbb{Z}_2^{N_i}} (-1)^{f^{(i)}(\mathbf{x})} \\ &= \frac{1}{2^N} (2^{N-1} - 2F^{(i)}),\end{aligned}\tag{48}$$

where we defined  $N_i$  as the number of neighbours of vertex  $i$ ,  $f^{(i)}$  as the boolean function  $f^{(i)} = \bigoplus_{e \in E^{(i)}} \prod_{j \in e} x_j$ , and  $F^{(i)}$  as the cardinality of its support, i.e.  $F^{(i)} = |\text{supp}(f^{(i)})|$ . By the same reasoning as before,  $f^{(i)}$  corresponds again to a hypergraph which contains the maximal edge (here of cardinality  $N - 1$ ), and is thus also not balanced and  $F^{(i)} \neq 2^{N-2}$  for any  $i$ . Hence, none of the single-qubit reduced states is proportional to the identity. Moreover,  $f$  not balanced also implies that  $\hat{f}_\pm(\mathbf{0}) \neq 0$ , and therefore  $|\text{supp}(\hat{f}_\pm)| = 2^N$ , that is  $\hat{f}_\pm$  is never vanishing. This means that a hypergraph state with the edge of maximal cardinality is a generic LME state, which leads to the corollary:

**Corollary 7.** *Let  $|\psi\rangle$  and  $|\phi\rangle$  be  $N$ -qubit hypergraph states such that the associated hypergraphs contain the edge of maximum cardinality  $N$ . Then  $|\psi\rangle$  and  $|\phi\rangle$  are generic LME states and  $|\psi\rangle \simeq_{\text{LU}} |\phi\rangle$  if and only if  $|\psi\rangle$  and  $|\phi\rangle$  are equivalent under the action of local Pauli operators (in the  $Z$  basis).*

## 5. Nonclassicality of hypergraph states

In this section, we will investigate whether the correlations present in hypergraph states can be used to demonstrate contradictions between quantum physics and the

classical world view. Classical models obey by definition the constraint of realism: Any observable has a given value and this value is independent of whether the observable is indeed measured or not. In order to arrive at a contradiction to quantum mechanics, further assumptions on a classical model are needed. One possible assumption is noncontextuality. This means that the value of one measurement is independent of which other compatible measurement is carried out jointly with it. To give an example, one may consider the situation where the measurements  $A$  and  $B$  commute, and  $A$  and  $C$  commute. Then, the outcome of  $A$  is assumed to be independent of whether it is measured together with  $B$  or with  $C$ . A different type of assumption is the locality assumption. Here, one considers a system consisting of several particles and demands that an observable on one particle has a value that is independent of other observables at distant particles, measured at the same time. Clearly, the locality assumption can be viewed as the noncontextuality assumption applied to special observables.

Both assumptions are in conflict with the quantum mechanical prediction. For noncontextuality, this statement is known as the Kochen-Specker theorem [28, 29], while for locality this fact is called Bell's theorem [30]. It is also known that for usual graph states the stabilizer formalism can be used to derive arguments and inequalities to demonstrate these contradictions. For locality, the most famous of the arguments is the GHZ reasoning [9], but a plethora of further results exists [31–33]. For noncontextuality, the most known argument is the Mermin star [10], but recently many other contradictions have been systematically investigated [34, 35]. We will show now that similar contradictions can be found employing the nonlocal stabilizer of hypergraphs. We will first derive an argument and an inequality for noncontextuality, then we will show that it can be rephrased as a Bell inequality.

### 5.1. A GHZ-like argument for the hypergraph formalism

To start, let us recall the GHZ argument and the Mermin inequality for the three-qubit GHZ state. The three-qubit GHZ state is a graph state, where the graph is the fully connected graph. Its stabilizing operators are therefore given by  $g_1 = X_1Z_2Z_3$ ,  $g_2 = Z_1X_2Z_3$ , and  $g_3 = Z_1Z_2X_3$ . Then one considers the operator

$$\mathcal{M} = g_1 + g_2 + g_3 + g_1g_2g_3 \quad (49)$$

$$= X_1Z_2Z_3 + Z_1X_2Z_3 + Z_1Z_2X_3 - X_1X_2X_3. \quad (50)$$

The GHZ state is an eigenstate with the eigenvalue +1 for all the operators in the sum in Eq. (49), so the expectation value for this state is  $\langle \mathcal{M} \rangle = 4$ . On the other hand, if one considers the  $X_i$  and  $Z_i$  in the second line as classical quantities with values  $\pm 1$ , the product of the first three terms in Eq. (50) equals the last term, up to the sign. Therefore it is impossible to assign values to the  $X_i$  and  $Z_i$  such that all four terms take the value +1. It follows that classical models have to obey the constraint  $\langle \mathcal{M} \rangle \leq 2$ , which is known as Mermin inequality.

The question arises, whether a similar argument can be derived from the hypergraph formalism. Since the hypergraph stabilizer consists of nonlocal operators, such an argument will, in the first place, lead to a noncontextuality inequality. Later we will discuss whether this can be translated to a Bell inequality.

To derive an inequality in the hypergraph formalism, we aim at finding a hypergraph state whose stabilizer operators fulfill the following relation:

$$\sum_{i=1}^N g_i + \prod_{i=1}^N g_i = \sum_{i=1}^N X_i \left( \prod_{e \in E(i)} C_{e \setminus \{i\}} \right) - \prod_{i=1}^N X_i. \quad (51)$$

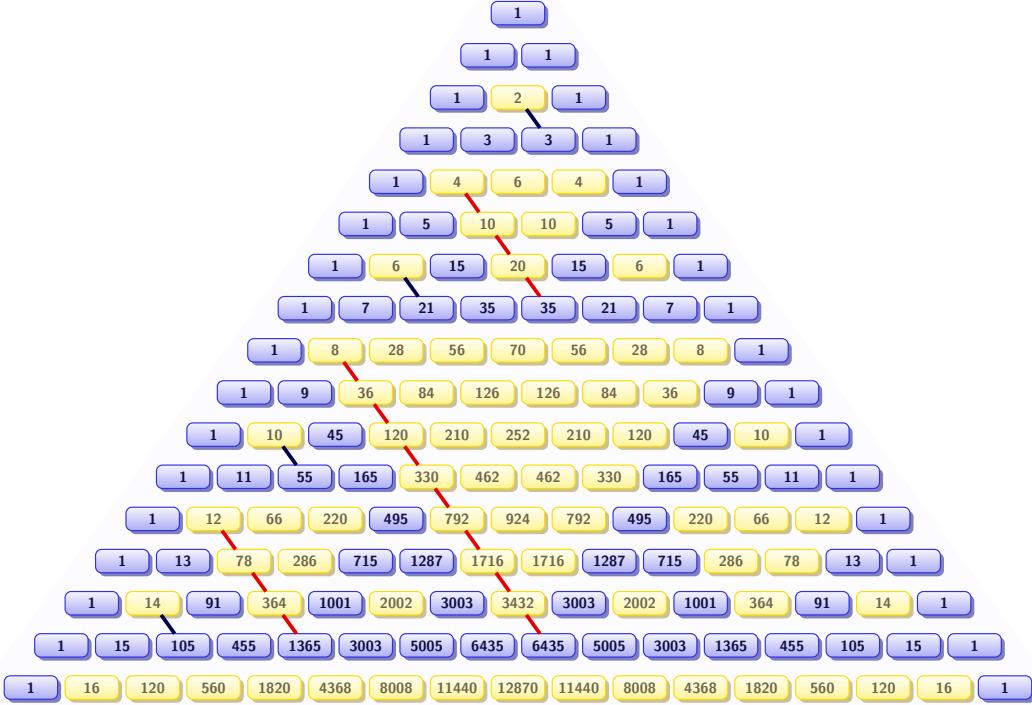
In this case, any classical assignment of  $\pm 1$  to the  $X_i$  as well as to the operators  $C_{e \setminus \{i\}}$  (which commute) cannot reproduce the quantum mechanical predictions. In order to make this ansatz work, we consider the subset of  $k$ -uniform fully connected hypergraph states. These are the hypergraphs where any possible  $k$ -edge is present. An example is the graph No. 14 in Fig. 3, which is the fully connected three-uniform four-vertex graph.

There are several conditions which have to be fulfilled by the stabilizer generated by  $\{g_i\}$  in order to fulfill Eq. (51):

- (i) First, if we want to apply the same trick as in the GHZ argument, the product of the first terms on the right-hand side of Eq. (51) has to equal the last term, up to a sign. This means that in this product each  $C_{e \setminus \{i\}}$  has to occur an even number of times. For  $k$ -uniform fully connected hypergraphs each of the  $C_{e \setminus \{i\}}$  occurs  $N - (k - 1)$  times, so this number has to be even.
- (ii) For the last term on the right-hand side of Eq. (51) there has to be a minus sign. We write  $\prod_{i=1}^N g_i = (\prod_{e \in E} C_e)(\prod_{i=1}^N X_i)(\prod_{e \in E} C_e)$  and with the help of Lemma 2 one finds that pulling each  $C_e$  from the left to the right results in a minus sign. It follows that the total number of  $C_e$  must be odd, so  $\binom{N}{k}$  must be odd.
- (iii) Finally, when applying Lemma 2 to the term  $\prod_{i=1}^N g_i$ , all the further  $C_j$  for  $j \neq \emptyset$  and  $j \neq e$  have to cancel. If  $j = \{j_1\}$  consists of a single element, the term  $C_j$  arises from a  $C_e$  if  $j_1 \in e$ . For fully-connected  $k$ -uniform hypergraphs, this happens  $\binom{N-1}{k-1}$  times, so this number must be even. By considering  $j = \{j_1, j_2\}$  one finds that  $\binom{N-2}{k-2}$  must be even. In general, any  $\binom{N-\alpha}{k-\alpha}$  must be even for any  $\alpha < k$ . Note that for  $\alpha = k - 1$  this implies the first condition explained above.

Considering the possible values for  $N$  and  $k$  fulfilling the conditions above, one finds the first possible choice to be  $(N, k) = (3, 2)$ , which is the original Mermin inequality (see Fig. 5). Further examples are  $(N, k) = (3 + 4r, 2)$ . These are, however, just known Bell inequalities for usual graph states. The first example for a hypergraph is the  $(N, k) = (7, 4)$ , i.e. a 7-qubit 4-uniform fully connected hypergraph state. This leads to the operator

$$\mathcal{M} = \sum_{i=1}^7 g_i + \prod_{i=1}^7 g_i = \sum_{i=1}^7 X_i \left( \prod_{e \in E(i)} C_{e \setminus \{i\}} \right) - \prod_{i=1}^7 X_i. \quad (52)$$



**Figure 5.** Pascal's triangle allows for a visualization of the conditions for obtaining a noncontextuality inequality in the hypergraph formalism. For that, one has to find a tuple  $(N, k)$  where  $\binom{N}{k}$  is odd, while  $\binom{N-\alpha}{k-\alpha}$  is even for any  $\alpha < k$ . Obvious solutions are of the type  $(N, k) = (3 + 4r, 2)$ , denoted by black lines. These correspond to the usual Mermin argument for standard graph states. Examples of solutions for hypergraph states are  $(7, 4)$ ,  $(15, 4)$ , or  $(15, 8)$ , see the lower ends of the red lines. The structure of odd and even binomial coefficients (marked in blue and yellow, respectively) is known to approximate the fractal of the Sierpiński triangle. From this one directly finds an arbitrary number of noncontextuality inequalities [e.g., for  $(N, k) = (31, 16)$ ]. The figure was generated with code from Ref. [36].

Note that here each  $(\prod_{e \in E(i)} C_{e \setminus \{i\}})$  contains 20 operators  $C_f$ . For any classical model which assigns to the  $X_i$  and  $C_{e \setminus \{i\}}$  the values  $\pm 1$ , we have  $\langle \mathcal{M} \rangle \leq 6$ , but for the corresponding hypergraph state, we have  $\langle \mathcal{M} \rangle = 8$ . This shows that the hypergraph formalism can be used to develop novel Kochen-Specker inequalities.

For an experimental test of this inequality, the experimenter should measure each of the eight correlation terms from Eq. (52). For each of them, he has to prepare the corresponding hypergraph state and then measure jointly or in a sequence the observables  $X_i$  and  $C_{e \setminus \{i\}}$ , which is possible, as these observables commute. The results are multiplied and averaged over many repetitions of the experiment, to compute  $\langle \mathcal{M} \rangle$ .

Two remarks should be added here. First, it is remarkable that the conditions to obtain a noncontextuality argument lead to the fractal structure of the Sierpiński triangle (see Fig. 5) and from this one can directly read off an infinite number of further noncontextuality arguments. In fact, one can directly see that if we take an arbitrary

$r \geq 1$  and  $s \geq 0$  and choose

$$k = 2^r \text{ and } N = (2^{r+1} - 1) + 2sk, \quad (53)$$

the corresponding  $(N, k)$  fully-connected  $k$ -uniform hypergraph state can be used to derive a noncontextuality inequality in the same way as before.

Second, we introduce for the case  $(N, k) = (7, 4)$  the observables

$$A_i = \prod_{e \text{ with } i \in e \text{ and } |e|=3} C_e \quad (54)$$

as the product of all possible  $C_e$  where  $e$  are 3-edges that contain  $i$ . Then we have  $A_2 A_3 A_4 A_5 A_6 A_7 = \prod_{e \in E(1)} C_{e \setminus \{1\}}$ , so the product of the six  $A_i$  contains all  $C_e$ , where  $e$  are 3-edges that do *not* contain  $i = 1$ . Then we can write  $g_1 = X_1 A_2 A_3 A_4 A_5 A_6 A_7$  and the noncontextuality inequality takes the form

$$\langle \mathcal{M} \rangle = \langle X_1 A_2 A_3 A_4 A_5 A_6 A_7 \rangle + \text{permutations} - \langle X_1 X_2 X_3 X_4 X_5 X_6 X_7 \rangle \leq 6, \quad (55)$$

while for the hypergraph state we have  $\langle \mathcal{M} \rangle = 8$ . This form shows the close relation to the original Mermin inequality in Eq. (50). Note, however, that this is only a formal similarity and that in this form the  $A_i$  are not the appropriate observables to measure, since  $X_i$  and  $A_j$  for  $i \neq j$  do not commute.

### 5.2. Bell inequalities in the hypergraph formalism

So far, we have shown how the hypergraph formalism can be used to derive noncontextuality inequalities for nonlocal observables. It would be very desirable, however, to find also Bell inequalities for local observables. To demonstrate that this is indeed possible, one can decompose the nonlocal observables into local ones, and can try to show that a local assignment of classical values for these local observables cannot lead to the same result as quantum physics.

To start, let us consider Eq. (52). We can write the first term in  $\mathcal{M}$  as

$$\begin{aligned} g_1 &= X_1 \otimes \left( \prod_{e \in E(1)} C_{e \setminus \{1\}} \right) \\ &= \frac{1}{128} [X_1 \otimes (48 \cdot \mathbb{1}^{\otimes 6} + 16 \cdot [Z_2 Z_3 \mathbb{1} \mathbb{1} \mathbb{1} \mathbb{1} + \text{permutations}] \\ &\quad - 16 \cdot [Z_2 Z_3 Z_4 Z_5 \mathbb{1} \mathbb{1} + \text{permutations}] + 80 \cdot Z^{\otimes 6})], \end{aligned} \quad (56)$$

and the other terms can be represented similarly. In this way, we can express the correlation  $\mathcal{M}$  only in terms of local measurements  $X_i$  and  $Z_i$ . The question is, whether the bound  $\langle \mathcal{M} \rangle \leq 6$  still holds, if we assign to these local observables the values  $\pm 1$  in a local manner.

This is indeed the case and it can be seen as follows: Any local assignment of  $\pm 1$  to three observables  $Z_i, Z_j$ , and  $Z_k$  gives a value for the nonlocal observable  $C_{\{i,j,k\}}$  as

this can be expressed as a classical function in terms of the  $Z_i$ ,  $Z_j$ , and  $Z_k$ . Moreover, one can directly check that from a local assignment to  $Z_i$ ,  $Z_j$ , and  $Z_k$  the observable  $C_{\{i,j,k\}}$  can only take the values  $\pm 1$ . Therefore, a local assignment to the  $Z_i$  leads to a noncontextual assignment of  $C_{e \setminus \{i\}}$  in Eq. (52) and the bound  $\langle \mathcal{M} \rangle \leq 6$  holds. In this way, all the noncontextuality inequalities from the previous section can be interpreted as Bell inequalities, if the nonlocal observables  $C_e$  are decomposed into local observables  $Z_i$ .

Finally, we note that it is not clear how to construct a Bell or noncontextuality inequality with the help of the stabilizer for arbitrary hypergraph states. The simple method for graph states from Ref. [33] is not successful, since multiplying the elements of the stabilizer of the hypergraph state does not necessarily result in different signs. We believe that finding more general Bell inequalities for hypergraph states is a topic worth of further investigation.

## 6. Conclusions

In conclusion we have investigated the entanglement properties and nonclassical features of hypergraph states. We have characterized the local unitary equivalence classes up to four-qubits and have provided general conditions under which the local unitary equivalence of hypergraph states can simply be decided by considering the finite set of local Pauli transformations. Finally, we have shown that the stabilizer formalism of hypergraph states can be used to derive various inequalities for testing the Kochen-Specker theorem or Bell's theorem.

There are many questions which are worth to be addressed in the future. First, it would be highly desirable to find applications of hypergraph states, e.g. for quantum error correction. Second, it would be interesting to see whether the stabilizer formalism of hypergraph states can also be used to derive Bell inequalities with an increasing violation. Finally, proposals for the experimental generation of hypergraph states with photons or ions are still missing.

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## 7. Appendix

In Table 2 we present the 24 classes of three-uniform six-qubit hypergraph states, where all single-qubit reduced density matrices are maximally mixed.

Class	Edges
1	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 3, 6\}, \{2, 3, 4\}, \{2, 3, 5\}, \{2, 3, 6\}\}$
2	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 6\}, \{2, 3, 4\}, \{2, 3, 5\}, \{2, 4, 6\}\}$
3	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 3, 5\}, \{1, 4, 6\}, \{1, 5, 6\}, \{2, 3, 6\}, \{2, 4, 5\}, \{2, 5, 6\}, \{3, 4, 5\}, \{3, 4, 6\}\}$
4	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 4, 5\}, \{1, 4, 6\}, \{2, 3, 4\}, \{2, 4, 5\}, \{2, 4, 6\}, \{3, 5, 6\}\}$
5	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 3, 6\}, \{1, 4, 5\}, \{2, 3, 4\}, \{2, 3, 5\}, \{2, 3, 6\}, \{2, 4, 5\}\}$
6	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 5\}, \{1, 4, 6\}, \{2, 3, 4\}, \{2, 4, 5\}, \{2, 4, 6\}, \{3, 5, 6\}\}$
7	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 6\}, \{1, 5, 6\}, \{2, 3, 4\}, \{2, 3, 5\}, \{2, 4, 6\}, \{2, 5, 6\}\}$
8	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 6\}, \{1, 5, 6\}, \{2, 3, 4\}, \{2, 3, 5\}, \{2, 4, 6\}, \{3, 5, 6\}\}$
9	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 4, 5\}, \{1, 4, 6\}, \{2, 3, 4\}, \{2, 4, 5\}, \{2, 5, 6\}, \{3, 4, 6\}, \{3, 5, 6\}\}$
10	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 4, 5\}, \{1, 5, 6\}, \{2, 3, 4\}, \{2, 4, 5\}, \{2, 5, 6\}, \{3, 4, 6\}, \{3, 5, 6\}\}$
11	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 5\}, \{1, 4, 6\}, \{2, 3, 4\}, \{2, 3, 5\}, \{2, 4, 5\}, \{2, 4, 6\}, \{3, 5, 6\}\}$
12	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 6\}, \{1, 5, 6\}, \{2, 3, 4\}, \{2, 4, 6\}, \{2, 5, 6\}, \{3, 4, 5\}, \{3, 5, 6\}\}$
13	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 3, 6\}, \{1, 4, 5\}, \{2, 3, 4\}, \{2, 3, 6\}, \{2, 4, 5\}, \{2, 4, 6\}, \{3, 4, 5\}, \{3, 4, 6\}\}$
14	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 5\}, \{1, 4, 6\}, \{2, 3, 4\}, \{2, 3, 5\}, \{2, 4, 5\}, \{2, 4, 6\}, \{3, 4, 5\}, \{3, 5, 6\}\}$
15	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 5\}, \{1, 4, 6\}, \{2, 3, 4\}, \{2, 3, 5\}, \{2, 4, 6\}, \{2, 5, 6\}, \{3, 4, 5\}, \{3, 5, 6\}\}$
16	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 5\}, \{1, 4, 6\}, \{2, 3, 4\}, \{2, 3, 5\}, \{2, 5, 6\}, \{3, 4, 5\}, \{3, 4, 6\}, \{3, 5, 6\}\}$
17	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 6\}, \{1, 5, 6\}, \{2, 3, 4\}, \{2, 3, 5\}, \{2, 4, 6\}, \{2, 5, 6\}, \{3, 4, 5\}, \{3, 4, 6\}\}$
18	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 5\}, \{1, 4, 6\}, \{2, 3, 5\}, \{2, 3, 6\}, \{2, 4, 6\}, \{2, 5, 6\}, \{3, 4, 5\}, \{3, 4, 6\}, \{3, 5, 6\}\}$
19	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 5\}, \{1, 4, 6\}, \{2, 3, 4\}, \{2, 3, 5\}, \{2, 4, 5\}, \{2, 5, 6\}, \{3, 4, 5\}, \{3, 4, 6\}, \{3, 5, 6\}\}$
20	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 5\}, \{1, 4, 6\}, \{2, 3, 5\}, \{2, 3, 6\}, \{2, 4, 5\}, \{2, 4, 6\}, \{3, 4, 5\}, \{3, 4, 6\}, \{3, 5, 6\}\}$
21	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 4, 5\}, \{1, 4, 6\}, \{2, 3, 5\}, \{2, 3, 6\}, \{2, 4, 6\}, \{2, 5, 6\}, \{3, 4, 5\}, \{3, 4, 6\}, \{3, 5, 6\}\}$
22	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 3, 4\}, \{1, 3, 6\}, \{1, 4, 5\}, \{1, 4, 6\}, \{1, 5, 6\}, \{2, 3, 5\}, \{2, 3, 6\}, \{2, 4, 5\}, \{2, 4, 6\}, \{2, 5, 6\}, \{3, 4, 6\}, \{3, 5, 6\}\}$
23	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 3, 4\}, \{1, 3, 6\}, \{1, 4, 5\}, \{1, 4, 6\}, \{1, 5, 6\}, \{2, 3, 5\}, \{2, 3, 6\}, \{2, 4, 5\}, \{2, 4, 6\}, \{2, 5, 6\}, \{3, 4, 5\}, \{3, 4, 6\}, \{3, 5, 6\}\}$
24	$\{\{1, 2, 3\}, \{1, 2, 4\}, \{1, 2, 5\}, \{1, 2, 6\}, \{1, 3, 4\}, \{1, 3, 5\}, \{1, 3, 6\}, \{1, 4, 5\}, \{1, 4, 6\}, \{2, 3, 5\}, \{2, 3, 6\}, \{2, 4, 5\}, \{2, 4, 6\}, \{2, 5, 6\}, \{3, 4, 5\}, \{3, 4, 6\}, \{3, 5, 6\}\}$

**Table 2.** The 24 classes of three-uniform six-qubit hypergraph states, where all the reduced single particle density matrices are maximally mixed.

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