Letter

Automated generation of arbitrarily many Kochen-Specker and other contextual sets in odd-dimensional Hilbert spaces

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The development of quantum computation and communication, recently shown to be supported by contextuality, arguably asks for a requisite supply of contextual sets. While that has been achieved in even-dimensional spaces, in odd-dimensional spaces only a dozen contextual critical Kochen-Specker (KS) sets have been found so far. In this Letter, we give three methods for the automated generation of arbitrarily many contextual KS and non-KS sets in any dimension for possible future application and implementation, and we employ them to obtain millions of KS and other contextual sets in dimensions 3, 5, 7, and 9 where previously only a handful of sets have been found. Also, we generate explicit vectors for the original Kochen-Specker set from 24 vector components.

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Contextuality is paving the road for applications in quantum computation [1,2], quantum steering [3], and quantum communication [4], as proved by the methods of processing, preparing, and measuring of *qudits* (quantum dits). Qudits are the units of quantum information carried by a quantum system whose number of states (d) is an integer greater than one. *Qubits* (quantum bits) are two-dimensional qudits ($d = 2$) and their tensor products build the corresponding even-dimensional Hilbert spaces. The smallest contextual sets from these spaces have been implemented in a series of experiments, while in Refs. [5–9] billions of contextual sets in 4-, 6-, 8-, 16-, and 32-dimensional Hilbert spaces, predominantly related to qubits, were generated by means of vector component algorithms (called method M3 below), particular symmetries, geometries, polytope correlations, parity filtering, Pauli operators, qubit states, and dimensional upscaling.

In contrast, far fewer contextual sets based on qudits in odd-dimensional spaces have been obtained so far. In particular, of Kochen-Specker contextual sets only four in the three-dimensional space [8,10], four in the five-dimensional space [11,12], five in the seven-dimensional space [11–13], two in the nine-dimensional space [12], and two in the 11-dimensional space [12]. General methods for the automated generation of sets of a chosen structure are lacking.

Since quantum communication and computation are supported by contextuality [1,2], the actual potential use of a large supply of contextual sets is twofold. First, quantum computation algorithms which would rely on contextual sets would arguably rely on a variety of such sets and on their automated generation. Second, structural properties of contextual sets differ according to their coordinatization, parities, dimensions, sizes, etc., and that can lead us to better understanding and applications of the sets.

In this Letter, we offer universal and general algorithms for the automated generation of arbitrarily many contextual sets in any dimension. In contrast to them, the programs we wrote to implement them are computationally demanding and therefore, here, we use them to generate sets that have not been generated so far: billions of KS and contextual non-KS sets in $n = 3, 5, 7, 9$-dimensional spaces. The programs themselves are freely available from our repository and technical details of their previous versions are given in Refs. [5–9].

To describe and handle contextual sets we make use of the McKay-Megill-Pavičić-hypergraph (MMPH) language [10,14]. An MMPH is a connected n-dimensional *hypergraph k-l* with k vertices and l hyperedges in which (i) every vertex belongs to at least one hyperedge; (ii) every hyperedge contains at least two and at most n vertices; (iii) no hyperedge shares only one vertex with another hyperedge; and (iv) hyperedges may intersect each other in at most $n - 2$ vertices. Graphically, vertices are represented as dots and hyperedges as (curved) lines passing through them.

We encode MMPHs by means of the following 90 ASCII characters: `1 2 ... 9 A B ... Z a b ... z ! " # $ % & ' ( ) * - / : ; < = > ? @ [ \ ] ^ _ ` { | } ~` [10]. When all 90 characters are exhausted, we reuse them prefixed by "+" (91st character), then again by "++," and so on. So encoded single ASCII characters (possibly prefixed by +'s) represent vertices, e.g., `1` or `+++A`. Put together they represent hyperedges, e.g., `123` or `1+1+++1Dd`. To represent an MMPH, hyperedges are organized in a string in which they are separated by commas; each string ends with a period, e.g., the string `123,345,567,789,9A1.` represents a noncontextual three-dimensional MMPH pentagon. There

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is no limit on the size of an MMPH. An MMPH is a special kind of a general hypergraph in the sense that none of the aforementioned points (i)–(iv) holds for it.

Of course, instead of ASCII characters we could have used Unicode characters or 16-bit integers but 20 years ago we decided to proceed with the ASCII characters to encode MMPH strings and design our algorithms and programs which in turn yield all properties and features of MMPHs as well as their figures within the MMPH language. All our papers since 2000 [15] make use of the ASCII characters for the purpose.

The MMPHs above are defined without a coordinatization. The meaning of coordinatization is that a vector is assigned to each vertex and that all vectors assigned to vertices belonging to a common hyperedge are orthogonal to each other. Thus, in the MMPHs above, neither their vertices nor their hyperedges are related to either vectors or operators. We say that an MMPH is in an n-dimensional space, called MMPH space, when either all its hyperedges contain n vertices or when we might add vertices to hyperedges so that each contains n vertices. Orthogonality between vertices in an MMPH space just means that they are contained in common hyperedges. Our programs may handle MMPHs without any reference to either vectors or projectors. In an MMPH with a coordinatization, i.e., with vectors assigned to vertices, an n-dimensional MMPH space becomes an n-dimensional Hilbert space spanned by a maximal number of (possibly added) vectors within hyperedges. Whether we speak about an MMPH without or with a coordinatization will be clear from the context.

A *nonbinary* MMPH (NBMMPH) is an n-dimensional ($n \geqslant 3$) k-l MMPH, whose ith hyperedge contains $\kappa(i)$ vertices $[2 \leqslant \kappa(i) \leqslant n,\ \ i = 1, \dots, l]$, to which it is impossible to assign 1s and 0s in such a way that the following rules hold: (I) No two vertices in any hyperedge are both assigned the value 1 and (II) in any hyperedge, not all of the vertices are assigned the value 0. A *binary* MMPH (BMMPH) is an MMPH for which such an assignment is possible. NBMMPHs are nonclassical and contextual since they do not allow assignments of predefined 0s and 1s to their vertices. BMMPHs are classical and noncontextual since they do allow such an assignment. A KS MMPH is an NBMMPH with $\kappa(i) = n,\ \forall i$. The assignments of 0s and 1s do not require a coordinatization but an implementation of (N)BMMPHs does require it as well as their filled MMPHs, i.e., those in which to all hyperedges with $\kappa(i) \leqslant n$ we add $n - \kappa(i)$ vertices so as to satisfy the mutual orthogonalities. An example of a non-KS NBMMPH without a coordinatization is the 33-27 in Fig. 1(d) in the Supplemental Material (SM) [16].

When either state-dependent or state-independent tests of operators defined on vertices of an NBMMPH with $\kappa(i) \leqslant n$ confirm the contextuality, e.g., Refs. [17–19], then the NBMMPH turns out to be contextual in all considered cases so far.

A *critical* NBMMPH is an NBMMPH which after removing any of its hyperedges becomes a BMMPH.

To generate (N)BMMPHs in the odd-dimensional spaces we make use of three methods, M1–M3.

M1 consists of an automated dropping of vertices contained in single hyperedges (multiplicity $m = 1$) [14] of MMPHs and a possible subsequent stripping of their hyperedges. The obtained smaller MMPHs are often NBMMPH although never KS.

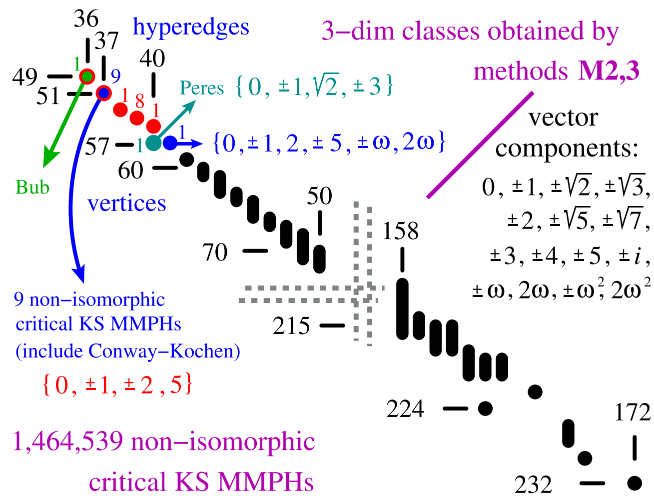

FIG. 1. The distribution of critical three-dimensional KS MMPHs obtained via M2 and M3 with the given vector components. Abscissa is l (number of hyperedges); ordinate is k (number of vertices). Dots represent (k, l). Consecutive dots (same l) are shown as strips. The same applies to Figs. 2 and 3. See text. MMPH strings, figures, and vectors are given in SM [16].

M2 consists of an automated random addition of hyperedges to MMPHs so as to obtain larger ones which then serve us to generate smaller KS MMPHs by stripping hyperedges randomly again.

M3 consists of combining simple vector components so as to exhaust all possible collections of n mutually orthogonal n-dimensional vectors. These form big *master* MMPHs which consist of single or multiple MMPHs of different sizes. Master MMPHs may or may not be NBMMPH, which we find out by applying filters to them. NBMMPHs serve us to massively generate a *class* of smaller MMPHs via our algorithms and programs.

We carry out methods M1–M3 by means of our programs MMPSSTRIP (for stripping and adding hyperedges), STATES01 (for verifying the contextuality), MMPSHUFFLE (for reorganizing MMPHs), and ONE (for evaluating the structural properties of MMPHs [14]).

We combine all three methods to obtain a large number of NBMMPHs in odd-dimensional spaces.

Three-dimensional case. So far there have been only four known KS MMPHs, and as we show in Ref. [8] none of their varieties with stripped $m = 1$ vertices is critical. Via M1, i.e., by stripping their edges, we can obtain thousands of smaller non-KS NBMMPHs and BMMPHs down to a pentagon [8]. But this means that they are limited in size by the size of four original MMPHs. To get larger MMPHs we have to apply M2 and M3. The final distribution of critical KS MMPHs we generated is given in Fig. 1.

M2 consists in adding hyperedges to Bub, Conway-Kochen, and Peres' KS MMPHs (for citations and figures, see Ref. [6]) using our program MMPSSTRIP, filtering out KS MMPHs, and stripping them to the critical KS MMPHs by

TABLE I. Some of smaller NBMMPHs obtained by methods M1–M3; "†" indicates that the MMPH is a non-KS NBMMPH—all the others are KS NBMMPHs; "?" indicates that obtaining the coordinatization is too demanding and that we were not able to carry it out on our supercomputers or that it might not exist at all.

Dimension	Smallest critical MMPHs	No. of nonisom. MMPHs	Methods	Smallest master	Vector components
3D MMPHs	5-5†	1	M1	40-23	$\{0, \pm 1, 2\}$
	19-13	1	M2	20-14	None
	39-27	1	M2	39-30	?
	49-36	1	M2 and M3	97-64	$\{0, \pm 1, \pm 2, 5\}$
	51-37	9	M2 and M3	97-64	$\{0, \pm 1, \pm 2, 5\}$
	53-38	1	M2 and M3	97-64	$\{0, \pm 1, \pm 2, 5\}$
	57-40	1	M2 and M3	81-52	$\{0, \pm 1, \sqrt{2}, \pm 3\}$
	69-50	3	M3	169-120	$(0, \pm\omega, 2\omega, \pm\omega^2, 2\omega^2\}$
5D	29-16	2	M3	105-136	$\{0, \pm 1\}$
7D	13-4	1	M1 and M2	24-6	?
	28-14†	1	M2 and M3	805-9936	$\{0, \pm 1\}$
	34-14	1	M3	805-9936	$\{0, \pm 1\}$
	207-97	1	M3	805-9936	$\{0, \pm 1\}$
9D	19-5	2	M2	20-6	?
	47-16	2	M3	9586-12068704	$\{0, \pm 1\}$
	7-6†	1	M1 and M3	9586-12068704	$\{0, \pm 1\}$

STATES01. The latter critical MMPHs build their coordinatization from the two vector component sets of the original three MMPHs.

These vector components also serve us to obtain the same critical KS MMPHs by employing M3 so as to exhaust all possible collections of three mutually orthogonal vectors representing hyperedges interwoven in MMPHs.

When applying M3 we obtain that Bub's is the only 49-36 NBMMPH and that there are no smaller KS ones for the considered vector components. There are no other critical KS MMPHs between 49-36 and 51-37; between 51-37 and Peres' 57-40 we obtained the following nonisomorphic MMPHs: one 53-38, eight 54-39, and one 55-40. Peres' 57-40 is generated from the components $\{0, \pm 1, \pm\sqrt{2}, 3\}$ and all the smaller ones from $\{0, \pm 1, \pm 2, 5\}$. When we apply M2 so as to add sufficiently many hyperedges to any of the three original MMPHs (Bub, Conway-Kochen, or Peres') and then strip them back down in a search for smaller critical MMPHs, we always obtain the other two among the generated critical KS MMPHs.

The more components we use with M3, the larger the master files and the more critical KS MMPHs we obtain. For instance, with the help of $\{0, \pm 1, \sqrt{2}, 3\}$ (Peres') components we obtain the master 81-52 which contains just one single critical set—Peres' 57-40; $\{0, \pm 1, \pm 2, 5\}$ yield the master 97-64 which generates 20 critical KS MMPHs from 49-36 to 55-40; in contrast, $\{0, \pm 1, \sqrt{2}, \pm 2, \pm 3, 5\}$ yield the master 301-184 which generates 81 critical KS MMPHs from 49-36 to 92-66; $\{0, \pm\omega, 2\omega, \pm\omega^2, 2\omega^2\}$, where$\omega = e^{2\pi i/3}$, yield 514 criticals from 69-50 to 106-79, etc. Several smallest MMPHs from these classes are shown in Table I and SM.

We did not find simple real vector components which would yield KS MMPHs smaller than 49-36, although we are able to generate many smaller KS MMPHs down to 19-13 or 39-27 shown in SM, although without a coordinatization based on components shown in Fig. 1.

The path taken in Ref. [20] is intractable for hundreds of small KS MMPHs we checked on our supercomputer since the number of free variables is too high. See Fig. 1(a) in SM [16].

Another path was taken in 2021 by Jean-Pierre Merlet who applied the interval analysis method of solving nonlinear equations to the 19-13 MMPH. The equations turned out not to have a real solution and complex ones were not calculable even on a supercomputer.

As for possible coordinatizations of smaller KS MMPHs, we draw a parallel with the original KS set 192-118 [21]. Its trigonometric formula in Ref. [21] looks simple, but its coordinatization is so complicated that a random search for them is infeasible. More specifically, the aforementioned trigonometric formula is not sufficient to provide a coordinatization. We therefore constructed a coordinatization of the original Kochen-Specker set from 24 components in SM [16].

Five-dimensional case. In contrast to the three-dimensional case, the five-dimensional KS MMPHs can be obtained from just three vector components $\{0, \pm 1\}$, which by method M3 generate the 105-136 master set and its 105-136 class of KS MMPHs. These include critical ones from the smallest 29-16 to the biggest 64-41, altogether 27 829 399 nonisomorphic MMPHs. The distribution of the MMPHs within the class is shown in Fig. 2(a) and the 29-16 in Fig. 2(b).

We also obtained the master (1185-3596) and a number of elements from its class from the five components $\{0, \pm 1, \pm 2\}$ but we stopped the generation of KS criticals after only 307 MMPHs. Their distribution is indicated in Fig. 2—if fully generated it would completely include the 105-136 class and would be continuously spread over the whole ranged of hyperedges and vertices.

Seven-dimensional case. We generated the seven-dimensional critical KS MMPHs from the vector components

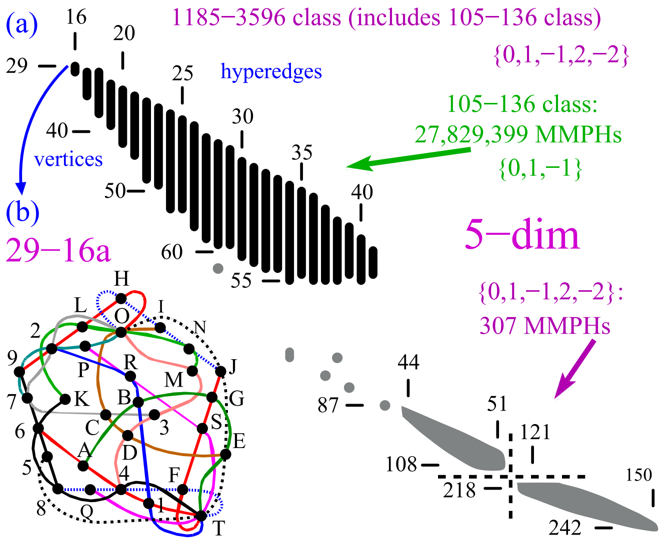

FIG. 2. (a) Distribution of the five-dimensional critical KS MMPHs obtained by M3; the generation of the 1185-3596 was demanding and CPU-time consuming, so we stopped it after obtaining the upper samples which enable us to estimate the size of the class. (b) One of the two smallest five-dimensional 29-16 critical KS MMPH; the other (29-16b) was previously obtained by the dimensional upscaling method in Ref. [12].

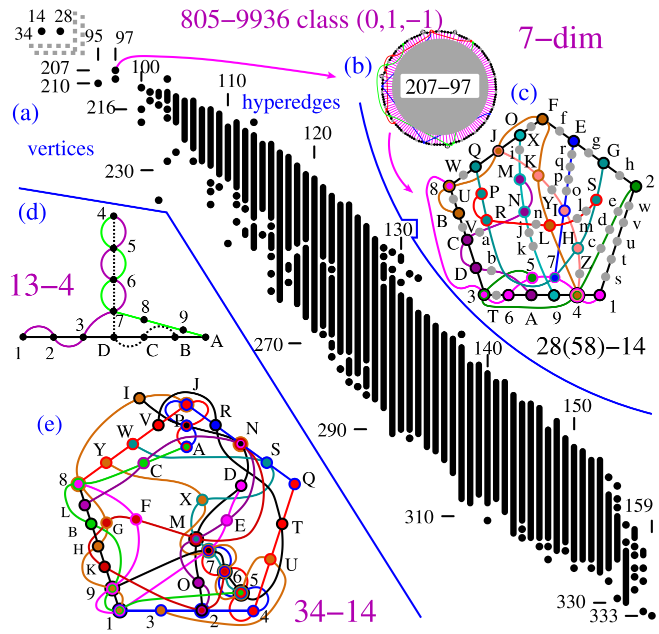

FIG. 3. (a) Distribution of 42 816 seven-dim critical KS MMPHs from the class 805-9936 generated by M2 and M3; the master is obtained from $\{0, \pm 1\}$. (b) 207-97; too interwoven to be graphically represented in detail. (c) The non-KS NBMMPH obtained from 207-97 via MMPSHUFFLE. (d) Critical KS 13-4 obtained by M1 and M2. (e) Critical KS 34-14 MMPH obtained by massive targeting MMPHs with 34 vertices—see text.

$\{0, \pm 1\}$ via M3 so as to first obtain the 805-9936 master which in turn generated the the 805-9936 class shown in Fig. 3(a). Their vectors were automatically generated from the master set by means of our programs MMPSTRIP, MMPSHUFFLE, and STATES01.

The generation provided MMPHs from 207-97 to 333-159 after running 200 parallel jobs on a supercomputer for 2 weeks. Longer runs would give us smaller MMPHs as proved by the 34-28 MMPH [see the top of Fig. 3(a)] obtained in Ref. [11]. Particular targeted runs might give us particular smaller KS MMPHs, e.g., the critical 34-14 [Figs. 3(a) and 3(e) and SM]; it required stripping the master down to the MMPHs with 34 vertices via MMPSTRIP and then filtering them for the KS feature via STATES01; since such a procedure is too CPU-time demanding, a search for further smaller MMPHs is out of the scope of this Letter. Instead, M1 can serve for a massive automated generation of smaller non-KS NBMMPHs with the help of MMPSHUFFLE and MMPSTRIP. An outcome (28-14) is shown in Fig. 3(c), as obtained from the 207-97 [Figs. 3(a) and 3(b)]. The procedure is analogous to stripping original three-dimensional MMPHs [8].

Yet another way of automated generation of seven-dimensional MMPHs is via M2 by means of MMPSTRIP, an example of which is 13-6 shown in Fig. 3(d); we were not able to find its coordinatization and we conjecture that it does not have any. We confirmed that it is not determined by the vector components $\{0, \pm 1\}$ and we work on a program which would calculate coordinatization for bigger instances of such MMPHs we generated.

Nine-dimensional case. Two entangled qutrits live in a nine-dimensional space and we generated the MMPH master from $\{0, \pm 1\}$ components. It consists of 9586 vertices and 12 068 705 hyperedges and that proved to be too huge for a direct generation of critical MMPHs (via stripping and filtering) from the master MMPH although the KS 47-16 given in SM proves that the master is a KS MMPH.

However, smaller critical KS MMPH can be obtained from simple BMMPHs via M2, in particular via an automated procedure of adding hyperedges and then generating critical KS MMPHs by stripping hyperedges via M1 and filtering them for the critical KS property. The critical KS MMPH 19-5 obtained in this way [Fig. 4(a)] has no coordinatization from $\{0, \pm 1\}$ and we conjecture that it does not have any, but it represents the proof of principle of how M2 works.

Also, a great many of MMPHs stripped of $m = 1$ vertices exhibit contextuality. Smaller ones can easily be implemented. The smallest one we obtained by M3 and M1 is shown in Fig. 2(c) of SM and referred to in Table I. Its filled MMPH is shown in Fig. 2(c) of SM. Their differences are discussed in SM.

To summarize, in this Letter, we give methods for generating KS as well as non-KS NBMMPHs in odd-dimensional Hilbert spaces. Our goal is not to find "record" smallest MMPHs but to establish general methods for automated

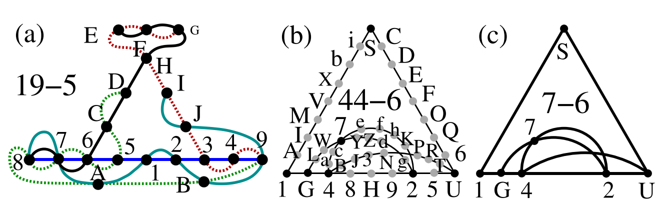

FIG. 4. (a) KS MMPH 19-5; no coordinatization was found. (b) BMMPH 44-6. (c) NBMMPH 7-6. MMPH strings (a)–(c) and vectors (b), (c) are given in SM.

generation of NBMMPHs in any dimension for any possible future application and implementation, e.g., in quantum computation and communication. The methods are especially needed in odd-dimensional Hilbert spaces since, in contrast to even-dimensional ones, we cannot make use of polytopes, Pauli operators, qubit states, parities, and other approaches specific to qubit spaces. We propose three such methods: M1 which consists in dropping vertices contained in single hyperedges, M2 consists in random addition of hyperedges to MMPHs, and M3 which consists in combining simple components so as to exhaust all possible collections of mutually orthogonal vectors. Automated generation is achieved by means of our algorithms and programs presented above.

In the three-dimensional space we generated roughly a million and a half nonisomorphic KS ones, ranging from MMPHs with 19 vertices and 13 hyperedges (19-13) without a coordinatization (via M3), over eleven 51-37s, up to a 232-172, all with coordinatizations, distributed as shown in Fig. 1. Special cases are given in Table I and SM. In SM we also give an explicit coordinatization of the original KS set.

In the five-dimensional space, from the vector components $\{0, \pm 1\}$, we generated roughly 28 million KS MMPHs whose distribution is shown in Fig. 2(a), ranging from 29-16 to 242-131.

In the seven-dimensional space the components $\{0, \pm 1\}$ generate roughly 30000 rather big and computationally demanding KS MMPHs shown in Fig. 3(a), ranging from 34-14 to 333-159.

The nine-dimensional MMPH master generated by $\{0, \pm 1\}$ has 9586 vertices and 12 068 705 hyperedges and it is computationally too demanding to yield critical KS MMPHs directly.

We also explain how a combination of methods M1–M3 can be employed to generate targeted smaller classes of non-KS NBMMPHs. This approach is important because the operator- and projector-based contextual sets, which are recently being used in the literature, are often built by means of such NBMMPHs.

Our programs are freely available from our repository [22].

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