

New class of 4-dim Kochen–Specker sets

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We find a new highly symmetrical and very numerous class (millions of nonisomorphic sets) of 4-dim Kochen–Specker (KS) vector sets. Due to the nature of their geometrical symmetries, they cannot be obtained from previously known ones. We generate the sets from a single set of 60 orthogonal spin vectors and 75 of their tetrads (which we obtained from the 600-cell) by means of our newly developed *stripping technique*. We also consider *critical KS subsets* and analyze their geometry. The algorithms and programs for the generation of our KS sets are presented. © 2011 American Institute of Physics. [doi:10.1063/1.3549586]

I. INTRODUCTION

Kochen–Specker (KS) sets have recently been studied extensively due to new theoretical results which have prompted new experimental and computational techniques. The theoretical results consider conditions under which such experiments are feasible,^{1,2} including single qubit KS setups.^{3,4} Such results and experiments are applicable to quantum computational rules of dealing with qubits and qutrits within a large number of quantum gates.

The experiments were carried out for spin-(1/2) \otimes (1/2) particles (correlated photons, or neutrons with spatial and spin degrees of freedom), and therefore, in this paper we provide results only for 4-dim KS vector sets of yes–no questions (KS sets for short). Recent designs⁵ and experiments^{6–11} deal with state-independent vectors. Such experiments can tell us a great deal more about quantum formalism and the geometry involved in obtaining new functional KS setups and quantum gate setups in general. On the other hand, a recent result of Cabello¹² connects noncontextuality and, therefore, the KS theorem with quantum nonlocality and opens the possibility of using KS sets in quantum information experiments.

For both of these applications, it is important to have many nonisomorphic critical (empirically distinguishable) KS sets. Before our work, only eight 4-dim ones were known (see below). In this work, we present thousands of new nonisomorphic 4-dim critical and millions of noncritical KS sets. This is also important for a better understanding of quantum systems. First, it seemed that quantum gates and system state configurations that would allow only quantum representations were very sparse. We show that they are actually abundant. Second, the configurations of Hilbert space vectors and subspaces in KS sets have interesting symmetries that have intrigued many authors since the discovery of the KS theorem.^{13–23} We now get many new symmetries because we obtain a new disjoint class of KS sets, none of which were previously known and none of which can be built up from previously known ones.

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Recently, we found that all known KS sets with up to 24 vectors and component values from the set $\{-1,0,1\}$ (including one with 18 vectors for which experiments have been carried out) can be obtained from a single KS set with 24 vectors and 24 tetrads (blocks) originally found by Peres.²⁴ The following is a brief summary of the techniques we used for that discovery.

When a KS set can be obtained from a larger one by stripping (removing) tetrads, the stripped tetrads correspond to redundant detections within a measurement of spin projections. “Critical” sets are the smallest empirically distinguishable KS sets in the sense that they cannot be reduced to each other by stripping tetrads. Instead, stripping any tetrad from a critical set will cause the set to cease to be a KS set.

Using the “stripping technique” (which we explain below), we exhaustively generated all possible 24–24 McKay-Megill-Pavicic (MMP) hypergraphs²⁵ [each vertex in a hypergraph represents a vector (state) in a Hilbert space and each tetrad (block) corresponds to four mutually orthogonal vectors] and found [after several months of computation on our 500 central processing unit (CPU) cluster *Isabela*] that among over 10^{10} nonlinear equations to which the hypergraphs correspond, only one has a solution.²⁶ The solution is, of course, isomorphic to Peres’ 24–24 KS set as mentioned above. Therefore, we named this set simply the “24–24 KS set” and the family of KS sets that can be obtained from it, the “24–24 KS class.”

We obtained KS subsets of the 24–24 set by a *stripping technique*, which consisted of stripping blocks off the initial 24–24 KS set then checking whether the resulting subset continued to be a KS set. There are altogether 1232 such KS subsets.²⁴ Looking at these sets as sets of vectors with component values from a $\{-1,0,1\}$ that do not allow a numerical evaluation (KS theorem!), we might not see any apparent reason why, among trillions of instances, there would not also be KS sets that are not subsets of the 24–24 set. But it turns out that there is none. We prove that by an exhaustive generation of KS sets with 18–23 vectors. They are isomorphic to the subsets of the 24–24 set.²⁶

When we strip off blocks, we eventually reach smallest KS sets in the sense that any of them ceases to be a KS set if we strip off an additional block. We call such smallest sets *critical sets*. This is the definition we used in Ref. 24, and it differs from the definition we used in Ref. 27, which is based on deleting vectors (directions, rays). In Ref. 24 we proved that there are altogether six critical KS subsets in the 24–24 KS class. These are: 18–9,²⁸ 20–11,²⁹ another 20–11,³⁰ two 22–13s,³⁰ and 24–15.²⁴

The main focus of this paper is to describe another isolated family of KS sets (the 60–75 KS class), which we discovered by means of our stripping technique applied to a KS set with 60 vectors and 75 blocks. This latter set was obtained from the 4-dim polytope called the 600-cell.³¹ We call this new family the “60–75 KS class.” It turns out that it contains millions of KS sets and thousands of critical sets, and this is what is novel in this paper.³² Previously, we found only several isolated examples from this class using a different technique.^{27,31} Being based on the geometry of the 600-cell, the 60–75 set provides us with highly symmetrical configurations of 60 rays, and this symmetry can be traced down to its smallest (with an estimated a confidence of over 95%) 26–13 KS subset (described in Sec. II). In particular, the smallest maximal loop of any KS set from the 60–75 class forms an octagon, while all sets from the 24–24 class have a hexagon maximal loop. The fact that the smallest KS set from the 60–75 class has 26 vectors, together with the fact that we could not build up to any subset of the 60–75 class with 24 vectors proves the disjointness of the two classes with a confidence of over 95%.

Below, we present some of many (several thousand) new critical sets from the 60–75 KS class, give the algorithms that enabled us to find them, and investigate their symmetry and geometry, comparing it with the ones of the 24–24 KS class.

II. CRITICAL SETS

A discovery we made for the 18–24 vector sets was that the maximal loop of edges in all their MMP hypergraphs was a hexagon and that in all of them there was only one hexagon. (In an MMP hypergraph vertices correspond to vectors and edges to tetrads. So, 1 denotes the 1st vector, . . . , 9

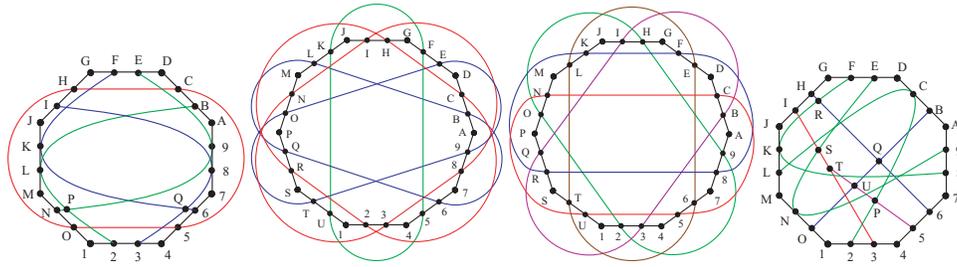


FIG. 1. (Color online) (a) The smallest critical KS set has shown with the help of MMP hypergraphs. It has 26 vertices, 13 edges, and a maximal loop of 8 edges (octagon). Vertices correspond to vectors and edges to orthogonal tetrads. (b)–(d) Critical sets with 30 vertices, 15 edges, and a maximal loop of 10 edges (decagon) for (b) and (c) and an octagon for (d). (b) is isomorphic to the first and (d) to the second of the two 30–15 critical sets found in Table 5 of Ref. 27.

the 9th, A the 10th, . . . , Z the 35th, at the 36th, . . . y the 60th.) That gave us the idea of the stripping technique because stripping the edges in a way that preserves the hexagon might give a comparatively small number of subsets and critical sets. That was confirmed in Ref. 24.

Since the 24–24 KS set is a single largest set of its class, we expected that sets and in particular critical ones of our new 60–75 class would be based on loops larger than hexagons. The conjecture was correct. Also, since by exhaustive generation of all MMP hypergraphs up to 23 vertices we have not found a single KS set with a loop larger than a hexagon, we concluded that these classes of KS sets do not overlap, i.e., the minimal critical sets of the 60–75 KS sets must have more than 24 vectors, see Fig. 1.

Figure 1 shows MMP hypergraph representations of the smallest critical subsets of the 60–75 KS set. The smallest one has 26 vectors and 13 tetrads. Each vector is represented by a vertex in the MMP hypergraph. Each tetrad, which consists of four mutually orthogonal vectors, is represented by an edge in the MMP hypergraph. The next smallest ones are three KS sets with 30 vectors and 15 tetrads. Their MMP hypergraphs have 30 vertices and 15 edges each, as shown in their figures. As we can see, the first three sets are highly symmetrical and might be suitable for setting up an experiment.

In the MMP notation described above, the 26–13 set has the following representation:

1234,4567,789A,ABCD,DEFG,GHIJ,JKLM,MNO1,5CHO,3Q8I,6QKF,NP9E,2PLB.

As we can see, there is a one-to-one correspondence between this notation and the figure. This is possible because in constructing a set, we only deal with orthogonalities between vectors and not with the values of the vector components. The values can always be ascribed later on by means of our program VECTORFIND.

The 60–75 (Refs. 27 and 31) in the MMP notation reads:

12341cKT,1Qtg,1Njo,1yYE,2Mmn,2vZD,2Pri,2bIV,3HWe,3kqO,3XGx,3shS,4Fwa,4UdJ,4fRu,4pLl,5678,5pSK,5XiN,5buE,5Wwm,9ABC,9fxK,9sVN,9PIE,9qdZ,AUOt,AHiy,Abao,AGRm,BFSj,BXnc,BvJg,BWlr,CpeY,CkDQ,CMuT,ChwI,6Fet,6kVy,6PJo,6hLZ,7Uxj,7sDc,7Mag,7qRI,8fOY,8HnQ,8vIT,8Gdr,FGDE,FqiT,UhnE,UWVT,fhig,fWDo,pGVg,pqno,HIJK,HZuj,kraK,klmj,XIlt,XZaY,srut,smJY,MLON,MdSy,vReN,vwxy,PRSQ,PwOc,bLxQ,bdec.

To obtain these results, we used an interactive procedure where we stripped one block at a time and then decided (based, e.g., on the size of the output) what steps to take next. The programs we used and their algorithms are described in Sec. III. We used the program MMPSTRIP to strip blocks from starting diagrams. In general, we attempted to set the parameters of MMPSTRIP (in particular, its increment parameter) so that we ended up with a sample of about 10 000 hypergraphs after colorable hypergraphs and isomorphic hypergraphs were removed.

The overall interactive procedure was as follows. We start with the MMP hypergraph for the 60–75 KS set.

- (1) From this set, new sets with less and less blocks were generated with MMPSTRIP. We used their increment parameter to keep the number of hypergraphs manageable, and we enabled the suppression of nonconnected hypergraphs.
- (2) Duplicate hypergraphs will result when one block is removed at a time (rather than multiple blocks combinatorially). These duplicates were removed.
- (3) Colorable hypergraphs were filtered out with STATES01, leaving only noncolorable ones (i.e., KS sets).
- (4) Isomorphic hypergraphs were removed with SHORTDL.

While it is not exhaustive, the advantage of the above technique is that the filtering quickly converges to give us a collection of nonisomorphic KS sets with the desired block count for further study. Typically, we first ran these steps on a small sample of the hypergraphs (a hundred or so) so that the increment parameter for MMPSTRIP in the first step above could be estimated, in order to end up with around 10 000 hypergraphs in the last step.

In order to determine, after the above process (i.e., after removing a single block then processing the output), which (noncolorable) hypergraphs were critical, we ran MMPSTRIP on one hypergraph at a time, then determined with STATES01 whether all of them became colorable. If any one was noncolorable, it meant that the hypergraph was noncritical. This procedure is somewhat CPU-intensive and for this study was done (in conjunction with the above process) only up to 19 blocks remaining (i.e., with 56 blocks or more blocks removed). We also did a more limited sampling of critical KS sets with higher block counts.

The following list summarizes the critical hypergraphs we found with up to 19 blocks, along with some sample MMP diagrams and figure references. “30–15 \times 3” means that we found three nonisomorphic critical diagrams with 30 vectors and 15 blocks (tetrads). This list resulted from testing several million hypergraphs using the procedure described above. The reader should keep in mind that the list is not necessarily exhaustive but is based on this limited sample.

- ≤ 12 blocks: None.
- 13 blocks: 26–13 \times 1. It is shown in Fig. 1, with a maximal loop of eight blocks (octagon). Its MMP representation is:
26–13: 1234,4567,789A,ABCD,DEFG,GHIJ,KLM,MNO1,5CHO,3Q8I,6QKF,NP9E,2PLB
- 14 blocks: None.
- 15 blocks: 30–15 \times 3. The first two sets in Fig. 1 have a maximal loop of order 10 (decagon) and the third one of order eight (octagon). They receive the following MMP representation:
30–15a: 1234,4567,789A,ABCD,DEFG,GHIJ,KLM,MNOP,PQRS,STU1,5FKU,2CHR,38I
N,9EOT,6BLQ.
30–15b: 1234,4567,789A,ABCD,DEFG,GHIJ,KLM,MNOP,PQRS,STU1,6ELT,8FKR,C5U
N,O29H,B3QI.
30–15c: 1234,4567,789A,ABCD,DEFG,GHIJ,KLM,MNO1,2PCL,3TSI,5PUT,6QRH,8KRF,
9NSE,BQUO.
30–15c is isomorphic to the first and 30–15a to the second of the two 30–15 critical sets found in Ref. 27.
- 16 blocks: None.
- 17 blocks: 32–17 \times 1, 33–17 \times 2, and 34–17 \times 5. The 32–17, 33–17b, and 34–17d have maximal loops nine (nonagon) and the maximal loops of 33–17a–c and 34–17e are decagons as shown in Figs. 2 and 3. Their MMP representations are
32–17: 1234,4567,789A,ABCD,DEFG,GHIJ,KLM,MNOP,PQR1,2SCK,3VIO,3WE8,3LTB,
5SGR,6WUH,9TGN,FUVQ.
33–17a: 1234,4567,789A,ABCD,DEFG,GHIJ,KLM,MNOP,PQRS,STU1,K2VF,3BIN,R5C
H,Q6WL,U8OH,9TXE,VWXH.

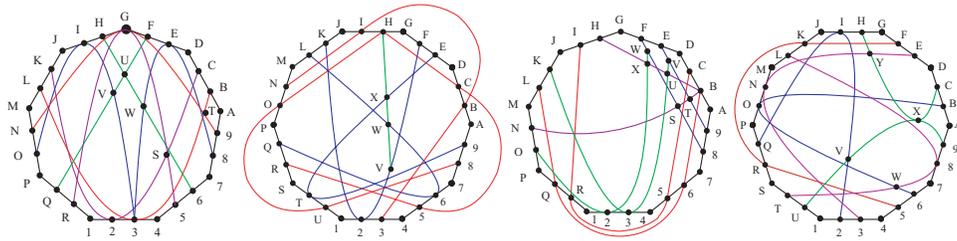


FIG. 2. (Color online) (a) 32–17 KS set; Maximal loop: nonagon; (b) and (c) 33–17a and b; decagon, nonagon; (d) 34–17a; decagon.

33–17b: 1234,4567,789A,ABCD,DEFG,GHIJ,JKLM,MNOP,PQR1,O2XW,K3UV,IR5C,LQ6B,8SWF,9TVE,BTSN,BUXH.

34–17a: 1234,4567,789A,ABCD,DEFG,GHIJ,JKLM,MNOP,PQRS,STU1,2VIQ,3NYE,5RK F,6WOB,TW8L,9XVU,CXYH.

34–17b: 1234,4567,789A,ABCD,DEFG,GHIJ,JKLM,MNOP,PQRS,STU1,2XHO,3CYR,5VKT,6BIN,8FWU,9ELQ,VWXY.

34–17c: 1234,4567,789A,ABCD,DEFG,GHIJ,JKLM,MNOP,PQRS,STU1,2WIN,3XHC,5FKU,6RVB,8YTO,9ELQ,VWXY.

34–17d: 1234,4567,789A,ABCD,DEFG,GHIJ,JKLM,MNOP,PQR1,O2T9,NS38,5UCH,6YBI,ELVQ,FKXR,XWUT,VSZY.

34–17e: 1234,4567,789A,ABCD,DEFG,GHIJ,JKLM,MNOP,PQRS,STU1,2VXI,3WYH,5FKU,6BOT,8VWR,9ELQ,CXYN.

- 18 blocks: None.
- 19 blocks: 36–19×11, 37–19×9, and 38–19×6. Three of them have the maximal loops of order 11.
- 20 blocks: None
- 21 and higher: The number of critical KS sets per block increases to a maximum of over 1700 sets with 38 blocks, then decreases. Even numbers of blocks in a KS set start at 24. Odd numbers of vectors with an odd number of blocks start to appear at 17 blocks (33 vectors) and with an even number of blocks at 24 blocks. The 33–17 set is given above, and an MMP representation of a 42–24 set (with 14 blocks in a maximal loop) reads:

42–24: 1234,5678,9ABC,DEF8,GHIJ,KLMJ,NOPQ,RSTM,UVI4,WXYF,ZaE3,bcLC,dTHB,eaYQ,ecVD,fbPG,gUSO, gfeA,ZTN7,XU97,bWR2,dWO6,fK63,eJ72.

An exhaustive generation proves that there are no critical sets with more than 63 blocks. We conjecture that the first critical sets will appear at 60 blocks, i.e., for 60–60 KS sets and smaller, in analogy to the 24–24 class, assuming that picking up new tetrads (61st–63rd) of the already recorded 60 vector/state values would not make a set empirically distinguishable from the 60–60 one we started with. The size of maximal loops steadily rises with the number of blocks. (Detailed presentation of additional KS sets we obtained by two other techniques will be given elsewhere, because the algorithms we use for higher numbers of blocks are too involved to be presented here. Besides, many massive computations that take months on our clusters are under way.)

Since our sampling was not exhaustive—for example, there are 290 quadrillion (2.9×10^{17}) hypergraphs with 19 blocks—it is likely that there are many more critical KS sets than suggested above, particularly at block counts higher than 19. When repeating the above procedure with independent random samples, some critical diagrams (up to isomorphism) recurred frequently, whereas others occurred only once or twice, indicating that their distribution and symmetries are far

from uniform. An exhaustive generation of all sets from the 60–75 KS class, that we might be able to carry out in the future, would give us the complete list.

III. ALGORITHMS

Our study makes use of algorithms and computer programs from several disciplines (quantum mechanics, lattice theory, graph theory, and geometry). Each has its own terminology, which we will sometimes keep when discussing an algorithm from that discipline. To avoid confusion, the reader should keep in mind that in the context of the MMP diagrams used for this study, the terms “vertex,” “atom,” “ray,” “1-dim subspace,” and “vector” are synonymous, as are the terms “edge,” “block,” and “tetrad (of mutually orthogonal vectors).” Similarly, “MMP hypergraph” and “MMP diagram” mean the same thing.

For the purpose of the KS theorem, the vertices of an MMP hypergraph are interpreted as rays, i.e., 1-dim subspaces of a Hilbert space, each specified by a representative (nonzero) vector in the subspace. The vertices on a single edge are assumed to be mutually orthogonal rays or vectors. In order for an MMP hypergraph to correspond to a KS set, first there must exist an assignment of vectors to the vertices such that the orthogonality conditions specified by the edges are satisfied. Second, there must not exist an assignment (sometimes called a “coloring”) of 0/1 (nondispersive or classical) probability states to the vertices such that each edge has exactly one vertex assigned to 1 and other vertices assigned to 0.

For a given MMP hypergraph, we use two programs to confirm these two conditions. The first one, VECTORFIND, attempts to find an assignment of vectors to the vertices that meets the above requirement. This program is described in Ref. 24. The second program, STATES01, determines whether or not a 0/1 coloring is possible that meets the above requirement. The algorithm used by STATES01 is described in Ref. 30.

The 60-vertex, 75-edge MMP hypergraph based on the 600-cell described above (which we refer to as 60–75) has been shown to be a KS set.³¹ However, we can remove blocks from it and it will continue to be a KS set. The purpose of this study was to try to find subsets of the 60–75 hypergraph that are critical, i.e., that are minimal in the sense that if any one block is removed, the subset is no longer a KS set.

While the program VECTORFIND independently confirmed that 60–75 admits the necessary vector assignment, such an assignment remains valid when a block is removed. Thus it is not necessary to run VECTORFIND on subsets of 60–75. However, a noncolorable (KS) set will eventually admit a coloring when enough blocks are removed, and the program STATES01 is used to test for this condition.

The basic method in our study was to start with the 60–75 hypergraph and generate successive subsets, each with one or more blocks stripped off of the previous subset, then keep the ones that continued to admit no coloring and discard the rest. Of these, ones isomorphic to others were also discarded.

The program MMPSTRIP was used to generate subsets with blocks stripped off. The user provides the number of blocks k to strip from an input MMP hypergraph with n blocks, and the program will produce all $\binom{n}{k}$ subsets with a simple combinatorial algorithm. Partial output sets can be generated with start and end parameters, and if the full output is too large to be practical, an increment parameter i will skip all but every i th output line in order to partially sample the output subsets. Given an input file with MMP hypergraphs, the program can calculate in advance how many output hypergraphs will result, so that the user can plan which parameter settings to use.

The MMPSTRIP program will also optionally suppress MMP hypergraphs that are not connected, such as those with isolated blocks or two unconnected sections, since these are of no interest. Finally, all output lines are by default renormalized (assigned a canonical atom naming), so that there are no gaps in the atom naming as is required by some other MMP processing programs.

In order to detect isomorphic hypergraphs, one of two programs was used. For testing small sets of hypergraphs, we used the program SUBGRAPH described in Ref. 24, which has the advantage of displaying the isomorphism mapping for manual verification. For a large number

of hypergraphs, we used Brendan McKay’s program SHORTDL, which has a much faster run time.

IV. DISCUSSION

In this paper, we describe the 60–75 class of Kochen–Specker set with a focus on its smallest critical sets, as defined in the Introduction. The smallest critical sets we find are shown in Figs. 1–3. The order of their maximal loops of edges (blocks and tetrads) is eight and more. Since the order of the maximal loop of all subsets that form the lower KS 24–24 class is 6, this is an additional aspect of the disjointness of 24–24 and 60–75 classes, for which we have shown to have a statistical confidence of over 95%. More details on the latter results are given in Introduction.

The high symmetry of the smallest critical KS sets shown in the first three figures of Fig. 1 and in the figures of Fig. 3 suggests that spin KS experiments might be designed for them. Therefore, we would like to discuss geometrical features of the sets we obtained in Sec. II.

Each of the sets shown in Figs. 1–3 involves an odd number of bases (blocks, edges, and tetrads) (13, 17, or 17), with each ray (vertex, vector, and direction) occurring exactly twice over these bases. This observation, by itself, gives an immediate “parity proof” of the BKS (Bell–Kochen–Specker) theorem without the need for any further calculation or analysis (and, in particular, without the need to use program STATES01 mentioned in Sec. III). The reason is the following: on the one hand, because each tetrad must have exactly one ray assigned the value 1, there must be an odd number of occurrences of 1’s over all the tetrads; but, on the other hand, because each ray is repeated twice, there must be an even number of 1’s over all the tetrads. This contradiction shows that a 1/0 assignment is impossible and so proves that these are indeed KS sets. The argument, of course, does not go through for those sets where a ray appears in an odd number of tetrads as, e.g., ray 2 in the set 42–24 whose MMP representation is given at the end of Sec. II.

An interesting difference between the 26–13 and 30–15 cases is that the latter are isogonal (or vertex transitive), whereas the former is not. A set of rays is said to be isogonal if there is a symmetry operation that will take any ray into any other one while keeping the structure as a whole invariant. The 60 rays of the 600-cell are isogonal as a whole, and this might encourage the belief that subsets yielding parity proofs must also be isogonal. The 26–13 set shows this supposition to be false in the case of the 600-cell, or the 60–75 set.

In addition to the methods outlined in the previous sections, alternative methods were used to arrive at some of the possible critical sets. The idea, which followed the “parity proof” above, was to look for N rays forming T complete tetrads, with T odd, in such a way that each ray occurred in exactly two of the tetrads. Such a set, which we will refer to as a N – T set (e.g., 26–13 and 30–15) is a KS set. An N – T set that obeys the “parity proof” satisfies the numerical constraint $N = 2T$, so it involves only one free parameter. (Of course, there are other critical sets such as 33–17 that will not be found by this method.) Starting from small values of N and proceeding upwards, we looked for KS sets. It is easily seen that no set of this type can exist for N less than 16.

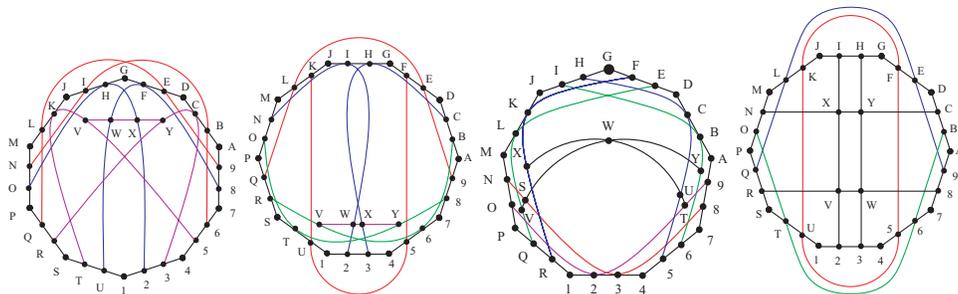


FIG. 3. (Color online) (a) 34–17b (Max. loop: decagon); (b) 34–17c (decagon); (c) 34–17d (nonagon); and (d) 34–17e (decagon).

The reason has to do with the structure of the tetrads for the 600-cell. Inspection shows that each ray occurs in exactly five tetrads and that it occurs exactly once in these tetrads with each of the 15 rays it is orthogonal to. Suppose a particular tetrad is chosen as the “seed” for a $N-T$ set. Then each ray in that tetrad must occur in one other tetrad, and so there must be at least four other tetrads involved. However, each of those tetrads must involve three new rays, and so the total number of rays, including the four we began with, is 16. Starting with $N = 18$ and proceeding upwards (remembering that $T = N/2$ must be an odd integer) shows, through slightly more involved arguments (which differ from those for the smallest critical set (18–9) of the 24–24 class), that solutions with $N = 18$ and 22 are impossible. The first solution that is possible is for $N = 26$, and it explains the 26–13 set shown in Fig. 1. There are actually 1800 different sets of 26 rays that lead to such a solution, but they are all geometrically isomorphic to one another, in the sense that there is a four-dimensional orthogonal transformation that will take any one such set into any other. In the Introduction, we give a statistical argument showing, with over 95% confidence, that there are no smaller sets than 26–13 in the 60–75 class that do not follow the parity proof.

All the other results we obtained, together with the presentation of the algorithms and programs we used, is given in Ref. 33. There we give a detailed analysis of the results, complete statistics of the obtained sets, and a review of their features. All that is outside of the scope of the present paper.

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