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A linear time algorithm for finding a maximum independent set of a fullerene*

Sean Daugherty and Wendy Myrvold

A *fullerene* is an all carbon molecule that can be represented by a 3-regular planar graph with face sizes five or six. A subset S of the vertices of a graph forms an *independent set* if the vertices of S are pairwise non-adjacent. The problem of finding the size of a maximum independent set of a graph is NP-complete when restricted to 3-regular graphs. In contrast, for fullerenes we have designed an algorithm that solves the problem in linear time.

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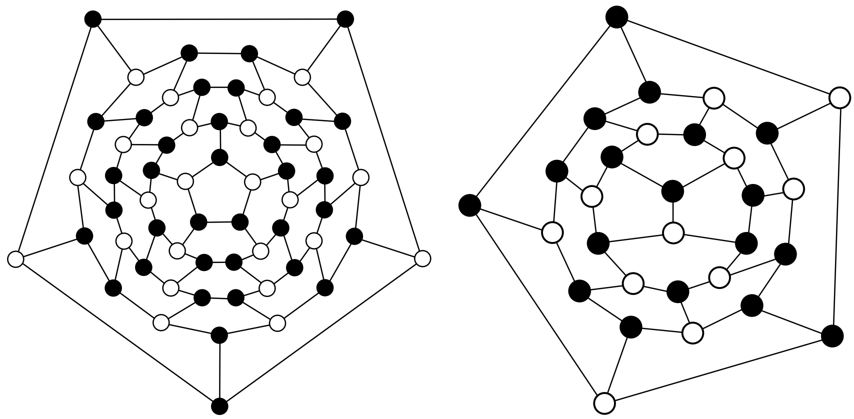
1. Independent sets of fullerenes

An *independent set* of a graph is a subset S of the vertices that are pairwise non-adjacent. A *maximum independent set* for a graph is a largest independent set. The *independence number of a graph* is the number of vertices in a maximum independent set.

Fullerenes are all-carbon molecules whose molecular structures correspond to 3-regular planar graphs that have face sizes equal to five or six. Euler's formula enforces that there must be exactly twelve pentagons in any fullerene. The Atlas of Fullerenes [13] is an excellent starting point for researchers interested in fullerenes and related graph theory questions.

*Dedication from Wendy Myrvold: I would like to dedicate this paper to my mentor, Adrian Bondy. I took my very first graph theory class (on the graph reconstruction problem) from him at the University of Waterloo in 1983. The class was life changing. Because I fell so madly in love with graph theory research, I ended up switching my Master's program research area from numerical analysis to graph theory. The passion for graph theory research that he inspired lead to the completion of a Ph.D. followed by a job as a professor at the University of Victoria. I would like to thank Adrian for setting me on this path that leaves me still having fun and passionate about doing research.



(a) C_{60} (b) $C_{30}:2$

Figure 1: Maximum independent sets (white vertices) of two fullerenes.

The face spiral conjecture for fullerenes [13, p. 24] is that the surface of a fullerene polyhedron can be unwound in a continuous strip of edge-sharing pentagons and hexagons such that each new face in the spiral after the second one shares an edge with both (a) its immediate predecessor in the spiral and (b) the first face in the preceding spiral that has an open edge. It has been shown that a smallest counterexample to this conjecture has 380 vertices [4]. A fullerene face spiral can be represented by a sequence of 5's and 6's that give the sizes of the faces it has. Chemists number the n-vertex fullerenes by first choosing a lexicographically smallest sequence for each of the n-vertex fullerenes. Then the n-vertex fullerenes are sorted according to these sequences. The n-vertex fullerene that appears in position k when the minimum face spiral sequences are sorted is denoted by $C_n : k$. This numbering scheme gives names to all of the fullerenes having less than 380 vertices since all have at least one face spiral.

The fullerene that is easiest to synthesize is C_{60}, the unique isomer on 60 vertices with isolated pentagons. A fascinating observation is that when the C_{60} fullerene reacts with bromine, the end product is such that the locations of the bromine atoms correspond to a maximum independent set in the fullerene [12]. A picture of C_{60} showing the independent set that corresponds to the positions of the bromine atoms in the molecule $C_{60}Br_{24}$ is shown in Figure 1(a). A second example of a maximum independent set of a fullerene is shown in Figure 1(b).

Many practical algorithms for finding a maximum independent set (equivalent to finding a maximum clique in the complement graph) have been published including [1, 2, 5, 19, 20, 21], and this problem was the subject of a DIMACS challenge [17]. The problem of finding the independence number is NP-Complete for cubic planar graphs [15, A1.GT20], a class that contains fullerenes.

An *icosahedral fullerene* [13, pp. 18–21] is a fullerene that has the same symmetries as an icosahedron. The smallest icosahedral fullerene is the dodecahedron (the dual of an icosahedron). The famous Buckminster fullerene (with 60 vertices) is an icosahedral fullerene (it has the same structure as a soccer ball). The seven smallest ones have 20, 60, 80, 180 and 240 vertices. Graver showed that for icosahedral fullerenes, the independence number can be calculated from a formula in $O(1)$ time [16]. The results here build on his ideas [16] that apply to general fullerenes to describe an algorithm for finding the independence number in $O(n)$ time.

2. Basic definitions

It is assumed that a fullerene graph is represented by a rotation system (an adjacency list where the order of the neighbors represents the clockwise order in a planar embedding). A rotation system for the dual of a planar graph can be obtained from the primal in $O(n)$ time. The primal and dual graphs are undirected, but computationally, it is useful to think of their corresponding directed graphs that have two arcs (u, v) and (v, u) corresponding to each edge (u, v) of the undirected graph.

A *walk* in a directed graph of length k from v_0 to v_k consists of an alternating sequence of vertices and arcs of the form: $v_0, (v_0, v_1), v_1, (v_1, v_2), v_2, \ldots,$ $v_{k-1}, (v_{k-1}, v_k), v_k$. Walks can repeat vertices or arcs. A *circuit* is a walk that start and ends on the same vertex.

A *dual walk* is a walk in the dual graph. When a dual walk enters a vertex v of degree six from arc (u, v), it is said to continue in the *straight* direction if it leaves v using the arc that is three clockwise positions after arc (v, u). The straight direction is not defined for a vertex of degree five. A walk makes a *sharp right turn* at vertex v of degree five or six if it exits v using the arc that is one counter-clockwise position after arc (v, u). A *wide right turn* occurs when the walk exits using the arc that is two counter-clockwise positions Figure 2 shows a pentagon in the primal with the arcs indicating the turn types in the dual graph.

A *quintant* of a vertex v of degree five in the dual consists of a pair of arcs from v, the *x-arc* and the *y-arc*, such that the x-arc is 1 clockwise position after the y-arc. Figure 3 gives an example. Each degree five vertex has five quintants. A walk along the x-axis (y-axis) of a quintant starts with the

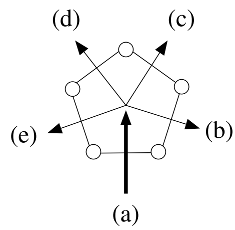


Figure 2: Entering at (a) means (b) is a sharp right turn, (c) is a wide right turn, (d) is a wide left turn, and (e) is a sharp left turn.

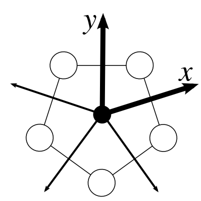


Figure 3: The x- and y-arcs of a quintant.

x-arc (y-arc) and continues straight (since straight is not defined for degree five vertices, the walk must terminate when it hits a degree five vertex).

3. Graver's results and clear fields

In a maximum independent set of a fullerene, each hexagon would ideally contribute three vertices. However, because the pentagons contribute at most two independent set vertices each, this can create some disruptions in the hexagons. Graver [16] showed that a maximum independent set of a fullerene can be obtained by finding a way to pair the twelve pentagons of the fullerene so that all the disruptions occur within six parallelogram-shaped regions (clear fields) between the pairs of pentagons. The term clear field was chosen because he proved that these regions must be free of pentagons other than the two being paired [16, Lemma 7].

Definition 3.1 (Clear Field). *A* clear field *with dimensions* (x, y)*,* $x \geq 1$*,* $y \geq 0$*, is a circuit in the dual graph of a fullerene that has* $2x + 2y$ *arcs such that the circuit and its internal region (the region on the right side of the circuit) contain exactly two vertices* a *and* b *of degree five. When* $y = 0$*, the walk starts at* a*, traverses the* x*-axis using* x *arcs to get to* b *then uses the reverses of these arcs to return to* a*. When* $y > 0$*, the walk starts at* a *and* *traverses y arcs along the y-axis of a quintant, makes a wide right turn then walks straight using x arcs to get to b. At b the walk makes a sharp right turn and follows y arcs in the straight direction, and then takes a wide right turn and walks straight along x arcs to return to a.*

Figure 4 shows a subgraph of a fullerene overlaid with arcs indicating the dual edges in a clear field with dimensions $(5, 3)$. Note that the walks for the clear fields are always along edges of the dual graph; the Coxeter coordinization introduced in [6] does not impose this constraint. The *clear field subgraph* for a given clear field is the primal subgraph induced by the faces that correspond with either a dual vertex that is part of the clear field or a dual vertex on the inside (right side) of the clear field. As per Graver [16], the independent set vertices are colored *white*, a maximum independent set of the rest is colored *black*, and the remaining vertices are *gray*.

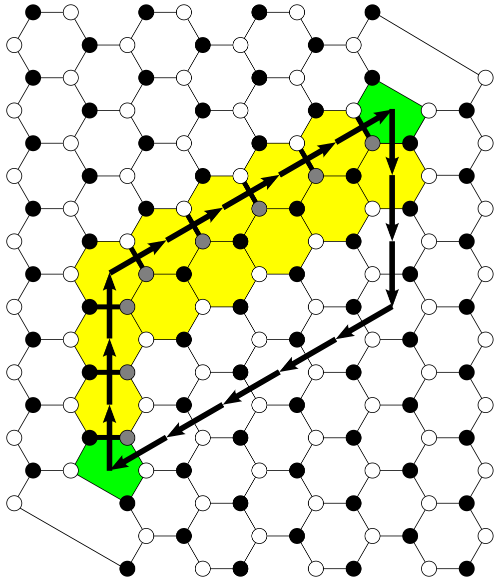
In the final section of [16], Graver comments that to find a maximum independent set on any fullerene, one could consider the independent sets that correspond to each of the possible pairings of the pentagons that give clear fields and select an independent set of maximum size. That is the general approach taken by our algorithm. But there are several tricky issues that make designing an algorithm harder than it sounds.

The first problem is that there is more than one way to cause disruption in a clear field subgraph. The amount of disruption depends on how the independent set vertices are selected from the boundary of the clear field. This causes some hexagons to be deficient, i.e. they contain fewer than three white vertices. The *penalty* assigned to an independent set of a clear field is equal to one plus the number of hexagonal deficiencies. With this definition of the penalties, the number α of independent set vertices satisfies

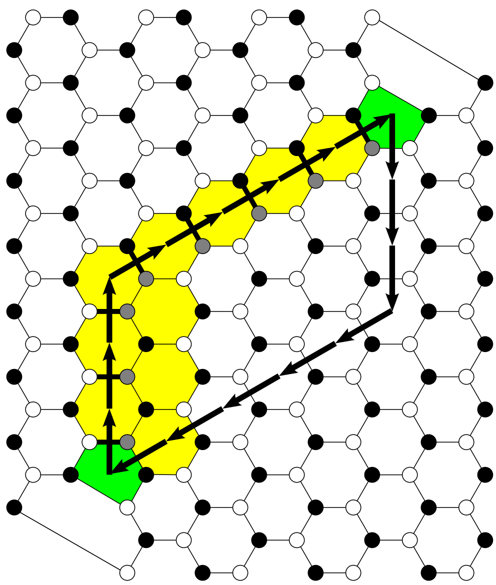
(1) $\alpha = n/2 - (\text{the sum over all the clear fields of the penalties})/3.$

To see why this formula holds, first observe that if none of the hexagons are deficient, then each 5-face has two independent set vertices and each 6-face has three. Since the number of 5-faces is 12 and the number of 6-faces is $n/2-10$, the independent set order in this case would be $[24+3(n/2-10)]/3$ (the division by three is because each vertex is in three faces) which is equal to $n/2-2$. The formula based on the penalties gives the same result because each of the six clear fields has penalty one. Subtracting off 1/3 times the number of deficient hexagons gives the required correction for cases where some of the hexagons have only two independent set vertices instead of three. In Figure 4, two independent sets and their penalties are shown.

Another barrier to finding a fast algorithm is that there can be as many as a linear number of clear fields between one pair of pentagons. To illustrate



(a) One independent set for a $(5, 3)$ clear field: penalty is $2 \cdot 5 + 3 = 13$



(b) Another independent set for a $(5, 3)$ clear field: penalty is $5 + 2 \cdot 3 = 11$

Figure 4: Examples of clear fields. The arcs of the clear fields are denoted by arrows. Hexagons with fewer than three independent set vertices are gray (yellow in the online version).

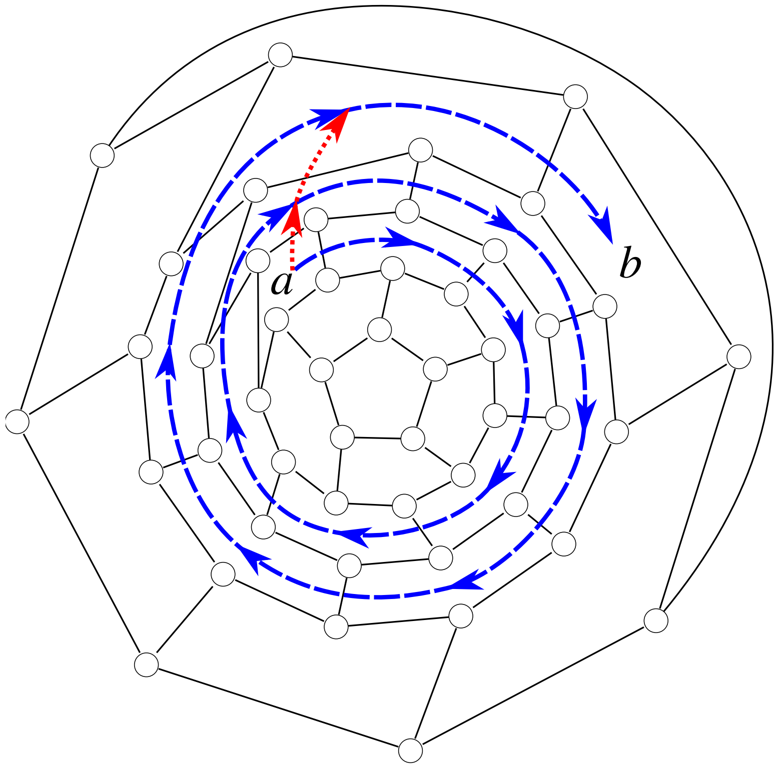


Figure 5: A member of an infinite family with a linear number of clear fields: the case when $k = 2$ ($n = 48$), with clear fields of dimensions $(13, 0)$, $(7, 1)$, and $(1, 2)$.

this, consider the infinite family of fullerenes defined for each $k \geq 0$ with $n = 24 + 12k$ vertices and pentagons at positions

$$0,\ 1,\ 2,\ 3,\ 4,\ 6,\ n/2-5,\ n/2-3,\ n/2-2,\ n/2-1,\ n/2,\ n/2+1$$

of a face spiral. Figure 5 shows the case $k = 2$. Such a fullerene has $k + 1$ clear fields between the same two quintants: one quintant of the pentagon at position 6 (labeled a in Figure 5) and one quintant of the pentagon at position $n/2-5$ (labeled b). The $k+1$ clear fields have dimensions $(6i+1, k-i)$ for $0 \leq i \leq k$.

Theorem 3.2. *The number of clear fields is at most* $3n/2$.

Proof. Each clear field with $y = 0$ corresponds uniquely to a choice of one edge from some pentagon a and one edge from another pentagon b of the primal graph. Hence the number with $y = 0$ can be at most 30 (the graph has 12 pentagons, and $30 = 12 \cdot 5/2$). The other clear fields correspond to two wide right turns in two hexagons. The number of hexagons is $n/2 - 10$ which means there is at most $6(n/2 - 10)/2 = 3n/2 - 30$ of these. □

4. Proper clear fields

As noted earlier, Graver showed that for any maximum independent set of a fullerene, the disruption in the hexagons falls into a set of exactly six clear fields. This section includes some theorems about the six clear fields that arise from selecting a maximum independent set. The proofs of these results are technical and rely on a deeper understanding of Graver's results. In order to not detract from the presentation of the algorithm, the detailed proofs have been included in the appendices. The first result is that when a maximum independent set is chosen, the clear fields cannot overlap each other.

Theorem 4.1. *[For a proof, refer to Theorem B.3] The six clear field subgraphs that arise from some maximum independent set of a fullerene have no faces in common.*

The idea of the proof is that if the clear fields overlap, then there is a way to choose a larger independent set. This contradicts the original assumption that the chosen independent set was a maximum independent set.

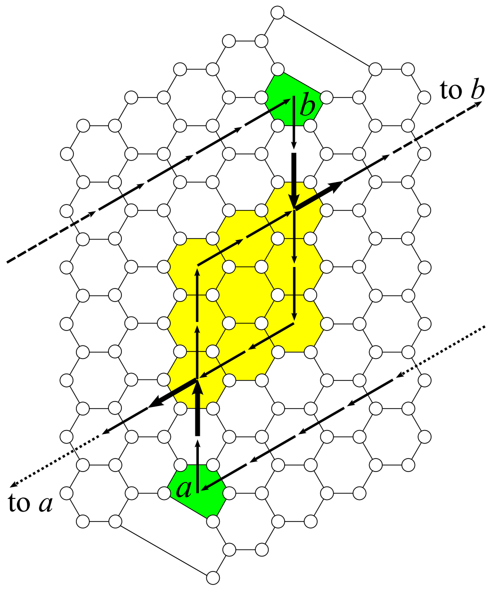
Clear fields can overlap themselves as shown in Figure 6. A clear field that does not overlap itself is called a *proper clear field*. Or equivalently, a clear field with dimensions (x, y) is a *proper clear field* if its clear field subgraph contains $(x + 1)(y + 1)$ unique faces.

Theorem 4.2. *[For a proof, refer to Theorem B.4] The clear fields that correspond to a maximum independent set of a fullerene must be proper clear fields.*

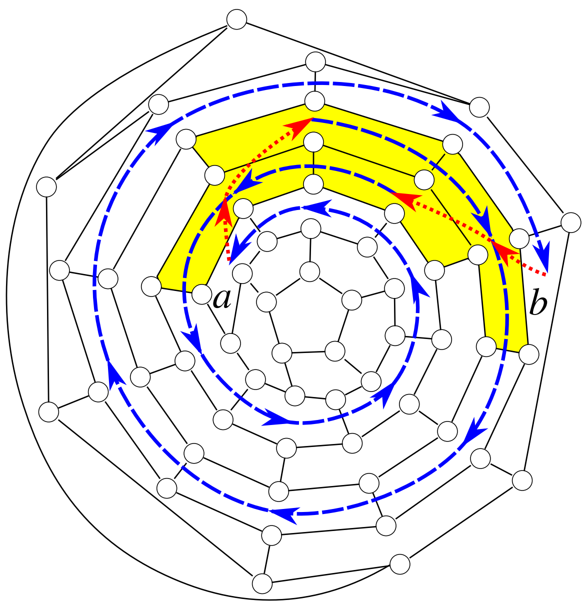
The next theorem is critical for achieving an $O(n)$ running time for our new algorithm.

Theorem 4.3. *[For a proof, refer to Theorem B.6] The number of proper clear fields is in $O(\log_2 n)$.*

The idea of the proof for this is to show that for any pair of quintants, the number k of proper clear fields for those two quintants satisfies $2^{k-1} < n/2$. The number of pairs of quintants is a constant so this proves the theorem. A key idea that is used both in the proof and in our algorithm is that



(a) A generic example.



(b) A specific example, $n = 60$, $x = 7$ (large dashes, blue in online version), $y = 2$ (smaller dashes, red in online version).

Figure 6: Clear fields that are not proper.

because clear fields have no pentagons in their interiors, when considering the dimensions of the proper clear fields for a given quintant, the y values are distinct, the x values are distinct, and ordering the clear fields by increasing y-values implies that they are ordered by decreasing x-values.

5. Finding all the proper clear fields

The first step of the algorithm is to identify all the proper clear fields. The quintants of the fullerene are numbered from 0 to 59. For each clear field, its two quintants and its dimensions are recorded.

The trick used to accomplish this in linear time is that we start by doing a walk in the dual graph along the x-axis of each quintant. A walk continues either until it reaches a degree five vertex or until just before some dual vertex is repeated (since continuing would result in clear fields that are not proper). The quintant number plus the number of arcs walked so far for this quintant are recorded on the arcs traversed. An arc of the graph can be on the x-axis for at most one quintant, so the amount of information recorded is $O(n)$ in total. The graph has 60 quintants and walking each one takes at most $O(n)$ time for a total of $O(n)$.

Some of these walks end in degree five vertices and correspond to clear fields with $y = 0$. The information regarding the other clear fields can be determined by examining the wide right turns of the hexagons. If one corresponds to a corner of a clear field then the two quintants and the distance to the pentagons can be recovered with the information stored with the arcs.

To ensure that the interiors are free of other pentagons as required by the definition of a clear field, it suffices to realize that this condition means that if the clear fields are sorted by increasing x value that the y values must be strictly decreasing.

But which of these clear fields are proper clear fields? Since there can be $3n/2$ possibilities to check, it is critical that this question can be answered in $O(1)$ time. The trick used to do this also enables us to check later if two clear fields share a face or not in $O(1)$ time.

The data structure used to solve this problem is an array:

$$\text{min\_intersection}[q_1][q_2][s]$$

where q_1 and q_2 are quintant numbers (values from 0 to 59) and s is the number of steps (edges traversed) taken along the x-axis of q_1 ($0 \leq s \leq d_1$, where d_1 is the length of the x-axis for q_1). For the segment of length s that lies along the x-axis for q_1, the value of min_intersection$[q_1][q_2][s]$ is computed so that it is equal to the minimum distance along the x-axis for q_2 to a dual vertex that corresponds to one of the first $s + 1$ vertices along the x-axis of q_1 (or infinity if the x-axis for q_2 does not include any of the initial $s+1$ vertices of the x-axis of q_1).

The values can be computed by one more traversal of each of the axes. The initial value of min_intersection$[q_1][q_2][0]$ is infinity. After following the kth arc along q_1 to a vertex w, the value of min_intersection$[q_1][q_2][k]$ is set to the minimum of min_intersection$[q_1][q_2][k-1]$ and any distance value to quintant q_2 associated with one of the entering arcs for w.

A clear field with $y = 0$ is always a proper clear field. A clear field with $y > 0$ is a proper clear field if its four boundary segments only intersect in four places: at the degree five vertices and the two locations of the wide right turns.

To test that a clear field is a proper clear field, the four segments that make up the boundary should be checked to ensure that there are no crossings that occur too early. Suppose that the four segments corresponding to the boundary are the x-axis of a pentagon p corresponding to q_1 of length d_1, the y-axis of pentagon p corresponding to q_2 of length d_2, the x-axis of a pentagon q corresponding to q_3 of length d_1, and the y-axis of pentagon q corresponding to q_4 of length d_2. There is an intersection that occurs too early in the pairs of segments that intersect to give the wide right turns of the clear field (the x-axis of p and the y-axis of q or the y-axis of p and the x-axis of q) if min_intersection$[q_1][q_4][d_1] < d_2$, or min_intersection$[q_2][q_3][d_2] < d_1$. The other pairs of segments should not intersect. They intersect if

$$\text{min\_intersection}[q_1][q_2][d_1] \le d_2, \text{min\_intersection}[q_1][q_3][d_1] \le d_1,$$
$$\text{min\_intersection}[q_2][q_4][d_2] \le d_2, \text{ or } \text{min\_intersection}[q_3][q_4][d_1] \le d_2.$$

6. Determining the independent set order

The next challenge in designing the algorithm is finding an approach for determining the independent set order that results from a fixed choice of six proper clear fields. This can be computed from the penalties of the clear fields. A clear field of dimensions (x, y) has two choices for a penalty for the clear field: either $2x + y$ or $2y + x$. It should be noted that the choices for the clear field penalties are not independent: making a choice for one forces choices for the rest of then.

The pentagons are numbered from 0 to 11 (arbitrarily). The vertices of each pentagon are numbered 0 to 4. The idea for finding all the penalties for a given selection of six clear fields is that given the status of vertex 0 in pentagon 0 (either white meaning it is in the independent set or black if it is not), we compute whether vertex 0 of the remaining pentagons should be white or black and this is sufficient to determine the penalties of the clear fields. The *color* of a clear field is defined to be the color of its vertex number 0 (that is, it is either *white* or *black*.

Examining Figure 4 reveals that many paths in the primal graph alternate white vertices and black vertices. If a walk from a vertex u to a vertex v does not use any of the primal arcs that correspond to the arcs of the dual defining the left-hand or upper segments of the clear field, then the color of v depends only on the distance between u and v. Vertex u is the same color as v if the distance is even and otherwise it is a different color.

Complications arise when a walk from u to v uses some of the edges shown in bold. For the purpose of this discussion, assume that the gray vertices are recolored so that they are the same color as the neighbor connected to it by the bold edge. If r bold edges are traversed on the walk from u to v then vertex u is the same color as v if the distance plus r is even and otherwise it is a different color.

The first step in creating the data structure is to perform a breadth first search of the primal graph starting at vertex 0 of pentagon 0 whose aim is to determine the distance to the vertex numbered 0 for each of the other pentagons.

The next step is to again walk the x-axes of the quintants, this time keeping track of 11 values (one for each pentagon p that is not pentagon 0). Each arc of the dual has a constant sized array to record this information; num_arcs_used[q][pentagon_number] where the quintant q is from 0 to 59 and the pentagon_number is between 1 and 11.

The value of num_arcs_used[q][p] associated with an arc which is the *kth* arc used in walking the x-axis for quintant q is the number of dual arcs on the walk so far whose corresponding primal edges were used in the BFS tree to get from pentagon 0 to pentagon p.

The value num_arcs_used[q][p] for an arc is equal to num_arcs_used[q][p] for the previous arc on the walk with 1 added on if the current dual arc corresponds to a primal arc on the BFS tree on the path to vertex 0 to pentagon p.

When $y = 0$ the number of bold arcs that correspond to BFS tree edges from pentagon 0 to pentagon p is equal to num_arcs_used[q][p] for the last arc on the x-axis of quintant q. For a clear field with $y > 0$, the required information can be looked up using data stored with the two arcs defining the upper left-hand corner of the clear field.

7. Determining an optimal selection of 6 clear fields

Once the $O(\log_2 n)$ proper clear fields have been identified, it suffices to use a backtracking approach to consider each viable choice for six of them since the number of ways to choose six is in $O((\log_2 n)^6)$ which is in $O(n)$. For each choice, the min_intersection data structure (as described in Section 4) is used to first check that the clear fields have no faces in common (or equivalently, that for each pair of clear fields, the boundary segments of one do not intersect the boundary segments of the other one). The tactic described in Section 6 is used to compute the number of independent set vertices resulting from each of the two ways to select penalties for the selection of clear fields. The maximum independent set order corresponds to the case resulting in a maximum number of independent set vertices.

8. Computational checks

To ensure correctness of our implementation, four versions were implemented: a very simple exponential time backtracking algorithm, an approach that ignores the speed ups discussed earlier that takes time in $O(n^6)$, and two variants of a linear time approach. The program fullgen [3] was used to generate the 10,190,782 fullerenes on up to 120 vertices. The information fullgen provides gives a rotation system for a planar embedding without requiring access to an algorithm for planar embedding. For the last three approaches, in addition to checking for a correct maximum independent set order, we ensured that the number of proper clear fields identified were the same.

9. Future research

When bromine reacts with C_{60} to form $C_{60}Br_{24}$, the final product is a compromise between a combination of steric constraints (bulky atoms cannot be placed close together) and electronic constraints [12]. It is important that each connected component of the graph induced by the carbons not bonded to bromines is *closed shell*; that is, each of these components has even order and has an adjacency matrix for which exactly half the eigenvalues are strictly positive. Notice that the components induced by the black vertices in Figure 1(a) each consist of two black vertices connected by an edge (these components are closed-shell). In contrast, it is easy to check that the components in Figure 1(b) are not all closed-shell (a component which is an isolated vertex is not closed shell because the number of vertices is odd).

The *closed-shell independence number* [7, 12, 14] is defined to be the maximum order of an independent set S such that the graph induced by $V - S$ has closed-shell components. This graph parameter encapsulates this combination of steric and electronic constraints. The most effective algorithm discovered so far for computing the closed-shell independence number of a fullerene is an exponential approach that works reasonably well in practice [8]. One important open question is whether or not the closed-shell independence number can be computed in polynomial time.

Fullerenes are not far from being bipartite in that they only have a constant number of faces that are odd cycles. It is possible that the tactics applied in this paper could be applied to yield polynomial time algorithms for other classes of planar graphs that do not have too many odd faces.

Having the maximum independent set orders for fullerenes may lead to new conjectures regarding this graph parameter. The first step we plan to take is to modify our program for visualizing fullerenes [18] so that the clear fields and a Graver coloring can be shown on the picture of the fullerene.

Since the penalties of the clear fields must add up to a value that is six or more, equation 1 in Section 3 gives an upper bound for the maximum independent set order of $n/2-2$. It is not hard to construct infinite families of fullerenes realizing this upper bound.

The result of Dvořák, Lidický and Škrekovski [10] (who show that the removal of at most $\sqrt{n}$ vertices is required to leave a bipartite graph) implies that a maximum independent set has cardinality at least $n/2-O(\sqrt{n})$ (take out the $O(\sqrt{n})$ vertices then take the largest half of the bipartition of the remaining vertices). Our computational results lead to a conjecture in 2009 [9] that all fullerenes have maximum independent set order at least $n/2 - \sqrt{3n/5}$ and this conjecture was subsequently shown to be correct in 2012 by Faria, Klein, and Stehlík [11].

An interesting avenue of future research is to determine other graph parameters that are difficult to compute for planar graphs but can be determined in polynomial time for fullerenes. A *dominating set* D of a graph G is a subset of the vertices of G such that each vertex is either in D or has an neighbor in D. A 3-regular graph has an obvious lower bound of $\lceil n/4 \rceil$ on the order of a minimum dominating set since each vertex dominates four vertices. Since an infinite hexagonal grid can be dominated by using $1/4$ of the vertices, it seems reasonable to assume that falling short of the bound arises again due to disruptions caused by the pentagons. But preliminary computational results indicate that the minimum dominating set order is at most two off from the lower bound instead of possibly something on the order of $\sqrt{n}$. A promising avenue of future research is to search for a polynomial time algorithm for finding a minimum dominating set of a fullerene.

Appendix A. Graver's results

This appendix contains the proofs omitted from the main body of the paper. Some of the theorem statements are a little different in order to facilitate the exposition of the proofs.

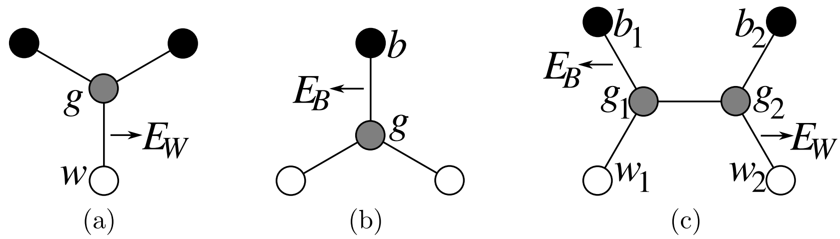


Figure 7: The three possible configurations involving gray vertices [16, Fig. 1].

An explanation of Graver's colorings and his theorems are required to understand the material that follows. Let W be a maximum independent set of a fullerene F, let B be a maximum independent set of $F - W$ and let G be the remaining vertices $(V - W - B)$. Color the vertices in W white, those in B black, and those in G gray. The following property arises:

Lemma A.1. *[16, Lemma 1] For every maximum independent set, every gray vertex is adjacent to a black vertex and a white vertex.*

Definition A.2 (Graver Coloring)**.** *A* Graver coloring *of a fullerene $F = (V, E)$ consists of a partitioning of the vertices into sets of white vertices W, black vertices B and gray vertices G and a partitioning of the edges into white edges E_W, black edges E_B and gray edges E_G, such that W is a maximum independent set of F, B is a maximum independent set of $F - W$, G is $V - W - B$, and E_W, E_B, and E_G are defined as follows:*

[Figure 7(a)]: *If gray vertex g is adjacent to two black vertices and one white vertex w, then edge (g, w) is assigned to E_W.*

[Figure 7(b)]: *If gray vertex g is adjacent to two white vertices and one black vertex b, then edge (g, b) is assigned to E_B.*

[Figure 7(c)]: *For each pair of adjacent gray vertices, arbitrarily label one as g_1 and the other as g_2. Vertex g_1 is adjacent to one white vertex w_1 and one black vertex b_1 and g_2 is adjacent to one white vertex w_2 and one black vertex b_2. Assign (g_1, b_1) to E_B and (g_2, w_2) to E_W.*

The edge set E_G is defined to be $E - E_W - E_B$.

With the sets defined in this manner, each gray vertex is incident with exactly one edge of either E_W or E_B. Note that this definition of E_G differs from Graver's set E_G in [16] in order to simplify some of the discussion.

Lemma A.3. *[16, Lemma 2] For any Graver coloring,* $|E_W| + |E_B| = |G|$ *(where* G *is the set of gray vertices) and no two edges in* $E_W \cup E_B$ *have a common endpoint.*

Lemma A.4. *[16, Lemma 3] A Graver coloring will satisfy the following:*

(i) Each pentagonal face contains exactly one edge from $E_W \cup E_B$*.*
(ii) Each hexagonal face contains either exactly two edges from $E_W \cup E_B$ *or no edges from* $E_W \cup E_B$*. If two edges from* $E_W \cup E_B$ *are opposite one another on a hexagon, then they are either both from* E_W *or both from* E_B*. If two edges from* $E_W \cup E_B$ *are on a hexagon and are not opposite one another, then one is from* E_W *and one is from* E_B*.*

An important relationship exists between $|W|$, $|E_W|$ and $|E_B|$, which is shown by the next lemma.

Lemma A.5. *[16, Lemma 4] Given a Graver coloring, the independence number can be computed as*

$$|W| = |V|/2 - (2|E_W| + |E_B|)/3. \tag{2}$$

The next theorem allows one to view a correspondence between a maximum independent set and a pairing of the twelve pentagons.

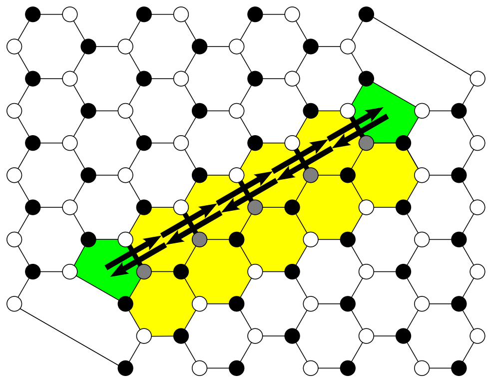
Theorem A.6. *[16, Theorem 1] Given a Graver coloring, the dual subgraph induced by the dual edges corresponding to the primal edges in* $E_W \cup E_B$ *is disconnected with six components, each of which is a simple path between a different pair of vertices of degree five.*

The paths in Theorem A.6 cannot make a sharp turn at any hexagon due to Lemma A.4(ii). The next lemma introduces a restriction on the wide turns that can be made.

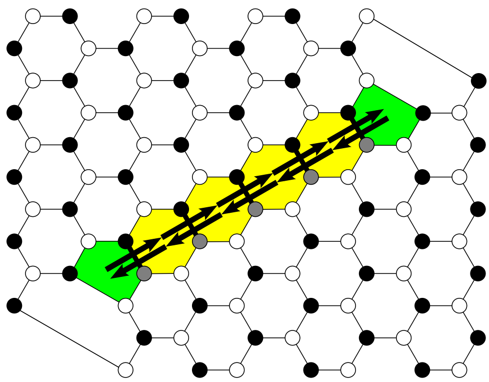
Lemma A.7. *[16, Lemma 6] If any particular one of the six paths in Theorem A.6 is viewed as a dual walk from one degree five vertex to its mate, then if the walk has a wide right (left) turn then the next turn cannot be another wide right (left) turn.*

Figures 4 and 8 show sample regions that may occur in a Graver coloring of a fullerene. If a hexagon has fewer than three vertices from W then it is shaded. The (primal) edges in $E_W \cup E_B$ are shown in bold. In each of the four subfigures, the edges of the dual graph that correspond to the bold primal edges induce a path that pairs the pentagons.

Two different colorings of a fullerene are said to be *color-equivalent* if they have the same values for $|W|$, $|B|$, $|E_W|$ and $|E_B|$. The colorings that



(a) A white $(5,0)$ clear field: penalty is $2 \cdot 5 + 0 = 10$



(b) A black $(5,0)$ clear field: penalty is $5 + 2 \cdot 0 = 5$

Figure 8: Examples of clear fields. The arcs of the clear fields are denoted by arrows. A Graver coloring is shown in each case. Bold primal edges denote the edges in $E_W \cup E_B$. If fewer than three vertices in W are on a hexagon then it is shaded.

induce different paths in the clear field are color-equivalent and in particular "any two [such] paths in the clear field between paired pentagons will have the same contribution to $2|E_W|+|E_B|$; hence that contribution is a property of the pairing" [16, p. 861]. A proof of this fact is given later by Theorem B.2. The contribution that a clear field makes to $2|E_W|+|E_B|$ is called the *penalty* of a clear field because in Equation (2), the sum of the penalties divided by three gives the difference between $|V|/2$ and the independence number. In the example in Figure 4(a), the clear field contains five edges in

E_W and three edges in E_B for a penalty of $2 \cdot 5 + 3 = 13$. Any Graver coloring that results in this clear field with the boundary colored as indicated will have a path in the dual corresponding to the edges of $E_W \cup E_B$ that gives the same penalty. Similarly, in Figure 4(b), the clear field contains three edges in E_W and five edges in E_B for a penalty of $5 + 2 \cdot 3 = 11$.

Appendix B. Extensions of Graver's results

This section proves some new results that expand on Graver's work in order to build a theoretical foundation for the algorithm. The first result uses the Graver coloring properties to examine how the colors of two vertices are related by examining primal walks that connect them.

Theorem B.1. *Given a fullerene with a Graver coloring, let P be a primal walk of length k from vertex v_0 to v_k such that v_0 and v_k are not gray. Let ℓ be the number of arcs of P that correspond to some edge in $E_W \cup E_B$. If $k \equiv \ell \mod 2$ then v_0 and v_k are the same color, otherwise they are different colors.*

Proof. The possible internal vertex colorings are considered by cases.

Case 1 $[k < 2]$**:** If $k = 0$ then the result holds trivially. If $k = 1$ then the single arc must connect a white and a black vertex and the edge it corresponds to is hence not in $E_W \cup E_B$, so the result holds.

Case 2 $[k \geq 2$ and all internal vertices of P are gray$]$**:** There are two subcases.

Case 2.1 $[k = 2]$**:** The Graver coloring properties illustrated in Figure 7 show that v_0 and v_2 are the same color if and only if neither arc on the path corresponds to an edge in $E_W \cup E_B$ or if both arcs correspond to the same edge in $E_W \cup E_B$. Otherwise, v_0 and v_2 are different colors.

Case 2.2 $[k \geq 3]$**:** No gray vertex has more than one gray neighbor, so the situation must be the one shown in Figure 7(a). The $k-2$ arcs of P that are not the first or last arc must correspond with the edge that connects the two gray vertices (recall that walks can have repeated arcs). Only the first and last arcs of P can correspond with an edge in $E_W \cup E_B$. If k is odd, then v_0 and v_k are the same color if and only if exactly one of the arcs corresponds with an edge in $E_W \cup E_B$. If k is even, then v_0 and v_k are the same color if and only if zero or two of the arcs correspond with an edge in $E_W \cup E_B$. Otherwise, v_0 and v_k are different colors.

Case 3 [$k \geq 2$ and not all internal vertices of P are gray]**:** Let v_i be a vertex in P that is not gray. Walk P can be decomposed into two smaller walks P_1 with length k_1 from v_0 to v_i and P_2 with length k_2 from v_i to v_k. Induction shows that if the result holds for P_1 and P_2, then the result holds for P. □

Some clear fields will be named as necessary in the discussions. Given a specific clear field, arbitrarily label its two vertices of degree five a and b and denote the clear field ▱ab having dimensions (x_{ab}, y_{ab}). Multiple clear fields may exist between two vertices of degree five and so it is important to note that given two such vertices a and b, the label ▱ab is not always sufficient to identify a unique clear field. When such notation is used, however, ambiguity will be avoided by identifying the clear field and then naming it. When a clear field is named ▱ab, let $\overrightarrow{ab}$ denote the subwalk of ▱ab from a to b and let $\overrightarrow{ba}$ denote the subwalk of ▱ab from b to a.

Given a Graver coloring, the six connected components of the dual subgraph induced by the edges of $E_W \cup E_B$ are called the *pairing paths*. A particular clear field ▱ab is said to correspond to a pairing path if the path pairs vertices a and b, all of the primal edges corresponding to the edges of the path are in the clear field subgraph of ▱ab, and the length of the path is $x_{ab} + y_{ab}$. A clear field is a *pairing clear field* if it corresponds to a pairing path.

The faces in a clear field subgraph and their corresponding dual vertices may be referred to using a coordinate system. Choose a clear field and label it ▱ab with degree five vertices a and b labeled arbitrarily. The two arcs of ▱ab that are incident with a correspond with one of the five quintants of a (Figure 9). This quintant is said to be the *quintant of a for* ▱ab. A coordinate system is defined for ▱ab such that a straight walk beginning with the x-arc of the quintant defines the *x-axis* of the quintant and the *y-axis* is similarly defined using the y-arc. A dual vertex corresponding to a face in the clear field subgraph of ▱ab receives the coordinate (x, y) if it may be reached by following the y-axis for y arcs and, if $x > 0$, then making a wide right turn (and following the appropriate arc) then taking $x-1$ more arcs in the straight direction, as in Figure 9. Vertex a is the origin at $(0, 0)$ and b is located at (x_{ab}, y_{ab}).

It is important to note that the faces of the clear field subgraph do not necessarily have unique coordinates, but each coordinate uniquely identifies a face. Figure 6 is an example of such a situation. If the face at coordinate (x_1, y_1) is the same face as the one at coordinate (x_2, y_2), then the notation $(x_1, y_1) \equiv (x_2, y_2)$ is used to express this fact.

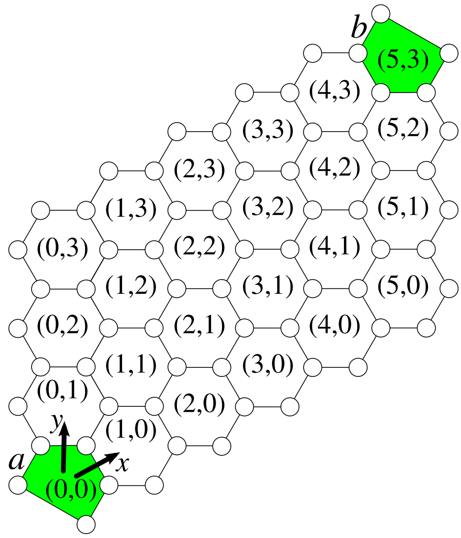


Figure 9: The faces in a clear field region may be labeled with coordinates using one of the pentagons (a) as the origin $(0, 0)$.

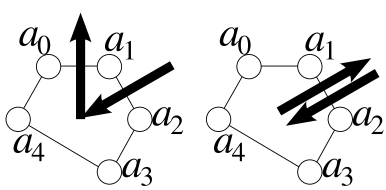


Figure 10: A numbering system for the vertices of a pentagon with the clear field arcs shown.

Given a particular quintant, an *x-direction walk at y* is a straight dual walk with its first arc from the dual vertex at $(0, y)$ to the one at $(1, y)$. Similarly, a *y-direction walk at x* is a straight dual walk with its first arc from the dual vertex at $(x, 0)$ to the one at $(x, 1)$.

For a Graver coloring, each vertex has a color and a pentagon is now defined to have a color of white or black as follows. Let ▱ab be the clear field that pairs degree five vertices a and b given some Graver coloring. As in Figure 10, number the primal vertices on the pentagon corresponding to a in clockwise order as $a_0, \ldots, a_4$ such that the dual arc of ▱ab that enters a crosses primal edge (a_1, a_2). Define the *pentagon color* of the pentagon for a to be the color of a_2, unless a_2 is gray, in which case the pentagon receives the color of a_1. In Figures 4(a) and 8(a), the pentagons are white and in Figures 4(b) and 8(b), the pentagons are black.

Exactly one of (a_0, a_1) and (a_1, a_2) is in $E_W \cup E_B$ because $\varangle ab$ pairs a and b. Note that if a_2 is gray, then $(a_1, a_2) \in E_W \cup E_B$ so a_1 has a different color than the other two neighbors of a_2 (see Figure 7) and a color-equivalent coloring may be obtained by swapping the colors of a_1 and a_2. Similarly, if $(a_0, a_1) \in E_W \cup E_B$ then a color-equivalent coloring may be obtained by swapping the colors of a_0 and a_1. Equivalently, the color of the pentagon for a is white if $(a_1, a_2) \in E_W$ or $(a_0, a_1) \in E_B$ and is black if $(a_1, a_2) \in E_B$ or $(a_0, a_1) \in E_W$.

Theorem B.2. *Let a and b be two degree five vertices that are paired by a Graver coloring and let $\varangle ab$ be their pairing clear field with dimensions (x, y). Let $F' = (V', E')$ be the clear field subgraph of $\varangle ab$.*

(i) There are exactly $2^{x+y}\binom{x+y}{x}$ ways to color the vertices of F' such that a pairing path exists between a and b and the pentagon for a is the same color as in F.

(ii) If the pentagon for a is white then $|E_W \cap E'| = x$ and $|E_B \cap E'| = y$, otherwise $|E_W \cap E'| = y$ and $|E_B \cap E'| = x$.

(iii) The colors of the pentagons for a and b are the same.

Proof. Label the vertices of the pentagon corresponding with a as a_0 through a_4 as in Figure 10. Similarly, label b_0 through b_4.

(i) The paths in the dual of F' that pair a and b correspond to walks of length $x + y$ from a to b within the clear field region of $\varangle ab$ such that no two consecutive wide turns are made in the same direction. Counting these walks is equivalent to the classical problem of counting the number of lattice walks from the origin $(0, 0)$ to (x, y) using steps in the north and east directions only. The north direction corresponds with the y-direction from a (taking the dual arc from a that crosses (a_0, a_1) and continuing straight). Likewise, the east direction corresponds with the x-direction and (a_1, a_2). The number of such lattice walks is $\binom{x+y}{x}$.

Once a pairing path P has been selected, it is easy to generate a coloring of F' that induces the pairing path. Let E_P be the edges in P. For each primal edge corresponding to an edge in E_P, select one incident vertex and color it gray. Color a_1 and/or a_2 (whichever is not gray) black or white as appropriate such that the pentagon for a is the same color in F' as in F. The graph $F' - E_P$ is bipartite so there is a unique way that the remaining uncolored vertices of F' can be colored with black and white.

Each of these possible paths pairing a with b contains $x + y$ edges in $E_W \cup E_B$. No two edges in $E_W \cup E_B$ are adjacent so the colors of the vertices on the endpoints of an edge in $E_W \cup E_B$ may be swapped, for a total of 2^{x+y} ways to color each pairing path. Each coloring induces exactly one pairing path, so $2^{x+y}\binom{x+y}{x}$ counts each coloring exactly once.

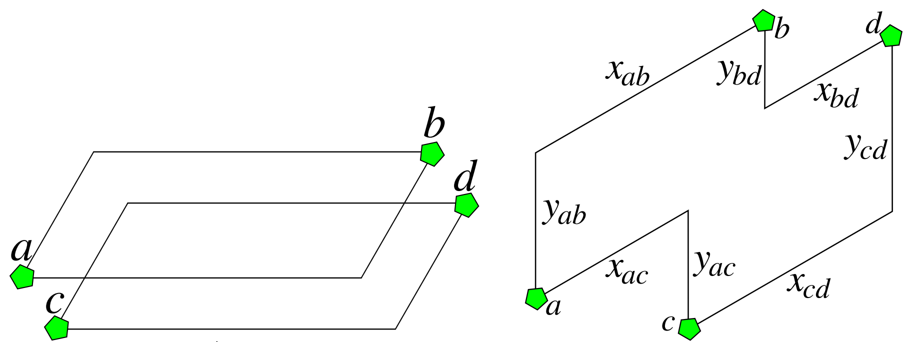
(ii) Let $e_1, e_2, \ldots, e_{x+y}$ be the arcs of the walk from a to b for some pairing path and let $v_0, v_1, \ldots, v_{x+y}$ be the vertices of the walk. Let $e'_1, e'_2, \ldots, e'_{x+y}$ be the edges in $E_W \cup E_B$ such that e'_i is the primal edge crossed by e_i. If the walk follows the straight direction at v_i $(0 < i < x+y)$, then e'_i and e'_{i+1} are either both in E_W or both in E_B (Lemma A.4). Conversely, if the walk makes a turn at v_i, then one of e'_i and e'_{i+1} is in E_W and the other is in E_B (Lemma A.4). When the walk is viewed as a walk on the lattice from the origin $(0,0)$ to (x,y), each step in the north direction indicates an edge in one of E_W or E_B and each step in the east direction indicates an edge in the other set. If the pentagon for a is white then either $(a_1,a_2) \in E_W$ or $(a_0,a_1) \in E_B$, so $|E_W \cap E'| = x$ and $|E_B \cap E'| = y$. If the pentagon for a is black then either $(a_1,a_2) \in E_B$ or $(a_0,a_1) \in E_W$, so $|E_B \cap E'| = x$ and $|E_W \cap E'| = y$.

(iii) Continuing the argument from (ii), if the pentagon for a is white and the final step of the walk from a to b is in the east direction, it crosses (b_1,b_2) so $(b_1,b_2) \in E_W$. If the final step is in the north direction, it crosses (b_0,b_1) so $(b_0,b_1) \in E_B$. In either case, the pentagon for b is white. If the pentagon for a is black then either $(b_1,b_2) \in E_B$ or $(b_0,b_1) \in E_W$, so the pentagon for b is black. □

Graver's claim that each clear field will have the same contribution to $2|E_W|+|E_B|$ is backed up by Theorem B.2. Furthermore, it gives the ability to replace one pairing path corresponding to a clear field with any other pairing path corresponding to the same clear field without affecting the independent set order.

The *clear field color* is defined as the color the clear field's corresponding pentagons. Figures 4(a) and 8(a) show white clear fields and Figures 4(b) and 8(b) show black clear fields. If a clear field is white, then the primal edges crossed by the edges of the pairing path in the x-direction are in E_W and if the clear field is black, these edges are in E_B. Because the contribution of a clear field to $2|E_W| + |E_B|$ is the penalty of the clear field, it follows from Theorem B.2(ii) that if a clear field with dimensions (x,y) is white, its penalty is $2x+y$ and if it is black, the penalty is $x+2y$. Equation (2) may be rewritten as

$$|W| = \frac{|V(G)|}{2} - \frac{1}{3} \sum_{\text{clear fields}} (\text{clear field penalties}). \tag{3}$$



(a) Example of $\overrightarrow{ba}$ sharing dual vertices with $\overrightarrow{cd}$

(b) Distance labels when two clear fields overlap

Figure 11: Situation when two clear fields overlap in the proof of Theorem B.3.

Theorem B.3. *[Equivalent to Theorem 4.1] Given a Graver coloring of a fullerene, let a and b be two dual vertices of degree five paired by the coloring and let ▱ab be their pairing clear field. Similarly, c and d are paired by pairing clear field ▱cd. The clear field subgraphs of ▱ab and ▱cd have no faces in common.*

Proof. For contradiction, assume the clear field subgraphs of ▱ab and ▱cd has a face in common, so at least one of $\overrightarrow{ab}$ and $\overrightarrow{ba}$ have a dual vertex in common with at least one of $\overrightarrow{cd}$ and $\overrightarrow{dc}$. By Theorem A.6, the pairing paths of ▱ab and ▱cd have no dual vertices in common. For such pairing paths to exist, at least one of $\overrightarrow{ab}$ and $\overrightarrow{ba}$ must not share a dual vertex with either $\overrightarrow{cd}$ nor $\overrightarrow{dc}$ and at least one of $\overrightarrow{cd}$ and $\overrightarrow{dc}$ must not share a dual vertex with either $\overrightarrow{ab}$ nor $\overrightarrow{ba}$. Therefore, by interchanging labels a and b and/or c and d if necessary, it can be assumed without loss of generality that $\overrightarrow{ba}$ shares at least one dual vertex with $\overrightarrow{cd}$, as illustrated in Figure 11(a). It will be shown that a better coloring exists by pairing a, b, c, and d differently, which implies the coloring is not optimal and provides a contradiction.

Some distances in the graph are labeled in Figure 11(b). The length of the pairing path between a and b is $x_{ab} + y_{ab}$. The distance from c to a using the arcs of the clear fields involves the first y_{ac} arcs of $\overrightarrow{cd}$ followed by the last x_{ac} arcs of $\overrightarrow{ba}$. The other distances are similarly defined. Figure 12(a) shows an example with ▱ab with dimensions $(7, 5)$, ▱cd with dimensions $(6, 6)$, $x_{ac} = 5$, $y_{ac} = 4$, $x_{bd} = 4$, and $y_{bd} = 3$.

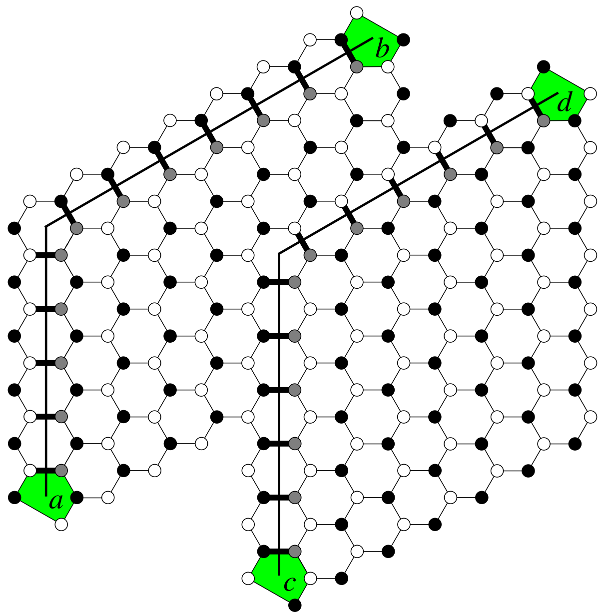
It can be assumed that no other pairing path uses any of the dual vertices on the dual walk from c to a, nor on the walk from b to d. This is because if some other pairing path did cross between c and a, it must also cross between b and d since it cannot share a dual vertex with the path pairing a and b nor with the path pairing c and d. Such a path would indicate that a third clear field shares dual vertices with ▱ab and ▱cd. Without loss of generality, the third clear field can be renamed to be ▱cd, repeating as necessary, so as to assume that no pairing path shares a dual vertex with c to a or b to d.

Label the vertices of the pentagon at a with a_0 through a_4 as per Figure 10 and similarly label the pentagons at b, c, and d. Consider the primal walk from c_2 to a_2 around the boundary of the subgraph induced by the clear field subgraphs of ▱ab and ▱cd. This walk includes an odd number of arcs (three if $x_{ac} = y_{ac} = 1$ and $1 + 2(y_{ac} - 1) + 2(x_{ac} - 1)$ otherwise), none of which are in $E_W \cup E_B$ because no pairing path crosses them. By Theorem B.1, ▱ab and ▱cd have opposite colors. Figure 12(a) shows an example in which ▱ab is black and ▱cd is white. This may be assumed without loss of generality because the other option is obtained by interchanging labels a and d as well as b and c.

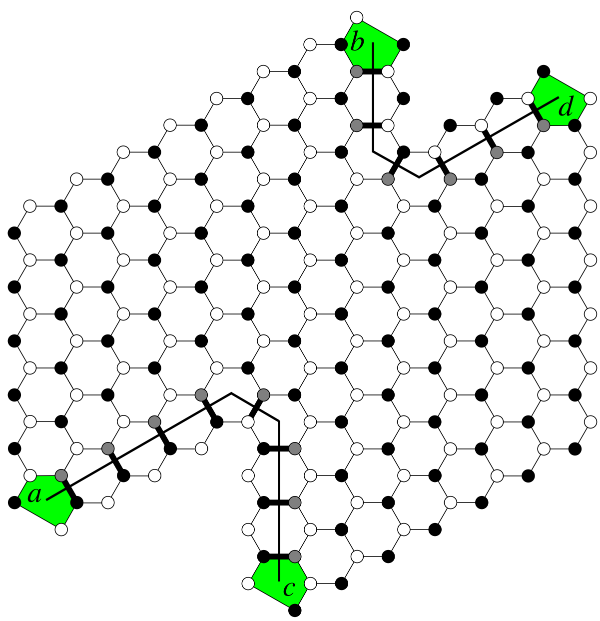
Define a dual walk W_{ca} from c to a as follows. If $y_{ac} > 1$, W_{ca} begins at c and uses the first $y_{ac} - 1$ arcs of $\overrightarrow{cd}$, then it makes a wide left turn to reach a dual vertex on ▱ab. If $y_{ac} = 1$, W_{ca} begins at c and uses the arc that crosses primal arc (c_0, c_4). In either case, if $x_{ac} > 1$, W_{ca} continues by following the last $x_{ac} - 1$ arcs of $\overrightarrow{ba}$ to reach a. The total length of W_{ca} is $x_{ac} + y_{ac} - 1$. Similarly, define W_{bd} from b to d having length $x_{bd} + y_{bd} - 1$. Figure 12(b) shows these walks on an example.

For the original coloring pairing of a with b and c with d, the clear field subgraphs of ▱ab and ▱cd contribute $y_{ab} + x_{cd}$ edges to E_W and $x_{ab} + y_{cd}$ edges to E_B. Obtain a new coloring by instead pairing a with c and b with d. Assign the primal edges crossed by W_{ca} and W_{bd} to E_W or E_B and color the clear field subgraphs of ▱ab and ▱cd such that a and b remain white and c and d remain black. In this new coloring, the clear field subgraphs of ▱ab and ▱cd contribute $x_{bd} + y_{bd} - 1$ edges to E_W and $x_{ac} + y_{ac} - 1$ edges to E_B. The new coloring is better (it provides a larger $|W|$) because $x_{ac} \leq x_{ab}$, $y_{ac} \leq y_{cd}$, $x_{bd} \leq x_{cd}$, and $y_{bd} \leq y_{ab}$. Note that if the new pairings make two consecutive left turns (they do when $x_{ac} + y_{ac} > 2$ or $x_{bd} + y_{bd} > 2$), then the new coloring is not optimal (Lemma A.7); however it is better than the original coloring, which is sufficient for a contradiction. □

The previous lemma shows that the clear field subgraphs of two clear fields that pair pentagons cannot share a face with each other. The next lemma extends that idea to a single clear field by showing that the clear field subgraph of a pairing clear field cannot share a face with itself.



(a) $|E_W| = 11$ and $|E_B| = 13$



(b) $|E_W| = 6$ and $|E_B| = 8$

Figure 12: Colorings of the subgraphs of two clear fields that share faces.

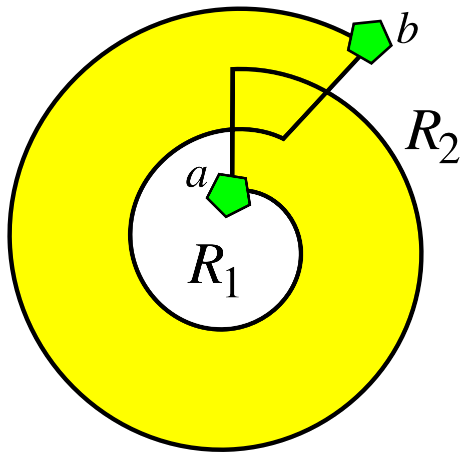
Theorem B.4. *[Equivalent to Theorem 4.2] Given a Graver coloring of a fullerene, let a and b be two dual vertices of degree five paired by the coloring and let $\varparallelogram ab$ be their pairing clear field with dimensions (x, y). If $y = 0$, then the $x + 1$ dual vertices of $\varparallelogram ab$ from a to b are unique. If $y > 0$, then all the dual vertices of $\varparallelogram ab$ are unique. That is, the clear field subgraph of $\varparallelogram ab$ contains $(x + 1)(y + 1)$ unique faces.*

Proof. For contradiction, suppose $\varparallelogram ab$ contains a repeated dual vertex. Walk $\overrightarrow{ab}$ does not contain a repeated dual vertex because if it did, the clear field subgraph of $\varparallelogram ab$ could be recolored using the primal edges crossed by $\overrightarrow{ab}$ to induce a pairing path that is not a simple path and would violate Theorem A.6. Likewise, $\overrightarrow{ba}$ does not contain a repeated dual vertex. It must be that a repeated dual vertex in $\varparallelogram ab$ is found once in $\overrightarrow{ab}$ and once in $\overrightarrow{ba}$.

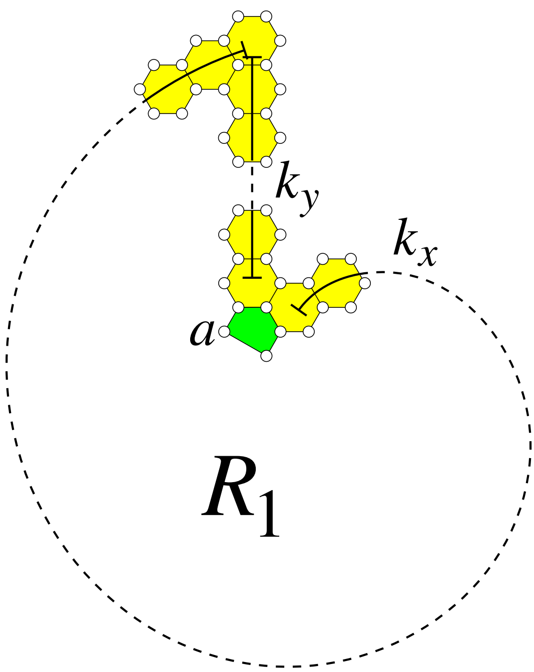
The above gives the result for the case where $y = 0$. Henceforth, assume $y > 0$.

Let $u_0, u_1, \ldots, u_{x+y}$ be the dual vertices visited by $\overrightarrow{ab}$ and let $v_0, v_1, \ldots,$ v_{x+y} be the dual vertices visited by $\overrightarrow{ba}$. Note that $a \equiv u_0 \equiv v_{x+y}$ and $b \equiv v_0 \equiv u_{x+y}$. Walks $\overrightarrow{ab}$ and $\overrightarrow{ba}$ make their wide right turns at u_y and v_y, respectively. Let $w_0, w_1, \ldots, w_k$ be the dual vertices of an arbitrary straight dual walk. Because $\overrightarrow{ab}$ makes a wide right turn at u_y, it is not possible for the straight walk to "cut the corner" of $\overrightarrow{ab}$. That is, w_i and w_j $(i < j)$ cannot exist such that w_i is a vertex in $\{u_1, \ldots, u_{y-1}\}$, w_j is a vertex in $\{u_{y+1}, \ldots, u_{x+y-1}\}$, and $\{w_i, \ldots, w_j\}$ all correspond to faces in the clear field subgraph of $\varparallelogram ab$. Therefore, if $\overrightarrow{ab}$ and $\overrightarrow{ba}$ share a vertex, it must be the situation pictured in Figure 6(a). That is, $\overrightarrow{ba}$ must "enter" $\varparallelogram ab$ by meeting $\overrightarrow{ab}$ at a vertex u_y through u_{x+y-1} and then make its turn and "exit" $\varparallelogram ab$ by meeting $\overrightarrow{ab}$ at a vertex u_1 through u_y. More specifically, there is a choice of $1 \le k_1 \le y$ and $y \le \ell_1 \le x + y - 1$ such that $u_{k_1} \equiv v_{\ell_1}$ and arc $(v_{\ell_1}, v_{\ell_1+1})$ is 1 clockwise position after arc (u_{k_1-1}, u_{k_1}) and there is a choice of $y \le k_2 \le x+y-1$ and $1 \le \ell_2 \le y$ such that $u_{k_2} \equiv v_{\ell_2}$ and arc (u_{k_2}, u_{k_2+1}) is 1 clockwise position after $(v_{\ell_2-1}, v_{\ell_2})$. Figure 6(b) shows an example of a complete fullerene exhibiting the situation in Figure 6(a). Such a situation is common in larger fullerenes.

Figure 13(a) shows an abstract drawing of a clear field that exhibits the situation in Figure 6(a). Because the three-dimensional surface of the fullerene is being drawn in two dimensions, one part of each of $\overrightarrow{ab}$ and $\overrightarrow{ba}$ is drawn with a curved line, even though they represent the straight direction. The faces not in the clear field subgraph of $\varparallelogram ab$ induce two fullerene subgraphs R_1 and R_2, which are also identified in Figure 6(a). Figure 13(b)



(a) An abstract diagram with the clear field region shaded



(b) Boundary of the interior white region in (a)

Figure 13: More diagrams of the situation pictured in Figure 6.

shows a more detailed drawing of the faces in the clear field subgraph of $\varparallelogram ab$ that are adjacent to subgraph R_1.

The clear field subgraph of $\varparallelogram ab$ contains two of the twelve pentagons, leaving ten pentagons to be distributed between subgraphs R_1 and R_2. Five of these pentagons are in R_1 due to the following. Refer to Figure 13(b) and note that the x-axis and y-axis of the quintant of a for $\varparallelogram ab$ meet at the hexagon that has both coordinates $(0, k_y)$ and $(k_x, 0)$ when the origin is defined at a. Subgraph R_1 has a large outer face bordered by the faces shown in the figure. This outer face of R_1 has two vertices of degree three from a, one from each of the first $k_x - 2$ hexagons on the x-axis and one from each of the first $k_y - 2$ hexagons on the y-axis for a total of $k_x + k_y - 2$ vertices of degree three. The remaining $k_x + k_y - 1$ vertices on the outer face of R_1 have degree two. There are $2k_x + 2k_y - 3$ edges on the outer face of R_1. Let p be the number of pentagonal faces in R_1 and h be the number of hexagonal faces in R_1. The total number of faces, edges, and vertices, respectively, are:

$$\begin{aligned}
f &= p + h + 1 \\
e &= (5p + 6h + (2k_x + 2k_y - 3))/2 \\
v &= (5p + 6h - \underbrace{(k_x + k_y - 1)}_{\text{outer vert. of deg. 2}} + \underbrace{(k_x + k_y - 2)}_{\text{outer vert. of deg. 3}})/3 + \underbrace{(k_x + k_y - 1)}_{\text{total vert. of deg. 2}} \\
&= (5p + 6h - 1)/3 + k_x + k_y - 1.
\end{aligned}$$

Euler's formula ($v - e + f = 2$) gives:

$$((5p + 6h - 1)/3 + k_x + k_y - 1) - ((5p + 6h - 3)/2 + k_x + k_y) + (p + h + 1) = 2$$

that simplifies to $p = 5$.

Five pentagons are in R_1, which implies that five are in R_2. The dual vertices of degree five corresponding to these ten pentagons are paired up by the Graver coloring using clear fields, which implies that at least one of these dual vertices, c, corresponding to a pentagon in R_1 must be paired with another dual vertex, d, corresponding to a pentagon in R_2. This implies that pairing clear field $\varparallelogram cd$ must share a dual vertex with $\varparallelogram ab$, but this cannot happen by Theorem B.3. □

Definition B.5 (Proper Clear Field)**.** *A clear field with dimensions* (x, y) *is called a* proper clear field *if its clear field subgraph contains* $(x+1)(y+1)$ *unique faces.*

The previous theorem shows that all pairing clear fields are proper clear fields. The next two theorems consider clear fields on a fullerene whether or not they pair two vertices of degree five for some coloring. The first shows that there is a simple linear upper bound on the number of clear fields. The second shows that there is a logarithmic upper bound for the number of proper clear fields.

Theorem B.6. *[The same as Theorem 4.3] The number of proper clear fields is in* $O(log_2 n)$.

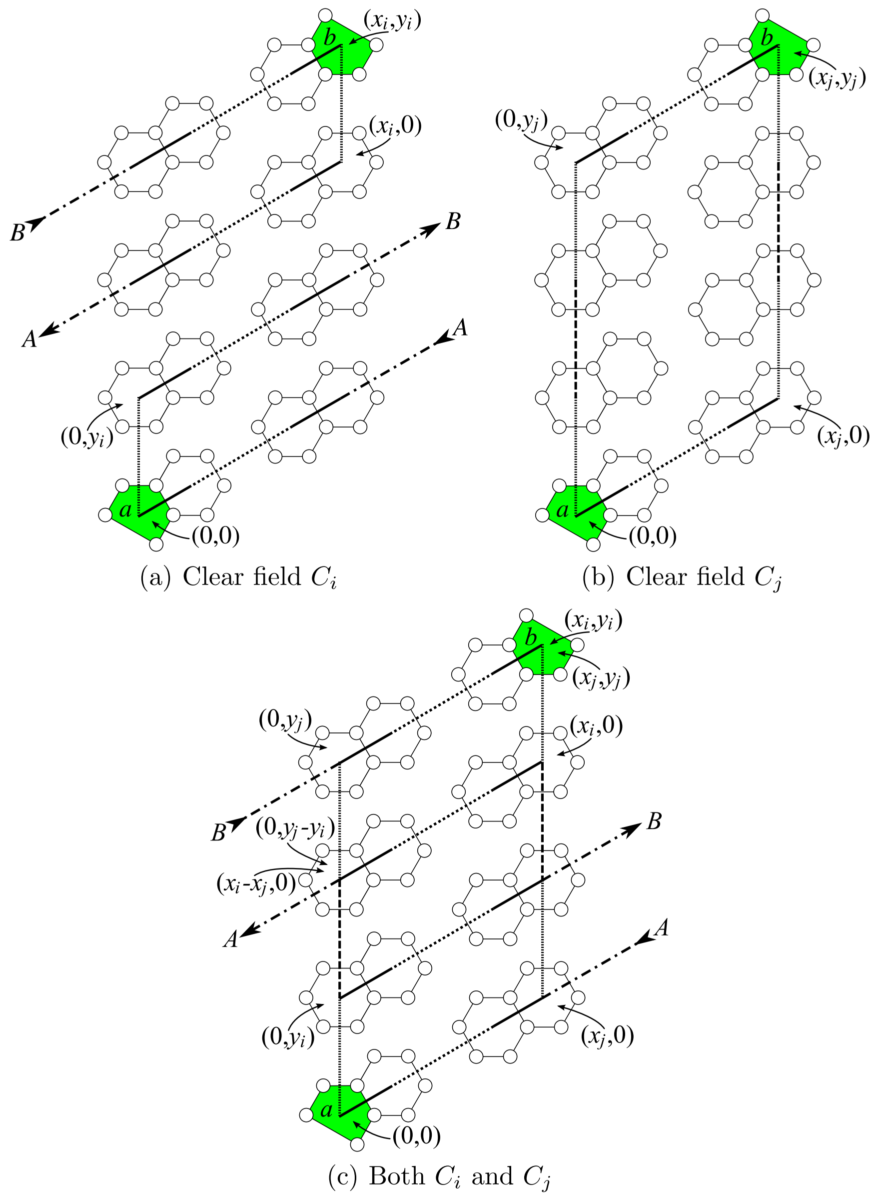
Proof. Let k be the number of proper clear fields between a quintant Q_a of a vertex a of degree five and a quintant Q_b of another vertex b of degree five. Denote these k clear fields as $C_1, C_2, \ldots, C_k$ with C_i having dimensions (x_i, y_i). Fixing a as the origin $(0, 0)$ and using Q_a, assign coordinates to the dual vertices (see Figure 9). A counter-intuitive situation emerges. Because C_1 pairs a and b using Q_a with dimensions (x_1, y_1), b receives coordinate (x_1, y_1). Similarly, C_2 pairs a and b using Q_a with dimensions (x_2, y_2), so b also receives coordinate (x_2, y_2). This also holds for clear fields $C_3, C_4, \ldots C_k$, so b receives coordinates $(x_1, y_1), (x_2, y_2), \ldots, (x_k, y_k)$.

The y-dimensions of clear fields $C_1, C_2, \ldots C_k$ must be unique because no two clear fields may share a wide right turn, as in the proof of Theorem 3.2. Likewise, the x-dimensions must be unique. Order the clear fields such that $y_1 < y_2 < \ldots < y_k$.

Consider two of these clear fields with y-dimensions y_i and y_j such that $y_i < y_j$. This non-intuitive situation is shown in Figure 14. Figure 14(a) shows clear field C_i that starts at a with coordinate $(0, 0)$, goes straight to $(0, y_i)$ where it makes a wide right turn and continues straight along the path marked B to b at (x_i, y_i). At b, C_i makes a sharp right turn and continues straight to $(x_i, 0)$ where it makes a wide right turn and continues straight along the path marked A to return to a at $(0, 0)$. Figure 14(b) shows clear field C_j in a more typical illustration that shows the tight right turns at a $(0, 0)$ and b (x_j, y_j) and the wide right turns at $(0, y_j)$ and $(x_j, 0)$. Figure 14(c) combines these figures to show the full picture, which must be as shown because C_i and C_j both share quintants Q_a and Q_b.

To show that $x_i > x_j$, assume for contradiction that $x_i < x_j$. In this case, the dual vertex at (x_i, y_i) is in the interior of C_j, which implies the dual vertex at (x_i, y_i) has degree six. Because C_i pairs a and b, the dual vertex at (x_i, y_i) is b, which has degree five, which provides the contradiction. Therefore, $x_i > x_j$.

The subwalk of C_i from b to a makes its wide right turn at $(x_i, 0)$. Therefore, the x-axis of a meets the y-axis of a at the dual vertex at coordinate



(a) Clear field C_i

(b) Clear field C_j

(c) Both C_i and C_j

Figure 14: Diagram for the proof of Theorem B.6. Some coordinates are labeled, using a as the origin. Lines of the same style represent the same distance. Arrows represent the continuation of a straight walk with the matched ends identified by letters A and B.

$(x_i - x_j, 0)$, which is also $(0, y_j - y_i)$ because C_i and C_j share Q_a and Q_b (see Figure 14(c)). Clear field C_i is a proper clear field, so it contains no repeated dual vertices. Therefore the vertex at $(0, y_j - y_i)$ is not one of the dual vertices at coordinates $(0,0)$ through $(0, y_i)$, so $y_j - y_i > y_i$, which implies $2y_i + 1 \leq y_j$. This gives $2^{k-1}(y_1 + 1) - 1 \leq y_k$, which simplifies to $2^{k-1} - 1 \leq y_k$ because $y_1 \geq 0$. Clear field C_k is a proper clear field, so $y_k \leq n/2 - 10$, the number of vertices of degree six. Therefore, $2^{k-1} < n/2$, which gives $k < \lg n$.

There is a constant number of quintant pairs so the total number of proper clear fields is in $O(\lg n)$. □

This completes the necessary background to describe an algorithm to find a maximum independent set of a fullerene.

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Sean Daugherty
Department of Computer Science
University of Victoria
Canada
E-mail address: daughe@gmail.com

Wendy Myrvold
Department of Computer Science
University of Victoria
Canada
E-mail address: wendym@cs.UVic.ca

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