

# Bipartizing fullerenes\*

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## Abstract

A fullerene graph is a cubic bridgeless planar graph with twelve 5-faces such that all other faces are 6-faces. We show that any fullerene graph on  $n$  vertices can be bipartized by removing  $O(\sqrt{n})$  edges. This bound is asymptotically optimal.

**Keywords:** Fullerene graph; Fullerene stability; Bipartite spanning subgraph

## 1 Introduction

*Fullerenes* are carbon-cage molecules comprised of carbon atoms that are arranged on a sphere with pentagonal and hexagonal faces. The icosahedral  $C_{60}$ , well known as Buckminsterfullerene was found by Kroto et al. [10], and later confirmed by experiments by Krätschmer et al. [9] and Taylor et al. [12].

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Since the discovery of the first fullerene molecule, the fullerenes have been objects of interest to scientists all over the world.

From the graph theoretical point of view, the fullerenes can be viewed as cubic 3-connected graphs embedded into a sphere with face lengths being 5 or 6. Euler's formula implies that each fullerene contains exactly twelve pentagons, but provides no restriction on the number of hexagons. In fact, it is not difficult to see that mathematical models of fullerenes with precisely  $\alpha$  hexagons exist for all values of  $\alpha$  with the sole exception of  $\alpha = 1$ . See [3, 5, 6, 11] for more information on chemical, physical, and mathematical properties of fullerenes.

The question of stability of fullerene molecules receives a lot of attention. The goal is to obtain a graph-theoretical property whose value influences the stability. Different properties, like the number of perfect matchings [7] or the independence number [4] were considered. The property investigated in this paper is how far the graph is from being a bipartite graph, which was suggested by Došlić [1] and further considered in [2]. Despite of the effort none of the so far considered parameters works in all cases. Hence more research is still needed.

For a plane graph  $H$ , let  $F(H)$  be the set of the faces of  $H$ . Let  $H$  be a fullerene graph, and let  $K_H$  be the weighted complete graph whose vertices correspond to the 5-faces of  $H$  and the weight of the edge joining two 5-faces  $f_1$  and  $f_2$  is equal to the distance from  $f_1$  to  $f_2$  in the dual of  $H$ . Let  $b(H)$  be the size of the minimum set  $S \subseteq E(H)$  such that  $H - S$  is bipartite. Došlić and Vukičević [2] proved the following:

**Theorem 1.** *If  $H$  is a fullerene graph, then  $b(H)$  is equal to the minimum weight of a perfect matching in  $K_H$ .*

A corollary of the above theorem is a polynomial-time algorithm for finding a set of edges  $S$  whose removal makes the graph bipartite.

Došlić and Vukičević [2] conjectured that  $b(H) = O(\sqrt{|V(H)|})$ . In fact, they gave the following stronger conjecture.

**Conjecture 2.** *If  $H$  is a fullerene graph with  $n$  vertices, then  $b(H) \leq \sqrt{12n/5}$ .*

The main result of this paper is an upper bound on  $b(H)$ , confirming the weaker version of the conjecture.

**Theorem 3.** *If  $H$  is a fullerene graph with  $n$  vertices, then  $b(H) = O(\sqrt{n})$ .*

## 2 Proof of Theorem 3

Let  $H$  be a fullerene graph. A *patch with boundary  $o$*  is a 2-connected subgraph  $G \subseteq H$  such that  $o \in F(G)$  (usually, we consider  $o$  to be the outer face of  $G$ ) and  $F(G) \setminus F(H) \subseteq \{o\}$  (but it is possible for the boundary  $o$  to be also a face of  $G$ ). Let  $v$  be a vertex incident with  $o$ . If  $\deg_G(v) = 3$ , then  $v$  is a *3-vertex (with respect to  $o$ )*, otherwise  $v$  is a *2-vertex (with respect to  $o$ )*. An edge  $e$  incident with  $o$  is a *22-edge* (resp. a *33-edge*) if both vertices incident with  $e$  are 2-vertices (resp. 3-vertices) with respect to  $o$ . If  $e$  is neither a 22-edge nor a 33-edge, then it is a *23-edge*. The *description  $D(o)$*  of the boundary  $o$  is the cyclic sequence in that  $A$  represents a 33-edge,  $B$  represents a 22-edge, and a maximal consecutive segment of 23-edges is represented by the integer giving its length. For example, the boundary of the patch consisting of a 5-face and a 6-face sharing an edge is described as  $BB2BBB2$ .

Let  $s(o)$  and  $t(o)$  be the numbers of 22-edges and 33-edges of  $o$ , respectively, and let  $s_2(o)$  be the number of pairs of consecutive 22-edges of  $o$ . Let  $p(G)$  be the number of 5-faces of  $G$  distinct from  $o$ . In the example of the previous paragraph, we have  $s(o) = 5$ ,  $t(o) = 0$ ,  $s_2(o) = 3$  and  $p(G) = 1$ . The following lemma relates the number of 22- and 33-edges; a similar relation was derived by Kardoš and Škrekovski [8].

**Lemma 4.** *If  $G$  is a patch with boundary  $o$ , then  $s(o) = 6 - p(G) + t(o)$ .*

*Proof.* Suppose that the length of  $o$  is  $\ell$ . Let  $n = |V(G)|$ ,  $m = |E(G)|$  and  $f = |F(G)|$ . Since each edge of  $G$  is incident with two faces,

$$2m = 6(f - p(G) - 1) + 5p(G) + \ell,$$

i.e.,  $\ell = 2m + p(G) + 6 - 6f$ . Note that the number of 2-vertices is  $(\ell + s(o) - t(o))/2$ , which can be easily seen from the modification of the boundary by adding  $s(o)$  and deleting  $t(o)$  3-vertices so that there is no 33-edge or 22-edge. Thus

$$2m = 3n - (\ell + s(o) - t(o))/2.$$

Substituting for  $\ell$ , we obtain

$$3m = 3n + 3f - 6 + \frac{6 - p(G) + t(o) - s(o)}{2}.$$

By Euler's formula,  $m = n + f - 2$ , thus  $6 - p(G) + t(o) - s(o) = 0$  and the claim of the lemma follows.  $\square$

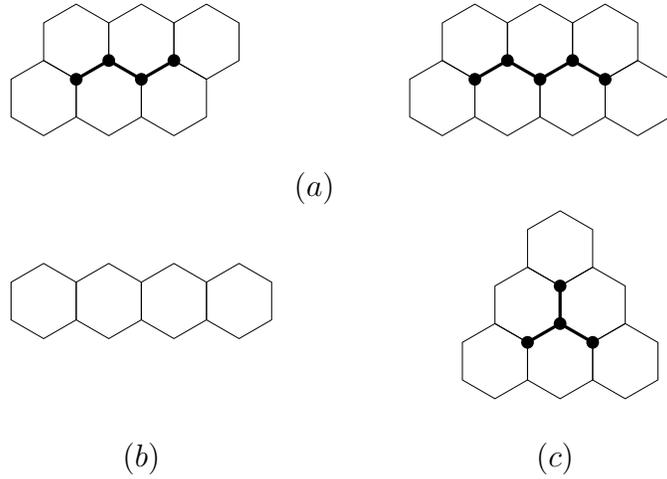


Figure 1: A fat worm, a slim worm and the shell.

A patch  $G$  with boundary  $o$  is a *fat worm* if  $p(G) = 0$ , the subgraph of  $G$  induced by  $V(G) \setminus V(o)$  is a path  $P$ , and the edges of  $E(G) \setminus E(P)$  incident with each two consecutive inner vertices of  $P$  are not incident to a common face of  $G$ . See Figure 1(a). Note that in this case, the description of  $o$  is

- $BB2B(2k + 2)BB2B(2k + 2)$  if  $P$  has length  $2k + 1$  and
- $BB2B(2k + 2)B2BB(2k + 4)$  if  $P$  has length  $2k + 2$ .

We consider the patch with exactly one vertex not incident with  $o$  (and boundary  $BB2BB2BB2$ ) to be a fat worm as well (in this case,  $P$  has length 0). The patch  $G$  is a *slim worm* if  $p(G) = 0$ ,  $V(G) = V(o)$  and  $t(o) = 0$ . Geometrically, it is a straight line of hexagons, see Figure 1(b). Note that  $D(o) = BBB(2k)BBB(2k)$  for some  $k$  (or  $D(o) = BBBBBB$ , when  $k = 0$  and  $o$  is a 6-face). The patch  $G$  is a *worm* if it is a fat worm or a slim worm. The *shell* is the patch  $G$  with boundary  $o$  such that  $p(G) = 0$  and  $D(o) = BB4BB4BB4$  (having 4 internal vertices). See Figure 1(c).

An  $\ell$ -chord of a cycle  $C$  in a patch  $G$  is a path of length  $\ell$  with distinct endvertices belonging to  $V(C)$  such that the inner vertices and edges of the path do not belong to  $C$ . We say a chord instead of a 1-chord. Consider an  $\ell$ -chord  $Q$  of the boundary  $o$  of a patch  $G$ . Let  $G_1$  and  $G_2$  be the two patches into that  $Q$  splits  $G$  (i.e., the subgraphs such that  $G_1 \cup G_2 = G$ ,  $G_1 \cap G_2 = Q$

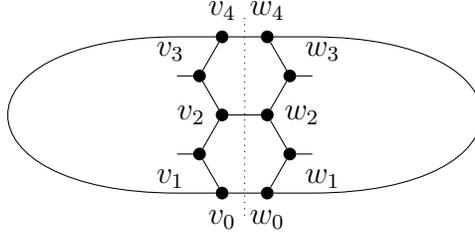


Figure 2: Two 4-chords.

and  $G_1 \neq Q \neq G_2$ ), and  $o_1$  and  $o_2$  their boundaries. We say that  $Q$  *splits off a face* if  $G_1 = o_1$  or  $G_2 = o_2$ . The patch  $G$  is *decomposable* if it contains a *simplifying cut*, that is

- an  $\ell$ -chord  $Q$  of  $o$  with  $\ell \leq 3$  such that  $t(o_1) + t(o_2) < t(o)$ , or
- two 4-chords  $Q_1 = v_0v_1v_2v_3v_4$  and  $Q_2 = w_0w_1w_2w_3w_4$  such that  $v_0w_0$ ,  $v_2w_2$  and  $v_4w_4$  are edges of  $G$ . See Figure 2.

Otherwise, we call  $G$  *indecomposable*. We say that  $G$  is a *normal patch* if  $G$  is indecomposable, no 5-face of  $G$  distinct from  $o$  shares an edge with  $o$  and  $G$  is neither a worm nor the shell.

**Lemma 5.** *Let  $G$  be a normal patch with boundary  $o$  and  $Q$  an  $\ell$ -chord of  $o$ , with  $\ell \leq 3$ . Then  $\ell \geq 2$  and  $Q$  splits off a face. Furthermore, the number of 33-edges incident with the endvertices of  $Q$  is most  $\ell - 2$ .*

*Proof.* Let  $G_1$  and  $G_2$  with boundaries  $o_1$  and  $o_2$ , respectively, be the patches into that  $Q$  splits  $G$ . Let  $Q = q_0q_1 \dots q_\ell$  and  $o_2 = q_0v_1v_2 \dots v_aq_\ell q_{\ell-1} \dots q_0$ .

Suppose first that  $\ell = 1$ . Since  $G$  is not a slim worm, there exists an edge  $e \in E(G)$  that either is a 33-edge of  $o$  or is incident with a vertex in  $V(G) \setminus V(o)$ . Let us choose the chord  $Q$  and the patches  $G_1$  and  $G_2$  so that  $e \in E(G_2)$  and  $G_2$  is minimal. As  $G$  is indecomposable, each 33-edge of  $G$  is also a 33-edge in  $G_1$  or  $G_2$ . It follows that  $v_1$  and  $v_a$  are 2-vertices, and since the internal face incident with  $q_0v_1$  has length six,  $v_2$  and  $v_{a-1}$  must be adjacent. Since  $e \in E(G_2)$ , we have  $G_2 \neq o_2$ ; hence,  $v_2v_{a-1}$  is a chord of  $o$ . The chord  $v_2v_{a-1}$  splits  $G$  into patches  $G'_1$  and  $G'_2$  with  $G'_2 \subset G_2$ . However, this contradicts the choice of  $Q$ , since it is easy to see that  $e \in E(G'_2)$ . We conclude that  $o$  is an induced cycle.

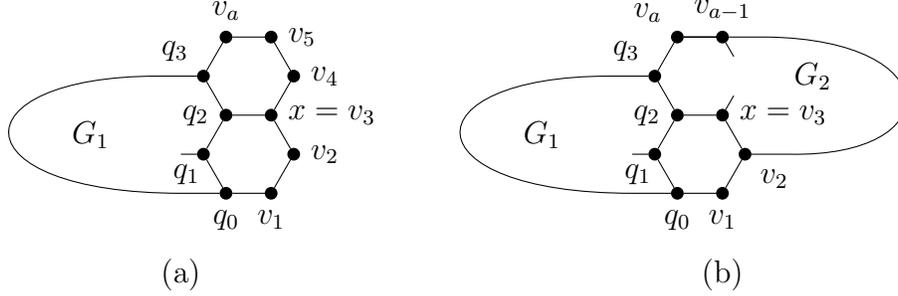


Figure 3: 3-chords from Lemma 5.

Suppose now that  $\ell = 2$ . By symmetry between  $G_1$  and  $G_2$ , we may assume that  $q_1$  is a 2-vertex in  $G_2$ . Since  $t(o_1) + t(o_2) \geq t(o)$ , we have that  $v_1$  and  $v_a$  are 2-vertices, and it follows that  $G_2 = o_2$  is a face split off by  $Q$ .

Finally, suppose that  $\ell = 3$ . Suppose first that both  $q_1$  and  $q_2$  are 2-vertices in  $G_2$ , and thus  $q_1q_2$  is a 33-edge with respect to  $o_1$ . Since  $t(o_1) + t(o_2) \geq t(o)$ , at least one of  $v_1$  and  $v_a$  (say  $v_1$ ) is a 2-vertex. Thus,  $V(Q) \cup \{v_1, v_2, v_a\}$  are all incident with a common face, which is only possible if  $a = 2$  and  $G_2$  consists of a single face. It follows that  $Q$  splits off a face.

The case that both  $q_1$  and  $q_2$  are 2-vertices in  $G_1$  is symmetrical. Hence, without loss of generality, we assume that  $q_1$  is a 2-vertex and  $q_2$  is a 3-vertex in  $G_2$ . As  $t(o_1) + t(o_2) \geq t(o)$ , we infer that both  $v_1$  and  $v_a$  are 2-vertices. Let  $x \notin \{q_1, q_3\}$  be the third neighbor of  $q_2$ . Observe that  $x$  and  $v_2$  are adjacent. Furthermore,

- if  $x \in V(o)$ , then both  $xq_2q_3$  and  $xq_2q_1q_0$  split off a face (for the former, note that the edge joining  $v_{a-1}$  with a neighbor of  $x$  is not a chord, since we already proved that  $o$  is an induced cycle). See Figure 3(a).
- if  $x \notin V(o)$ , then  $v_1v_2xq_2q_1q_0$  is a face and we may apply the same observations to the 3-chord  $v_2xq_2q_3$ . See Figure 3(b).

By symmetry, this argument also holds for  $o_1$ . Hence by repeating the argument we conclude that  $G$  is a fat worm, contradicting the assumption that  $G$  is a normal patch.

Furthermore, note that if  $Q$  splits off a face, then  $t(o) = t(o_1) + t(o_2) - (\ell - 2) + k$ , where  $k$  is the number of 33-edges incident with  $q_0$  or  $q_\ell$ . Since  $G$  is indecomposable, it follows that  $k \leq \ell - 2$ .  $\square$

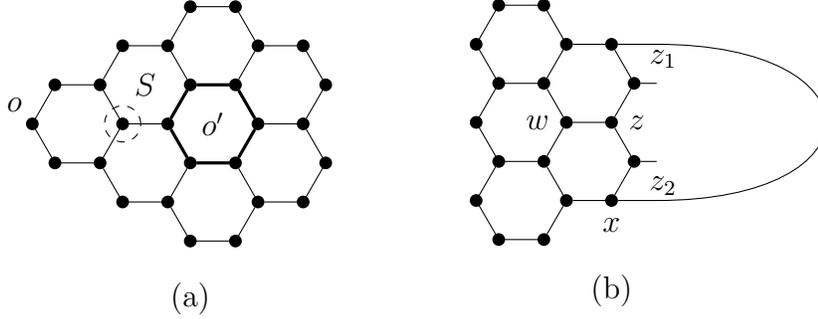


Figure 4: Patch  $G$  and  $o'$  and a configuration from Lemma 6.

For a patch  $G$  with boundary  $o$ , let  $G' \subseteq G$  be the subgraph consisting of the outer layer of the faces of  $G$ ; that is,  $e$  is an edge of  $G'$  if and only if it is incident with a face that shares an edge with  $o$ . Let  $S$  be the set of vertices in  $V(G) \setminus V(o)$  that have at least two neighbors in  $o$ . Let  $o' = G' - (V(o) \cup S)$ . See Figure 4(a). For a cycle  $o$ , let  $\ell(o)$  denote its length.

**Lemma 6.** *If  $G$  is a normal patch with boundary  $o$ , then  $o'$  is a cycle, and the patch bounded by  $o'$  satisfies  $t(o') = t(o)$ ,  $s(o') = s(o)$  and  $s_2(o') \geq s_2(o)$ . Furthermore,  $\ell(o') = \ell(o) + 2p(G) - 12 - 2s_2(o)$ .*

*Proof.* Since  $G$  is not a fat worm, we have  $|V(G) \setminus V(o)| > 1$ . If two vertices of  $S$  were adjacent, then  $|V(G) \setminus V(o)| = 2$  by Lemma 5 and  $G$  would be a fat worm, thus  $S$  is an independent set and hence  $o'$  is not empty. Lemma 5 also implies that  $G - V(o)$  is connected, and since  $S$  only contains vertices whose degree in  $G - V(o)$  is one,  $o'$  is connected as well.

Suppose that a vertex  $w$  of  $o'$  is adjacent to more than one vertex of  $S$ . Since  $G$  is not the shell,  $w$  is adjacent to exactly two vertices in  $S$ ; let  $z$  be the neighbor of  $w$  not in  $S$ . Since  $G$  is not a fat worm, we have  $z \notin V(o)$ . Let  $z_1$  and  $z_2$  be the neighbors of  $z$  distinct from  $w$ ; since  $z \notin S$ , we may assume that  $z_2 \notin V(o)$ . Let  $f$  be the face of  $G$  incident with  $w, z$  and  $z_2$ , and let  $x$  be the neighbor of  $z_2$  in  $f$  distinct from  $z$ . Note that  $f$  is incident with a neighbor of  $w$  that belongs to  $S$ , and thus  $f$  shares an edge with  $o$ . Hence  $f$  is a 6-face and we have  $x \in V(o)$ . If  $z_1 \in V(o)$ , then the 3-chord  $z_1 z z_2 x$  contradicts Lemma 5. Otherwise, by a symmetric argument we conclude that a face  $f'$  incident with  $w, z$  and  $z_1$  is also a 6-face sharing an edge with  $o$ , see Figure 4(b). However,  $f \cup f'$  forms a simplifying cut (a pair of 4-chords)

in  $G$ , which is a contradiction. Therefore, each vertex of  $o'$  has at most one neighbor in  $S$ .

By Lemma 5, no vertex of  $o'$  has a neighbor both in  $S$  and in  $o$ , since at least one of the two resulting 3-chords would not split off a face. If  $v$  is a vertex of  $o'$  that has a neighbor in  $o$  or  $S$ , then  $v$  has two neighbors in  $o'$ , and thus  $o'$  has at least three vertices.

Suppose that  $o'$  contains a bridge  $e = uv$ . Note that both faces  $f_1$  and  $f_2$  of  $G$  incident with  $e$  share an edge with  $o$ . As  $u, v \notin S$ , these two vertices do not lie on 2-chords. Note that  $f_1 \cup f_2$  contains an  $\ell_u$ -chord  $P_u$  of  $o$  such that  $u \in V(P_u)$  and  $v \notin V(P_u)$ , where  $3 \leq \ell_u \leq 5$ . Similarly, let  $P_v$  be an  $\ell_v$ -chord of  $o$  such that  $v \in V(P_v)$  and  $u \notin V(P_v)$ . As neither  $P_u$  nor  $P_v$  splits off a face, Lemma 5 implies that  $\ell_u, \ell_v \geq 4$ . Since  $f_1$  and  $f_2$  are 6-faces, we conclude that  $P_u$  and  $P_v$  are 4-chords. Lemma 5 further implies that  $u$  and  $v$  are middle vertices of  $P_u$  and  $P_v$ , thus  $f_1$  and  $f_2$  is a pair of 4-chords forming a simplifying cut. This is a contradiction; therefore,  $o'$  is 2-edge-connected. Since  $o' \subset G'$ , every edge of  $o'$  is incident with a face that shares an edge with  $o$ . We conclude that  $o'$  is a cycle.

Consider now a 33-edge  $x_1x_2$  in  $o$ . Since  $G$  is a normal patch, there exists a 6-face incident with  $x_1x_2$  distinct from  $o$ ; let  $x_1x_2x_3x_4x_5x_6$  be the cycle bounding this face. Lemma 5 implies that each of  $x_3$  and  $x_6$  has only one neighbor in  $o$ , as otherwise one of them would belong to a 2-chord whose endpoint is incident with the 33-edge  $x_1x_2$ . Therefore,  $x_3, x_6 \notin S$  and  $x_3x_4x_5x_6$  is a part of  $o'$ , and  $x_4x_5$  is a 33-edge with respect to  $o'$ . It follows that  $t(o') \geq t(o)$ . On the other hand, consider a 33-edge  $y_4y_5$  of  $o'$ , and let  $y_3y_4y_5y_6$  be a part of the boundary of  $o'$ . As  $y_4$  and  $y_5$  are 3-vertices in  $o'$ , there exists a 6-face  $y_1y_2y_3y_4y_5y_6$  in  $G$ , and  $y_1y_2$  is a 33-edge in  $o$ . Hence, we have  $t(o') = t(o)$  and by Lemma 4,  $s(o') = s(o)$ .

Similarly, consider a part  $z_0z_1z_2z_3z_4z_5z_6$  of  $o$ , where  $z_2z_3$  and  $z_3z_4$  are 22-edges. The common neighbor  $z$  of  $z_1$  and  $z_5$  belongs to  $S$ , and its neighbor  $z'$  distinct from  $z_1$  and  $z_5$  belongs to  $o'$ . As we observed before, both neighbors  $z'_1$  and  $z'_2$  of  $z'$  distinct from  $z$  belong to  $o'$ . Furthermore, by Lemma 5, the endpoints of the 2-chord  $z_1zz_5$  are incident with no 33-edges, thus  $z_0$  and  $z_6$  are 2-vertices. It follows that both  $z'_1$  and  $z'_2$  have a neighbor in  $o$ , and  $z'_1z'$  and  $z'_2z'$  are 22-edges with respect to  $o'$ . Hence, we conclude that  $s_2(o') \geq s_2(o)$ .

In fact,  $D(o')$  can be obtained from  $D(o)$  in the following way: Add 0 between each two consecutive letters in  $D(o)$ . Since endvertices of a 2-chord of  $o$  are not incident with 33-edges, if  $B0B$  appears in the resulting

sequence, then it is as a part of a subsequence  $n_1B0Bn_2$ , where  $n_1, n_2 \geq 3$ . We construct  $D(o')$  by

- for each  $n_1B0Bn_2$  subsequence, decreasing each of  $n_1$  and  $n_2$  by 3,
- for each  $B$  not contained in such a subsequence, decreasing each of the neighboring integers by 1,
- for each  $A$ , increasing each of the neighboring integers by 1, and
- suppressing any zeros.

Note that the increases/decreases are cumulative, e.g., if  $D(o)$  contains a subsequence  $A3B2B$ , then the sequence  $D(o')$  contains a subsequence  $A3B0B$  (or  $A3BB$  after suppressing zeros). By Lemma 4,  $t(o) - s(o) = p(G) - 6$ , and the formula for the length of  $o'$  follows:

$$\begin{aligned} \ell(o') &= \ell(o) + 2t(o) - 2(s(o) - 2s_2(o)) - 6s_2(o) \\ &= \ell(o) + 2p(G) - 12 - 2s_2(o). \end{aligned}$$

□

Consider a patch  $G$  with boundary  $o_1$ . A sequence of cycles  $o_1, o_2, \dots, o_k$  (with  $k \geq 2$ ) is called an *uninterrupted peeling* if for  $1 \leq i < k$ , the subpatch of  $G$  bounded by  $o_i$  is normal and  $o_{i+1} = o'_i$ .

**Lemma 7.** *Let  $o$  be the boundary of a patch  $G$  such that  $p(G) \neq 6$ . If  $o = o_1, o_2, \dots, o_k$  is an uninterrupted peeling, then the number of vertices of  $G$  outside of (and not including)  $o_k$  is at least  $4k^2/9$ .*

*Proof.* By Lemma 6, we have  $s_2(o_1) \leq s_2(o_2) \leq \dots \leq s_2(o_k)$ . Moreover, Lemma 6 also implies that the sequence  $\ell(o_1), \dots, \ell(o_k)$  is concave.

Let  $a$  be the largest index such that  $\ell(o_1) < \dots < \ell(o_a)$  and let  $b$  be the smallest index such that  $\ell(o_b) > \dots > \ell(o_k)$ . Note that if the whole sequence is decreasing then  $a = b = 1$  and similarly if the whole sequence is increasing then  $a = b = k$ , hence  $a \leq b$  in all the cases. We compute a lower bound on the number of vertices of  $G$  outside of  $o_k$  as follows:

$$\sum_{i=1}^{k-1} \ell(o_i) = \sum_{i=1}^{a-1} \ell(o_i) + \sum_{i=a}^{b-1} \ell(o_i) + \sum_{i=b}^{k-1} \ell(o_i).$$

First, we deal with the middle term. Let  $m = b - a$ . Suppose that  $a < b$ . By concavity, we have  $\ell(o_a) = \ell(o_{a+1}) = \dots = \ell(o_b)$ ; let  $r = \ell(o_a)$ . By Lemma 6,  $s_2(o_i) = p(G) - 6$  for  $a \leq i < b$ . Since  $p(G) \neq 6$ , we conclude that  $s_2(o_a) \geq 1$ , i.e.,  $o_a$  contains two consecutive 22-edges. Equivalently,  $D(o_a)$  contains a subsequence  $n_1 B B n_2$  (note that Lemma 5 implies that  $D(o_a)$  does not contain three consecutive  $B$ 's and that  $n_1, n_2 \geq 3$ ). By Lemma 4,  $t(o_a) - s(o_a) = p(G) - 6 = s_2(o_a)$ . Again using the fact that  $D(o_a)$  does not contain three consecutive  $B$ 's, we have  $s(o_a) \geq 2s_2(o_a)$ , and consequently  $t(o_a) \geq 3$ . It follows that  $n_1 + n_2 + 5 \leq r$ . By symmetry, assume that  $2n_1 \leq r - 5$ . As observed in the proof of Lemma 6,  $D(o_{a+1})$  contains a subsequence  $n'_1 B B n'_2$ , where  $n'_1 \leq n_1 - 2$  (the equality is achieved if  $n_1$  is adjacent to  $A$  in  $D(o_a)$ ). The same observation applies to  $o_{a+1}, \dots, o_{b-2}$ . In the normal patch  $o_{b-1}$ , the integers adjacent to  $BB$  are greater or equal to three, thus  $n_1 \geq 2m + 1$  and  $r \geq 4m + 7$ . It follows that  $\sum_{i=a}^{b-1} \ell(o_i) = mr \geq m(4m + 7)$ . In the case where  $a = b$ , we have  $\sum_{i=a}^{b-1} \ell(o_i) = 0 = m(4m + 7)$ , since  $m = 0$ .

Now we deal with the other terms of the sum. If  $a > 1$ , then the sequence  $\ell(o_1), \ell(o_2), \dots, \ell(o_{a-1})$  dominates the arithmetic sequence of step 2 with first element  $\ell(o_1) \geq 5$  due to Lemma 6 and the fact that  $p(G) - 6 - s_2(o_i) \geq 1$  for  $1 \leq i \leq a - 1$ . Hence  $\sum_{i=1}^{a-1} \ell(o_i) \geq \sum_{i=1}^{a-1} (3 + 2i) = (a - 1)(a + 3)$ . If  $a = 1$  then  $\sum_{i=1}^{a-1} \ell(o_i) = 0 = (a - 1)(a + 3)$ .

Similarly, the sequence  $\ell(o_b), \ell(o_{b+1}), \dots, \ell(o_{k-1})$  dominates the arithmetic sequence of step  $-2$  with last element  $\ell(o_{k-1}) \geq 7$ , hence  $\sum_{i=b}^{k-1} \ell(o_i) \geq \sum_{i=1}^{k-b} (5 + 2i) = (k - b)(k - b + 6)$ .

Note that  $(a - 1) + m + (k - b) = k - 1$ . Summing these inequalities, we obtain

$$\begin{aligned} \sum_{i=1}^{k-1} \ell(o_i) &\geq (a - 1)(a + 3) + m(4m + 7) + (k - b)(k - b + 6) \\ &\geq (a - 1)^2 + 4m^2 + (k - b)(k - b + 2) + 1 \\ &\geq 4k^2/9, \end{aligned}$$

where the lower bound in the last inequality is achieved for  $a - 1 = 4k/9$ ,  $k - b = 4k/9 - 1$  and  $m = k/9$ . Since all the cycles  $o_1, \dots, o_{k-1}$  are strictly outside of  $o_k$ , the claim follows.  $\square$

**Lemma 8.** *Let  $H$  be a fullerene with  $n$  vertices and  $f$  a 5-face of  $H$ . There exist at least five 5-faces distinct from  $f$  whose distance to  $f$  in the dual of  $H$  is at most  $\sqrt{63n/2} + 14$ .*

*Proof.* We define a rooted tree  $T$  with each vertex of  $T$  corresponding to a patch  $G \subseteq H$  such that  $p(G) \neq 0$  and  $p(G) \neq 6$ . Furthermore, we assign a weight  $d(e)$  to each edge  $e$  of  $T$ . The root of  $T$  is the patch  $G_0 = H$  whose boundary is the cycle bounding  $f$ , i.e.,  $p(G_0) = 11$ . Suppose that a patch  $G$  with boundary  $o$  is a vertex of  $T$ . Let us note that  $G$  is neither a worm nor the shell, since  $p(G) > 0$ . The sons of  $G$  in the tree are defined as follows:

- (a) If  $p(G) \in \{1, 7\}$  and  $o$  shares an edge with a 5-face of  $G$ , then  $G$  is a leaf of  $T$ .
- (b) If  $G$  is a normal patch, then  $G$  has a single son  $G'$ , equal to the last element of the maximal uninterrupted peeling starting with  $o$ . The weight of the edge  $e$  joining  $G$  with  $G'$  is equal to the length (number of patches) of the uninterrupted peeling. Note that  $G'$  is not a normal patch.
- (c) If  $G$  has a simplifying cut, then let  $o_1$  and  $o_2$  be the boundaries of the two patches  $G_1$  and  $G_2$  into that it splits  $G$ . Note that  $t(o_1) + t(o_2) < t(o)$ . The patch  $G_i$  (with  $i \in \{1, 2\}$ ) is a son of  $G$  if  $p(G_i) \neq 0$  and  $p(G_i) \neq 6$ . In that case, the edge between  $G$  and  $G_i$  has weight 1. Since  $0 < p(G) < 12$  and  $p(G) \neq 6$ ,  $G$  has at least one son.
- (d) Finally, if  $G$  is indecomposable,  $p(G) \notin \{1, 7\}$  and  $o$  shares an edge with a 5-face  $f'$ , note that there exists an  $\ell$ -chord (with  $\ell \leq 4$ ) splitting off  $f'$  (otherwise  $f'$  would be incident with a chord and a 2-chord and both of them would witness the decomposability of  $G$ ). We let the son  $G'$  of  $G$  with boundary  $o'$  be the patch obtained from  $G$  by removing edges incident to both  $f'$  and  $o$  and by removing isolated vertices. We let the edge of  $T$  between  $G$  and  $G'$  have weight 1.

The *type* of  $G$  is defined according to the rule ((a) to (d)) in that its sons are described.

Observe that at least five 5-faces distinct from  $f$  share edges with boundaries of the patches forming the vertices of  $T$  of type (a) or (d). Indeed, either all 5-faces are reachable in this way, or there are exactly six potentially unreachable 5-faces contained in a single patch that is a leaf of  $T$ , or split off by a simplifying cut from an internal vertex of  $T$ . Let  $T_1$  be a subtree of  $T$  of smallest possible depth that contains five vertices of type (a) or (d). We choose  $T_1$  to be minimal, i.e., all leaves of  $T_1$  are of type (a) or (d).

Consider a vertex  $G_1$  with a son  $G_2$  in  $T_1$ , and let  $o_1$  and  $o_2$  be the boundaries of these patches. If  $G_1$  is of type (b), then  $p(G_1) = p(G_2)$  and  $t(o_1) = t(o_2)$  by Lemma 6. If  $G_1$  is of type (c), then  $p(G_1) \geq p(G_2)$  and  $t(o_1) > t(o_2)$ . If  $G_1$  is of type (d), then  $p(G_1) > p(G_2)$  and  $t(o_1) \geq t(o_2) - 1$ .

Let  $P = p_1 p_2 \dots p_m$  be the path in  $T$  joining the root  $G_0 = p_1$  with a leaf  $G = p_m$  whose boundary is incident with a 5-face  $f'$ . Observe that the distance between  $f$  and  $f'$  in the dual of  $G$  is at most the sum of the weights of the edges of  $P$ , plus 1. Let  $o_0$  and  $o$  be the boundaries of  $G_0$  and  $G$ , respectively. Let  $m_b$ ,  $m_c$  and  $m_d$  be the numbers of vertices of types (b), (c) and (d) in  $P$  distinct from  $G$ , respectively. By the observations in the previous paragraph, we have  $t(o) \leq t(o_0) + m_d - m_c = 5 + m_d - m_c$ . By the choice of  $T_1$ , we have  $m_d \leq 4$ , and since  $t(o)$  is nonnegative,  $m_c \leq 9$ . Therefore,

$$\sum_{p_i \text{ is non-normal}} d(p_i p_{i+1}) \leq m_c + m_d \leq 13.$$

Let  $d_1, d_2, \dots, d_{m_b}$  be the sequence of the weights of all edges  $p_i p_{i+1}$  of  $P$  such that  $p_i$  is a normal patch; by the construction of  $T$ ,  $p_{i+1}$  is not a normal patch in this case, hence  $m_b \leq m_c + m_d + 1 \leq 14$ . Using Lemma 7, we obtain

$$n \geq \frac{4}{9} \sum_{i=1}^{m_b} d_i^2 \geq \frac{4}{9m_b} \left( \sum_{i=1}^{m_b} d_i \right)^2.$$

Therefore, the total weight of these edges is at most  $\sqrt{63n/2}$ , and the distance between  $f$  and  $f'$  is at most  $\sqrt{63n/2} + 14$ .  $\square$

**Lemma 9.** *Every graph  $G$  on 12 vertices with minimum degree 5 such that  $K_{5,7} \not\subseteq G$  has a perfect matching.*

*Proof.* If  $G$  does not have a perfect matching, then there exists a set  $S \subseteq V(G)$  such that  $G - S$  has more than  $|S|$  components of odd size. Consider such a set  $S$ , and observe that  $|S| < 6$ . As  $\delta(G) \geq 5$ , either  $G$  is  $2K_6$  (and thus has a perfect matching) or  $G$  is connected. Therefore,  $|S| \geq 1$ .

If  $|S| < 5$ , then since  $\delta(G) \geq 5$ , no component of  $G - S$  may consist of a single vertex, and hence  $G - S$  has at most three odd components and  $|S| \leq 2$ . Since  $\delta(G) \geq 5$ , each component of  $G - S$  has size at least 4. However,  $G - S$  must have at least two components of odd size, thus it would have exactly two components of size 5. However, then  $|S| = 2$ , which is not smaller than the number of odd components.

Therefore,  $|S| = 5$  and  $G - S$  has at least 6 components of odd size. However, this is possible only if each component of  $G - S$  consists of a single vertex, and hence  $K_{5,7} \subseteq G$ .  $\square$

*Proof of Theorem 3.* Let  $K'_H$  be the subgraph of  $K_H$  consisting of edges with weight at most  $\sqrt{63n/2} + 14$ . By Lemma 8,  $\delta(K'_H) \geq 5$ , and thus  $K'_H$  either has a perfect matching or  $K_{5,7}$  as a subgraph, by Lemma 9. In the former case, the weight of each perfect matching in  $K'_H$  (and thus of the minimum-weight perfect matching in  $K_H$ ) is at most  $6(\sqrt{63n/2} + 14) = \sqrt{1134n} + 84$ . In the latter case, note that the weights in  $K_H$  satisfy the triangle inequality, thus the weight of any edge in  $K_H$  is at most  $2(\sqrt{63n/2} + 14)$ , and we conclude that  $K_H$  has a perfect matching of weight at most  $(5 + 2)(\sqrt{63n/2} + 14) = \sqrt{3087n/2} + 98$ . By Theorem 1,  $b(H) = O(\sqrt{n})$ .  $\square$

The multiplicative constant  $\sqrt{3087/2} \approx 39.29$  is likely to be far from the best possible. Indeed, it can be somewhat improved by a more complicated analysis of our argument (e.g., observing that not all 5-faces can appear in  $T$  on the lowest possible level, indicating that some of the edges of  $K_H$  are much shorter than we estimated). Nevertheless, we could not improve it enough to approach the best known lower bound of  $\sqrt{12/5} \approx 1.549$  of Došlić and Vukičević [2].

## References

- [1] T. Došlić, *Bipartivity of fullerene graphs and fullerene stability*, Chemical Physics Letters **412** (2005), 336–340.
- [2] T. Došlić, D. Vukičević, *Computing the bipartite edge frustration of fullerene graphs*, Discrete Applied Mathematics **155** (2007), 1294–1301.
- [3] M. S. Dresselhaus, G. Dresselhaus, P. C. Eklund, *Science of Fullerenes and Carbon Nanotubes*, Academic Press, New York (1996).
- [4] S. Fajtlowicz, C. E. Larson, *Graph-theoretic independence as a predictor of fullerene stability*, Chemical Physics Letters **377** (2003), 485–490.
- [5] P. W. Fowler, D. E. Manolopoulos, *An Atlas of Fullerenes*, Oxford Univ. Press, Oxford (1995).

- [6] I. Gutman, S. J. Cyvin, *Introduction to the Theory of Benzenoid Hydrocarbons*, Springer-Verlag, Berlin (1989).
- [7] F. Kardoš, D. Král', J. Miškuf, J.-S. Sereni, *Fullerene graphs have exponentially many perfect matchings*, Journal Mathematical Chemistry **46** (2009), 443–447.
- [8] F. Kardoš, R. Škrekovski, *Cyclic edge-cuts in fullerene graphs*, Journal Mathematical Chemistry **22** (2008), 121–132.
- [9] W. Krätschmer, L. D. Lamb, K. Fostiropoulos, D. R. Huffman, *Solid  $C_{60}$ : a new form of carbon*, Nature **347** (1990) 354–358.
- [10] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, R. E. Smalley,  *$C_{60}$  Buckminsterfullerene*, Nature **318** (1985) 162–163.
- [11] J. Malkevitch, *Geometrical and Combinatorial Questions About Fullerenes*, in: P. Hansen, P. Fowler, M. Zheng (Eds.), Discrete Mathematical Chemistry, DIMACS Series in Discrete Mathematics and Theoretical Computer Science **51** (2000) 261–266.
- [12] R. Taylor, J. P. Hare, A. K. Abdul-Sada, H. W. Kroto, *Isolation, separation and characterisation of the fullerenes  $C_{60}$  and  $C_{70}$ : the third form of carbon*, Journal of the Chemical Society, Chemical Communications (1990) 1423–1425.