

# Saturation number of fullerene graphs

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Saturation number of a graph  $G$  is the minimum possible size of a maximal matching in  $G$ . We establish improved upper and lower bounds on the saturation number in fullerene graphs and discuss their sharpness and quality.

**KEY WORDS:** saturation number, maximal matching, fullerene graph, fullerene

## 1. Introduction

Since the very beginning of the chemical graph theory various matching-related concepts and invariants have been used to study the properties of wide classes of chemically interesting compounds. The earliest research in this area was motivated by the observed correlation between the stability of certain aromatic molecules and the number of perfect matchings in the corresponding graphs [9]. This line of research has been vigorously followed over the course of several decades and has led to accumulation of a vast number of results, mostly concerned with enumerating perfect matchings in benzenoids [2, 18], and, more recently, also in fullerene graphs [3, 5, 22]. The non-perfect matchings came in the focus in early 1970s, by introduction of the so-called Hosoya index and Hosoya polynomial, and their subsequent use in investigation of structure-related properties of chemical compounds [13, 19]

In this paper, we are concerned with another matching-related invariant, the saturation number of a graph. Unlike the previously mentioned invariants, this one is not of enumerative, but of a structural nature. We present here improved lower and upper bounds on this quantity in the class of fullerene graphs, and discuss the quality and sharpness of the obtained bounds.

## 2. Mathematical preliminaries

All graphs considered here will be finite, simple, and connected. For all graph-theoretical terms and concepts used, but not defined here, we refer the reader to any of several standard monographs, such as [12, 16, 20].

We consider a graph  $G$  with the vertex set  $V$  and the edge set  $E$ . A set  $I \subseteq V$  is **independent** if no two vertices of  $I$  are adjacent. The largest cardinality of an independent set in  $G$  is called the **independence number** of  $G$  and denoted by  $\alpha(G)$ .

A **matching** in  $G$  is a subset  $M$  of  $E$  such that no two edges of  $M$  have a vertex in common. If every vertex  $v \in V$  is incident with an edge  $e \in M$ , we say that the matching  $M$  is **perfect**.

A subgraph  $H$  of  $G$  is **nice** if the graph that remains after removing from  $G$  the vertices of  $H$  and all edges incident with them still has a perfect matching.

A matching  $M$  of  $G$  is **maximum** if  $|M| \geq |N|$  for any other matching  $N$  in  $G$ . (Here  $|M|$  denotes the **size** of matching  $M$ , i.e., the number of elements in the set  $M$ .) The size of any maximum matching in  $G$  is called the **matching number** of  $G$  and denoted by  $\nu(G)$ . For a graph  $G$  with  $p$  vertices one always has  $\nu(G) \leq p/2$ , and  $\nu(G) = p/2$  if and only if  $G$  has a perfect matching. A maximum matching in a graph  $G$  (and hence also  $\nu(G)$ ) can always be found in a polynomial time [6].

A matching  $M$  in  $G$  is **maximal** if for every  $e \in E \setminus M$ , the set  $M \cup e$  is not a matching. In other words, a matching  $M$  is maximal if it is not a subset of some other matching in  $G$ . Obviously, any maximum matching in  $G$  is also a maximal matching. Hence, the largest number of edges in a maximal matching in  $G$  is  $\nu(G)$ . Much more interesting quantity is the smallest possible number of edges in a maximal matching of  $G$ . This number is called the **saturation number** of  $G$ . We denote it here by  $s(G)$ . Unlike the case of  $\nu(G)$ , the problem of determining  $s(G)$  is NP-hard [21]. This is completely in line with the fact that the theory behind maximal matchings is much less developed than the theory for maximum matchings. As a consequence, the maximal-matching-related problems are less researched and less well understood.

Obviously, the set of vertices not covered by a maximal matching  $M$  in  $G$  must be independent. This gives us an obvious lower bound on the saturation number of  $G$ ,  $s(G) \geq \frac{1}{2}(p - \alpha(G))$ . However, the independence number of a graph is notoriously difficult to compute, and this lower bound is often not very useful.

In a chemical context maximal matchings appear, e.g., when one considers adsorption of dimers (diatomic molecules) on a larger molecule, where each dimer binds to a pair of adjacent atoms in the large molecule. Obviously, any adsorption pattern corresponds to a matching in the graph representing the large molecule, and the situation when no further adsorption is possible since there are no free pairs of adjacent atoms in the large molecule is represented by a maximal matching in the corresponding graph.

### 3. Maximal matchings in fullerene graphs

In this paper, we consider the case when the role of a large molecule is played by a fullerene. A fullerene molecule is modeled by a fullerene graph.

A **fullerene graph** is a planar, 3-regular and 3-connected graph, 12 of whose faces are pentagons, and any remaining faces are hexagons. It is well known that fullerene graphs on  $p$  vertices exist for  $p = 20$  and for all even  $p \geq 24$  [11]. Fullerene graphs without abutting pentagons (the so-called IP-fullerenes) exist for  $p = 60$  and for all even  $p \geq 70$  [14].

Every fullerene graph admits a perfect matching [14], and the lower bounds on the number of perfect matchings have been presented in a number of recent papers [3, 5, 22]. Maximal matchings in fullerenes have been so far considered only briefly in [4], where the following bounds were established.

**Proposition 1** [4]. Let  $G$  be a fullerene graph on  $p$  vertices. Then

$$\left\lceil \frac{p}{4} + 1 \right\rceil \leq s(G) \leq \frac{p}{2} - 2.$$

The only property of fullerene graphs used to establish the bounds of proposition 1 was their 2-extendibility. (A graph  $G$  on  $p \geq 2(n + 1)$  vertices is  $n$ -extendable if it contains a set of  $n$ -independent edges and if any such set can be extended to a perfect matching in  $G$ .) The lower bound follows directly from theorem 4.3 of Ref. [17], while the upper one was derived considering certain nice subgraphs of fullerene graphs. It turns out that using another property of fullerene graphs, their 3-regularity, yields a better lower bound on  $s(G)$ . We will need the following result.

**Proposition 2** [24]. Let  $G$  be a  $d$ -regular graph. Then the size of any maximal matching in  $G$  is at most  $\left(2 - \frac{1}{d}\right) s(G)$ .

Our first main result now follows immediately.

**Theorem 3.** Let  $G$  be a fullerene graph on  $p$  vertices. Then  $s(G) \geq \frac{3p}{10}$ .

*Proof.* Every fullerene graph contains a perfect matching, i.e., a matching of size  $p/2$ . As any perfect matching is also maximal, from proposition 2 one has  $\frac{p}{2} \leq \frac{5}{3}s(G)$ , and the claim follows.  $\square$

The lower bound of theorem 3 is considerably better than the one from proposition 1, but again, it relies only on one particular property of fullerene graphs, their 3-regularity. It would be natural to expect that the quality of this lower bound will not be particularly high. However, the following result shows that the

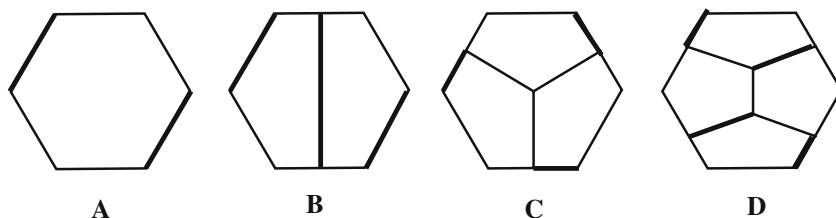


Figure 1. Maximal matchings in Grünbaum–Motzkin caps.

regularity of fullerene graphs in fact provides quite good lower bound, and is much more important for their saturation number than the 2-extendibility.

**Theorem 4.** For each even integer  $p \geq 24$  there is a fullerene graph  $G$  on  $p$  vertices such that  $s(G) \leq \lceil p/3 \rceil$ .

*Proof.* Let  $p \geq 24$  be an even integer. Then  $p$  is of the form  $p = 12(m + 1) + k$ , where  $k = 0, 2, 4, 6, 8, 10$ . Grünbaum and Motzkin showed [11] that it is always possible to construct a fullerene on  $p$  vertices by choosing two of the caps shown in figure 1 and connecting them by a nanotube composed of  $m$  rings (or layers) of 12 vertices. An example of such nanotube is shown in figure 2. The caps are chosen in such way that the total number of vertices in them is congruent to  $p \pmod{12}$ . We denote the number of vertices in cap  $X$  by  $|X|$ , for  $X = A, B, C$ , and  $D$ . Hence,  $|A| = 6$ ,  $|B| = 8$ ,  $|C| = 10$ , and  $|D| = 12$ . Obviously, the edges shown in bold in figure 1 make maximal matchings in the respective caps, and the cardinality of such a maximal matching in the cap  $X$  does not exceed  $\lceil |X|/3 \rceil$ . Now, the bold lines in the segment of the nanotube shown in figure 2 are a maximal matching in that segment, and it is obvious that in a nanotube of  $m$  layers (and hence with  $12m$  vertices) there is a maximal matching with  $4m$  edges. By combining a nanotube and two suitably chosen caps we obtain a fullerene with a given number of vertices, and the union of the exhibited maximal matchings in the nanotube and in the caps is a maximal matching in the whole fullerene graph. As the cardinality of this maximal matching does not exceed  $\lceil p/3 \rceil$ , the claim of the theorem follows.  $\square$

Hence, our lower bound from theorem 3 is of surprisingly good quality, given the fact that it does not use any other property of the fullerene architecture except its 3-regularity. Moreover, it is not very likely that it can be significantly improved. Namely, in a recent paper concerned with small maximal matchings in random graphs [23], the author provides a probabilistic argument that the cardinality of the smallest maximal matching in a random 3-regular graph on  $p$  vertices is at least  $0.315812p$  for almost all such graphs. (We refer the reader to the standard Ref. [1] for the precise meaning of the term “almost all” and for other random-graph-related terminology.) In other words, almost all cubic graphs on

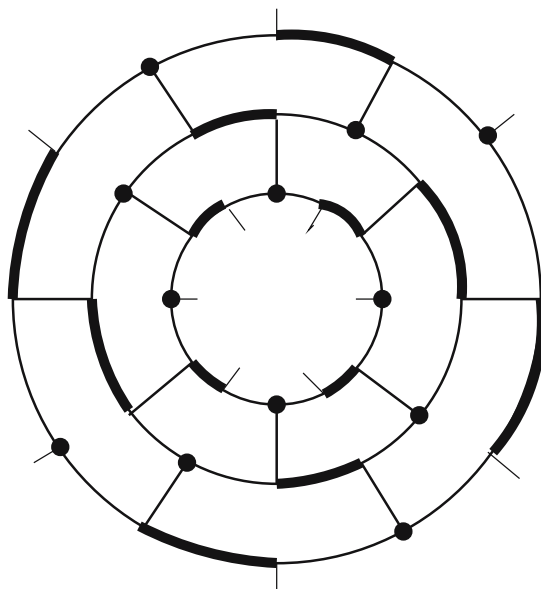


Figure 2. A maximal matching in a nanotube segment.

$p$  vertices have the saturation number at least  $0.315812p$ , and it should be very improbable that a fullerene graph has the saturation number between our lower bound  $0.3p$  and  $0.315812p$ . Improbable as it may be, it turns out that there are at least two fullerene graphs whose saturation number satisfies the lower bound of theorem 3 exactly. One of them is buckminsterfullerene isomer of  $C_{60}$ , the other one is the dodecahedron  $C_{20}$ . Both of them are in many ways exceptional –  $C_{20}$  is the smallest (mathematically) possible fullerene, and the only one without hexagons, while buckminsterfullerene is the smallest isomer with isolated pentagons, the most stable, and the most abundant one. Also, both of them possess the highest possible symmetry – their symmetry group is the full icosahedral group  $\mathcal{I}_h$ . We do not know if there are any other, less symmetrical, fullerenes with  $s(G) = 0.3p$ , but we can prove that there are no other such graphs with icosahedral symmetry.

It is well known (see, e.g. [7], pp. 10–21) that an icosahedral fullerene on  $p$  vertices can be constructed using the **Coxeter construction** for each  $p$  satisfying  $p = 20(i^2 + ij + j^2)$ , where  $i$  and  $j$  are integers,  $i \geq j \geq 0$  and  $i > 0$ . Here each distinct pair of Coxeter parameters  $(i, j)$  gives rise to a distinct isomer, and the geometric meaning of the parameters  $i$  and  $j$  is given by the distances between the pentagons in two directions on hexagonal lattice. When  $i = j$  or  $j = 0$ , the fullerene has the full icosahedral symmetry group  $\mathcal{I}_h$ , while for  $0 < j < i$  its symmetry group is the rotational subgroup  $\mathcal{I}$ . All icosahedral fullerenes except the smallest one ( $C_{20}$ , generated by  $i = 1, j = 0$ ) have isolated pentagons.

The independence number of an icosahedral fullerene can be neatly expressed in terms of its Coxeter coordinates. We refer the reader to Graver [10] for the proof of the following result.

**Proposition 5.** [10]. Let  $G$  be an icosahedral fullerene on  $p$  vertices with Coxeter parameters  $(i, j)$ . Then  $\alpha(G) = \frac{p}{2} - (2i + 4j)$ .

Now we can prove that the lower bound of proposition 1 is sharp for only two icosahedral fullerenes.

**Theorem 6.** Let  $G$  be an icosahedral fullerene on  $p$  vertices such that  $s(G) = 0.3p$ . Then  $G$  is either the dodecahedron  $C_{20}$  or buckminsterfullerene  $C_{60}$ .

*Proof.* Let us first consider the case  $i = j$ . Then  $p = 60i^2$  and  $\alpha(G) = \frac{p}{2} - 6i = \frac{p}{2} - \sqrt{\frac{3p}{5}}$ . Then a maximal matching in  $G$  must contain at least  $\frac{1}{2}(p - \alpha(G)) = \frac{p}{4} + \sqrt{\frac{3p}{20}}$  edges. Let us suppose that such a maximal matching exists. From the condition  $\frac{p}{4} + \sqrt{\frac{3p}{20}} \geq \frac{3p}{10}$  it follows  $p \leq 60$ , and our fullerene must be the buckminsterfullerene.

The case  $j = 0$  follows in a similar manner. Here  $p = 20i^2$  and  $\alpha(G) = \frac{p}{2} - \sqrt{\frac{p}{5}}$ . Hence, the minimum cardinality of a maximal matching in  $G$  must be at least  $\frac{p}{4} + \sqrt{\frac{p}{20}}$ . If such a maximal matching exists, the condition  $\frac{p}{4} + \sqrt{\frac{p}{20}} \geq \frac{3p}{10}$  yields  $p \leq 20$ , and  $G$  must be the dodecahedron  $C_{20}$ .

Finally, we consider the general case  $i \neq j, j > 0$ . Then the fullerene has  $20(i^2 + ij + j^2)$  vertices and proposition 5 implies that  $\alpha(G) = 10(i^2 + ij + j^2) - (2i + 4j)$ . Hence, the minimum number of edges in a maximal matching of  $G$  is at least  $5(i^2 + ij + j^2) + i + 2j$ . If there is a maximal matching in  $G$  with this cardinality, the condition  $s(G) \geq \frac{3p}{10}$  yields the inequality  $i + 2j \geq i^2 + ij + j^2$ . By dividing both sides by  $ij$  we obtain

$$\frac{1}{j} + \frac{2}{i} \geq \frac{i}{j} + 1 + \frac{j}{i}.$$

Since the quantity  $\frac{i}{j} + \frac{j}{i}$  is strictly greater than 2 for  $i \neq j$ , the right-hand side of the above inequality is strictly greater than 3. On the other hand, the left-hand side is always strictly less than 3, since the condition  $i > j > 0$  implies  $\frac{1}{i} < 1$ . Hence, the graph  $G$  cannot contain a maximal matching with exactly  $\frac{1}{2}(p - \alpha(G))$  edges, and the lower bound  $s(G) \geq \frac{3p}{10}$  cannot be sharp.  $\square$

Let us now turn our attention to the upper bounds. The upper bound of proposition 1 can be strengthened by exhibiting an independent set of certain cardinality such that all its neighbors are covered by a maximal matching. We prove

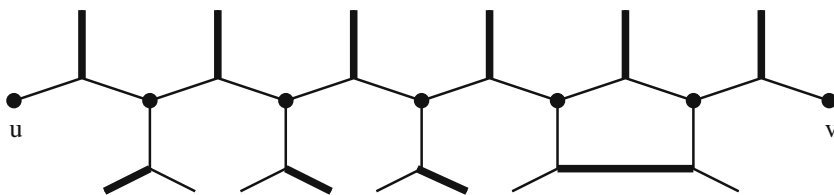


Figure 3. An independent set with  $c \log_2 p$  vertices.

that in a sufficiently large fullerene graph one can always find an independent set with this property whose cardinality grows at least logarithmically with the number of vertices. The key role in our proof is played by the relationship between the number of vertices in a fullerene graph and its diameter, i.e., the maximum distance between two vertices. For the proof of the following result we refer the reader to Friedman and Pratt [8] and to general literature on the degree–diameter problem for planar graphs.

**Lemma 7** [8]. Let  $G$  be a planar graph with maximum degree 3 and a given diameter  $D$ . Then  $G$  has at most  $2^{D+1} - 1$  vertices.  $\square$

Hence, in planar graphs with maximum degree 3 we have the following lower bound on their diameter in terms of number of vertices:

$$D \geq \lceil \log_2(p + 1) - 1 \rceil.$$

Now we can state and prove an upper bound on the saturation number valid for all fullerene graphs.

**Theorem 8.** There exists an absolute constant  $c > 0$  such that  $s(G) \leq \frac{p}{2} - c \log_2 p$ , for any fullerene graph  $G$  on  $p$  vertices.

*Proof.* Let  $G$  be a fullerene graph on  $p$  vertices. Then for its diameter  $D$  we have the following lower bound:

$$D \geq D_0 = \lceil \log_2(p + 1) - 1 \rceil = \lceil \log_2 p \rceil.$$

Let us take two vertices,  $u$  and  $v$ , such that the distance between them is equal to  $D_0$ . On a path  $P$  of length  $D_0$  connecting  $u$  and  $v$  we can take an independent set  $I_0$  of cardinality  $\lceil (D_0 + 2)/2 \rceil$  in the manner shown in figure 3. Let  $M_0$  be a maximal matching in  $G - I_0$  that covers all vertices adjacent to the vertices of  $I_0$ . It is obvious that such a maximal matching always exists, due to the defining properties of fullerene graphs. The cardinality of such a matching cannot exceed  $(p - |I_0|)/2$ . This quantity is roughly of the order of  $\frac{p}{4} - \frac{1}{4} \log_2 p$ . Since  $M_0$  is also a maximal matching in  $G$ , the claim of the theorem follows.  $\square$

The logarithmic correction in the upper bound of theorem 8 is a significant improvement compared with the constant offset of 2 from proposition 1, but it is not very likely that it is the best possible. In [23], the author presents a probabilistic algorithm that yields a maximal matching of the size at most  $0.47563p$  for almost all 3-regular graphs. Hence, it is very likely that for all fullerene graphs their saturation number is bounded from above by  $\gamma p$ , where  $\gamma < 1/2$  is a positive absolute constant. At the present time we are able to prove an upper bound of this type only for the fullerene graphs of sufficiently high symmetry. For the sake of clarity of exposition, we present the details only for the icosahedral fullerenes with Coxeter parameters  $(3m, 0)$ , where  $m \geq 1$ .

**Theorem 9.** Let  $G$  be an icosahedral fullerene on  $p$  vertices with Coxeter parameters  $(3m, 0)$  for some  $m \geq 1$ . Then

$$s(G) \leq \frac{p}{3} + \frac{\sqrt{5}}{10} \sqrt{p} - 36 = \frac{p}{3} + O(\sqrt{p}).$$

*Proof.* An icosahedral fullerene  $G$  with Coxeter parameters  $(3m, 0)$  has  $180m^2$  vertices. The claim of the Theorem will follow if we exhibit a nice independent set of sufficiently large cardinality. We start by noting that  $G$  is composed of 20 triangular patches, such as the one shown in bold in figure 4, and 12 pentagons. Each triangular patch has  $(3m - 1)(3m - 2)/2$  hexagons and  $9m^2 - 3$  vertices. As the patches are vertex disjoint from each other, as well as from the pentagons, our task is reduced to finding a nice independent set in a patch that will contain roughly one-third of its vertices. An example of such independent set is shown by black circles in figure 5. It can be constructed as follows.

First we choose one of two possible perfect matchings of the border cycle of the patch. By doing so, we avoid the problem of assembling patches together, and ensure that the union of independent sets in patches will be an independent set in the whole fullerene. We start by selecting  $3(m - 1)$  independent vertices in the lower-most row of hexagons and proceed toward the top, selecting at each level as many vertices as possible while maintaining nicety of the independent set. It is easy to notice the regularity in decrease of the number of vertices that are selected at each subsequent level: it decreases alternately by 3 and by 0. From there one easily obtains the total number of vertices in the nice independent set in one patch as

$$3(m - 1) + 2 \sum_{j=2}^m (3m - 3j) = 3(m - 1)^2.$$



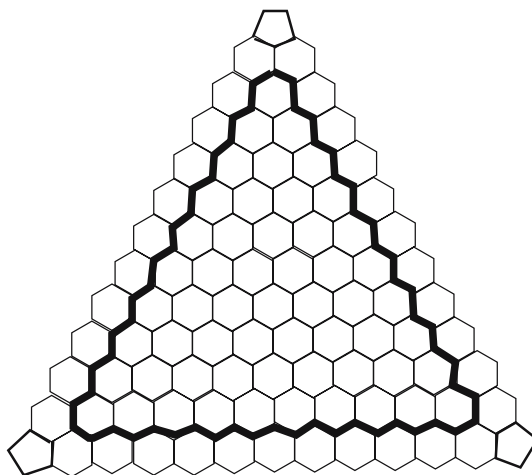


Figure 4. Basic triangular patch in an icosahedral fullerene.

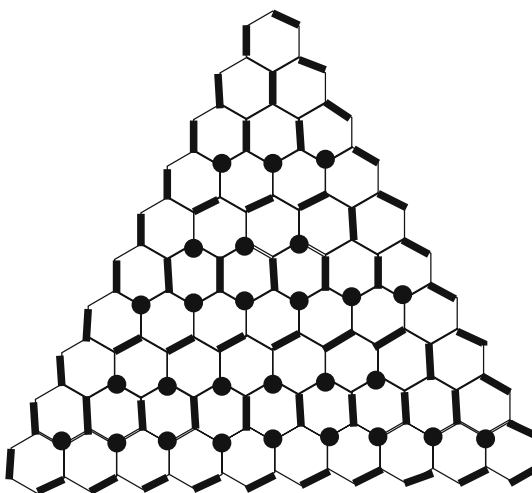


Figure 5. A large independent set and the corresponding maximal matching in a triangular patch.

Hence, each patch contains a maximal matching with  $3(m^2 + m - 1)$  edges. (Such maximal matching is shown in bold in figure 5.) By summing over all 20 patches and adding two edges for each of 12 pentagons, it follows that  $G$  contains a maximal matching with  $60m^2 + 60m - 36$  edges. Hence,  $s(G) \leq 60m^2 + 60m - 36$ , and the claim of the theorem follows by expressing the quantity  $60m^2 + 60m - 36$  in terms of the number of vertices  $p$ .  $\square$

The upper bound of theorem 9 is most likely not the best possible, and it is quite probable that taking into account the edges connecting different patches

would improve it by eliminating the  $\sqrt{p}$  term, but we wanted to keep the derivation as simple as possible.

By a similar argument one could establish linear upper bounds on  $s(G)$  for other icosahedral fullerenes, and also for tetrahedral fullerenes and certain classes of tubular fullerenes with high-enough symmetry, such as  $\mathcal{D}_{ih}$  and  $\mathcal{D}_{id}$ , where  $i = 5$  or  $6$ . However, highly symmetric fullerenes become increasingly rare with the increase of the number of vertices. Hence, we believe that a better insight into the quality of the bounds established in this paper could be obtained by computing the saturation number for all fullerene isomers on a given number of vertices and analyzing the results for the isomers of low symmetry. We are inclined to believe that the saturation number of most, if not all, fullerenes on  $p$  vertices will be close to the value of  $p/3$ . Arguments in support of such guess are provided by Theorems 4 and 9 that deal with extreme fullerene shapes. As for both extreme cases the saturation number is close to  $p/3$ , it is reasonable to expect that for the intermediate shapes the value of  $s(G)$  will not fluctuate much.

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