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Matchings in m-generalized fullerene graphs

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Abstract

A connected planar graph is called m-generalized fullerene if two of its faces are m-gons and all other faces are pentagons and hexagons. In this paper we first determine some structural properties of m-generalized fullerenes and then use them to obtain new results on the enumerative aspects of perfect matchings in such graphs. We provide both upper and lower bounds on the number of perfect matchings in m-generalized fullerene graphs and state exact results in some special cases.

Keywords: Perfect matching, Pfaffian graph, fullerene graph, Hadamard-Fischer inequality.

Math. Subj. Class.: 05C30, 05C70, 15A15

1 Introduction

Classical fullerene graphs have been intensely researched since the discovery of buckminsterfullerene in the fundamental paper [20], which appeared in 1985. This paper gave rise to the whole new area of fullerene science. Most of the research has been driven by a need

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to find a reliable predictor of fullerene stability. It became clear very early that the most stable (i.e., the experimentally observed) isomers all have isolated pentagons (IP). The main focus since has been on the invariants that could further distinguish between the isolated pentagon isomers. Several graph-theoretic invariants have been tested in this capacity and none of them was found completely satisfactory. In the meantime, the experimental evidence appeared indicating that for larger number of atoms some non-IP isomers might be energetically preferable to the IP ones, and even that some non-classical cages (i.e., with faces that are neither pentagons nor hexagons) are favored over the classical ones. Those observations motivated various generalizations of fullerene graphs. One such generalization is the subject of the present study.

A **fullerene graph** is a cubic, planar, 3-connected graph with only pentagonal and hexagonal faces. It follows easily from the Euler's formula that there must be exactly 12 pentagonal faces, while the number of hexagonal faces can be zero or any natural number greater than one. The smallest possible fullerene graph is the dodecahedron on 20 vertices, while the existence of fullerene graphs on an even number of vertices greater than 22 follows from a result by Grünbaum and Motzkin [12] obtained long before the discovery of fullerenes. Analogous results for IP fullerenes was obtained by Klein *et al.* [18].

A connected 3-regular planar graph $G = (V, E)$ is called an **m-generalized fullerene** if exactly two of its faces are m-gons and all other faces are pentagons and/or hexagons. (We also count the outer (unbounded) face of G.) In the rest of the paper we only consider $m \geq 3$; note that for $m = 5, 6$ an m-generalized fullerene graph is a classical fullerene graph. As for the classical fullerenes it is easy to show that the number of pentagons is fixed, while the number of hexagons is not determined. The smallest m-generalized fullerene has $4m$ vertices and no hexagonal faces. Such graphs are sometimes called **m-barrels**. They have two m-gons and $2m$ pentagons and they can be elongated by inserting $k \geq 0$ layers of m hexagons between two half-barrels. The elongated barrels are one of the main subjects of the present paper, since their highly symmetric structure allows for obtaining good bounds and even exact results on the number of perfect matchings in them.

A **matching** M in a graph G is a collection of edges of G such that no two edges of M share a vertex. If every vertex of G is incident to an edge of M, the matching M is called **perfect**. Perfect matchings have played an important role in the chemical graph theory, in particular for benzenoid graphs, where their number correlates with the compound's stability. Although it turned out that for fullerenes they do not have the same role as for benzenoids, there are many results concerning their structural and enumerative properties.

The paper is organized as follows. In the next section we state and prove some structural results about m-generalized fullerene graphs. In particular, we show that the number of hexagons is not necessarily an integer multiple of m. In section 3 we examine the diameter, the hamiltonicity and the leapfrog transformation of the elongated barrels, while in section 4 we obtain the upper bounds on the number of their perfect matchings. In section 5 we refine the results of section 4 by using the transfer matrix method. Finally, in the concluding section we state some conjectures about the entropy of the family of elongated barrels.

2 m-generalized fullerene graphs

In this introductory section we consider some structural properties of m-generalized fullerenes. For the beginning, we show that the number of pentagonal faces must be fixed.

Lemma 2.1. *Let $m \geq 3$ be a non-negative integer different from 5. Then an m-generalized*

fullerene $G = (V, E)$ has exactly $2m$ pentagonal faces.

Proof. Let v, e, f be the number of vertices, edges and faces, respectively, of an m-generalized fullerene G. From the Euler formula, $v - e + f = 2$, and 3-regularity of G we obtain $3v = 2e$. Let p and h denote the number of pentagonal and hexagonal faces, respectively, of G. Since every edge appears in exactly two faces, and every vertex in exactly 3 faces, we have the equality $2e = 2m + 5p + 6h$. By plugging it into Euler formula we obtain

$$\frac{2m + 5p + 6h}{3} - \frac{2m + 5p + 6h}{2} + (2 + p + h) = 2,$$

and hence $p = 2m$. □

The above proof works also for the case $m = 5$, yielding the familiar value of 12 pentagonal faces for classical fullerenes.

It is clear from the definition of elongated barrels that the number of hexagons in such graphs must be divisible by m. Here we show that there are also m-generalized fullerenes in which this is not the case. Take a hemi-dodecahedral cap shown in Fig. 1 left and truncate it at two non-adjacent vertices of the central pentagon. (A hemi-dodecahedral

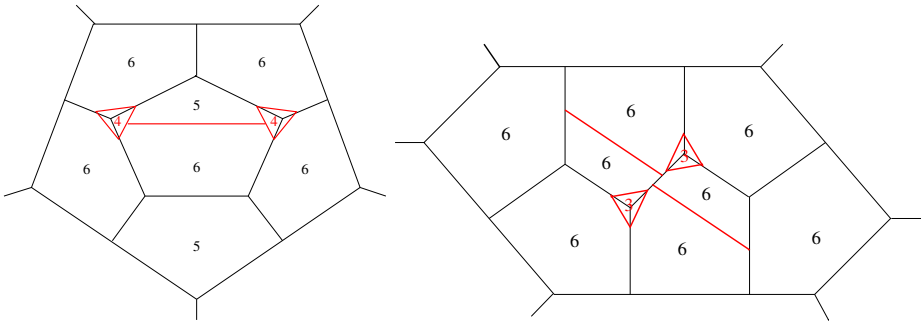

Figure 1: Nanotube caps with the number of hexagons not divisible by m.

cap is a pentagon surrounded by five other pentagons. Without any hexagons, two such caps make a dodecahedron, while by inserting a number of hexagonal layers one obtains a narrow nanotube.) The central pentagon now becomes a heptagon, and four out of five surrounding pentagons become hexagons. Now insert a vertex on both new edges in the heptagon and join them by an edge. The heptagon gives rise to a pentagon and a hexagon. We have obtained a cap with 21 vertices consisting of 2 quadrangles, 2 pentagons and 5 hexagons. We can now construct an infinite sequence of m-generalized fullerenes by taking another hemi-dodecahedral cap and connecting it with our cap using $\ell \neq 4i - 1$ layers of hexagons. The total number of hexagons in such a graph will not be divisible by $m = 4$. Another example, this time of a cap with two triangles and eight hexagons giving rise to an infinite sequence of nanotubes of circumference six, is shown in Fig. 1 right.

Lemma 2.2. *Let $G = (V, E)$ be an m-generalized fullerene with h hexagons. If G has an m-gonal face surrounded by m pentagons, then there exists an m-generalized fullerene G' with $h + m$ hexagons in which one m-gonal face is surrounded by m pentagons.*

Proof. Add additional m vertices in the middle of each edge of the m-gon to make it C_{2m}. Each of the m surrounding pentagons becomes a hexagon. Now connect the new m vertices to a new m-gon. □

So if there exists G satisfying the above lemma, where $h \neq 0$ modulo m, then we can create a sequence of generalized m-fullerene with $h + lm$ hexagons for $l \in \mathbb{N}$.

From a given fullerene graph G its **leapfrog transform** $Le(G)$ is obtained by first taking the dual of G and then truncating it. It is easy to see that $Le(G)$ is again a fullerene graph, with the number of vertices three times that of the original graph. Leapfrog fullerenes have many important properties; in particular, they are always IP, and they are rich in perfect matchings [7, 8]. It follows from the above results that the class of m-generalized fullerenes is also closed under the leapfrog transform.

Lemma 2.3. *The leapfrog of an m-generalized fullerene is again an m-generalized fullerene.*

3 The elongated barrels $F(m, k)$

In this section we describe a special family of m-generalized fullerenes, the elongated barrels, and list their properties. Recall that an **elongated barrel** $F(m, k)$ is obtained from the corresponding barrel by inserting $k \geq 0$ layers (or rings) of m hexagons between two halves of the barrel. For $m = 5$ and $m = 6$ we obtain classical fullerene nanotubes. Most of the nanotube properties are also preserved by elongated barrels. Note that $F(m, k)$ has $n = 2m(k + 2)$ vertices.

Elongated barrels can be neatly represented graphically using a sequence of $k + 3$ concentric circles with monotonically increasing radii such that the innermost and the outermost circle each have m vertices (representing, hence, two m-gons), while all other circles have $2m$ vertices each. An example is shown in Fig. 3. It follows that all elongated barrels are circular graphs in the sense of ref. [5]. (A graph G is **circular** if all its vertices can be placed on a number of concentric circles with increasing radii so that the edges are either arcs of the circles or connect vertices on neighboring circles without intersections between circles. A graph is **semi-circular** if there is a set V_0 of its vertices that cannot be placed on the circles in the above manner; instead, the subgraph induced by V_0 is placed

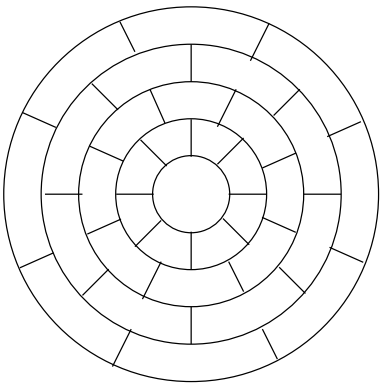

Figure 2: Elongated barrel $F(8, 2)$.

within the innermost circle. Since any connected planar graph without bridges is trivially semi-circular, of interest are graphs for which V_0 is either empty or small.)

Theorem 3.1. *Let $m \geq 3$ and k be non-negative integers. Then the diameter $d(F(m,k))$ of the elongated barrel $F(m,k)$ is given by $d(F(m,k)) = 2k+3$ for large enough k.*

Proof. It is clear that for $k = 0$ the diameter is equal to m and that it is achieved along the circumference. The effect of circumference is still felt for small k; for large k, however, (where large means $k \geq m$), the effect vanishes as the diameter is achieved between two vertices in antipodal caps. So, take a vertex v in one of antipodal m-gons. There are three vertices at distance one from v, one of them already at the first layer of hexagons, the other two in the same m-gon. Two more steps are needed to reach the second layer of hexagons; however, two more steps from other vertices at distance one from v will also advance along the m-gon and along the concentric circle of the first layer of hexagons. It is clear that after some (roughly) $2m$ steps the advances along concentric circles will meet on the opposite side, and from there on, all vertices on the i-th concentric circle will be at the distance of either $2i$ or $2i+1$ from v. The antipodal ring of pentagon is reached after $2k+1$ steps, and additional two steps are needed to reach any vertex in the antipodal m-gon. □

For $m = 5, 6$, i.e., for fullerene nanotubes, the above result is consistent with results of [2, 3].

The problem of hamiltonicity of fullerene graphs had been open for a long time. There were several partial results [17, 19, 21], until this special case of Barnette's conjecture was settled by Kardoš, who provided a computer-assisted proof [15].

Theorem 3.2. *For all natural numbers $m \geq 3$ and k, $F(m,k)$ is Hamiltonian.*

Proof. We construct a Hamiltonian cycle in $F(m,k)$ in the following way. Start from the innermost m-gon. Label its vertices clockwise by $v_{0,1}, \ldots, v_{0,m}$. Connect them by the path $P_0 = v_{01}v_{02}\ldots v_{0,m-1}v_{0,m}$. Each of the end-vertices of this path has exactly one neighbor not in the m-gon. Moreover, those neighbors both lie in the same pentagon and they are not adjacent. Hence, they both lie on C_{2m}. Label the vertices of C_{2m} by

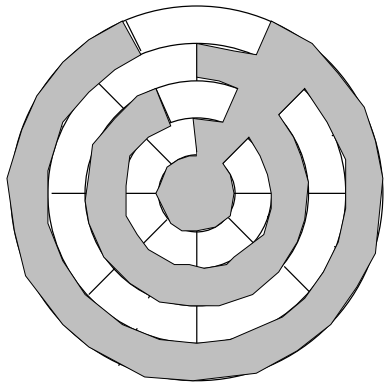

Figure 3: A Hamilton cycle in $F(8,2)$.

$v_{1,1}, \ldots, v_{1,2m-1}, v_{1,2m}$ clockwise so that $v_{1,1}$ is adjacent to $v_{0,1}$ and $v_{1,2m-1}$ is adjacent to $v_{0,m}$. Extend the path on one end by edges $v_{0,m}v_{1,2m-1}$ and $v_{1,2m-1}v_{1,2m}$, and on the

other side by the path $v_{0,1}v_{1,1}v_{1,2}\dots v_{1,2m-2}$ and denote the new path by P_1. Proceed in the same manner toward next concentric circle. After $k+1$ steps the end-vertices of P_{k+1} will be adjacent each to one of two adjacent vertices, $v_{k+2,1}$ and $v_{k+2,m}$, on the outer C_m, and hence, those two edges, together with all edges of the outer C_m except $v_{k+2,m}v_{k+2,1}$, will form a Hamilton cycle when added to P_{k+1}. □

The existence of Hamiltonian cycles has several consequences important for matchings-related properties of elongated barrels.

Corollary 3.3. *$F(m,k)$ has at least three different perfect matchings. Moreover, each edge of $F(m,k)$ is contained in some perfect matching of $F(m,k)$.*

The first claim is obvious – there are two perfect matchings formed by taking every other edge in a Hamiltonian cycle, and the third one formed by the edges that do not participate in it. The second claim of the above corollary says that all elongated barrels are 1-extendable. (A graph G is 1-extendable if each its edge is contained in a perfect matching of G.) This fact gives us a linear lower bound on the number of perfect matchings in $F(m,k)$, but we will derive much better lower bounds later. A bit better linear bounds would also follow for $m \geq 5$ by using the fact that all $F(m,k)$ are also 2-extendable, i.e., that any two independent edges are contained in (and hence can be extended to) a perfect matching. The 2-extendability follows from the fact that for $m \geq 5$ all $F(m,k)$ are cyclically 5-edge connected, i.e., they cannot be separated into two components, each containing a cycle, by deleting fewer than 5 edges [6], and result by Holton and Plummer [14] which claims that a cubic 3-connected planar graph which is cyclically 4-edge connected and has no faces of size 4 is 2-extendable.

Another consequence is 3-edge-colorability of $F(m,k)$. It means that its edges can be partitioned into 3 perfect matchings. As perfect matchings are also known as 1-factors, we have the following result.

Corollary 3.4. *$F(m,k)$ is 1-factorizable.*

An interesting perspective of elongated barrels has been offered by recently introduced concept of **altans**. Let G be a planar graph and S a cyclically ordered set of k vertices of degree 2 incident with its unbounded side. Altan $A(G)$ is obtained by encircling G by C_{2k} and connecting every other vertex of C_{2k} to a vertex of S respecting the cyclical order. The obtained graph can serve itself as input for another round of the altan transform; in that way we obtain iterated altans $A^n(G)$ for $n \geq 0$. The above definition is very informal, but it captures the most important aspects; we refer the reader to [4, 13] for formal definition of altans and exhaustive survey of their properties.

Starting from $G = C_m$ and taking $S = V(C_m)$, the altan transform will result in one half of barrel $F(m,0)$. Further iterations will result in adding successive layers of hexagons, so that $k+1$ iterations will give us $F(m,k)$ without one of its two caps.

An interesting property of altan transform is that it exactly doubles the number of perfect matchings of the starting graph [4].

Theorem 3.5. *Let $\Phi(G)$ denote the number of perfect matchings in G. Then $\Phi(A(G)) = 2\Phi(G)$. Hence, $\Phi(A^n(G)) = 2^n\Phi(G)$.*

The above result gives us an exponential lower bound on the number of perfect matchings in $F(m,k)$ for an even m.

Corollary 3.6. *Let m be even. Then*

$$\Phi F(m,k) \geq 2^{k+3}.$$

It is clear that the above result underestimates $\Phi(F(m,k))$, since it does not take into account perfect matchings containing some (or even all) edges connecting $A^{k+1}(C_m)$ with the other cap. We will later compare this bound with some more precise bounds obtained using transfer matrices. For odd m the above result is of no use, since all iterated altans of C_m have an odd number of vertices for odd m.

It would be interesting to see if similar exponential lower bounds could be established for all m-generalized fullerenes. A similar long-standing open problem for fullerenes was settled recently in [16].

Another consequence of being Hamiltonian is the following upper bound on the number of perfect matchings in $F(m,k)$. It is a direct consequence of Corollary 11 of [5].

Corollary 3.7. *Let $\Phi(F(m,k))$ denote the number of perfect matchings in $F(m,k)$. Then $\Phi(F(m,k)) \leq 8^{n/8}$ for mk even and $\Phi(F(m,k)) \leq \sqrt{3} \cdot 8^{(n-2)/8}$ for mk odd. Here n denotes the number of vertices of $F(m,k)$.*

Since $8^{1/8} \approx 1.29684 < 1.34801 \approx 6^{1/6}$, our result improves the upper bound of $6^{n/6}$ of reference [1].

The last result of this section shows that the property of circularity is preserved under the leapfrog transform for even k and not preserved for odd k.

Theorem 3.8. *The leapfrog transform of $F(m,k)$ is circular if and only if k is even. In that case, the circular structure of $Le(F(m,k))$ is as follows. The first inner circle is C_m, the second circle is C_{3m}, then there are $\frac{3k}{2}+1$ circles C_{4m}, then follows the circle C_{3m}, and the last circle is C_m. If k is odd then $Le(F(m,k))$ is semi-circular and has the following structure. The first circle is C_m, then the next $\frac{3k+3}{2}$ circles are C_{4m}. The next to the last circle is C_{3m}, and the last circle is C_m. Inside the first circle there are m vertices.*

The proof follows along the same lines as for Theorem 15 of [5] and we omit the details.

4 Improved upper bounds on the number of perfect matchings in $F(m,k)$

In this section we use the Hadamard–Fischer inequality to improve the upper bounds on $\Phi(F(m,k))$ from the previous section. To this end, we consider two orientations of C_m. In the first one, all edges are oriented clockwise; in the second one, one edge is oriented anti-clockwise, while all other edges are oriented clockwise. The first orientation we denote by $1 \to 2 \to \ldots \to n \to 1$, the second one by $1 \to 2 \to \ldots \to n, 1 \to n$. Let $T_{n,-}, T_{n,+}$ be the skew symmetric matrices obtained from the first and from the second orientation, respectively. We will need the following result (Lemma 18 of ref. [5]).

Lemma 4.1. *For $n \geq 3$*

$$\begin{cases} \det(I_n - T_{n,+}^2) = \det(I_n - T_{n,-}^2) = ((\frac{1+\sqrt{5}}{2})^n + (\frac{1-\sqrt{5}}{2})^n)^2 & \text{if } n \text{ is odd;} \\ \det(I_n - T_{n,+}^2) = ((\frac{1+\sqrt{5}}{2})^n + (\frac{1-\sqrt{5}}{2})^n + 2)^2 & \text{if } n \text{ is even;} \\ \det(I_n - T_{n,-}^2) = ((\frac{1+\sqrt{5}}{2})^n + (\frac{1-\sqrt{5}}{2})^n - 2)^2 & \text{if } n \text{ is even.} \end{cases}$$

Furthermore, for $n \geq 3$ the odd-indexed subsequence of $(\det(I_n - T^2_{n,+}))^{\frac{1}{n}}$ is increasing, while the even-indexed subsequence is decreasing. Both subsequences converge to $(\frac{1+\sqrt{5}}{2})^2 \approx 2.6180$.

Now we combine the lemma with the Hadamard-Fischer inequality to establish an upper bound on $\Phi(F(m,k))$ better than those of the previous section.

Theorem 4.2. *The number of perfect matchings in $F(m,k)$ is bounded from above by*

$$\begin{cases} \left(\left(\frac{1+\sqrt{5}}{2}\right)^m + \left(\frac{1-\sqrt{5}}{2}\right)^m\right)\left(\left(\frac{1+\sqrt{5}}{2}\right)^{2m} + \left(\frac{1-\sqrt{5}}{2}\right)^{2m} + 2\right)^{\frac{k+1}{2}} & \text{if } m \text{ is odd;} \\ \left(\left(\frac{1+\sqrt{5}}{2}\right)^m + \left(\frac{1-\sqrt{5}}{2}\right)^m + 2\right)\left(\left(\frac{1+\sqrt{5}}{2}\right)^{2m} + \left(\frac{1-\sqrt{5}}{2}\right)^{2m} + 2\right)^{\frac{k+1}{2}} & \text{if } m \text{ is even.} \end{cases}$$

Proof. The proof is along the lines of the proof of Theorem 9 of [5]. We use the Hadamard-Fischer inequality to estimate from above the determinant of $B := -S^2(F(m,k))$, which is equal to $\Phi(F(m,k))^4$. Let $V_i, i \in [k+3]$ be all vertices of $F(m,k)$ on the $i-th$ circle. So V_1 and V_{k+3} have m vertices, while all other V_i have $2m$ vertices. Recall the Hadamard-Fischer inequality

$$\det B \leq \prod_{i \in [k+3]} \det B[V_i].$$

Note that since the path of distance 2 between any two edges on each V_i can be obtained only using the edges on the cycle $F(m,k)(V_i)$, it follows that $B[V_i] = I_{|V_i|} - S(F(m,k+1)(V_i))^2$. Here $S(F(m,k)(V_i))$ is a skew symmetric matrix induced by the Pfaffian orientation of $F(m,k)$ on the cycle $F(m,k)(V_i)$. (See [24] for more on Pfaffian graphs.) The arguments in Section 5 of [5] yield that $\det B(V_i) = \det(I_{|V_i|} - T^2_{|V_i|,+})$. The theorem now follows by applying Lemma 4.1. □

Theorem 4.2 gives better upper bounds than Corollary 3.7. It is only to be expected, since it fully draws on the information stored in the structure of $F(m,k)$, while Corollary 3.7 uses only its hamiltonicity and regularity. While the asymptotic behavior of Corollary 3.7 is of the type $8^{n/8} \approx 1.29684^n$ and does not depend on m, Theorem 4.2 yields the asymptotic $(\varphi^{2m}+2)^{\frac{n}{4m}}$, that is roughly of the order of $\sqrt{\varphi}^n \approx 1.2720^n$ for large m.

5 The transfer matrix method for counting perfect matchings in $F(m,k)$

In this section we provide some explicit formulas and some asymptotics result of the type $\Phi(F(m,k)) \sim C\rho(m)^k$, where $\rho(m)$ is the spectral radius of certain nonnegative irreducible matrix associated with $F(m,k)$. We use the transfer matrix method to count the matchings as in [10].

Consider the cycle C_{2m}. Fix a vertex on C_{2m} and call this vertex 1. View 1 as colored in white. Then color other vertices of C_{2m} black and white so we get a bipartite partition of C_{2m}, where the edges connect white and black vertices. Delete a black neighbor vertex to the left of 1 on C_{2m} to obtain the path P_{2m-1}. Then the vertex i for $i = 2, \ldots, m$ is the white vertex of distance $2(i-1)$ from 1 on P_{2m-1}. The black vertex i on C_{2m} is located to the right of the white vertex i. So the distance between the white vertex 1 and the black vertex $i \in [m-1]$ is $2i-1$ on P_{2m-1}. The distance between the white vertex 1 and the

black vertex m is 1 on C_{2m}. Let $S \subset [m] = \{1, 2, \ldots, m\}$. Then $\alpha(S), \beta(S)$ are the sets of those white vertices and black vertices on C_{2m} whose indices belong to S, respectively.

Let $A(m) = [a_{ST}]$ be the following $2^m \times 2^m$ matrix with nonnegative integer entries. Each S, T is a subset of $[m] = \{1, \ldots, m\}$. (S, T are allowed to be empty.) Then a_{ST} is the number of perfect matchings in the subgraph of C_{2m} obtained by deleting the vertices $\alpha(S) \cup \beta(T)$. We assume that $a_{[m][m]} = 1$.

Lemma 5.1. *Let $m \geq 3$ be an integer, and assume that $A(m) = [a_{ST}]_{S,T \subset [m]}$ is defined as above. Then $a_{ST} = 0$ if $|S| \neq |T|$. In particular, A is a direct sum of $m+1$ submatrices $A_{i,m} = [a_{ST}]_{S,T \subset [m], |S|=|T|=i}$ for $i = 0, \ldots, m$.*

Proof. Let $S, T \subset [m]$. Delete the vertices from $\alpha(S), \beta(T)$ in C_{2m} to obtain the subgraph G. Then G has $m - |S|, m - |T|$ white and black vertices, respectively. To have a perfect matching in G we need the equality $|S| = |T|$. Hence $A(m) = \mathrm{diag}(A_{0,m}, \ldots, A_{m,m})$. □

As an illustration, we construct matrix A for the smallest case $m = 3$. Here by $i \pm 1$ we mean modulo 3. So $3 + 1 = 1$ and $1 - 1 = 3$. Note that $a_{ST} = 0$ if $|S| + |T|$ is odd. Then the following elements of A are nonzero:

$$a_{\emptyset\emptyset} = 2, a_{\{i\}\{i\}} = a_{\{i\}\{i+1\}} = a_{\{i\}\{i+2\}} = a_{\{i,j\}\{i,j\}} = a_{\{i,j\}\{i-1,j-1\}} = a_{[3][3]} = 1.$$

Hence $A(3)$ is an 8×8 matrix whose rows and columns are indexed by the subsets of $[3]$ in the following way: $\emptyset, \{1\}, \{2\}, \{3\}, \{1,2\}, \{1,3\}, \{2,3\}, \{1,2,3\}$.

$$A(3) = \begin{bmatrix} 2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

We can see that $A(3)$ is the direct sum of the following matrices:

$$A_{0,3} = [2],\ A_{1,3} = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix},\ A_{2,3} = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix},\ A_{3,3} = [1].$$

Let now $m \geq 3$ and k be nonnegative integers. In $F(m, k)$ we label each vertex on O_i for $i = 1, \ldots, k + 3$ as follows. Choose a vertex on O_1, which is C_m, and call it vertex 1. Then the right neighbor of i is $i+1$ for $i = 1, \ldots, m-1$. Assume that all m vertices of C_m are colored in black. Now the white vertex indexed i on O_2, which is C_{2m}, is connected to the vertex i in O_1. Now label the black vertices on O_2 as above and connect black vertices in O_2 to white vertices in O_3, which have the same index $i \in [m]$. Continue in the same manner until we color and label all vertices of $F(m, k)$. Note that the color of all vertices on O_{k+3}, which is C_m, is white. Furthermore, the only edges that connect two vertices with the same color in $F(m, k)$ lie on O_1 and O_{k+3}.

Let $\mathbf{x} = (x_S), S \subset [m]$ be the following vector with $0, 1, 2$ coordinates. Consider the cycle C_m, which is either O_1 or O_{k+3}, where the vertices are marked as above. Then x_S is the number of perfect matchings in the subgraph of C_m induced by the set of vertices $[m] \setminus S$.

Theorem 5.2.

$$\Phi(F(m,k)) = \mathbf{x}^\top A(m)^{k+1}\mathbf{x}.$$

Proof. The right-hand side of the above formula can be written as

$$\mathbf{x}^\top A(m)^{k+1}\mathbf{x} = \sum_{S_1,\ldots,S_{k+2}\subset[m]} x_{S_0}x_{S_{k+2}} \prod_{j\in[k]} a_{S_jS_{j+1}}. \tag{5.1}$$

One summand $x_{S_1}x_{S_{k+1}} \prod_{i\in[k]} a_{S_iS_{i+1}}$ counts perfect matchings in which S_1 vertices in C_m are matched with S_1 corresponding white vertices in the adjacent C_{2m}, while the remaining vertices on C_m are matched between themselves. The number of such matchings is x_{S_1}. The black vertices i, where $i \in S_2$, in C_{2m}, are matched with the white vertices next level in C_{2m}, which is the third circle of the circular graph $F(m,k)$. (We assumed for simplicity that $k > 1$.) Continue in this way until the last white vertices in the set S_{k+2} of O_{k+2}, which is C_{2m}, are matched with the black vertices in the set S_{k+1} of O_{k+1}. The set of black vertices on O_{k+2}, denoted by S_{k+2} are connected to the cycle C_m, which is the last circle O_{k+3}. Observe that $a_{S_kS_{k+1}}$ is the number of perfect matchings in the subgraph C_{2m} when we remove the white vertices S_k and the black vertices S_{k+1}. Finally, $x_{S_{k+3}}$ is the number of perfect matchings in the subgraph C_m after removing vertices S_{k+3}. To summarize, the summand $x_{S_1}x_{S_{k+1}} \prod_{i\in[k]} a_{S_iS_{i+1}}$ counts the total number of perfect matchings in $F(m,k)$ where for each $j \in [k+2]$, S_j is the set of white vertices on O_{j+1} which is matched to the black vertices in O_j. □

Now we use the above result to count perfect matchings in $F(m,k)$ for small values of m.

Corollary 5.3. $\Phi(F(3,k)) = 3^{k+2} + 1$.

Proof. Note that $\mathbf{x}$ has 8 coordinates. There are 4 nonzero coordinates. First $x_{[3]} = 1$. This corresponds to the situation where we match all three vertices in C_3 in the circle O_1 to 3 vertices in C_6 in the circle O_2. But then to have a nonzero perfect matching we need to match the remaining 3 vertices on C_6 to 3 vertices in the next level. Continuing in this fashion we deduce that we have only one such perfect matching corresponding to the matching whose edges consist of all edges between different circles. The corresponding summand in the right hand side of formula (5.1) is the contribution of the matrix $A_{3,3} = [1]$ in $A(3)$. The three nonzero coordinates correspond to $x_{\{i\}} = 1$ for $i = 1, 2, 3$. These 3 coordinates correspond to the matrix $A_{1,3}$ in $A(3)$. Clearly $A_{1,3}^k = 3^{k-1}A_{1,3}$. Hence the contribution of all such terms in (5.1) is equal to 3^{k+2}. □

Corollary 5.4.

$$\Phi(F(4,k)) = 2(2+\sqrt{2})^{k+1} + 2(2-\sqrt{2})^{k+1} + 2^{k+3} + 1.$$

Proof. We need to consider only the cases when S has cardinality $0, 2, 4$. If $S_1 = \emptyset$, then $x_{S_1} = 2$. In this case we need to choose $S_1 = \ldots = S_{k+2} = \emptyset$. So we match the edges on the circles $O_1, \ldots, O_{k+3}$. The number of perfect matchings for each even cycle is 2.

Hence the total number of such matchings is 2^{k+3}. Now suppose that $S_1 = [4]$. Then $S_1 = \ldots = S_{k+1}$. So we match only the vertices between the circles $O_1, \ldots, O_{k+3}$. The number of such perfect matchings is 1. Suppose finally that $|S_1| = 2$. So $x_{S_1} = 1$ if and only if the two vertices in S_1 are neighbors. In other words, two vertices in S_1 form an edge in C_4. Let us write down the 6×6 matrix $A_{2,4}$ with rows and columns indexed by 2-element subsets of $[4]$ in the following order: $\{1,2\}, \{1,3\}, \{1,4\}, \{2,3\}, \{2,4\}, \{3,4\}$.

$$A_{2,4} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \end{bmatrix} \tag{5.2}$$

So $A_{2,4}$ is an irreducible matrix with a positive diagonal. Its characteristic polynomial $x^6 - 6x^5 + 14x^4 - 24x^3 + 28x^2 - 24x + 8$ factors as $(x^2 - 4x + 2)(x^2 - 2x + 2)(x^2 + 2)$. It has two real eigenvalues, $2 + \sqrt{2}$ and $2 - \sqrt{2}$, and two pairs of conjugated complex eigenvalues. Hence, $\Phi(F(4,k))$ will be dominated by the $(k+1)$-st power of the spectral radius, $(2 + \sqrt{2})^{k+1}$, with the correction term $(2 - \sqrt{2})^{k+1}$. The claim now follows by adding all contributions. □

Corollary 5.5.

$$\Phi(F(5,k)) = 5^{k+2} + 5\left[\left(\frac{5+\sqrt{5}}{2}\right)^k + \left(\frac{5-\sqrt{5}}{2}\right)^k\right] + 1.$$

Proof. Note that $x_S > 0$ if and only if $|S| = 1, 3, 5$. For $|S| = 5$, i.e. $S = [5]$ we deduce that the number of perfect matchings is 1, which is achieved by matching the adjacent vertices on different circles. This gives us the last term in the right hand side. Consider now the case $|S| = 1$. First choose any vertex on O_1, which is C_5. There are 5 choices. Connect this vertex to a white vertex on O_2, which is C_{10}. Now choose any black vertex on O_2. Delete these two vertices. We obtain one or two paths of even length which have 1 perfect matching. That is, $a_{\{i\},\{j\}} = 1$ for any $i, j \in [5]$. Continuing in this manner we obtain the number of perfect matchings to be 5^{k+2}, the dominant term on the right hand side. The middle term is obtained by considering the eigenvalues of $A_{3,5}$, the 10 by 10 matrix whose row and columns are indexed by lexicographically ordered 3-element subsets of $[5]$.

$$A_{3,5} = \begin{bmatrix} 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 1 \end{bmatrix} \tag{5.3}$$

□

Corollary 5.6.

$$\Phi(F(6,k)) \sim (2(2+\sqrt{3}))^{k+2}.$$

Proof. The dominant term is the power of the spectral radius of $A_{2,6}$, a matrix of order 15 that we omit. □

Results of Corollaries 5.3 and 5.4 are new. Corollary 5.5 is in agreement with results of Sachs, Hansen and Zheng from [23], while Corollary 5.6 agrees with findings in [22].

6 The entropy of the family $F(m,k), k \in \mathbb{N}$

Recall that the graph $F(m,k)$ has $2m(k+2)$ vertices. The **dimer entropy** $h(m)$ of the family $F(m,k)$ is defined as

$$h(m) := \limsup_{k\to\infty} \frac{\log \Phi(F(m,k))}{2m(k+2)}.$$

(See [9–11].) From the previous section we deduce

$$h(m) = \frac{\log \rho(m)}{2m}.$$

Equivalently, it says that the number of perfect matchings in $F(m,k)$ for m fixed and $k \gg 1$ is of order $e^{kh(m)}$.

Empirical results suggest that narrow nanotubes have the largest number of perfect matchings among all fullerene graphs on $10k$ vertices. That motivates us to advance the following conjecture.

Let n be an integer number greater than 11 so that there is a fullerene with $2n$ vertices. Denote by μ_{2n} the maximal number of perfect matchings in all fullerene graphs with $2n$ vertices. Define

$$h_F := \limsup_{n\to\infty} \frac{\log \mu_{2n}}{2n}.$$

We conjecture that $h_F = h(5)$.

Similar claim seems plausible also for m-generalized fullerenes. Fix an integer $m \geq 3, m \neq 5, 6$. Let $\mu_{2m(k+2),m}$ be the maximal number of perfect matchings in all m-generalized fullerene graphs with $2m(k+2)$ vertices. Define

$$h_F(m) := \limsup_{k\to\infty} \frac{\log \mu_{2m(k+2),m}}{2m(k+2)}.$$

We conjecture that $h_F(m) = h(m)$.

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