MATCH
Communications in Mathematical and in Computer Chemistry

no. 50, February 2004
MATCDY (50) 63- 72 (2004)

ISSN 0340 - 6253

Spectral moments of fullerene graphs

Dragoš Cvetković[a], Dragan Stevanović[b]

[a] *Faculty of Electrical Engineering, P.O. Box 35-54, 11120 Belgrade, Serbia and Montenegro*

[b] *Faculty of Science and Mathematics, Višegradska 33, 18000 Niš, Serbia and Montenegro*

(Received July 21, 2003)

Abstract

Let G be a fullerene on n vertices having width w. We prove that the k-th spectral moment of G depends only on n, w and k for $k \leq 2w+6$ and its value is denoted by $W(n, w, k)$. We study the properties of the function $W(n, w, k)$ and derive some bounds for the width w in terms of eigenvalues of G.

0 Introduction

Let G be a simple graph on n vertices with an adjacency matrix A and eigenvalues $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_n$.

The k-th *spectral moment* of G is defined as $S_k = \sum_{i=1}^{n} \lambda_i^k$, and it is equal to the number of all closed walks of length k in G (see [2, 4]). If we know S_0, S_1, ..., S_{n-1}, we can compute eigenvalues λ_1, λ_2, ..., λ_n.

We have $S_0 = n$, $S_1 = 0$, $S_2 = 2m$, $S_3 = 6t$, where m is the number of edges and t the number of triangles of G.

Fullerenes, which are 3-regular planar graphs with faces being only pentagons and hexagons, have attracted much attention in chemical and mathematical literature. From the point of view of spectral graph theory, the most important question regarding fullerene graphs is whether they are characterized by their spectra.

It is studied in [3] to what extent the structure of a fullerene graph can be reconstructed from its eigenvalues and graph angles. It is noted that among fullerene graphs no two with $n \leq 100$ have the same spectrum.

Here we determine some further properties of a fullerene graph using only eigenvalues, i.e., spectral moments, which is a step ahead in resolving the question whether fullerenes are characterized by their spectra.

By above general formulas for spectral moments, for a fullerene graph on n vertices we have $S_0 = n, S_1 = 0, S_2 = 3n, S_3 = 0$. It is known from the literature (c.f., e.g., [6]) that the spectral moments S_k for $k \leq 11$ under some conditions are either constant or depend only on n. Expressions for S_k for a few values of k above 11 under some conditions are known as well.

Using the notion of the *width* of a fullerene graph (see Section 3 for the definition), we are able to extend the formulas for the spectral moments S_k for k much above 11 under additional conditions.

The plan of the paper is as follows. Basic facts from the theory of graph spectra which are relevant for fullerene graphs are summarized in Section 1. Some results, obtained in [3], on hexagonal nets and on pentahex subnets, which will be used later, are presented in Sections 2 and 3, respectively. Finally, our results on spectral moments of fullerene graphs are described in Section 4.

1 Information derived from eigenvalues

Based on the classic knowledge from the spectral graph theory, given the eigenvalues of a fullerene only, we can

- establish that the fullerene graph is connected and regular of degree 3 [2, p. 94],
- determine the girth g ($g = 5$ for fullerene) and the number of circuits of length g (12 for fullerene) [2, p. 95, Theorem 3.26],
- determine the number of circuits of lengths $6, 7, 8$ and 9 [2, p. 97, Theorem 3.27].

From the last item mentioned, we conclude that we can recognize whether the fullerene has *disjoint pentagons*. In the sequel we shall consider only fullerenes with disjoint pentagons.

The distance of the vertex j to the nearest pentagon is called *pentadistance* of a vertex. Let P_s be the set of vertices at the distance s from the nearest pentagon. Let t be the largest pentadistance of a vertex. The vertex set is then partitioned into subsets P_0, P_1, $\ldots$, P_t. Obviously, since the pentagons are disjoint, we have that $|P_0| = 60$.

Let $N_k(j)$ be the number of closed walks of length k starting and terminating at vertex j. The sequences $N_k(j)$ ($j = 1, 2, \ldots, n$) were used in [3] as a basic tool for detecting details of the structure of a fullerene graph.

For any vertex j of the fullerene F we have that

$$N_0(j) = 1, \quad N_1(j) = 0, \quad N_2(j) = 3, \quad N_4(j) = 15.$$

If j is a vertex of a pentagon, then $N_5(j) = 2$ and, otherwise, $N_5(j) = 0$. If we allow pentagons to have common vertices, then $N_5(j)$ is twice the number of pentagons to which the vertex j belongs.

If j does not belong to any pentagon, then we can find its distance to the nearest pentagon. Suppose that the nearest pentagon is at distance s from j. The $(s+2)$-neighborhood of j does not contain odd cycles and it is bipartite, so that $N_{2k+5}(j) = 0$ for $k < s$. The pentadistance of a vertex j is obtained from the eigenvalues and angles as the smallest s for which $N_{2s+5}(j) > 0$.

Of course, the sum of numbers $N_k(j)$ for all vertices j yields the k-th spectral moment S_k. Unfortunately, the numbers $N_k(j)$ cannot be determined from eigenvalues. Nevertheless, we shall use these numbers in our study of spectral moments.

However, the numbers $N_k(j)$ can be calculated provided we know eigenvalues and the angles of the graph [4, pp. 82–83]. This fact was used in [3]. In particular, from the eigenvalues and angles we can obtain the partition $P_0, P_1, \ldots, P_t$ and the numbers $|P_0|, |P_1|, \ldots, |P_t|$ which can tell us a lot about the structure of the fullerene.

2 Coordinates and closed walks in hexagonal nets

The $(s+2)$-neighbourhood of a vertex j at the distance s from the nearest pentagon is isomorphic to a subgraph of the infinite, 3-regular, hexagonal net. In this section we give the number of closed walks starting and terminating at a vertex of such net.

In a geometric representation of the hexagonal net, each edge in the net has the same unit length and one of three directions. Denote the unit vectors having these directions with u, v and w, as done on Fig. 1. Note that there are two kinds of vertices: vectors u, v and w leave the vertices of *the first kind* and enter the vertices of *the second kind*. Note also that edges in the net always connect vertices of different kinds.

All shortest paths from a fixed vertex A to all other vertices may be divided into classes based on the set of vectors they contain:

$$\begin{array}{ll} \{u, v, -w\}, & \{-u, -v, w\}, \\ \{u, -v, w\}, & \{-u, v, -w\}, \\ \{-u, v, w\}, & \{u, -v, -w\}. \end{array}$$

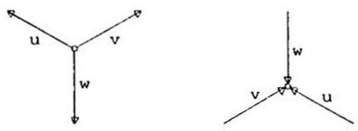

Figure 1: Two kinds of vertices in hexagonal net.

These classes divide the hexagonal net into six hexagonal subnets starting from A, as it is shown in Fig. 2. There are two kinds of hexagonal subnets. We will call the hexagonal subnet having only one edge with an end in A the *hex subnet of the first kind*, while the hexagonal subnet having two edges with ends in A will be called the *hex subnet of the second kind*.

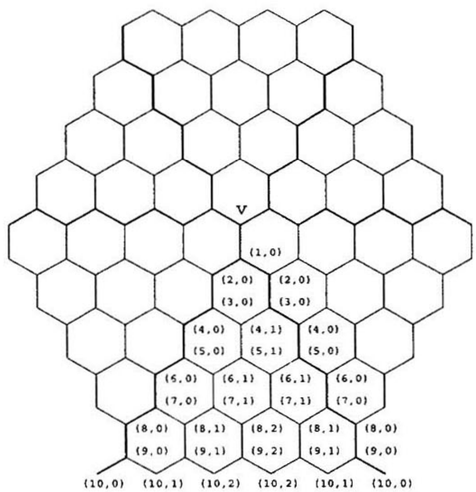

Figure 2: Hexagonal subnets of the hexagonal net.

Suppose A is the vertex of first kind, such that u, v and w leave the vertex A. Consider the vertex B from the hex subnet of the first kind corresponding to the set of vectors $\{-u, -v, w\}$. Let d be the distance between A and B. Let a_x be the number of edges on the shortest path from A to B along the vector $x \in \{-u, -v, w\}$.

Returning to Fig. 2, let us coordinatize the hex subnet: vertex B is uniquely determined by the distance d and $\min\{a_{-u}, a_{-v}\}$. Thus d and $\min\{a_{-u}, a_{-v}\}$ may be viewed as the coordinates of B in this hex subnet. Other hex subnets may be coordinatized in the same manner.

The number of closed walks of given length in hexagonal net is calculated in [3]. Since the graph of this net is bipartite, the number of closed walks of an odd length is equal to 0. Let N_k be the number of closed walks of length k. The following proposition is proved in [3].

Proposition 1 *The number of closed walks of length* $2m$ *starting and terminating at a vertex in the hexagonal net is equal to* $N_{2m} = \sum_{l=0}^{m} \binom{m}{l}^2 \binom{2l}{l}$.

For any vertex j of a fullerene graph we can compare the sequences $N_k(j)$ and N_k. The smallest index k for which $N_k(j) \neq N_k$ indicates the presence of an object strange for hexagonal net in the $\left\lfloor \frac{k}{2} \right\rfloor$-neighborhood of j. In our case, it is of course a pentagon, as pointed out in Section 1. More details can be obtained in a similar way.

3 Penta-hex nets and subnets

We need to study the 3-regular, planar *penta-hexagonal net*, made of the central pentagon p surrounded by infinite number of hexagons, shown in Fig. 3.

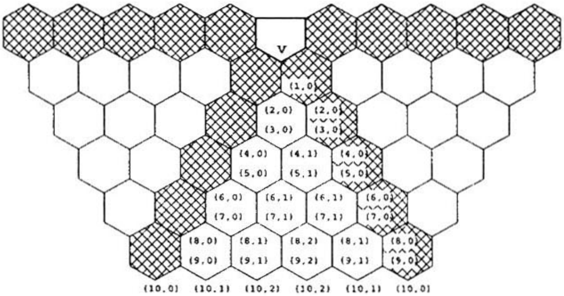

Figure 3: Part of penta-hexagonal net with pentagonal bands and penta-hex subnets.

The infinite sequence of hexagons $h_1, h_2, \ldots$ such that h_1 has a common edge with p, h_{i+1} has a common edge with h_i for $i \in N$ and the centers of pentagon p and all hexagons $h_1, h_2, \ldots$ are collinear is called a *pentagonal band*. The subnets made of hexagons between the two pentagonal bands (for which initial hexagons have a common edge) are called *penta-hex subnets*. There are five pentagonal bands and five penta-hex subnets. Notice that penta-hex subnets are disjoint and contain all vertices of the penta-hexagonal net. A penta-hex subnet is isomorphic to a hexagonal subnet and can be coordinatized in the same manner (cf. Fig. 3). We assume that vertices on pentagons have coordinates $(0,0)$.

The following lemma has been proved in [3].

Lemma 1 *The number of vertices at distance d from the pentagon in a penta-hexagonal net is equal to* $5\left\lfloor \frac{d}{2} \right\rfloor + 5$.

Since there are 12 pentagons in the fullerene, the number of vertices with pentadistance d is equal to $60\left\lfloor \frac{d}{2} \right\rfloor + 60$, in the case that d-neighborhoods of pentagons are disjoint.

Largest k for which $|P_k| = 60\left\lfloor \frac{k}{2} \right\rfloor + 60$ is called the *width* of fullerene F, as defined in [3]. The set of vertices of the pentadistance at most w is called the *regular part* of F, while the remaining vertices form the *irregular part* of F. If w is the width of F then w-neighborhoods of pentagons are clearly reconstructed. In particular, we have the following proposition.

Proposition 2 *The regular part of a fullerene graph with width w contains*

$$n_w = 60\left(\left\lfloor \frac{w}{2} \right\rfloor \left\lceil \frac{w}{2} \right\rceil + w + 1\right)$$

vertices.

Proof. By Lemma 1 we have

$$n_w = 12\sum_{s=0}^{w}\left(5\left\lfloor \frac{s}{2} \right\rfloor + 5\right).$$

Since $\sum_{s=0}^{w}\left\lfloor \frac{s}{2} \right\rfloor = \left\lfloor \frac{w}{2} \right\rfloor \left\lceil \frac{w}{2} \right\rceil$, we are done. ■

Let j be a vertex in a penta-hex subnet with coordinates (s,c). The number $H_k^{(s,c)}$ denotes the number of closed walks of length k in the penta-hexagonal net starting and terminating at j. Obviously, if $k < 2s+5$, then no closed walk of length k can embrace the pentagon and thus,

$$H_k^{(s,c)} = N_k, \quad \text{for } k < 2s+5.$$

In case $k \geq 2s+5$, we do not have an expression for the numbers $H_k^{(s,c)}$, but they can be calculated for given k, s, c using a computer program.

4 Width and spectral moments

Let j be a fixed vertex of F, and let s be its distance from the nearest pentagon, i.e., $j \in P_s$.

If $0 \leq s \leq w$, then let c be its coordinate in the penta-hex subnet of the nearest pentagon. Since j is at distance at least $w+1$ from any other pentagon, then for $k \leq 2w+6$ no closed walk of length k starting from j can embrace any other pentagon of a fullerene and thus, the number $N_k(j)$ is the same as if j is contained in a penta-hexagonal net, i.e., $N_k(j) = H_k^{(s,c)}$ if j has coordinates (s, c).

If $w < s \leq t$, then for $k \leq 2w + 6$, no closed walk of length k starting from j can embrace any pentagon of a fullerene and thus, the number $N_k(j)$ is the same as if j is contained in a hexagonal net, i.e., $N_k(j) = N_k$.

Since the numbers $H_k^{(s,c)}$ and N_k do not depend on the fullerene F, we can form the function $W(n, w, k)$ that is equal to the sum of the corresponding numbers of closed walks of length k, $k \leq 2w + 6$, in any fullerene with n vertices and width w, which can be determined at least by a computer program. Actually, we don't need to know values $H_k^{(s,c)}$ alone, but only their sum across the "layers" of a penta-hexagonal net. This sum might happen to be easier to calculate.

Let $\phi(s)$ be the family of coordinates c of vertices at pentadistance s in the penta-hexagonal net. We introduce the functions

$$\begin{aligned} f(s,k) &= \sum_{j \in P_s} N_k(j) = 12 \sum_{c \in \phi(s)} H_k^{(s,c)}, \\ g(w,k) &= \sum_{s=0}^{w} f(s,k). \end{aligned}$$

Then we can formulate our main result.

Theorem 1 *Let F be a fullerene graph on n vertices and having width w. For $k \leq 2w+6$ the k-th spectral moment of F is equal to*

$$W(n, w, k) = g(w, k) + \left(n - 60\left(\left\lfloor \frac{w}{2} \right\rfloor \left\lceil \frac{w}{2} \right\rceil + w + 1\right)\right) N_k. \quad \blacksquare$$

Although we do not know an explicit expression for $W(n, w, k)$, this function should be considered as known and can be tabulated for any range of values of n, w, k.

Using a sufficiently large finite part of the pentahex net we calculated the numbers $H_k^{(s,c)}$ by means of the package MATLAB. The results are given in Table 1, where in each

k	0	1	2	3	4	5	6	7	8	9	10	11	12
s c													
0 0	1	0	3	0	15	2	91	26	609	260	4325	2390	31965
1 0	1	0	3	0	15	0	93	2	637	38	4611	494	34583
2 0						0	93	0	639	4	4649	94	35067
3 0								0	639	0	4653	4	35165
4 0										0	4653	0	35169
1												0	35169

k	13	14	15	16	17	18
s c						
0 0	21218	243105	185362	1889123	1606848	14928081
1 0	5500	265957	56506	2084135	553868	16574037
2 0	1428	271187	17916	2136065	202352	17065187
3 0	122	272705	2268	2155215	33434	17280723
4 0	6	272829	222	2157525	4804	17314541
1	18	272817	570	2157153	11002	17307553
5 0	0	272835	6	2157753	272	17319553
1	0	272835	18	2157741	690	17319111
6 0			0	2157759	8	17319829
1			0	2157759	48	17319789
7 0					0	17319837
1					0	17319837

k	19	20	21	22	23
s c					
0 0	13879044	119555435	119707390	968041777	1032235820
1 0	5270282	133377007	49169432	1083882175	452520308
2 0	2142368	137885353	21733702	1124475981	214040922
3 0	430862	140146039	5091972	1147108355	56699904
4 0	80092	140576343	1142952	1152110809	14721384
1	168000	140472815	2235898	1150775985	27207542
5 0	6944	140660529	132890	1153313801	2132058
1	15622	140650921	273060	1153152505	4080518
6 0	428	140667621	12518	1153449557	268528
1	2028	140665941	49780	1153408783	931818
7 0	8	140668057	506	1153462473	17030
1	48	140668017	2368	1153460531	66452
8 0	0	140668065	10	1153462985	730
1	0	140668065	100	1153462895	5470
2	0	140668065	200	1153462795	10200
9 0			0	1153462995	10
1			0	1153462995	100
2			0	1153462995	200
10 0					0
1					0
2					0

Table 1: Values of function $H_k^{(s,c)}$ for small s and k.

k	$W(n,w,k)$	k	$W(n,w,k)$
0	n	1	0
2	$3n$	3	0
4	$15n$	5	120
6	$93n - 120$	7	1680
8	$639n - 1920$	9	18360
10	$4653n - 22680$	11	184800
12	$35169n - 240120$	13	1790880
14	$272835n - 2411640$	15	16996800
16	$2157759n - 23510400$	17	159254640
18	$17319837n - 224961960$	19	1479510240
20	$140668065n - 2125759320$		

Table 2: Values of function $W(n,w,k)$ for $k \leq 2w+6$.

of the columns, after the first repetition, the values continue to repeat indefinitely, so that only the first two repetitions are shown.

Using Theorem 1 we obtained from Table 1 the values of $W(n,w,k)$ as given in Table 2. The moments shown here in Table 2 agree with those from [6] for $k \leq 11$. They also agree for $k = 12$ and $k = 13$ if one supposes that $w \geq 1$.

Corollary 1 *Given a non-negative integer k, the k-th spectral moment S_k is constant if k is odd and is a linear function of n if k is even for all fullerene graphs with sufficiently large width.* ■

In fact, Theorem 1 can be extended to higher odd spectral moments.

Theorem 2 *Let F be a fullerene graph on n vertices and having width w. For k odd satisfying $k \leq 4w + 11$ the k-th spectral moment of F is equal to*

$$W(n,w,k) = g(2w+3,k).$$

Sketch of the proof. Closed walks of odd length not greater than $4w+11$ which embrace a pentagon P start and terminate at vertices belonging to the $(2w+3)$-neighbourhood of P. Such a walk cannot embrace any other pentagon and can be considered as a walk within the penta-hex net containing P. Of course, a vertex could be in $(2w+3)$-neighbourhoods of more than just one pentagon. Hence, for $k \leq 4w+11$ we have

$$S_k = 12 \sum_{s=0}^{2w+3} \sum_{c \in \phi(s)} H_k^{(s,c)} = \sum_{s=0}^{2w+3} f(s,k) = g(2w+3,k). \quad ■$$

Theorem 2 explains why values of S_7, S_9 and S_{11} from Table 2 are equal to those from [6]. The fact that S_8 and S_{10} from Table 2 are equal to the values of [6] suggest that Theorem 1 might be valid also for even k greater than $2w+6$ but we were not able to prove that in general.

Theorem 1 can be used to derive an upper bound for the width of a fullerene graph. If we know spectral moments S_k $(k = 0, 1, 2, \ldots)$ of a fullerene graph F, then we can find maximum w such that $S_k = W(n, w, k)$ for $k \leq 2w + 6$. The value w, found in this way, should represent the width of F.

At least we can formulate the following theorem.

Theorem 3 *Let F be a fullerene graph with eigenvalues λ_1, λ_2, $\ldots$, λ_n. Let w_0 be the largest positive integer w such that*

$$\sum_{i=1}^{n} \lambda_i^k = W(n, w, k) \quad (k = 0, 1, \ldots, 2w + 6).$$

Then the width of F is at most w_0. ∎

References

[1] D. Cvetković, *Some comments on the eigenspaces of graphs*, Publ. Inst. Math.(Beograd), 50(64) (1991), 24–32.

[2] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs-Theory and Application*, Deutscher Verlag der Wissenschaften, Berlin, Academic Press, New York, 1980; second edition 1982; Russian edition, Naukova Dumka, Kiev 1984; third edition, Johann Ambrosius Barth Verlag, 1995.

[3] D. Cvetković, P. Fowler, P. Rowlinson, D. Stevanović, *Constructing fullerene graphs from their eigenvalues and angles*, Linear Algebra Appl. 356 (2002), 37–56

[4] D. Cvetković, P. Rowlinson, S. Simić, *Eigenspaces of graphs*, Encyclopedia of Mathematics and Its Appl., Vol. 66, Cambridge University Press, Cambridge, 1997.

[5] P. Fowler, D. Manolopoulos, *An Atlas of Fullerenes*, Clarendon Press, Oxford, 1995.

[6] H. Zhang, K. Balasubramanian, *Analytical Expressions for the Moments and Characteristic Polynomials of Fullerenes Containing Isolated Pentagons*, J. Phys. Chem. 97 (1993), 10341–10345.