Technische Universität Ilmenau
Institut für Mathematik

Preprint No. M 05/07

On Maximum Matchings and Eigenvalues of Benzenoid Graphs

Fajtlowicz, Siemion; John, Peter E.;
Sachs, Horst

Mai 2005

Impressum:
Hrsg.: Leiter des Instituts für Mathematik
Weimarer Straße 25
98693 Ilmenau
Tel.: +49 3677 69 3621
Fax: +49 3677 69 3270
http://www.tu-ilmenau.de/ifm/

ISSN xxxx-xxxx

ilmedia

On Maximum Matchings and Eigenvalues of Benzenoid Graphs

Siemion Fajtlowicz [a], Peter E. John [b], and Horst Sachs [b]

[a] *Department of Mathematics, University of Houston, Texas 77204, U.S.A.*
E-mail: math0@bayou.uh.edu

[b] *Department of Mathematics, Ilmenau Technical University,*
98684 Ilmenau, Germany
E-mail: Peter.John@tu-ilmenau.de, Horst.Sachs@tu-ilmenau.de

Dedicated to Professor Edward C. Kirby on the occasion of his 70th birthday

Abstract: In August 2003 the computer program GRAFFITI made conjecture 1001 stating that for any benzenoid graph, the size of a maximum matching equals the number of positive eigenvalues. Later, the authors learned that this conjecture was already known in 1982 to I. Gutman (Kragujevac). Here we present a proof of this conjecture and of a related theorem. The results are of some relevance in the theory of (unsaturated) polycyclic hydrocarbons.

Key words: benzenoid graph, characteristic polynomial and spectrum of graphs,
hexagonal systems, Hückel-MO-Theory, resonance theory

1 Introduction

1.1 The results

All graphs G considered in this paper are undirected and finite, loops and multiple edges do not occur. The number of vertices of G is denoted by n.

Two vertices are *adjacent* iff they are connected by an edge; two edges are *adjacent* iff they have an end vertex in common.

A set of vertices, or edges, is called *independent* (or *stable*) iff its elements are pairwise nonadjacent.

a is the maximum number of pairwise nonadjacent vertices of G, often called the *vertex independence* (or *vertex stability*) *number* of G.

b is the maximum number of pairwise nonadjacent edges of G, often called the *edge independence* (or *edge stability*) *number* of G.

p and n are the numbers of **p**ositive and **n**egative eigenvalues of G, respectively (eigenvalues are counted regarding their multiplicities; for precise definitions see Section 1.2).

z is the multiplicity of the eigenvalue **z**ero of G. In a chemical context, this number is often denoted by h, and it is considered an indicator of instability of benzenoid molecules.

In general, there are no relations between b and p: b may be larger than, equal to, or smaller than p (see Section 1.4, Table 1 and Figure 4). However, the situation changes if G is restricted to the class of bipartite graphs, and even more so if G belongs to the subclass of hexagonal systems (benzenoid graphs). The aim of this paper is to prove the following propositions.

Theorem 1.

(i) *The number of positive (negative) eigenvalues of a bipartite graph B is not greater than the maximum number of pairwise nonadjacent edges contained in B, briefly:*

$$p(B) = n(B) \le b(B).$$

(ii) *For a hexagonal system H,* $p(H) = n(H) = b(H).$

For bipartite graphs the number n of negative eigenvalues equals the number p of positive eigenvalues, see Section 2, Theorem A, Observation 2.

Theorem 2.

(i') *The minimum of the numbers of nonnegative eigenvalues and of nonpositive eigenvalues of any graph G is not smaller than the maximum number of pairwise nonadjacent vertices contained in G; briefly:*

$$\min\{p(G), n(G)\} + z(G) \ge a(G).$$

(ii') *For a hexagonal system H,* $p(H) + z(H) = n(H) + z(H) = a(H).$

Part (i') of Theorem 2 is Cvetkovic' theorem[1] (see also *Inequalities obtained on the basis of the spectrum of the graph*[2] and the monograph *Spectra of graphs*[3], Theorem 3.14) who proved it in 1971 using Cauchy's interlacing theorem.

Corollary to Theorems 1 and 2.

(i'') *For a bipartite graph B,* $z(B) \ge a(B) - b(B)$.

(ii'') *For a hexagonal system H,* $z(H) = a(H) - b(H)$.

Part (ii) of Theorem 1 is of some significance for the chemistry of polycyclic hydrocarbons: b is a (structural) parameter of Kekulé's model (resonance theory) counting double bonds whereas p is an (analytical) parameter of Hückel's model (simple molecular orbital theory) counting bonding energy levels of delocalized electrons. Thus the equation $b = p$ once more confirms the close relationship between these two models.

For the discussion of some of I. Gutman's work that is closely related to our investigations see Section 5.

1.2 Some more definitions

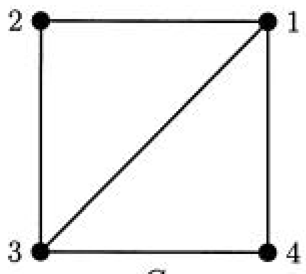
Let G be a graph with vertex set $\{v_1, v_2, \ldots, v_n\}$ and let

$$a_{ij} = \begin{cases} 1 & \text{if } v_i \text{ and } v_j \text{ are adjacent} \\ 0 & \text{otherwise.} \end{cases}$$

1.2.1 The matrix $A = A(G) = (a_{ij})$ is the *adjacency matrix* of G.

If every vertex of graph G' is also a vertex of G, and if two vertices of G' are adjacent in G' if and only if they are adjacent in G, then G' is an *induced subgraph* of G. Note that the adjacency matrix A' of G' is a principal minor of the adjacency matrix A of G; conversely, every principal minor A^* of A determines an induced subgraph G^* of G.

The *characteristic polynomial* $f_G(x)$ of G is the characteristic polynomial of the adjacency matrix of G: $f_G(x) = \det(xI - A)$ (Fig.1). Analogously we define the *eigenvalues* and the *spectrum* of G.



G

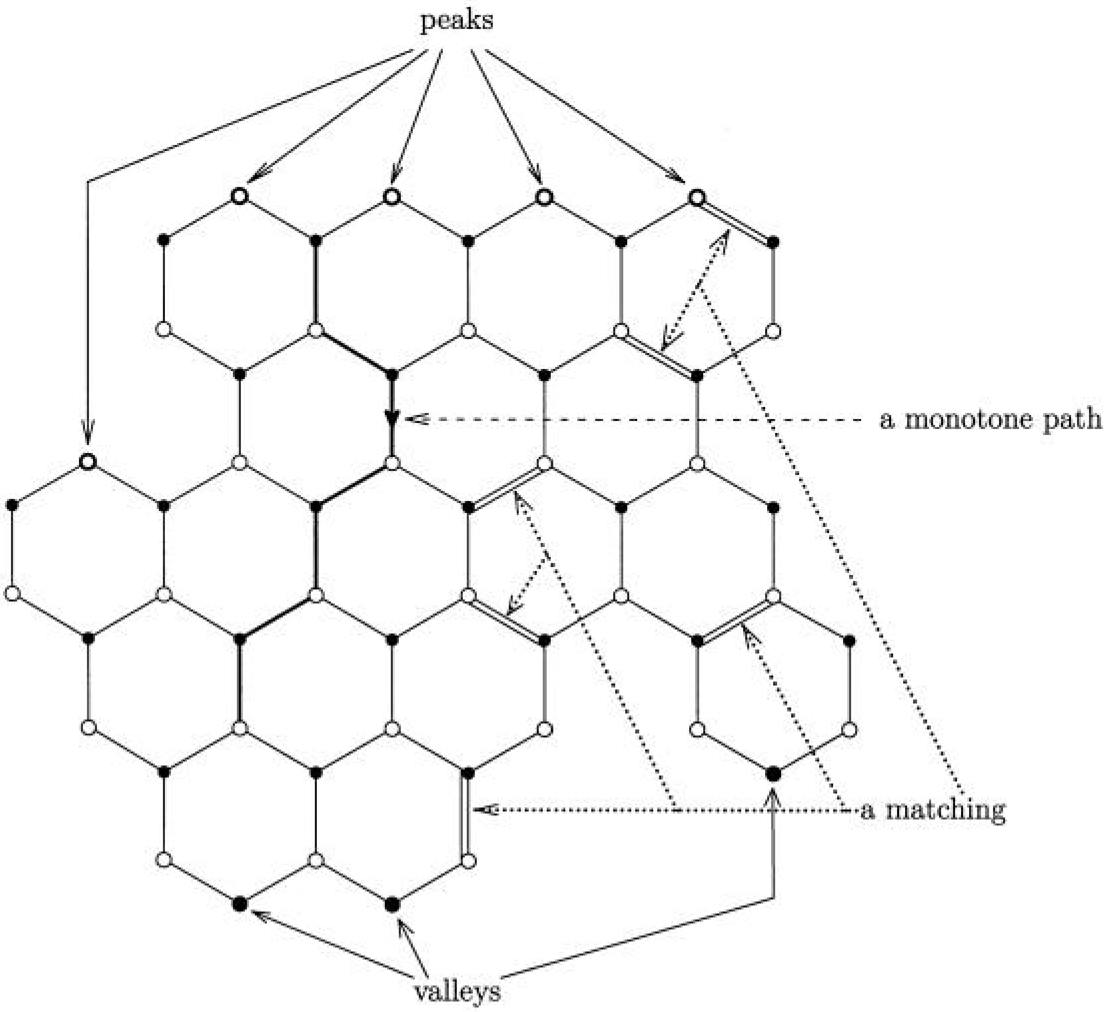
$$A = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \end{pmatrix}$$

$$f_G(x) = \det(xI - A) = x^4 - 5x^2 - 4x.$$

Figure 1: Graph G with adjacency matrix A and characteristic polynomial $f_G(x)$

1.2.2 A *dumbbell* consists of two distinct vertices and an edge joining them. A *matching* is a set of pairwise disjoint dumbbells, its *size* is the number of dumbbells (or edges) it contains. A vertex v is *covered* by matching M iff v belongs to some dumbbell of M (Fig. 2). A matching of G is *perfect* iff it covers all vertices of G.

The size of a maximum matching of G is often called the *matching number* and denoted by $m = m(G)$; note that $m(G) = b(G)$. For a comprehensive monograph on matching theory the reader is referred to the work of L. Lovász and M.D. Plummer[4] (1986).



A hexagonal system

Figure 2

1.2.3 A *hexagonal system* (also called *polyhex*, *honeycomb*, *benzenoid graph*, …) is a finite connected plane graph *H* that can be drawn such that

- all of its finite faces are regular hexagons of equal size,
- its boundary (that is the boundary of the infinite face) is a topological circuit (Fig. 2).

Note that a hexagonal system is 2-connected, every vertex on its boundary has valency 2 or 3, every interior vertex has valency 3.

In addition, we shall assume that some of the edges are perpendicular to a given straight line which is considered horizontal: with respect to this picture, we will freely use the concepts "up", “down”; “high”, “low”; “top”, “bottom”; etc. . A monotone path is always considered decreasing, i.e. running down, from top to bottom (Fig. 2). As each hexagonal system is bipartite, we will assume its vertices to be coloured black and white such that every edge connects a black vertex with a white one and, in addition, that the highest vertices of all finite faces are white (and the lowest are

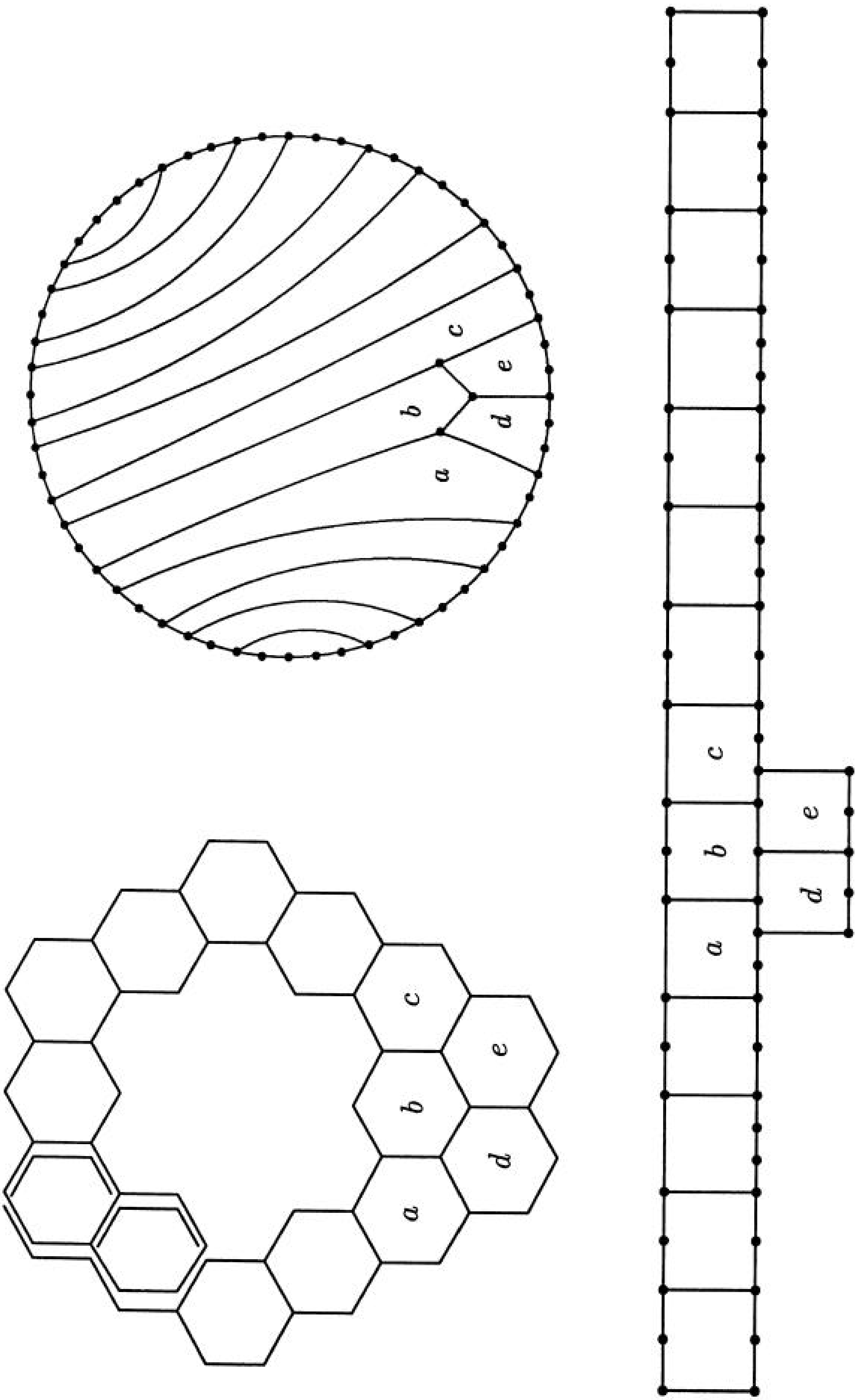


Figure 3: The graph of a helicene and two of its (topologically equivalent) plane representations

black). The locally highest [lowest] vertices of the graph H are called its *peaks* [*valleys*]; the peaks and valleys are the *extremal vertices* of H (Fig. 2).

A slightly more general concept is that of a *topological hexagonal system*: this is a finite two-connected plane graph whose finite faces are (topological) hexagons, whose vertices on the boundary circuit C of the infinite face have valencies 2 or 3, and whose vertices in the interior of C have valency 3. Such a graph can always be drawn on a suitably chosen Riemann surface such that the finite faces are realized by regular plane (schlicht) hexagons of equal size. A topological hexagonal system that cannot be realized this way in the plane (without overlapping) has sometimes been called a *helicene* graph (Fig. 3).

1.3 A remark on possible extensions

Part (ii) of Theorem 1 can easily be extended to a larger class of bipartite plane graphs including, in particular, the class of helicene graphs. However, for the sake of simplicity, we shall here restrict our considerations to the class of hexagonal systems as defined above.

1.4 Some simple examples

1) The spectrum of a circuit on n vertices consists of the numbers $2\cos\left(2p\cdot n/n\right)$, $n = 1,2,\ldots,n$, (Spectra of Graphs[3], p.72). For circuits the numbers $m = b$ and p can be taken from Table 1.

n	$a = b = m$	p
$4k$	$2k$	$2k-1$
$4k+1$	$2k$	$2k+1$
$4k+2$	$2k+1$	$2k+1$
$4k+3$	$2k+1$	$2k+1$

Table 1

2) The graphs of Fig. 4 both have $p = 3$, $b = m = 4$.

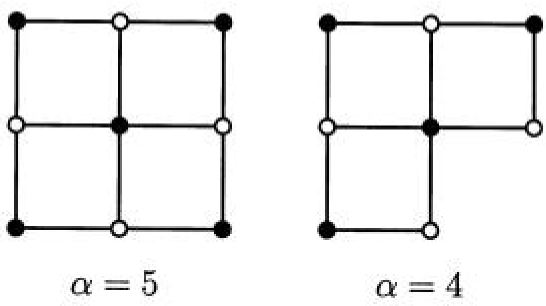


Figure 4

2 Preparation of the Proofs

We recall some known results and formulate a Lemma.

Theorem A lists some well-known general properties of bipartite graphs (see, e.g., *Spectra of Graphs*[3], p.87).

Theorem A. *Let B denote a bipartite graph on n vertices.*

Observation 1.

$$\begin{aligned} f_B(x) &= x^n + a_1 x^{n-1} + \cdots + a_n \\ &= x^n - b_2 x^{n-2} + b_4 x^{n-4} - + \cdots \end{aligned}$$

where $a_1 = a_3 = a_5 = \cdots = 0$ *and* $b_{2i} = (-1)^i a_{2i} \geq 0 \quad \left(i = 1,2,\ldots,\left\lfloor \frac{n}{2} \right\rfloor \right)$.

Observation 2. *The collection of eigenvalues of B, which are all real, is symmetric with respect to the zero point of the real axis.*

Observation 3. If $n = 2k$ then

$$\begin{aligned} a_n &= (-1)^k b_n = f_B(0) \\ &= \det A(B) = (-1)^k \left(\prod l\right)^2 \end{aligned}$$

where the product is taken over all non-negative eigenvalues of B.

The following theorem is a special case of a result obtained by D.M. Cvetkovic, I. Gutman and N. Trinajstic in 1974 (*Graph theory and molecular orbitals, VII. The role of resonance structures*[5]; see *Spectra of Graphs*[3], Theorem 8.13 on page 243; see also H. Sachs[6]); it also follows from a general theorem due to P.W. Kasteleyn (*Dimer statistics and phase transition*[7] (1963)); see also Kasteleyn's survey article[8] (1967). Orginally formulated for connected graphs, the theorem immediately extends to non-connected graphs, too.

Theorem B. *Let G be a plane graph on n vertices all of whose finite faces are hexagons. Then G is bipartite and the number of perfect matchings of G is equal to the product of all non-negative eigenvalues of G.*

Corollary. *If G has a perfect matching then*

$$m(G) = p(G) = \frac{n}{2}.$$

For the next theorem (the "coefficients theorem", H. Sachs[9] and L. Spialter[10] (1964); see *Spectra of Graphs*[3], Theorem 1.3 on page 32) we need another concept.

A *basic figure U* of a graph is a (not necessarily induced) subgraph that has only circuits and dumbbells as its components (Fig. 5). Let $q(U)$ and $c(U)$ denote the number of components of U, and the number of circuits among these components, respectively.

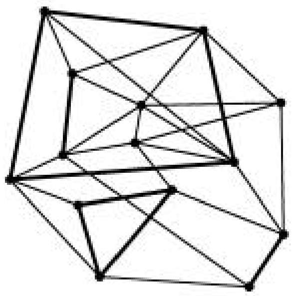


Figure 5: A graph G with one of its basic figures U where $q(U) = 4$, $c(U) = 2$.

Theorem C. *Let G be an arbitrary graph with characteristic polynomial*

$$f_G(x) = x^n + c_1 x^{n-1} + \cdots + c_n .$$

Then

$$c_i = \sum (-1)^{q(U)} 2^{c(U)} ,\ i = 1,2,\ldots,n$$

where the sum is taken over all basic figures U of G on precisely i vertices.

A set *R* of vertices of a graph *G represents* the edges of *G* iff, for every edge of *G*, at least one of its end vertices is contained in *R*.

In 1931 in his paper[11] *Graphs and Matrices* (Hungarian) D. König proved the following famous theorem (Theorem 14 in chapter XIV of the first monograph on graph theory (D. König[12], 1936)).

Theorem D. *In any bipartite graph B, the maximum number of pairwise nonadjacent edges,* b (*i.e. the size of a maximum matching, m*) *equals the minimum number of vertices representing the edges of* B.

We use Theorem D to prove the following well-known proposition.

Theorem E. *For any bipartite graph* B, $a(B) + b(B) = n(B)$.

Proof. Claim I: $a + b \le n$.

Proof of Claim I. Let S be a maximum independent vertex set. Then $|S| = a$, and the $n - a$ vertices not in S represent all edges of B, for an edge not so represented would have to have both of its end vertices in S - a contradiction. By Theorem D, $n - a \ge b$, thus $a + b \le n$.

Claim II: $a + b \ge n$.

Proof of Claim II. By theorem D, there is a vertex set R with $|R| = b$ representing all edges of B. The $n - b$ vertices not in R are pairwise nonadjacent for otherwise there were an edge not represented by some vertex of R. Therefore, $n - b \leq a$, thus $a + b \geq n$. $\square$

Remark. The ideas of the above proof may also be used to derive Theorem D from Theorem E. Thus König's theorem and Theorem E are equivalent.

The proof of the following lemma (which is crucial) is left to the reader (see Fig. 6).

Lemma. *Let H be a hexagonal system and let M denote a maximum matching of H. Colour all edges of H that belong to M red and the remaining edges blue; accentuate the red oblique edges and the blue perpendicular edges. Then the accentuated edges display a system* $\mathbf{P}$ *of disjoint monotone paths with the colours red and blue alternating on each path. The top vertex of a path $P \in \mathbf{P}$ is either a (white) peak covered by M and followed by a red edge or a non-extremal black vertex not covered by M and followed by a blue edge, its bottom vertex is either a (black) valley covered by M and preceded by a red edge or a non-extremal white vertex not covered by M and preceded by a blue edge.*

In $\mathbf{P}$ *there is no path connecting two non-extremal non-covered vertices.* (For otherwise an interchange of colours on such a path would result in a matching that has one edge more than M.)

Thus we distinguish between two types of paths P in $\mathbf{P}$:

Type 1. *Both end vertices of P are extremal* (P *connects a peak with a valley*).

Type 2. *Exactly only one end vertex of P is extremal* (Fig. 6a).

In each non-extremal black vertex that is not covered by M there originates, and in each non-extremal white vertex that is not covered by M there terminates, a path of type 2.

3 Proof of Theorem 1

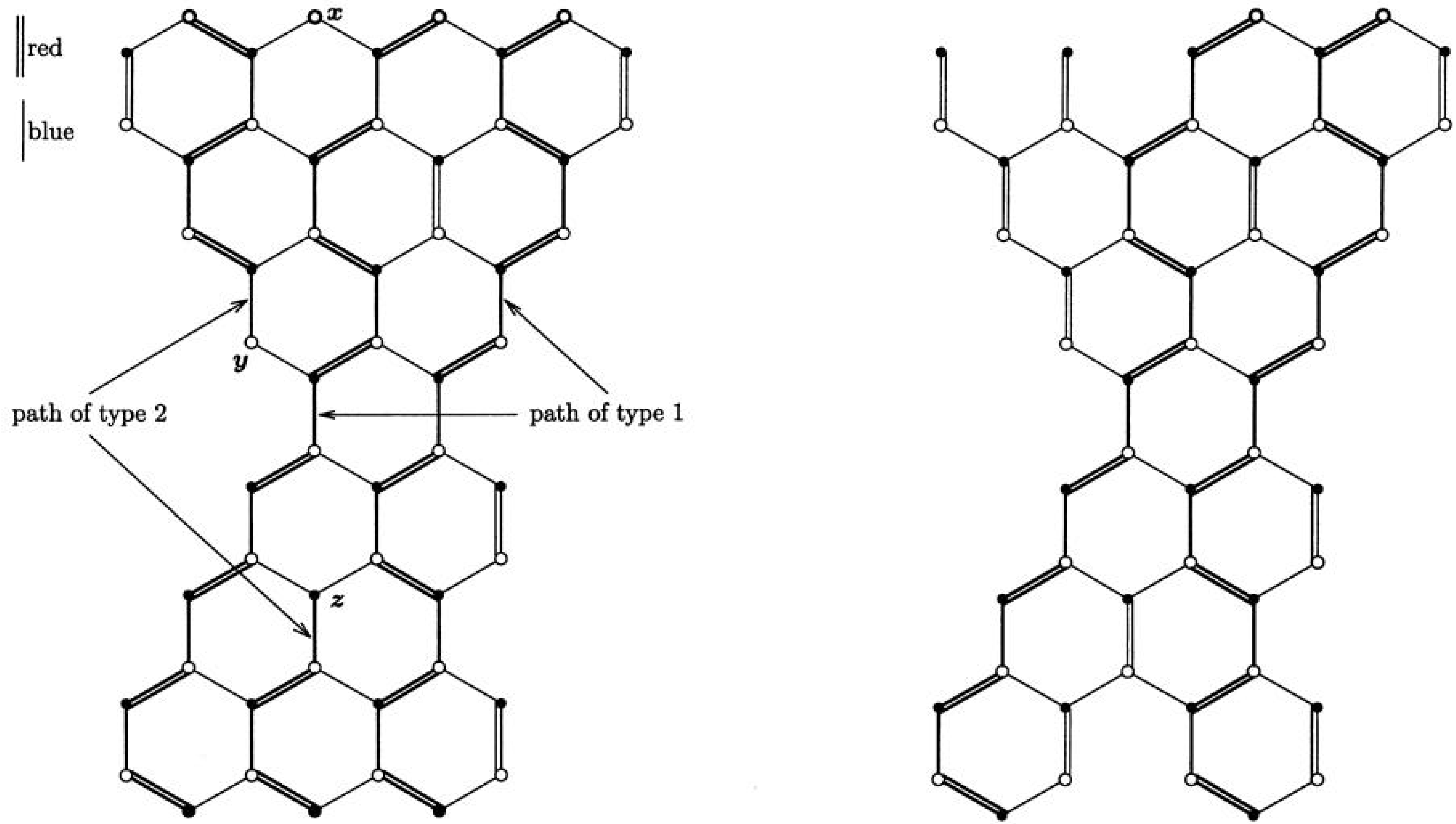
Recall Theorem A, Observations 1 and 2. By Vieta's theorem, a_{2p} is the product of all nonzero eigenvalues of B, and $a_{2i} = 0$ for $i > p$. Thus

$$b_{2p} > 0, \tag{1a}$$

$$b_{2i} = 0 \quad \text{for} \quad i > p \tag{1b}$$

3.1 Proof of Part (*i*)

Let $p = p(B)$, $m = m(B)$; we have to show that $p \leq m$.



a) Hexagonal system H with one of its maximum matchings M (‖).
Vertices x, y, z not covered by M.
$n = 55$, $m = 26$.

b) Induced subgraph H^* of H with perfect matching M^*.
$n^* = 52$, $m^* = m = 26$.

Figure 6

B being bipartite, each component of any basic figure of B is a circuit of even length or a dumbbell, thus any basic figure on $2i$ vertices contains as a subgraph some matching of size i. Consequently, for $i > m$ there is no basic figure on $2i$ vertices in B and therefore, by Theorem C (in connection with Theorem A, Observation 1), $b_{2i} = 0$. Assuming $p > m$ we obtain $b_{2p} = 0$ contradicting (1a).

3.2 Proof of Part (*i i*)

Let $p = p(H)$, $m = m(H)$. It remains to show that $p \geq m$. Recall Observation 1 of Theorem A. We shall prove that $a_{2m} \neq 0$, thus $b_{2m} \neq 0$ which, by (1b), implies $m \leq p$.

By a well-known theorem of matrix theory, a_{2m} is the sum of the determinants of all principal minors of $A(H)$ of size $2m$; equivalently, in terms of subgraphs,

$$a_{2m} = \sum \det A(H') \tag{2}$$

where the sum is taken over all induced subgraphs H' of H on $2m$ vertices (see 1.2.1).

Recall that $\det A(H')$ is the product of the eigenvalues of H'. Graph H being bipartite, so are the H'. By Theorem A, Observation 2, the nonzero eigenvalues of H' can be arranged in pairs $(m,-m)$ $(m > 0)$, thus the nonzero among the $\det A(H')$ (the terms of the sum in equation (2)) all have the same sign (namely, $(-1)^m$). Therefore, in order to show that $a_{2m} \neq 0$, it suffices to show that $\det A(H') \neq 0$ for at least one of the H'.

Consider any maximum matching M of H and colour the edges of H as described in the Lemma (for an example see Fig. 6). Interchange the colours red and blue on all paths of type 2: this results in a new colouring of H where

(*i*) the red edges again determine a maximum matching - M^*, say - of H,

(*ii*) all nonextremal vertices are covered by M^* (all paths in the corresponding set $\mathbf{P}^*$ are of type 1).

Deleting the vertices that are not covered by M^* (these are certain peaks and/or valleys, all lying on the boundary of H) we obtain an induced subgraph H^* of H on $2m$ vertices all of whose finite faces are hexagons; note that M^* is a perfect matching of H^*. By the Corollary to Theorem B, graph H^* has m positive eigenvalues; by Theorem A, Observation 2, zero is not an eigenvalue of H^*. Observation 3 of Theorem A now yields the desired result that $\det A(H^*) \neq 0$. $\square$

Remark. Once having established the existence of H^*, we immediately obtain that not only a_{2m} but all coefficients a_{2i} $(i = 1,2,\ldots,m)$ are different from zero, or, equivalently:

Theorem 3. *For a hexagonal system* H *,*

$$f_H(x) = x^n - b_2 x^{n-2} + b_4 x^{n-4} - + \cdots + (-1)^m b_{2m} x^{n-2m}$$

where $b_2, b_4, \ldots, b_{2m}$ *are positive.*

This in particular implies Theorem 1, Part (*ii*).

4 Proof of Theorem 2

As remarked above, Part (*i'*) is identical with Cvetkovic' theorem.

Part (*ii'*) is an immediate consequence of Part (*ii*) of Theorem 1 and König's theorem in the form of Theorem E: from $n = p = b$ and $n = z + p + n = a + b$ we obtain

$p + z = n + z = n - p = a + b - p = a$. □

5 Remark on a paper of I. Gutman

Already in 1982, in his paper *Characteristic and Matching Polynomials of Benzenoid Hydrocarbons*, I. Gutman[13] formulated a statement (Theorem 4 on page 341) that is equivalent to the following interesting assertion.

(**G1**) *Let* H *be a hexagonal system with characteristic polynomial*

$$f_H(x) = x^n - b_2 x^{n-2} + b_4 x^{n-4} - + \cdots$$

(see Theorem A in Section 2 above)

and let $p(H,k)$ *denote the number of matchings of size* k *contained in* H *. Then*

$p(H,1) = b_2$, $p(H,2) = b_4$,

$p(H,k) < b_{2k}$ for $k = 3,4,\ldots,m$,

$p(H,k) = b_{2k} = 0$ for $k > m$.

Using (*i*) of Theorem 1, (G1) immediately implies

(**G2**) $b_{2k} = 0$ *if and only if* $p(H,k) = 0$.

This is Theorem 3 in Gutman's paper.

Obviously, the last statement is equivalent to our Theorem 3 (Section 3).

Unfortunately, Gutman's proof of his Theorem 4 - and thus of (G1) and (G2) – is incomplete.

6 Miscellaneous remarks

For hexagonal systems, $z = n - p - n = n - 2b = n - 2m$ which means that *for a hexagonal system, the multiplicity of the eigenvalue zero equals the number of vertices left uncovered by a maximum matching.*

Graphs for which equality holds in Cvetcovic' inequalities (Theorem 2, Part (*i'*)) are called *plants* (there are two kinds, helio- and geo-tropic plants, see *Spectra of Graphs*[3] 3rd edition, p. 416) and surprisingly, there are many examples of these objects. They include, for example, all trees, and as we know now, all hexagonal systems.

Concluding remark

The main result of this paper may be summarized as follows.
In any hexagonal system, the edge independence number equals the number of positive eigenvalues, and the vertex independence number equals the number of nonnegative eigenvalues.

Acknowledgements

The authors thank I. Gutman (Kragujevac) for bringing his work to their attention, and Mrs. B. Hamann and Mrs. G. Käppler for their cooperation and technical support.

6 References

1. D.M. Cvetkovic, *Graphs and their spectra (Grafovi i njihovi spectri) (Thesis)*. Univ. Beograd Publ. Elektrotehn. Fak., Ser. Mat. Fiz., No. 354 - No. 356 (1971) 1-50.
2. D.M. Cvetkovic, *Studia Sci. Math. Hung.* **8** (1973) 433-436.
3. D.M. Cvetkovic, M. Doob and H. Sachs, *Spectra of Graphs -Theory and Application.* Deutscher Verlag der Wissenschaften, Berlin 1980, 1982; Academic Press, New York - San Francisco - London 1979; 3rd revised and enlarged edition, Johann Ambrosius Barth Verlag, Heidelberg - Leipzig 1995.
4. L. Lovász and M.D. Plummer, *Matching Theory.* Akadémiai Kiadó, Budapest 1986; North-Holland (Ann. Discr. Math. **29**), Amsterdam 1986.
5. D.M. Cvetkovic, I. Gutman and N. Trinajstic, *J. Chem. Phys.* **61** (1974) 2700-2706.
6. H. Sachs, *On the number of perfect matchings in bipartite plane graphs.* In: *Algebra und Graphentheorie (Beiträge der Jahrestagung „Algebra und Grenzgebiet", Siebenlehn,* 28.10.-1.11.1985), Bergakademie Freiberg, Freiberg 1986.
7. P.W. Kasteleyn, *J. Math. Phys.* **4** (1963) 287-293.
8. P.W. Kasteleyn, *Graph theory and crystal physics*. In: *Graph Theory and Theoretical Physics* (ed. F. Harary), Academic Press, London - New York 1967, pp. 43-110.
9. H. Sachs, *Publ. Math. Debrecen* **11** (1964) 74-84.
10. L. Spialter, *J. Chem. Doc.* **4** (1964) 269-274.
11. D. König, *Mat. és Fiz. Lapok* **38** (1931) 116-119.

12. D. König, *Theorie der endlichen und unendlichen Graphen.* Akademische Verlagsgesellschaft, Leipzig 1936; Chelsea, New York 1950; B.G. Teubner Verlagsgesellschaft, Leipzig 1986. English Translation: Theory of Finite and Infinite Graphs. Birkhäuser, Boston - Basel - Berlin 1989.
13. I. Gutman, *J. Chem. Soc. Faraday Trans.* 2, **79** (1983) 337-345