Bulletin T.CXLI de l'Académie serbe des sciences et des arts − 2010
Classe des Sciences mathématiques et naturelles
Sciences mathématiques, № 35

HYPERENERGETIC GRAPHS AND CYCLOMATIC NUMBER

X. SHEN, Y. HOU, I. GUTMAN, X. HUI

(Presented at the 9th Meeting, held on December 18, 2009)

A b s t r a c t. *Let G be a graph with n vertices and m edges. Then its cyclomatic number is $c = m - n + 1$. If $\lambda_1, \lambda_2, \ldots, \lambda_n$ are the eigenvalues of G, then its energy is $E(G) = \sum_{i=1}^{n} |\lambda_i|$. The graph G is said to be hyperenergetic if $E(G) > E(K_n) = 2n - 2$. It is known [Nikiforov, J. Math. Anal. Appl.* **327** *(2007) 735–738] that almost all graphs are hyperenergetic. We now show that for any $c < \infty$, there is only a finite number of hyperenergetic graphs with cyclomatic number c. In particular, there are no hyperenergetic graphs with $c \leq 8$.*

AMS Mathematics Subject Classification (2000): 05C50
Key Words: energy (of graph), spectrum (of graph), hyperenergetic

1. *Introduction*

Let G be a simple graph with n vertices and m edges. Then the cyclomatic number of G is $c = m - n + 1$. Throughout this paper, without loss of generality, we assume that G is connected. If so, then a graph with $c = 0$ is called a tree. Graphs with $c = 1, 2, 3, 4, \ldots$ are said to be unicyclic, bicyclic, tricyclic, tetracyclic,..., respectively.

Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of the graph G [3, 5]. Then the *energy* of G is defined as

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| \ .$$

Details on the mathematical theory of graph energy can be found in the recent reviews [7, 10, 20]; for the chemical background and applications of E see [8, 12].

Earlier empirical studies (especially those restricted to molecular graphs) showed that the energy can be approximated by [13, 14, 15, 21] or bounded by [2, 21] expressions in which the only variables are n and m, and in which E is a monotonically increasing function of m. This observation lead to the conjecture that the complete graph K_n, possessing the greatest possible number of edges, has maximum energy. The conjecture was found to be false [2]. In [2] it was shown that for $n \leq 7$ the n-vertex graph with maximal energy is K_n. However, for $n \geq 8$ there exist graphs with energy exceeding $2n-2$. Graphs whose energy exceeds the energy of the complete graph, i. e., n-vertex graphs for which $E(G) > E(K_n) = 2n-2$, were named *hyperenergetic graphs* [6].

The first systematic construction of hyperenergetic graphs was discovered by Walikar et al. [27]. After that, hyperenergeticity was verified for numerous classes of graphs [1, 11, 16, 19, 23, 24, 25]. Some other graphs were shown to be not hyperenergetic [9, 26]. Researches along these lines were much slowed down after Nikiforov discovered that almost all graphs are hyperenergetic [22]. In fact, Nikiforov proved a much stronger result:

Theorem 1. [22] *For almost all graphs*

$$\left(\frac{1}{4} + o(1)\right) n^{3/2} < E(G) < \left(\frac{1}{2} + o(1)\right) n^{3/2} \ .$$

2. *Hyperenergetic graphs with fixed cyclomatic number*

Bearing in mind Theorem 1, it is somewhat surprising that the number of hyperenergetic graphs with any fixed value c of the cyclomatic number is limited. Namely, we have:

Theorem 2. *For any value of c, $0 \leq c < \infty$, the number of hyperenergetic graphs with cyclomatic number c is finite.*

In fact, there is an even stronger restriction:

Theorem 3. *No graph with cyclomatic number c and more than c vertices is hyperenergetic.*

P r o o f. The energy of any graph G with n vertices and m edges is bounded from above by [17, 18]

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{m}\right)^2\right]} \,.$$

Therefore, if

$$\frac{2m}{n} + \sqrt{(n-1)\left[2m - \left(\frac{2m}{m}\right)^2\right]} \leq 2n - 2 \tag{1}$$

then the respective graph cannot be hyperenergetic.

Inequality (1) can be transformed into

$$2\,m^2 - m(n-1)(n+4) - 2n(n-1)^2 \geq 0$$

whose solutions are $m \geq n(n-1)/2$ and $m \leq 2(n-1)$. It cannot be $m > n(n-1)/2$, since an n-vertex graph has at most $n(n-1)/2$ edges. Therefore, the graphically feasible solutions of (1) are $m = n(n-1)/2$ and $m \leq 2(n-1)$. The solution $m = n(n-1)/2$ is not interesting, since then $G \cong K_n$. Thus $m \leq 2(n-1)$ i. e., $m < 2n-1$ is a sufficient condition for non-hyperenergeticity of the graph G. Now,

$$m < 2n - 1 \quad \Longleftrightarrow \quad m - n + 1 < n \quad \Longleftrightarrow \quad n > c$$

which implies Theorem 3, which in turn implies Theorem 2. $\square$

3. *Applications to graphs with small cyclomatic number*

Lemma 4. *A graph with cyclomatic number c has at least* $\left\lceil \dfrac{3+\sqrt{1+8c}}{2} \right\rceil$ *vertices.*

P r o o f. The cyclomatic number of the complete graph is $c(K_n) = (n-1)(n-2)/2$, from which

$$n(K_n) = \frac{3 + \sqrt{1 + 8\,c(K_n)}}{2} \ .$$

Lemma 4 follows now from the fact that if $c(K_n) < c \leq c(K_{n+1})$, then the graph with cyclomatic number c must have at least $n(K_{n+1})$ vertices. □

According to Lemma 4, a graph with cyclomatic number 0, 1, 2, 3, 4, 5, and 6 must have at least 1, 3, 4, 4, 5, 5, and 5 vertices, respectively. This implies:

Theorem 5. (a) *There are no hyperenergetic trees.*
(b) *There are no hyperenergetic unicyclic graphs.*
(c) *There are no hyperenergetic bicyclic graphs.*
(d) *There are no hyperenergetic tricyclic graphs.*
(e) *There are no hyperenergetic tetracyclic graphs.*
(f) *There are no hyperenergetic pentacyclic graphs.*
(g) *There are no hyperenergetic hexacyclic graphs.*

P r o o f. According to Theorem 3, in order that a tree, unicyclic, bicyclic, tricyclic, and tetracyclic graph be hyperenergetic, these must have less than 1, 2, 3, 4, and 5 vertices, respectively. By Lemma 4, this is impossible. This proves (a), (b), (c), (d), and (e).

By Theorem 3, in order that a pentacyclic graph be hyperenergetic, it must have less than 6 vertices. By Lemma 4, a pentacyclic graph must have at least 5 vertices. Therefore, we need to examine pentacyclic graphs with 5 vertices, i. e., graphs with $n = 5$ and $m = 9$. The only such graph is $K_5 - e$, obtained by deleting an edge from K_5. Since $E(K_5 - e) = 7.2915\ldots < 2 \cdot 5 - 2$, this graph is not hyperenergetic. This proves (f).

By Theorem 3, in order that a hexacyclic graph be hyperenergetic, it must have less than 7 vertices. By Lemma 4, a hexacyclic graph must have at least 5 vertices. Therefore, we need to examine hexacyclic graphs with 5 and 6 vertices. The only hexacyclic graph with 5 vertices is K_5, which by definition is not hyperenergetic. We therefore have to examine the hexacyclic graphs with 6 vertices, i. e., graphs with $n = 6$ and $m = 11$. From the available tables of six-vertex graphs [4] we get that there exist exactly nine such graphs. These are depicted in Fig. 1, together with the calculated energies. None of these graphs has energy greater than 10, implying that none of these are hyperenergetic. This proves (f). □

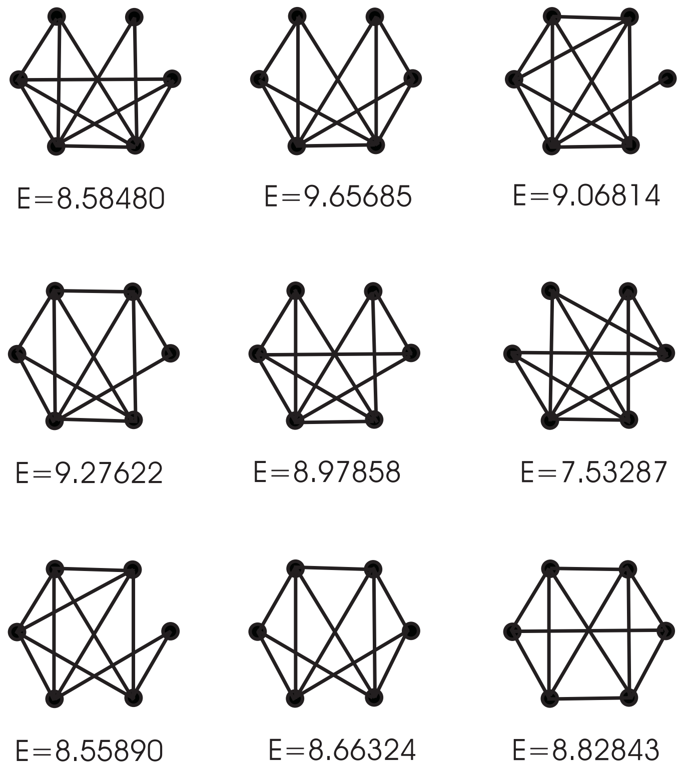
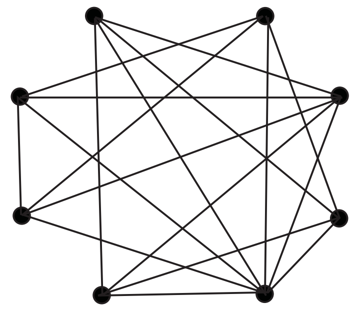


Fig. 1. Graphs needed for in the proof of part (g) of Theorem 5

By an analogous way of reasoning, but assisted by use of computers, we could extend Theorem 5 also to the cases $c = 7$ and $c = 8$. If $c = 7$ then all heptacyclic graphs with 6 and 7 vertices need to be constructed and their energies calculated. If $c = 8$ then all octacyclic graphs with 6, 7, and 8 vertices need to be constructed and their energies calculated. After this has been done we found that none is hyperenergetic. This leads to:

Proposition 6. (h) *There are no hyperenergetic heptacyclic graphs.*
(i) *There are no hyperenergetic octacyclic graphs.*

For greater values of c, the considerations become so complicated that, without a massive use of computers, are not feasible. Anyway, at some point we must reach a value of c for which there exist c-cyclic hyperenergetic graphs. This value of the cyclomatic number is less than or equal to 11, as seen from the example shown in Fig. 2.



E=14.18599

Fig. 2. A hyperenergetic graph with cyclomatic number 11

In the work [2], by means of a computer–aided combinatorial optimization method (called "variable neighborhood search"), it was found that for $n \leq 7$ there are no hyperenergetic graphs, and that there exist hyperenergetic graphs with $n = 8$. If we would accept this finding as mathematically correct, then both Theorem 5 and part (h) of Proposition 6 would follow immediately. In addition, in order to verify part (i) of Proposition 6, it would be sufficient to check only the octacyclic graphs with 8 vertices.

Acknowledgment. This work was partially supported by the Serbian Ministry of Science through Grant no. 144015G.

REFERENCES

[1] S. A k b a r i, F. M o a z a m i, S. Z a r e, *Kneser graphs and their complements are hyperenergetic*, MATCH Commun. Math. Comput. Chem. **61** (2009) 361–368.

[2] G. C a p o r o s s i, D. C v e t k o v i ć, I. G u t m a n, P. H a n s e n, *Variable neighborhood search for extremal graphs. 2. Finding graphs with extremal energy*, J. Chem. Inf. Comput. Sci. **39** (1999) 984–996.

[3] D. C v e t k o v i ć, M. D o o b, H. S a c h s, *Spectra of Graphs – Theory and Application*, Barth, Heidelberg, 1995.

[4] D. C v e t k o v i ć, M. P e t r i ć, *A table of connected graphs on six vertices*, Discr. Math. **50** (1984) 37–49.

[5] D. C v e t k o v i ć, P. R o w l i n s o n, S. K. S i m i ć, *Introduction to the Theory of Graph Spectra*, Cambridge Univ. Press, Cambridge, 2010.

[6] I. G u t m a n, *Hyperenergetic molecular graphs*, J. Serb. Chem. Soc. **64** (1999) 199–205.

[7] I. G u t m a n, *The energy of a graph: Old and new results*, in: A. Betten, A. Kohnert, R. Laue, A. Wassermann (Eds.), *Algebraic Combinatorics and Applications*, Springer–Verlag, Berlin, 2001, pp. 196–211.

[8] I. G u t m a n, *Topology and stability of conjugated hydrocarbons. The dependence of total π-electron energy on molecular topology*, J. Serb. Chem. Soc. **70** (2005) 441–456.

[9] I. G u t m a n, Y. H o u, H. B. W a l i k a r, H. S. R a m a n e, P. R. H a m p i h o l i, *No Hückel graph is hyperenergetic*, J. Serb. Chem. Soc. **65** (2000) 799–801.

[10] I. G u t m a n, X. L i, J. Z h a n g, *Graph energy*, in: M. Dehmer, F. Emmert–Streib (Eds.), *Analysis of Complex Networks. From Biology to Linguistics*, Wiley–VCH, Weinheim, 2009, pp. 145–174.

[11] I. G u t m a n, L. P a v l o v i ć, *The energy of some graphs with large number of edges*, Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.) **118** (1999) 35–50.

[12] I. G u t m a n, O. E. P o l a n s k y, *Mathematical Concepts in Organic Chemistry*, Springer–Verlag, Berlin, 1988.

[13] I. G u t m a n, T. S o l d a t o v i ć, *(n, m)-Type approximations for total π-electron energy of benzenoid hydrocarbons*, MATCH Commun. Math. Comput. Chem. **44** (2001) 169–182.

[14] G. G. H a l l, *A graphical model of a class of molecules*, Int. J. Math. Educ. Sci. Technol. **4** (1973) 233–240.

[15] G. G. H a l l, *Eigenvalues of molecular graphs*, Publ. Inst. Math. Appl. *17* (1981) 70–72.

[16] Y. H o u, I. G u t m a n, *Hyperenergetic line graphs*, MATCH Commun. Math. Comput. Chem. **43** (2001) 29–39.

[17] J. K o o l e n, V. M o u l t o n, *Maximal energy graphs*, Adv. Appl. Math. **26** (2001) 47–52.

[18] J. H. K o o l e n, V. M o u l t o n, I. G u t m a n, *Improving the McClelland inequality for total π-electron energy*, Chem. Phys. Lett. **320** (2000) 213–216.

[19] J. H. K o o l e n, V. M o u l t o n, I. G u t m a n, D. V i d o v i ć, *More hyperenergetic molecular graphs*, J. Serb. Chem. Soc. **65** (2000) 571–575.

[20] S. M a j s t o r o v i ć, A. K l o b u č a r, I. G u t m a n, *Selected topics from the theory of graph energy: hypoenergetic graphs*, in: D. Cvetković, I. Gutman (Eds.), *Applications of Graph Spectra*, Math. Inst., Belgrade, 2009, pp. 65–105.

[21] B. J. M c C l e l l a n d, *Properties of the latent roots of a matrix: The estimation of π-electron energies*, J. Chem. Phys. **54** (1971) 640–643.

[22] V. N i k i f o r o v, *Graphs and matrices with maximal energy*, J. Math. Anal. Appl. **327** (2007) 735–738.

[23] I. S h p a r l i n s k i, *On the energy of some circulant graphs*, Lin. Algebra Appl. **414** (2006) 378–382.

[24] W. S o, *Remarks on some graphs with large number of edges*, MATCH Commun. Math. Comput. Chem. **61** (2009) 351–359.

[25] D. S t e v a n o v i ć, I. S t a n k o v i ć, *Remarks on hyperenergetic circulant graphs*, Lin. Algebra Appl. **400** (2005) 345–348.

[26] H. B. W a l i k a r, I. G u t m a n, P. R. H a m p i h o l i, H. S. R a m a n e, *Non–hyperenergetic graphs*, Graph Theory Notes New York **41** (2001) 14–16.

[27] H. B. W a l i k a r, H. S. R a m a n e, P. R. H a m p i h o l i, *On the energy of a graph*, in: R. Balakrishnan, H. M. Mulder, A. Vijayakumar (Eds.), *Graph Connections*, Allied Publishers, New Delhi, 1999, pp. 120–123.

College of Mathematics and Computer Science
Hunan Normal University
Hunan 410081
P. R. China
e-mail: xlshen20032003@yahoo.com.cn,
yphou@hunnu.edu.cn,
xiaohui0079@126.com

Faculty of Science
University of Kragujevac
P. O. Box 60
34000 Kragujevac
Serbia
e-mail: gutman@kg.ac.rs