Communications in Mathematical and in Computer Chemistry

ISSN 0340 - 6253

# **On Path Energy of Graphs**

## Saieed Akbari<sup>1,\*</sup>, Amir Hossein Ghodrati<sup>1</sup>, Ivan Gutman<sup>2</sup>, Mohammad Ali Hosseinzadeh<sup>3</sup>, Elena V. Konstantinova<sup>4,5</sup>

<sup>1</sup>Department of Mathematical Sciences, Sharif University of Technology, Tehran, Iran

s\_akbari@sharif.edu , amir.ghodrati1729@student.sharif.edu

<sup>2</sup>Faculty of Science, University of Kragujevac, P.O.Box 60, 34000 Kragujevac, Serbia gutman@kg.ac.rs

<sup>3</sup>Department of Mathematics, Faculty of Mathematical Sciences, Tarbiat Modares University, P.O. Box 14115-137, Tehran, Iran ma.hosseinzadeh@modares.ac.ir

<sup>4</sup>Sobolev Institute of Mathematics, Acad. Koptyug av. 4, Novosibirsk 630090, Russia

> <sup>5</sup>Novosibisk State University, Pirogova str. 2, Novosibirsk 630090, Russia e\_konsta@math.nsc.ru

> > (Received June 4, 2018)

#### Abstract

For a graph G with vertex set  $\{v_1, \ldots, v_n\}$ , let P(G) be an  $n \times n$  matrix whose (i, j)-entry is the maximum number of internally disjoint  $v_i v_j$ -paths in G, if  $i \neq j$ , and zero otherwise. The sum of absolute values of the eigenvalues of P(G) is called the path energy of G, denoted by PE. We prove that PE of a connected graph G of order n is at least 2(n-1) and equality holds if and only if G is a tree. Also, we determine PE of a unicyclic graph of order n and girth k, showing that for every n, PE is an increasing function of k. Therefore, among unicyclic graphs of order n, the maximum and minimum PE-values are for k = n and k = 3, respectively. These results give affirmative answers to some conjectures proposed in MATCH Commun. Math. Comput. Chem. **79** (2018) 387–398.

<sup>\*</sup>Corresponding author

### 1 Introduction

Let G be a graph with vertex set  $V(G) = \{v_1, \ldots, v_n\}$ . In the recent paper [10], the so-called *path matrix*  $\mathbf{P} = \mathbf{P}(G)$  of G was defined as the  $n \times n$  matrix whose (i, j)-entry is the maximum number of internally disjoint paths between the vertices  $v_i$  and  $v_j$  when  $i \neq j$  and is zero when i = j.

By definition, **P** is a real and symmetric matrix. Therefore its eigenvalues are real and we call them the *path eigenvalues* of G. The spectral radius of  $\mathbf{P}(G)$  will be denoted by  $\rho = \rho(G)$ . The sum of the absolute values of the path eigenvalues, denoted by PE = PE(G), is the *path energy* of the graph G.

The concept of path energy was introduced in [11] in analogy to a number of earlier conceived "graph energies". Namely, in the 1970s, the sum of the absolute values of the adjacency matrix of a graph was recognized as a mathematically interesting object, having applications in the quantum theory of conjugated molecules. Eventually, this graph energy became a popular topic of research, with hundreds of published papers; details are found in the book [9] and recent review [6]. Motivated by the success of the graph energy based on the adjacency matrix, several analogous graph energies were put forward, based on eigenvalues of other graph matrices. Some of these new graph energies proved to possess attractive mathematical properties and some found unexpected applications in various fields of science; details are found in the book [8] and recent review [7]. Until now, around 120 various graph energies have been considered in the literature.

In [11] it was established that several classes of graphs have a single positive path eigenvalue (equal to  $\rho$ ). For many other graphs,  $\rho$  is much greater than the other positive–valued path eigenvalues. Based on these findings, the following conjectures were proposed [11].

**Conjecture 1.** Let G be a connected graph of order n.

- (a)  $PE(G) \ge 2(n-1)$ , with equality if and only if G is a tree (any tree) of order n.
- (b)  $PE(G) \leq 2(n-1)^2$ , with equality if and only if G is the complete graph of order n.

**Conjecture 2.** If G is a connected unicyclic graph of order n and girth k, then PE(G) depends only on the parameters n and k. For fixed n, PE(G) is a monotonically increasing function of k.

-467-

**Conjecture 3.** Let G be a connected unicyclic graph of order n.

- (a) PE(G) is maximal if and only if G is the cycle (whose girth is n).
- (b) PE(G) is minimal if and only if G is any of the graphs with girth 3.

In the next section we confirm the correctness of part (a) of Conjecture 1 as well as Conjectures 2 and 3.

### 2 Proving the Conjectures

By  $\mathcal{U}_n$  we denote the set of connected unicyclic graphs with *n* vertices. In addition  $\mathcal{U}_{n,k}$  is the subset of  $\mathcal{U}_n$ , consisting of graphs whose (unique) cycle is of size k,  $3 \le k \le n$ .

By **j** and **J** we denote the all-one vector and all-one matrix, respectively.

A graph is k-connected if it has at least k + 1 vertices and the subgraph obtained by removal of each subset of its vertices of size k - 1 remains connected.

**Lemma 4.** (Menger's Theorem) [1, Theorem 9.1.] A graph is k-connected if and only if there are at least k internally disjoint paths between every two vertices.

**Theorem 5.** Let G be a connected graph of order n. Then  $PE(G) \ge 2(n-1)$  and the equality holds if and only if G is any tree of order n.

*Proof.* As noted in [11],  $PE(G) \ge 2\rho(G)$ . Since G is connected, every off-diagonal entry of the path matrix **P** is at least one. So,  $\mathbf{j}^T \mathbf{Pj} \ge n^2 - n$ . On the other hand, by the Rayleigh quotient,  $\rho(G) \ge \mathbf{j}^T \mathbf{Pj}/\mathbf{j}^T \mathbf{j}$ , which implies that

$$PE(G) \ge 2\rho(G) \ge 2\frac{\mathbf{j}^T \mathbf{P} \mathbf{j}}{\mathbf{j}^T \mathbf{j}} \ge 2\frac{n^2 - n}{n} = 2(n-1),$$

and the equality holds if and only if every off-diagonal entry of  $\mathbf{P}(G)$  is one, i.e., if G is a tree.

**Theorem 6.** Let  $n \ge k \ge 3$ . For every  $G \in \mathcal{U}_{n,k}$ ,

$$PE(G) = \begin{cases} 2(n+k-3) & 3 \le k \le n-3\\ \sqrt{(n-k+1)^2 + 4k(k-1)} + n+k-3 & n-2 \le k \le n \end{cases}$$

Thus, for every n, PE(G) is an increasing function of k.

-468-

*Proof.* Let  $\mathbf{P} = \mathbf{P}(G)$ . Note that for every two distinct vertices  $v_i, v_j$  of G, if  $v_i$  and  $v_j$  lie on the unique cycle of G, then the (i, j)-entry of  $\mathbf{P}$  is 2, otherwise this entry is equal to 1. So,

$$P = \begin{pmatrix} 2\mathbf{J}_{k\times k} - 2\mathbf{I} & \mathbf{J}_{k\times (n-k)} \\ \mathbf{J}_{(n-k)\times k} & \mathbf{J}_{(n-k)\times (n-k)} - \mathbf{I} \end{pmatrix},$$

where I stands for a unit matrix of appropriate order.

The first k rows of  $\mathbf{P} + 2\mathbf{I}$  are the same. Thus,  $rank(\mathbf{P} + 2\mathbf{I}) \leq n - k + 1$ , which implies that  $null(\mathbf{P} + 2\mathbf{I}) \geq k - 1$ . Therefore, -2 is an eigenvalue of  $\mathbf{P}$  with multiplicity at least k - 1. Similarly, the last n - k rows of  $\mathbf{P} + \mathbf{I}$  are the same, which implies that  $null(\mathbf{P} + \mathbf{I}) \geq n - k - 1$ . Hence, -1 is an eigenvalue of  $\mathbf{P}$  with multiplicity at least n - k - 1. Now, let a, b be the other two eigenvalues of  $\mathbf{P}$ . Since

$$tr(\mathbf{P}) = a + b + (k - 1)(-2) + (n - k - 1)(-1) = 0,$$

we have a + b = n + k - 3. Furthermore, since  $tr(\mathbf{P}^2) = \sum_{1 \le i,j \le n} p_{ij}^2$ , we find that,

$$a^{2} + b^{2} + (k-1)(-2)^{2} + (n-k-1)(-1)^{1} = n^{2} - n + 3k(k-1),$$

which implies that

$$ab = n(k-2) - k^2 + 2$$

If  $3 \le k \le n-3$ , then ab > 0, so both a and b are positive and we conclude that

$$PE(G) = a + b + (k - 1)(2) + (n - k - 1)(1) = 2(n + k - 3)$$

If  $k \in \{n-2, n-1, n\}$ , then ab < 0, so a and b have opposite signs and we conclude that

$$PE(G) = |a - b| + (k - 1)(2) + (n - k - 1)(1)$$
$$= \sqrt{(n - k + 1)^2 + 4k(k - 1)} + n + k - 3$$

which completes the proof.

By Theorems 5 and 6, the validity of Conjectures 1(a) and 2 has been confirmed. Then the claim of Conjecture 3 follows as an immediate consequence of Theorem 6.

Remains Conjecture 1(b). Although at the first glance it looks plausible, at this moment its verification (or refutation) remains an open task.

In [11] it has been proved that if  $k \ge 2$  and G is a k-connected graph of order 2k + 1, then  $\rho(G) \ge 4k$ . Here we improve this result as follows: **Theorem 7.** Let G be a k-connected graph of order n. Then,  $\rho(G) \ge k(n-1) \ge k^2$ .

*Proof.* By Menger's Theorem, there are at least k internally disjoint paths between every two distinct vertices of G. So,  $\mathbf{P}(G) \ge k(\mathbf{J} - \mathbf{I})$  which implies that  $\rho(G) \ge k(n-1)$ .

**Theorem 8.** Let G be a k-connected, k-regular graph of order n. Then  $\rho(G) = k(n-1)$ and PE(G) = 2k(n-1).

*Proof.* Let  $u, v \in V(G)$ . Since G is k-connected, there are at least k internally disjoint paths between u and v. On the other hand, since d(u) = k, there are at most k internally disjoint paths between u and v. Thus, the maximum number of internally disjoint paths between u and v is exactly k. Therefore,  $\mathbf{P}(G) = k(\mathbf{J} - \mathbf{I})$  and this gives the result.

By direct calculations we immediately have from Theorem 8 the following formulas for the complete graph  $K_n$ , the *n*-cycle, and the complete bipartite graph  $K_{n,n}$ :

- $\rho(K_n) = (n-1)^2$ ,  $PE(K_n) = 2(n-1)^2$ ;
- $\rho(C_n) = 2(n-1), PE(C_n) = 4(n-1);$
- $\rho(K_{n,n}) = n(2n-1), PE(K_{n,n}) = 2n(2n-1).$

By [2-4, 12] and [5, Chap. 27], a strongly regular or distance-regular or minimal Cayley graph of valency k is k-connected. Hence Theorem 8 gives the following result.

**Corollary 9.** Let G be a k-regular graph of order n. If G is a distance-regular (specially strongly regular) or minimal Cayley graph, then  $\rho(G) = k(n-1)$  and PE(G) = 2k(n-1).

Acknowledgement. The research of S. Akbari, A. H. Ghodrati and M. A. Hosseinzadeh was partly funded by the Iranian National Science Foundation (INSF) under the contract No. 96004167. M. A. Hosseinzadeh was also supported by the National Elites Foundation under Grant Number 15/89682. E. V. Konstantinova was supported by RFBR according to the research project 17-51-560008.

### References

- [1] J. A. Bondy, U. S. R. Murty, *Graph Theory*, Springer, New York, 2008.
- [2] A. E. Brouwer, J. H. Koolen, The vertex-connectivity of a distance-regular graph, *Eur. J. Comb.* **30** (2009) 668–673.

- [3] A. E. Brouwer, D. M. Mesner, The connectivity of strongly regular graphs, *Eur. J. Comb.* 6 (1985) 215–216.
- [4] C. D. Godsil, Connectivity of minimal Cayley graphs, Arch. Math. Basel 37 (1981) 473–476.
- [5] R. Graham, M. Grötschel, L. Lovász, *Handbook of Combinatorics*, Vol. 2, MIT Press, Cambridge, 1996.
- [6] I. Gutman, B. Furtula, The total π-electron energy saga, Croat. Chem. Acta 90 (2017) 359–368.
- [7] I. Gutman, B. Furtula, Survey of graph energies, *Math. Interdisc. Res.* 2 (2017) 85–129.
- [8] I. Gutman, X. Li (Eds.), Graph Energies Theory and Applications, Univ. Kragujevac, Kragujevac, 2016.
- [9] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2012.
- [10] S. C. Patekar, M. M. Shikare, On the path matrices of graphs and their properties, Adv. Appl. Discr. Math. 17 (2016) 169–184.
- [11] M. M. Shikare, P. P. Malavadkar, S. C. Patekar, I. Gutman, On path eigenvalues and path energy of graphs, *MATCH Commun. Math. Comput. Chem.* **79** (2018) 387–398.
- [12] M. E. Watkins, Connectivity of transitive graphs, J. Comb. Theory B 8 (1970) 23–29.