ISSN 2347-1921

Harmonic Matrix and Harmonic Energy

LI Bingjun[1,2]

[1]College of Mathematics, Central South University, Changsha, 410000, China.

[2]Department of Mathematics, Hunan Institute of Humanities Science and Technology, Loudi city, Hunan 417000, China.

E-mail: gfkdlbj@sina.com

Abstract

We define the Harmonic energy as the sum of the absolute values of the eigenvalues of the Harmonic matrix, and establish some of its properties, in particular lower and upper bounds for it.

Key words:

The RandiĆ index; Harmonic Matrix; Harmonic Energy; eigenvalues

2010 Mathematics Subject Classification: 05C70

Council for Innovative Research

Peer Review Research Publishing System

Journal: Journal of Advances in Mathematics

Vol 6, No. 1

editor@cirworld.com

www.cirworld.com, member.cirworld.com

1. Introduction: Randic matrix and Harmonic Matrix

Let G be a simple graph and let $v_1; v_2; \cdots v_n$ be its vertices. For $i = 1; 2; \cdots; n$, we denote the degree (the number of first neighbors) of the vertex v_i by d_i. Then the molecular structure descriptor, put forward in 1975 by Milan RandiĆ [11], is defined as

$$R = R(G) = \sum_{i \sim j} \frac{1}{\sqrt{d_i d_j}} \qquad (1)$$

Where $\sum_{i \sim j}$ indicates summation over all pairs of adjacent vertices $v_i; v_j$. Nowadays, R is referred to as the Randic index .

The summands on the right hand side of formula (1) may be understood as matrix elements. This observation may serve as a motivation for conceiving a symmetric square matrix, called the RandiĆ matrix.

$R = R(G) = (R_{ij})$ of order n , defined via

$$R_{ij} = \begin{cases} 0 & \text{if } i = j \\ \dfrac{1}{\sqrt{d_i d_j}} & \text{if the vertices } v_i \text{ and } v_j \text{ of G are adjacent} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ of G are not adjacent} \end{cases} \qquad (2)$$

Harmonic index and graph radius. The Harmonic index is defined by Fajtlowicz[3] as follows. Given any graph G, the Harmonic index of G is

$$H = H(G) = \sum_{i \sim j} \frac{2}{d_i + d_j}$$

where the sum is over all edges $v_i v_j$ of the graph G.

Then, we can a symmetric matrix (Hij) of order n , defined via

$$H_{ij} = \begin{cases} 0 & \text{if } i = j \\ \dfrac{2}{di + dj} & \text{if the vertices } v_i \text{ and } v_j \text{ of G are adjacent} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ of G are not adjacent} \end{cases}$$

At this point it is purposeful to recall the definition of the adjacency matrix A of the graph G. Its (i; j)-entry is defined as:

$$A_{ij} = \begin{cases} 0 & \text{if } i = j \\ 1 & \text{if the vertices } v_i \text{ and } v_j \text{ of G are adjacent} \\ 0 & \text{if the vertices } v_i \text{ and } v_j \text{ of G are not adjacent} \end{cases}$$

We can call (R_{ij}) and (H_{ij}) "weighted adjacency matrices".

2. Energies

Graph spectral theory, based on the eigenvalues of the adjacency matrix, has well and long known applications in chemistry [5-7]. One of the chemically (and also math- ematically) most interesting graph energy, defined as follows.

Let G be a simple graph on n vertices, and let A be its adjacency matrix. Let, $\lambda_1; \lambda_2; \cdots; \lambda_n$ be the eigenvalues of A. These are said to be the eigenvalues of the graph G and to form its spectrum. The energy E(G) of the graph G is defined as the sum of the absolute values of its eigenvalues

$$E = E(G) = \sum_{i=1}^{n} |\lambda_i| \qquad (3)$$

For details on graph energy see the reviews.

In view of the evident success of the concept of graph energy, and because of the rapid decrease of open mathematical problems in its theory, energies based of the eigenvalues of other graph matrices have been introduced. Of these, the Laplacian energy LE(G) , pertaining to the Laplacian matrix, seems to be the first [1, 2]. Burcu Bozkurt et al[9] defined the RandiĆ energy, as the sum of absolute values of the eigenvalues of the RandiĆ matrix. They studied the Bounds for Randic energy.

Along these lines of reasoning, we could think of the Harmonic energy, as the sum of absolute values of the eigenvalues of the Harmonic matrix. More formally: Let $\rho_1, \rho_2, \cdots, \rho_n$ be the eigenvalues of the Harmonic matrix H(G) . Knowing that these eigenvalues are necessarily real numbers, and that their sum is zero, the Harmonic energy can be defined as

$$HE = HE(G) = \sum_{I=1}^{N} |\rho_I| \qquad (4)$$

This definition is applicable to all graphs.

3 Bounds for Harmonic energy

In this section we first calculate tr(H^2) , tr(H^3) , and tr(H^4) , where tr denotes the trace of a matrix. Moreover, using these equalities we obtain an upper and a lower bound for Harmonic energy of the graph G.

In order to obtain our main results we give the following:

Lemma 1. Let G be a graph with n vertices and Harmonic matrix H. Then

$$tr(H)=0$$

$$tr(H^2)=4\sum_{i`\sim j}\frac{1}{(d_i+d_j)^2}$$

$$tr(H^3)=2\sum_{i\sim j}\frac{1}{d_id_j}\left(\sum_{k\sim i,k\sim j}\frac{1}{d_k}\right)$$

$$tr(H^4)=16\sum_{i\neq 1}^{n}\left(\sum_{i\sim j}\frac{1}{(d_i+d_j)^2}\right)^2+16\sum_{k\sim i,k\sim j}\left(\sum_{k\sim i,k\sim j}\frac{1}{d_k+d_j}\cdot\frac{1}{d_k+d_i}\right)^2$$

Proof. By definition, the diagonal elements of H are equal to zero. Therefore the trace of H is zero.

Next, we calculate the matrix H^2 . For $i=j$

$$(H)^2{}_{ii}=\sum_{j=i}^{n}H_{ij}H_{ji}=\sum_{j=1}^{n}(H_{ij})^2=\sum_{i\sim j}(H_{ij})^2=\sum_{i\sim j}\frac{4}{(d_i+d_j)^2}$$

Where as for $i \neq j$

$$(H^2)_{ij}=\sum_{k=1}^{n}H_{ik}H_{kj}=H_{ii}H_{ij}+H_{ij}H_{jj}+\sum_{k\sim i,k\sim j}H_{ik}H_{kj}=4\sum_{k\sim i,k\sim j}\left(\frac{1}{d_k+d_j}\cdot\frac{1}{d_k+d_i}\right)$$

Therefore

$$tr(H^2)=\sum_{i=1}^{n}\sum_{i\sim j}\frac{4}{(d_i+d_j)^2}=8\sum_{i\sim j}\frac{1}{(d_i+d_j)^2}$$

Since the diagonal elements of R^3 are

$$(H^3)_{ii}=\sum_{j=1}^{n}H_{ij}(H^2)_{jk}=\sum_{i\sim j}\frac{2}{d_i+d_j}(H^2)_{ij}=8\sum_{i\sim j}\frac{1}{d_i+d_j}\left(\sum_{k\sim i,k\sim j}\frac{1}{d_k+d_j}\cdot\frac{1}{d_k+d_i}\right)$$

We obtain

$$tr(H^3)=16\sum_{i\sim j}\frac{1}{d_i+d_j}\left(\sum_{k\sim i,k\sim j}\frac{1}{d_k+d_j}\cdot\frac{1}{d_k+d_i}\right)$$

ISSN 2347-1921

We now calculate tr(H^4) . Because tr(H^4) = $\| H^2 \|_F^2$, where $\| H^2 \|_F$ denotes the Frobenius norm of H^2 , we obtain

$$tr(H^4) = \sum_{i,j=1}^{n} |(H^2)_{ij}|^2 = \sum_{i=j}^{n} |(H^2)_{ij}|^2 + \sum_{i\neq j}^{n} |(H^2)_{ij}|^2 =$$

$$= 16\sum_{i\neq 1}^{n} \left(\sum_{i\sim j} \frac{1}{(d_i + d_j)^2} \right)^2 + 16 \sum_{k\sim i, k\sim j} \left(\sum_{k\sim i, k\sim j} \frac{1}{d_k + d_j} \cdot \frac{1}{d_k + d_i} \right)^2$$

Theorem 2. Let G be a graph with n vertices. Then

$$HE \leq 2\sqrt{2n\sum_{i\sim j} \frac{1}{(d_i + d_j)^2}} \qquad (7)$$

Proof. The variance of the numbers $|\rho_i|, i=1;2,\cdots,n$, is equal to

$$\frac{1}{n}\sum_{i=1}^{n} |\rho_i|^2 - \left(\frac{1}{n}\sum_{i=1}^{n} |\rho_i| \right)^2$$

and is greater than or equal to zero. Now,

$$\sum_{i=1}^{n} |\rho_i|^2 = \sum_{i=1}^{n} \rho_i^2 = tr(H^2)$$

and therefore

$$\frac{1}{n} tr(H^2) - (\frac{1}{n} HE)^2 \geq 0 \Leftrightarrow HE \leq \sqrt{n\,tr(H^2)}$$

Inequality (7) follows from Lemma 1.

Theorem 3 Let G be a graph with n vertices and at least one edge. Then

$$RE(G) \geq \sqrt{\frac{\sum_{i`\sim j} \frac{1}{(d_i + d_j)^2}}{\sum_{i \neq 1}^{n} \left(\sum_{i \sim j} \frac{1}{(d_i + d_j)^2} \right)^2 + \sum_{k \sim i, k \sim j} \left(\sum_{k \sim i, k \sim j} \frac{1}{d_k + d_j} \cdot \frac{1}{d_k + d_i} \right)^2}}$$

Proof. Our starting point is the Holder inequality

$$\sum_{i=1}^{n} a_i b_i \leq \left(\sum_{i=1}^{n} a_i^p \right)^{1/p} \left(\sum_{i=1}^{n} a_i^p \right)^{1/q}$$

which holds for any non-negative real numbers $a_i, b_i;\ i = 1, 2, \cdots, n$. Setting $a_i = |\rho_i|^{2/3}, b_i = |\rho_i|^{4/3}, p = 3/2$, and q = 3 , we obtain

$$\sum_{i=1}^{n} |\rho_i|^2 = \sum_{i=1}^{n} |\rho_i|^{2/3} (|\rho_i|^4)^3 \leq \left(\sum_{i=1}^{n} |\rho_i| \right)^{2/3} \left(\sum_{i=1}^{n} |\rho_i|^4 \right)^{1/3}$$

If G has at least one edge, then not all ρ_i 's are equal to zero. Then $\sum_{i=1}^{n} |\rho_i|^4 \neq 0$ and (8) can be rewritten as

$$PE(G) = \sum_{i=1}^{n} |\rho_i| \geq \sqrt{\frac{\left(\sum_{i=1}^{n} |\rho_i|^2 \right)^3}{\sum_{i=1}^{n} |\rho_i|^4}} = \sqrt{\frac{\left(\sum_{i=1}^{n} \rho_i^{\,2} \right)^3}{\sum_{i=1}^{n} \rho_i^{\,4}}}$$

Theorem 3 is now obtained from Lemma 1.

We conclude this section by a simple identity for the Harmonic energy of regular graphs.

Theorem 4. If the graph G is regular of degree r ; r > 0 , then

$$HE(G) = \frac{1}{r} E(G)$$

If, in addition r = 0 , then HE = 0 .

Proof. Since G is regular of degree r, then $\frac{2}{d_i + d_j} = \frac{1}{\sqrt{d_i d_j}}$

Hence, R(G)=H(G). Theorem 4 follows from theorem 6 of [9]

REFERENCES

[1] I. Gutman, B. Zhou, Laplacian energy of a graph, Lin. Algebra Appl. 414 (2006)29-37.

[2] B. Zhou, I. Gutman, On Laplacian energy of graphs, MATCH Commun. Math.Comput. Chem. 57 (2007) 211-220.

[3] S. Fajtlowicz, On conjectures of Graffiti, Discrete Math. 72 (1988) 113-118.

[4] V. Consonni, R. Todeschini, New spectral indices for molecule description, MATCH Commun. Math. Comput. Chem. 60 (2008) 3-14.

[5] V. Nikiforov, The energy of graphs and matrices, J. Math. Anal. Appl. 326 (2007) 1472-1475.

[6] M. R. Jooyandeh, D. Kiani, M. Mirzakhah, Incidence energy of a graph, MATCHCommun. Math. Comput. Chem. 62 (2009) 561-572.

[7] F. R. K. Chung, Spectral Graph Theory, Am. Math. Soc., Providence, 1997.

[8] J. Rada, A. Tineo, Upper and lower bounds for the energy of bipartite graphs, J. Math. Anal. Appl. 289 (2004) 446-455.

[9] Bozkurt S B, Güngör A D, Gutman I. Randic matrix and Randic energy[J]. MATCH Commun. Math. Comput. Chem, 2010, 64: 239-250.

[10] X. Li and I. Gutman, Mathematical Aspects of Randic-Type Molecular Structure Descriptors, Mathematical Chemistry Monographs No.1, Kragujevac, 2006.

[11] M. RandiĆ, On characterization of molecular branching, J. Amer. Chem. Soc. 97 (1975), 6609-6615.

ACKNOWLEDGMENTS

The project was supported by Hunan Provincial Natural Science Foundation of China(13JJ4103) and The Education Department of Hunan Province Youth Project(12B067)

Author' Biography

Li Bingjun

is an associate professor of Applied Mathematics at Hunan Institute of Humanities Science and Technology, China. He got his doctoral degree from National University of Defense Technology at 2009. His research interests include Algebra and (chemical) graph theory.