MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **79** (2018) 287-301

ISSN 0340 - 6253

New Upper Bounds on the Energy of a Graph

Noor Alawiah[1], Nader Jafari Rad[2], Akbar Jahanbani[2], Hailiza Kamarulhaili[1]

[1]*School of Mathematical Sciences, Universiti Sains Malaysia*
11800 USM Penang, Malaysia
hailiza@usm.my

[2]*Department of Mathematics, Shahrood University of Technology*
Shahrood, Iran
n.jafarirad@gmail.com

(Received June 14, 2017)

Abstract

The energy of a graph G, denoted by $\mathcal{E}(G)$, is defined as the sum of the absolute values of all eigenvalues of G. In this paper, we present various new upper bounds for the energy of graphs in terms of several graph variants such as the number of vertices, number of edges, maximum degree and Zagreb indices of the graph. We also characterize graphs achieving equality in each new bound. Our bounds improve several previous bounds given in [B.J. McClelland, Properties of the latent roots of a matrix: The estimation of π-electron energies, J. Chem. Phys. 54 (1971), 640-643], [J.H. Koolen, V. Moulton, Maximal energy graphs, Adv. Appl. Math. 26. 47-52 (2001)] and [J.H. Koolen and V. Moulton, Maximal energy bipartite graphs, Graphs Combin. 19 (2003), 131-135].

1 Introduction

Let $G = (V, E)$ be a simple undirected graph with vertex set $V = V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $E(G)$, $\mid E(G) \mid= m$. The *order* and *size* of G are $n = |V|$ and $m = |E|$, respectively. For a vertex $v_i \in V$, the *degree* of v_i, denoted by $\deg(v_i)$ (or just d_i), is the number of edges incident to v. We denote by $\Delta(G)$ the *maximum degree* among the vertices of G, and by $\delta(G)$ the *minimum degree* among the vertices of G. A *walk* from a vertex u to a vertex v is a finite alternating sequence $v_0(=u)e_1v_1e_2\ldots v_{k1}e_kv_k(=v)$ of vertices and edges such that $e_i = v_{i-1}v_i$ for $i = 1, 2, \ldots, k$. The number k is the *length* of the walk. In particular, if the vertex $v_i, i = 0, 1, ..., k$ in the walk are all distinct then the walk is called a *path*. A path of order n is denoted by P_n. A *closed path* or *cycle*, is obtained from a path $v_1, \ldots, v_k$ (where $k \geqslant 3$) by adding the edge v_1v_k. A cycle of order n is denoted by C_n. A graph is *unicyclic* if it contains precisely one cycle. A graph is *connected* if each pair of vertices in a graph is joined by a walk. A *bipartite* graph is a graph such that its vertex set can be partitioned into two sets X and Y (called the partite sets) such that every edge meet both X and Y. A *complete bipartite graph* is a bipartite such that any vertex of a partite set is adjacent to all vertices of the other partite set. A complete bipartite graph with partite set of cardinalities p and q is denoted by $K_{p,q}$. The graph $K_{1,n-1}$ is also called a *star* of order n, denoted by S_n. A simple undirected graph in which every pair of distinct vertices is connected by a unique edge, is the *complete graph* and is denoted by K_n. For other graph theory notation and terminology we refer to [19].

The *first* and *second Zagreb indices* of a graph G are defined as $M_1(G) = \sum_{u\in V} d_u^2$ and $M_2(G) = \sum_{uv\in V} d_ud_v$, respectively. For further study on the Zagreb indices and their properties, we refer to [10, 21, 22].

The *adjacency matrix* $A(G)$ of a graph G is defined by its entries as $a_{ij} = 1$ if $v_iv_j \in E(G)$ and 0 otherwise. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{n-1} \geqslant \lambda_n$ denote the *eigenvalues* of $A(G)$. Then λ_1 is called the *spectral radius* of G. When more than one graphs are under consideration, then we write $\lambda_i(G)$ instead of λ_i. The *energy* of a graph G is defined as

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

This concept was introduced by I. Gutman and is intensively studied in chemistry, since it can be used to approximate the total π-*electron* energy of a *molecule* (see, e.g. [7], [8]). In 1971, McClelland [18] discovered the first upper bound for $\mathcal{E}(G)$ as follows:

$$\mathcal{E}(G) \leq \sqrt{2mn}. \tag{1}$$

Since then, numerous other bounds for $\mathcal{E}(G)$ were found (see, e.g. [1], [6]- [7], [9]- [16]). Here we just state some upper bounds for $\mathcal{E}(G)$ which were obtained recently. Koolen and Moulton [13] showed that if $2m \geqslant n$ and G is a graph with n vertices, m edges, then

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

with equality if and only if G is either $\frac{n}{2}K_2$, K_n or a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{(2m-(\frac{2m}{n})^2)}{(n-1)}}$. The same authors showed then that if $2m \geqslant n$ and G is a bipartite graph with $n > 2$ vertices, m edges, then

$$\mathcal{E}(G) \leq 2(\frac{2m}{n}) + \sqrt{(n-1)\left(2m - 2(\frac{2m}{n})^2\right)}, \tag{3}$$

with equality if and only if G is either $\frac{n}{2}K_2$, a complete bipartite graph, or the incidence graph of a symmetric 2-(ν, k, λ)-design with $k = \frac{2m}{n}$ and $\lambda = \frac{k(k-1)}{\nu-1}(n = 2\nu)$. Zhou [20] proved that if G is a graph with n vertices, m edges and degree sequence $d_1, d_2, \ldots, d_n$, then

$$\mathcal{E}(G) \leq \sqrt{\frac{M_1}{n}} + \sqrt{(n-1)\left(2m - \frac{M_1}{n}\right)}, \tag{4}$$

with equality if and only if G is either $\frac{n}{2}K_2$, a complete bipartite graph, a non-complete connected strongly regular graph with two non-trivial eigenvalues both with absolute value $\sqrt{\frac{2m-(\frac{2m}{n})^2}{(n-1)}}$ or nK_1. Zhou [20] also showed that if G is a bipartite graph with $n > 2$ vertices, m edges and degree sequence $d_1, d_2, \ldots, d_n$, then

$$\mathcal{E}(G) \leq 2\sqrt{\frac{M_1}{n}} + \sqrt{(n-2)\left(2m - \frac{2M_1}{n}\right)}, \tag{5}$$

with equality if and only if G is either $\frac{n}{2}K_2$, a complete bipartite graph, the incidence graph of a symmetric $2-(\nu, \kappa, \lambda)$-design with $\kappa = \frac{2m}{n}$ and $\lambda = \frac{\kappa(\kappa-1)}{\nu-1}(n = 2\nu)$.

In this paper, we present various new upper bounds for the energy of graphs in terms of several graph variants such as the number of vertices, number of edges, maximum degree and Zagreb indices of the graph. We improve the bounds given in (1) by McClelland, and in (2) and (3) by Koolen and Moulton, and present bounds similar to those given in (4) and (5) in terms of the second zagreb indices. We also characterize graphs achieving equality in each new bound. The organization of the paper is as follows. In the Section 2, we give a list of some previously known results. In the Section 3, we present our upper bounds for the energy of a graph G. We divide the section into five subsections depending on the kind of graphs under study which are: general graphs, connected graphs, connected unicyclic graphs, bipartite graphs, and connected bipartite graphs.

2 Preliminaries and known results

In this section, we list some previously known results that will be needed in the next sections. We first state some results on the spectral radius of a graph.

Lemma 1 ([5]) *If G is a non-empty graph with maximum degree Δ, then $\lambda_1 \geqslant \sqrt{\Delta}$, with equality if and only if G is $\frac{n}{2}K_2$.*

Lemma 2 ([5]) *If G is a graph with n vertices, m edges and degree sequence $d_1, d_2, \ldots,$ d_n, then*

$$\lambda_1 \geqslant \frac{1}{m}\sum_{ij\in E}\sqrt{d_i d_j} = \frac{\sum_{ij\in E}\sqrt{d_i d_j}}{m} \geqslant \frac{\sqrt{\sum_{ij\in E} d_i d_j}}{m} = \frac{\sqrt{M_2}}{m}. \tag{6}$$

Lemma 3 ([11]) *If G is a connected unicyclic graph, then $\lambda_1 \geq 2$, with equality if and only if G is a cycle C_n.*

Lemma 4 ([3]) *If G is a connected graph with n vertices, then*

$$\lambda_1 \geq 2\cos(\frac{\pi}{(n+1)}), \tag{7}$$

with equality if and only if G is a cycle P_n.

We next state some results on the Zagreb index of a graph.

Lemma 5 ([17]) *If G is a graph with n vertices and m edges, then $\frac{M_2}{m} \geqslant \frac{4m^2}{n^2}$.*

The next lemma provides a bound for the energy of a graph.

Lemma 6 ([2]) *If G is a graph with m edges, then $\mathcal{E}(G) \geqslant 2\sqrt{m}$, with equality if and only if G is a complete bipartite graph plus arbitrarily many isolated vertices.*

Lemma 7 ([4]) *A graph G has only one eigenvalue if and only if G is an empty graph. A graph G has two distinct eigenvalues $\mu_1 > \mu_2$ with multiplicities m_1 and m_2 if and only if G is the direct sum of m_1 complete graphs of order $\mu_1 + 1$. In this case, $\mu_2 = -1$ and $m_2 = m_1\mu_1$.*

We end this section by stating the energy and the Zagreb indices of a complete graph. It is well known that the complete graph K_n has two distinct eigenvalues which are $n-1$ with multiplicity 1 and -1 with multiplicity $n-1$. Thus, $\mathcal{E}(K_n) = n-1+(n-1)\times 1 = 2n-2$. Furthermore, a simple calculation shows that $M_1(K_n) = n(n-1)^2$ and $M_2(K_n) = m(n-1)^2$, where $m = n(n-1)/2$.

3 Upper Bounds for the Energy of Graphs

In this section, we obtain some new upper bounds for the energy of graphs. We deal with general graphs, connected graphs, connected unicyclic graphs, bipartite graphs, connected bipartite graphs, and connected bipartite unicyclic graphs. We divide this section into six subsection depending on the kind of graphs we study.

3.1 Upper bounds in general graphs

We begin with the following upper bound in terms of order, size, maximum and minimum degree of a graph.

Theorem 8 *Let G be a non-empty graph with n vertices, m edges and maximum vertex degrees Δ. Then*

$$\mathcal{E}(G) \leq \sqrt{\Delta} + \sqrt{(n-1)(2m-\Delta)}, \tag{8}$$

equality holds if and only if $G \cong \frac{n}{2}K_2$, $(n = 2m)$.

Proof. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{n-1} \geqslant \lambda_n$ be the eigenvalues of G. By the $Cauchy-Schwartz$ inequality,

$$\sum_{i=2}^{n} | \lambda_i | \leqslant \sqrt{(n-1)\sum_{i=2}^{n} \lambda_i^2} = \sqrt{(n-1)(2m-\lambda_1^2)}.$$

Hence

$$\mathcal{E}(G) \leqslant \lambda_1 + \sqrt{(n-1)(2m-\lambda_1^2)}.$$

Note that the function $F(x) = x + \sqrt{(n-1)(2m-x^2)}$ decreases for $\sqrt{\frac{2m}{n}} \leqslant x \leqslant \sqrt{2m}$. By Lemma 1, we have $\lambda_1 \geqslant \sqrt{\Delta}$, equality holds if and only if G is $\frac{n}{2}K_2$. Clearly, $\Delta \geqslant \frac{2m}{n}$. By Lemma 1, we have

$$\lambda_1 \geqslant \sqrt{\Delta} \geqslant \sqrt{\frac{2m}{n}}.$$

So $F(\lambda_1(G)) \leqslant F(\sqrt{\Delta})$, which implies that

$$\mathcal{E}(G) \leq \sqrt{\Delta} + \sqrt{(n-1)(2m-\Delta)}.$$

If $G \cong \frac{n}{2}K_2$, then it is easy to check that the equality in (8) holds. Conversely, if the equality in (8) holds, then according to the above argument, we have $\lambda_1 = \sqrt{\Delta}$. Moreover, $| \lambda_i | = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$ $(2 \leqslant i \leqslant n)$. Since G is a non-empty graph, by Lemma 7, G has at least two distinct eigenvalues. We consider the following case.

Case 1. The absolute value of all eigenvalues of G are equal.

Then clearly $\lambda_1 =\mid \lambda_i \mid= \sqrt{\frac{2m-\lambda_1^2}{n-1}}$ $(2 \leqslant i \leqslant n)$, since G has at least two distinct eigenvalues. By Lemma 7, $\mid \lambda_i \mid= \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1 (2 \leqslant i \leqslant n)$. Hence $2m = n$ and also, $\lambda_1 =\mid \lambda_2 \mid= \cdots =\mid \lambda_n \mid= 1$. By applying Lemma 7 again, we obtain that $m_2 = m_1\lambda_1, \lambda_1 = 1$, and therefore $m_1 = m_2$. Then we obtain that $\lambda_1 = 1$ has multiplicity $\frac{n}{2}$, and $\lambda_i = -1$ $(2 \leqslant i \leqslant n)$ has multiplicity $\frac{n}{2}$. Therefore G is the direct sum of $m_1 = \frac{n}{2}$ complete graphs of order $\lambda_1 + 1 = 2$. Consequently, G is $\frac{n}{2}K_2$.

Case 2. The absolute value of all eigenvalues of G are not equal. Then G has two distinct eigenvalues with different absolute values. By Lemma 7, $\mid \lambda_i \mid= 1 (2 \leqslant i \leqslant n)$. Since, $\sum_{i=1}^{n} \lambda_i = 0$ and $\lambda_2 = \lambda_3 = \cdots = \lambda_n = -1$, we have, $\lambda_1 = n - 1$. Hence λ_1 has multiplicity 1 and $\lambda_i = -1$ has multiplicity $n - 1$. By Lemma 7, G is the direct sum of a complete graph of order $\lambda_1 + 1 = n$. Consequently, G is K_n. ■

We remark that since the function $F(x) = x + \sqrt{(n-1)(2m - x^2)}$ decreases for $\sqrt{\frac{2m}{n}} \leqslant x \leqslant \sqrt{2m}$, the bound of Theorem 8 is an improvement of the bound given in (2).

The next bound involves the second Zagreb index of a graph.

Theorem 9 *Let G be a non-empty graph with n vertices and m edges. Then*

$$\mathcal{E}(G) \leq \frac{\sqrt{M_2}}{m} + \sqrt{(n-1)(2m - \frac{M_2}{m^2})}, \tag{9}$$

equality holds if and only if $G \cong \frac{n}{2}K_2$, $(n = 2m)$.

Proof. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{n-1} \geqslant \lambda_n$ be the eigenvalues of G. By the Cauchy-Schwartz inequality,

$$\sum_{i=2}^{n} \mid \lambda_i \mid \leqslant \sqrt{(n-1)\sum_{i=2}^{n} \lambda_i^2} = \sqrt{(n-1)(2m - \lambda_1^2)}.$$

Hence

$$\mathcal{E}(G) \leqslant \lambda_1 + \sqrt{(n-1)(2m - \lambda_1^2)}.$$

Note that the function $S(x) = x + \sqrt{(n-1)(2m - x^2)}$ decreases for $\frac{2m}{n^2} \leqslant x \leqslant 2m$. By Lemma 2, we have

$$\lambda_1 \geqslant \frac{\sqrt{M_2}}{m},$$

with equality if and only if G is $\frac{n}{2}K_2$. By Lemmas 2 and 5, we have

$$\lambda_1 \geqslant \frac{\sqrt{M_2}}{m} \geqslant \frac{2m}{n^2}.$$

So $S(\lambda_1(G)) \leqslant S(\frac{\sqrt{M_2}}{m})$, which implies that

$$\mathcal{E}(G) \leq \frac{\sqrt{M_2}}{m} + \sqrt{(n-1)(2m - \frac{M_2}{m})^2}.$$

If $G \cong \frac{n}{2}K_2$, then it is easy to check that the equality in (9) holds. Conversely, if the equality in (9) holds, then according to the above argument, we have

$$\lambda_1 = \frac{\sqrt{M_2}}{m}.$$

Moreover, $\mid \lambda_i \mid = \sqrt{\frac{2m-\lambda_1^2}{n-1}} \quad (2 \leqslant i \leqslant n)$. Since G is a non-empty graph, by Lemma 7, G has at least two distinct eigenvalues.

Suppose that absolute value of all eigenvalues of G are not equal. Then G has two distinct eigenvalues with different absolute values. By Lemma 7, $\mid \lambda_i \mid = 1 (2 \leqslant i \leqslant n)$. Since, $\sum_{i=1}^{n} \lambda_i = 0$ and $\lambda_2 = \lambda_3 = \cdots = \lambda_n = -1$, we have, $\lambda_1 = n - 1$. Hence λ_1 has multiplicity 1 and $\lambda_i = -1$ has multiplicity $n - 1$. By Lemma 7, G is the direct sum of a complete graph of order $\lambda_1 + 1 = n$. Consequently, G is K_n. But $\mathcal{E}(K_n) = n - 1 + (n-1) \times 1 = 2n - 2$ and $M_2(K_n) = n(n-1)/2(n-1)^2$, and so the equality in (9) does not hold for K_n, a contradiction. We deduce that the absolute value of all eigenvalues of G are equal. Then clearly $\lambda_1 = \mid \lambda_i \mid = \sqrt{\frac{2m-\lambda_1^2}{n-1}} \quad (2 \leqslant i \leqslant n)$, since G has at least two distinct eigenvalues. By Lemma 7, $\mid \lambda_i \mid = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1 (2 \leqslant i \leqslant n)$. Hence $2m = n$ and also, $\lambda_1 = \mid \lambda_2 \mid = \cdots = \mid \lambda_n \mid = 1$. By applying Lemma 7 again, we obtain that $m_2 = m_1\lambda_1, \lambda_1 = 1$, and therefore $m_1 = m_2$. Then we obtain that $\lambda_1 = 1$ has multiplicity $\frac{n}{2}$, and $\lambda_i = -1 \quad (2 \leqslant i \leqslant n)$ has multiplicity $\frac{n}{2}$. Therefore G is the direct sum of $m_1 = \frac{n}{2}$ complete graphs of order $\lambda_1 + 1 = 2$. Consequently, G is $\frac{n}{2}K_2$. ■

3.2 An upper bound in connected graphs

In the following we consider connected graphs.

Theorem 10 *Let G be a non-empty, connected graph with n vertices and m edges. Then*

$$\mathcal{E}(G) \leq 2\cos(\frac{\pi}{n+1}) + \sqrt{(n-1)(2m - (2\cos(\frac{\pi}{n+1}))^2)}, \tag{10}$$

equality holds if and only if $G \cong P_2$.

Proof. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{n-1} \geqslant \lambda_n$ be the eigenvalues of G. By the Cauchy-Schwartz inequality,

$$\sum_{i=2}^{n} |\lambda_i| \leqslant \sqrt{(n-1)\sum_{i=2}^{n}\lambda_i^2} = \sqrt{(n-1)(2m-\lambda_1^2)}.$$

Hence

$$\mathcal{E}(G) \leqslant \lambda_1 + \sqrt{(n-1)(2m-\lambda_1^2)}.$$

Note that the function $L(x) = x + \sqrt{(n-1)(2m-x^2)}$ decreases for $\sqrt{\frac{2m}{n}} \leqslant x \leqslant \sqrt{2m}$. By Lemma 4, we have $\lambda_1 \geqslant 2\cos(\frac{\pi}{n+1})$, with equality if and only if G is P_2. Thus, $\lambda_1 \geqslant 2\cos(\frac{\pi}{n+1}) \geqslant \sqrt{\frac{2m}{n}}$. So $L(\lambda_1(G)) \leqslant L(2\cos(\frac{\pi}{n+1}))$, which implies that

$$\mathcal{E}(G) \leq 2\cos(\frac{\pi}{n+1}) + \sqrt{(n-1)(2m-(2\cos(\frac{\pi}{n+1}))^2)}.$$

If $G \cong K_2$, then it is easy to check that the equality in (10) holds. Conversely, if the equality in (10) holds, then according to the above argument, we have

$$\lambda_1 = 2\cos(\frac{\pi}{n+1}).$$

Moreover, $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$ $(2 \leqslant i \leqslant n)$. Since G is a non-empty graph, by Lemma 7, G has at least two distinct eigenvalues. Suppose that the absolute value of all eigenvalues of G are not equal. Then G has two distinct eigenvalues with different absolute values. By Lemma 7, $|\lambda_i| = 1 (2 \leqslant i \leqslant n)$. Since, $\sum_{i=1}^{n}\lambda_i = 0$ and $\lambda_2 = \lambda_3 = \cdots = \lambda_n = -1$, we have, $\lambda_1 = n-1$. Hence λ_1 has multiplicity 1 and $\lambda_i = -1$ has multiplicity $n-1$. By Lemma 7, G is the direct sum of a complete graph of order $\lambda_1 + 1 = n$. Consequently, G is K_n. But $\mathcal{E}(K_n) = n-1+(n-1)\times 1 = 2n-2$ and $-1 \leqslant \cos x \leqslant 1$ for $x \in R$, and so we observe that the equality in (10) does not hold, a contradiction. We deduce that the absolute value of all eigenvalues of G are equal. Then clearly $\lambda_1 = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$ $(2 \leqslant i \leqslant n)$, since G has at least two distinct eigenvalues. By Lemma 7, $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1 (2 \leqslant i \leqslant n)$. Hence $2m = n$ and also, $\lambda_1 = |\lambda_2| = \cdots = |\lambda_n| = 1$. By applying Lemma 7 again, we obtain that $m_2 = m_1\lambda_1, \lambda_1 = 1$, and therefore $m_1 = m_2$. Then we obtain that $\lambda_1 = 1$ has multiplicity $\frac{n}{2}$, and $\lambda_i = -1$ $(2 \leqslant i \leqslant n)$ has multiplicity $\frac{n}{2}$. Therefore G is the direct sum of $m_1 = \frac{n}{2}$ complete graphs of order $\lambda_1 + 1 = 2$. Consequently, G is $\frac{n}{2}K_2$. Since G is a connected graph, therefore, $G \cong K_2$. ■

Note that since the function $L(x) = x + \sqrt{(n-1)(2m-x^2)}$ decreases for $\sqrt{\frac{2m}{n}} \leqslant x \leqslant \sqrt{2m}$, the bound of Theorem 10 is another improvement of the bound given in (2) for connected graphs.

3.3 An upper bound in connected unicyclic graphs

We next give an upper bound for the energy in connected unicyclic graphs.

Theorem 11 *Let G be a non-empty, connected unicyclic graph with n vertices and m edges. Then*

$$\mathcal{E}(G) \leq 2 + \sqrt{(n-1)(2m-4)}, \tag{11}$$

equality holds if and only if $G \cong C_3$.

Proof. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{n-1} \geqslant \lambda_n$ be the eigenvalues of G. By the Cauchy-Schwartz inequality,

$$\sum_{i=2}^{n} |\lambda_i| \leqslant \sqrt{(n-1)\sum_{i=2}^{n}\lambda_i^2} = \sqrt{(n-1)(2m-\lambda_1^2)}.$$

Hence

$$\mathcal{E}(G) \leqslant \lambda_1 + \sqrt{(n-1)(2m-\lambda_1^2)}.$$

Note that the function $G(x) = x + \sqrt{(n-1)(2m-x^2)}$ decreases for $\sqrt{\frac{2m}{n}} \leqslant x \leqslant \sqrt{2m}$. By Lemma 3, we have $\lambda_1 \geqslant 2$, equality holds if and only if G is C_n. Thus, $\lambda_1 \geqslant 2 \geqslant \sqrt{\frac{2m}{n}}$. So $G(\lambda_1(G)) \leqslant G(2)$, which implies that

$$\mathcal{E}(G) \leq 2 + \sqrt{(n-1)(2m-4)}.$$

If $G \cong K_3$, then it is easy to check that the equality in (11) holds. Conversely, if the equality in (11) holds, then according to the above argument, we have $\lambda_1 = 2$. Since G is a non-empty graph, by Lemma 7, G has at least two distinct eigenvalues.

Suppose that the absolute value of all eigenvalues of G are equal. Then clearly $\lambda_1 = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$ $(2 \leqslant i \leqslant n)$, since G has at least two distinct eigenvalues. By Lemma 7, $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1 (2 \leqslant i \leqslant n)$. Hence $2m = n$ and also, $\lambda_1 = |\lambda_2| = \cdots = |\lambda_n| = 1$. By applying Lemma 7 again, we obtain that $m_2 = m_1\lambda_1, \lambda_1 = 1$, and therefore $m_1 = m_2$. Then we obtain that $\lambda_1 = 1$ has multiplicity $\frac{n}{2}$, and $\lambda_i = -1 \quad (2 \leqslant i \leqslant n)$ has multiplicity $\frac{n}{2}$. Therefore G is the direct sum of $m_1 = \frac{n}{2}$ complete graphs of order $\lambda_1 + 1 = 2$. Consequently, G is $\frac{n}{2}K_2$. This is a contradiction, since G is a unicyclic graph. We deduce that the absolute value of all eigenvalues of G are not equal. Then G has two distinct eigenvalues with different absolute values. By Lemma 7, $|\lambda_i| = 1 (2 \leqslant i \leqslant n)$. Since, $\sum_{i=1}^{n}\lambda_i = 0$ and $\lambda_2 = \lambda_3 = \cdots = \lambda_n = -1$, we have, $\lambda_1 = n-1$. Hence λ_1 has multiplicity

1 and $\lambda_i = -1$ has multiplicity $n-1$. By Lemma 7, G is the direct sum of a complete graph of order $\lambda_1+1 = n$. Consequently, G is K_n. Since G is a connected unicyclic graph, therefore, $G \cong K_3$. ■

Note that since the function $G(x) = x + \sqrt{(n-1)(2m-x^2)}$ is decreasing for $\sqrt{\frac{2m}{n}} \leqslant x \leqslant \sqrt{2m}$, a simple calculation shows that the bound of Theorem 11 is an improvement of the bound given in (1) for connected unicyclic graphs.

3.4 Upper bounds in bipartite graphs

In this subsection, we present upper bounds for the energy of a bipartite graph. In the following we give an upper bound is in terms of order, size, maximum and minimum degree of a graph.

Theorem 12 *Let G be a non-empty bipartite graph with $n \geqslant 2$ vertices, m edges and maximum vertex degrees Δ. Then*

$$\mathcal{E}(G) \leq 2\sqrt{\Delta} + \sqrt{(n-2)(2m-2\Delta)}, \tag{12}$$

equality holds if and only if one of the following statements holds:
(1) $G \cong \frac{n}{2}K_2$, $(n = 2m)$;
(2) $K_{1,r-1} \bigcup (n-1-r_{n-1})K_1$.

Proof. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{n-1} \geqslant \lambda_n$ be the eigenvalues of G. Since G is a bipartite graph, we have $\lambda_1 = -\lambda_n$. By the Cauchy-Schwartz inequality,

$$\sum_{i=2}^{n-1} |\lambda_i| \leqslant \sqrt{(n-2)\sum_{i=2}^{n-1}\lambda_i^2} = \sqrt{(n-2)(2m-2\lambda_1^2)}.$$

Hence

$$\mathcal{E}(G) \leqslant 2\lambda_1 + \sqrt{(n-2)(2m-2\lambda_1^2)}.$$

It is not diffcult to see that $H(x) = 2x + \sqrt{(n-2)(2m-2x^2)}$ decreases for $\sqrt{\frac{2m}{n}} \leqslant x \leqslant \sqrt{2m}$. By Lemma 1, we have $\lambda_1 \geqslant \sqrt{\Delta}$, with equality if and only if G is $\frac{n}{2}K_2$. Clearly, $\Delta \geqslant \frac{2m}{n}$. By Lemma 1, we have

$$\lambda_1 \geqslant \sqrt{\Delta} \geqslant \sqrt{\frac{2m}{n}}.$$

So $H(\lambda_1(G)) \leqslant H(\sqrt{\Delta})$, which implies that

$$\mathcal{E}(G) \leq 2\sqrt{\Delta} + \sqrt{(n-2)(2m-2\Delta)}.$$

If G is one of the two graphs shown in the second part of the theorem, then it is easy to check that the equality in (12) holds. Conversely, if the equality in (12) holds, then according to the above argument, we have $\lambda_1 = -\lambda_n = \sqrt{\Delta}$. Moreover, $|\ \lambda_i\ | = \sqrt{\frac{2m-\lambda_1^2}{n-2}}$ $(2 \leqslant i \leqslant n-1)$. Since G is a non-empty graph, by Lemma 7, G has at least two distinct eigenvalues. We consider the following case.

Case 1. The absolute value of all eigenvalues of G are equal.

Note that $\lambda_1 = -\lambda_n =|\ \lambda_i\ |= \sqrt{\frac{2m-\lambda_1^2}{n-2}}$ $(2 \leqslant i \leqslant n-1)$. By Lemma 7, $\lambda_n = -\sqrt{\frac{2m-\lambda_1^2}{n-2}} = |\lambda_i| = -1$ $(2 \leqslant i \leqslant n-1)$. Hence $2m = n$ and also, $\lambda_1 =|\ \lambda_2\ |= \cdots =|\ \lambda_n\ |= 1$. By Lemma 7, $m_2 = m_1\lambda_1, \lambda_1 = 1$, and therefore $m_1 = m_2$. Then we obtain that $\lambda_1 = 1$ has multiplicity $\frac{n}{2}$, and $\lambda_i = -1 \quad (2 \leqslant i \leqslant n)$ has multiplicity $\frac{n}{2}$. Therefore G is the direct sum of $m_1 = \frac{n}{2}$ complete graphs of order $\lambda_1 + 1 = 2$. Consequently, G is $\frac{n}{2}K_2$.

Case 2. The absolute value of all eigenvalues of G are not equal. If two eigenvalues of G have different absolute values, then by Lemma 7, $|\ \lambda_i\ | = -1 (2 \leqslant i \leqslant n)$. Noting that G is a bipartite graph, we have $\lambda_1 = -\lambda_n$, that is a contradiction, since the two eigenvalues of G have different absolute values. Thus assume that G has three distinct eigenvalues. Since G is a bipartite graph, we have that $\lambda_1 = -\lambda_n \neq 0$ and $\sum_{i=1}^{n} \lambda_i = 0$, and therefore, $\lambda_i = 0 (2 \leqslant i \leqslant n-1)$. Thus $\mathcal{E}(G) = 2\lambda_1$, and by Lemma 6, we have that $2\lambda_1 \geqslant 2\sqrt{m}$, and so $2\lambda_1^2 \geqslant 2m$. Notice that $2m = \sum_{i=1}^{n} \lambda_i^2 = 2\lambda_1^2$. Therefore $\lambda_1 = \sqrt{m}$ and $\mathcal{E}(G) = 2\sqrt{m}$. Hence by Lemma 6, G is a complete bipartite graph plus arbitrarily many isolated vertices. Thus, there exist integers $r_1 \geqslant 1$ and $r_2 \geqslant 2$ such that G is $K_{r_1,r_2} \cup (n - r_1 - r_2)K_1$. ■

We remark that since the function $H(x) = 2x + \sqrt{(n-2)(2m-2x^2)}$ is decreasing for $\sqrt{\frac{2m}{n}} \leqslant x \leqslant \sqrt{2m}$, the bound of Theorem 12 is an improvement of the bound given in (3) for bipartite graphs.

The next bound involves the first and the second zagreb indices.

Theorem 13 *Let G be a non-empty bipartite graph with $n \geqslant 2$ vertices and m edges. Then*

$$\mathcal{E}(G) \leq 2\frac{\sqrt{M_2}}{m} + \sqrt{(n-2)(2m - 2\frac{M_2}{m^2})}, \tag{13}$$

equality holds if and only $G \cong \frac{n}{2}K_2$, $(n = 2m)$.

Proof. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{n-1} \geqslant \lambda_n$ be the eigenvalues of G. By the *Cauchy* $-$

Schwartz inequality,

$$\sum_{i=2}^{n-1} \mid \lambda_i \mid \leqslant \sqrt{(n-2)\sum_{i=2}^{n-1} \lambda_i^2} = \sqrt{(n-2)(2m-2\lambda_1^2)}.$$

Hence

$$\mathcal{E}(G) \leqslant 2\lambda_1 + \sqrt{(n-2)(2m-2\lambda_1^2)}.$$

Note that the function $N(x) = 2x + \sqrt{(n-1)(2m-x^2)}$ decreases for $\frac{2m}{n^2} \leqslant x \leqslant 2m$. By Lemma 2, we have

$$\lambda_1 \geqslant \frac{\sqrt{M_2}}{m},$$

equality holds if and only if G is $\frac{n}{2}K_2$. By Lemmas 2 and 5, we have

$$\lambda_1 \geqslant \frac{\sqrt{M_2}}{m} \geqslant \frac{2m}{n^2}.$$

So $N(\lambda_1(G)) \leqslant N(\frac{\sqrt{M_2}}{m})$, which implies

$$\mathcal{E}(G) \leq 2\frac{\sqrt{M_2}}{m} + \sqrt{(n-2)(2m-2\frac{M_2}{m^2})}.$$

If $G \cong \frac{n}{2}K_2$ it is easy to check that the equality in (13) holds. Conversely, if the equality in (13) holds, according to the above argument, we have $\lambda_1 = -\lambda_n = \frac{\sqrt{M_2}}{m}$. Moreover, $\mid \lambda_i \mid = \sqrt{\frac{2m-\lambda_1^2}{n-2}}$ $(2 \leqslant i \leqslant n-1)$. Since G is a non-empty graph, by Lemma 7, G has at least two distinct eigenvalues. Suppose that the absolute value of all eigenvalues of G are not equal. If two eigenvalues of G have different absolute values, then by Lemma 7, $\mid \lambda_i \mid = -1 (2 \leqslant i \leqslant n)$. Noting that G is a bipartite graph, we have $\lambda_1 = -\lambda_n$, this is a contradiction. We deduce that the absolute value of all eigenvalues of G are equal. Note that $\lambda_1 = -\lambda_n = \mid \lambda_i \mid = \sqrt{\frac{2m-\lambda_1^2}{n-2}}$ $(2 \leqslant i \leqslant n-1)$. By Lemma 7, $\lambda_n = -\sqrt{\frac{2m-\lambda_1^2}{n-2}} = \|\lambda_i| = -1$ $(2 \leqslant i \leqslant n-1)$. Hence $2m = n$ and also, $\lambda_1 = \mid \lambda_2 \mid = \cdots = \mid \lambda_n \mid = 1$. By Lemma 7, $m_2 = m_1\lambda_1, \lambda_1 = 1$, and therefore $m_1 = m_2$. Then we obtain that $\lambda_1 = 1$ has multiplicity $\frac{n}{2}$, and $\lambda_i = -1 \quad (2 \leqslant i \leqslant n)$ has multiplicity $\frac{n}{2}$. Therefore G is the direct sum of $m_1 = \frac{n}{2}$ complete graphs of order $\lambda_1 + 1 = 2$. Consequently, G is $\frac{n}{2}K_2$. ■

3.5 An upper bounds in connected bipartite graphs

Theorem 14 *Let G be a non-empty connected bipartite graph with n vertices and m edges. Then*

$$\mathcal{E}(G) \leq 4\cos(\frac{\pi}{n+1}) + \sqrt{(n-2)(2m-2(2\cos(\frac{\pi}{n+1}))^2)}, \tag{14}$$

equality holds if and only if one of the following statements holds:

(1) $G \cong P_2(K_2)$*;*

(2) $G \cong P_3(K_{1,2})$*.*

Proof. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{n-1} \geqslant \lambda_n$ be the eigenvalues of G. By the Cauchy-Schwartz inequality,

$$\sum_{i=2}^{n-1} \mid \lambda_i \mid \leqslant \sqrt{(n-2)\sum_{i=2}^{n-1} \lambda_i^2} = \sqrt{(n-2)(2m-2\lambda_1^2)}.$$

Hence

$$\mathcal{E}(G) \leqslant 2\lambda_1 + \sqrt{(n-2)(2m-2\lambda_1^2)}.$$

Note that the function $D(x) = 2x + \sqrt{(n-1)(2m-x^2)}$ decreases for $\sqrt{\frac{2m}{n}} \leqslant x \leqslant \sqrt{2m}$. By Lemma 4, we have

$$\lambda_1 \geqslant 2\cos(\frac{\pi}{n+1}),$$

equality holds if and only if G is P_2. Then

$$\lambda_1 \geqslant 2\cos(\frac{\pi}{n+1}) \geqslant \sqrt{\frac{2m}{n}}.$$

So $D(\lambda_1(G)) \leqslant D(2\cos(\frac{\pi}{n+1}))$, which implies that

$$\mathcal{E}(G) \leq 2\cos(\frac{\pi}{n+1}) + \sqrt{(n-1)(2m-(2\cos(\frac{\pi}{n+1}))^2)}.$$

If G is one of the two graphs shown in the second part of the theorem, then it is easy to check that the equality in (14) holds. Conversely, if the equality in (14) holds, according to the above argument, we have that $\lambda_1 = -\lambda_n = 2\cos(\frac{\pi}{n+1})$. Moreover, $\mid \lambda_i \mid = \sqrt{\frac{2m-\lambda_1^2}{n-2}}$ $(2 \leqslant i \leqslant n-1)$. Since G is a non-empty graph, by Lemma 7, G has at least two distinct eigenvalues. We consider the following case.

Case 1. The absolute value of all eigenvalues of G are equal.
Note that $\lambda_1 = -\lambda_n = \mid \lambda_i \mid = \sqrt{\frac{2m-\lambda_1^2}{n-2}}$ $(2 \leqslant i \leqslant n-1)$. By Lemma 7, $\lambda_n = -\sqrt{\frac{2m-\lambda_1^2}{n-2}} = \||\lambda_i| = -1$ $(2 \leqslant i \leqslant n-1)$. Hence $2m = n$ and also, $\lambda_1 = \mid \lambda_2 \mid = \cdots = \mid \lambda_n \mid = 1$. By Lemma 7, $m_2 = m_1\lambda_1, \lambda_1 = 1$, and therefore $m_1 = m_2$. Then we obtain that $\lambda_1 = 1$ has multiplicity $\frac{n}{2}$, and $\lambda_i = -1 \quad (2 \leqslant i \leqslant n)$ has multiplicity $\frac{n}{2}$. Therefore G is the direct sum of $m_1 = \frac{n}{2}$ complete graphs of order $\lambda_1 + 1 = 2$. Consequently, G is $\frac{n}{2}K_2$. Since G is a connected bipartite graph, therefore $G \cong K_2$.

Case 2. The absolute value of all eigenvalues of G are not equal. If two eigenvalues of G have different absolute values, then by Lemma 7, $\mid \lambda_i \mid = -1 (2 \leqslant i \leqslant n)$. Noting that G is a bipartite graph, we have $\lambda_1 = -\lambda_n$, that is a contradiction, since the two eigenvalues of G have different absolute values. Thus assume that G has three distinct eigenvalues. Since G is a bipartite graph, we have that $\lambda_1 = -\lambda_n \neq 0$ and $\sum_{i=1}^{n} \lambda_i = 0$, and therefore, $\lambda_i = 0 (2 \leqslant i \leqslant n-1)$. Thus $\mathcal{E}(G) = 2\lambda_1$, and by Lemma 6, we have that $2\lambda_1 \geqslant 2\sqrt{m}$, and so $2\lambda_1^2 \geqslant 2m$. Notice that $2m = \sum_{i=1}^{n} \lambda_i^2 = 2\lambda_1^2$. Therefore $\lambda_1 = \sqrt{m}$ and $\mathcal{E}(G) = 2\sqrt{m}$. Hence by Lemma 6, G is a complete bipartite graph plus arbitrarily many isolated vertices. Thus, there exist integers $r_1 \geqslant 1$ and $r_2 \geqslant 2$ such that G is $K_{r_1,r_2} \cup (n-r_1-r_2)K_1$. Hence, for $r_1 = 1$ and $r_2 = 2$, we have $G \cong K_{1,2} \cup (n-r_1-r_2)K_1$. ■

Note that since the function $D(x) = 2x + \sqrt{(n-1)(2m-x^2)}$ is decreasing for $\sqrt{\frac{2m}{n}} \leqslant x \leqslant \sqrt{2m}$, the bound of Theorem 14 is another improvement of the bound given in (3) for conneted bipartite graphs.

Acknowledgements: We would like to thank the referee for his/her careful review of the paper and some helpful comments.

References

[1] D. Babić, I. Gutman, More lower bounds for the total π-electron energy of alternant hydrocarbons, *MATCH Commun. Math. Comput. Chem.* **32** (1995) 7–17.

[2] G. Caporossi, D. Cvetković, I. Gutman, P. Hansen, Variable neighbourhood search for extremal graphs. 2. Finding graphs with extremal energy, *J. Chem. Inf. Comput. Sci.* **39** (1999) 984–996.

[3] L. Collatz, U. Sinogowitz, Spektren Endlicher Grafen, *Abh. Math. Sem. Univ. Hamburg.* **21** (1957) 63–77.

[4] D. Cvetković, M. Doob, H. Sachs, *Spectra of Graphs Theory and Applications*, Academic Press, New York, 1980.

[5] O. Favaron, M. Mahéo, J. F. Saclé, Some eigenvalue properties in graphs, *Discr. Math.* **111** (1993) 197–220.

[6] I. Gutman, Bounds for total π-electron energy, *Chem. Phys. Lett.* **24** (1974) 283–285.

[7] I. Gutman, 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. Gutman, O. E. Polansky, *Mathatical Concepts in Organic Chemistry*, Springer, Berlin, 1986.

[9] I. Gutman, A. V. Teodorović, L. Nedeljković, Topological properties of benzenoid systems, bounds and approximate formula for total π-electron energy, *Theor. Chim. Acta.* **65** (1984) 23–31.

[10] I. Gutman, K. C. Das, The first Zagreb index 30 years after, *MATCH Commun. Math. Comput. Chem.* **50** (2004) 83–92.

[11] Y. Hong, On the spectra of unicyclic graph, *J. East China Norm. Univ. Natur. Sci. Ed.* **1** (1986) 31–34.

[12] A. Jahanbani, Some new lower bounds for energy of graphs, *Appl. Math. Comput.* **296** (2017) 233–238.

[13] J. H. Koolen, V. Moulton, Maximal energy graphs, *Adv. Appl. Math.* **26** (2001) 47–52.

[14] J. H. Koolen, V. Moulton, Maximal energy bipartite graphs, *Graphs Comb.* **19** (2003) 131–135.

[15] J. H. Koolen, V. Moulton, I. Gutman, Improving the McClelland inequality for total π-electron energy, *Chem. Phys. Lett.* **320** (2000) 213–216.

[16] X. Li, Y. Shi, I. Gutman, *Graph Energy*, Springer, New York, 2010.

[17] B. Liu, Z. You, A survey on comparing Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **65** (2011) 581–593.

[18] B. J. McClelland, Properties of the latent roots of a matrix: The estimation of π-electron energies, *J. Chem. Phys.* **54** (1971) 640–643.

[19] D. B. West, *Introduction to Graph Theory*, Prentice Hall, 2001.

[20] B. Zhou, Energy of a graph, *MATCH Commun. Math. Comput. Chem.* **51** (2004) 111–118.

[21] B. Zhou, I. Gutman, Further properties of Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **54** (2005) 233–239.

[22] B. Zhou, Remarks on Zagreb indices, *MATCH Commun. Math. Comput. Chem.* **57** (2007) 591–596.