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# Koolen–Moulton–Type Upper Bounds on the Energy of a Graph

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#### Abstract

The energy of a graph G, denoted by E(G), is defined as the sum of the absolute values of all eigenvalues of G. In this paper, using a Koolen and Moulton demonstration technique, new lower bounds are obtained for the energy of a graph G, that depends only the number of vertices, the number of edges, degree sequence and the spread of adjacency matrix of a graph given.

# 1 Introduction

Let  $G = (V, \mathbf{E})$  be a simple undirected graph with vertex set  $V = V(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set  $\mathbf{E}(G)$ . The order and size of G are n = |V| and  $m = |\mathbf{E}|$ , respectively. An independent set in G is a set of vertices, no two of which are adjacent. The size of the largest coclique (independent set of vertices) of G is denoted by  $\alpha(G)$ , short for  $\alpha$ . Let vertex degrees  $d_1, d_2, \ldots, d_n$  and  $d_1, d_n$  be the highest and the lowest degree of the vertices of G, respectively. 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 the end vertices of each edge in G are in distinct sets X and Y. 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  $K_n$ . A graph G is regular if there exists a constant k such that each vertex of G has

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degree k, such graphs are also called k-regular. A graph is said to be triangle-free if no two adjacent vertices are adjacent to a common vertex. For more graph theory notation and terminology we refer to [22]. The *adjacency matrix* A(G) of a graph G is defined by its entries as  $a_{ij} = 1$  if  $v_i v_j \in \mathbf{E}(G)$  and 0 otherwise. Let  $\lambda_1, \lambda_2, \ldots, \lambda_n$  denote the *eigenvalues* of A(G). The eigenvalue  $\lambda_1$  is called the *spectral radius* of G. For a matrix A of order n, the *spread*, S(A), of A is defined as the diameter of its spectrum, i.e.,

$$S(A) := \max_{i,j} |\lambda_i - \lambda_j|,$$

where the maximum is taken over all pairs of eigenvalues of A. Suppose A is the adjacency matrix of a simple graph G with n vertices. Since A is a real and symmetric matrix, we always assume the eigenvalues of A are ordering decreasing way, ie,  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$ . Then we can claim that the spread of graph G coincides with the spread of your adjacency matrix, ie;  $S(A) = \lambda_1 - \lambda_n$  and S(A) = S(G). When more than one graphs are under consideration, then we write  $\lambda_i(G)$  instead of  $\lambda_i$ .

The *energy* of a graph G is defined as

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

This concept was introduced by I. Gutman and is intensively studied in chemistry, since it can be used to approximate the total  $\pi$ -electron energy of a molecule (see, e.g. [10,11]). In 1971, McClelland [21], discovered the first upper bound for E(G)

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

Since then, numerous other bounds for E(G) were found (see, e.g. [1, 2, 9, 10, 13-15]and [12]- [19]). Here we just state some upper bounds for E(G) which were obtained recently. A fundamental bound for the theory of energy of a graph is due to Koolen and Moulton [16], they showed that if  $m \ge \frac{n}{2}$  and G is a graph with n vertices, m edges, then

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

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The same authors showed then that if  $m \ge \frac{n}{2}$  and G is a bipartite graph with n > 2 vertices, m edges, then

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

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- $(\nu, k, \lambda)$ -design with  $k = \frac{2m}{n}$  and  $\lambda = \frac{k(k-1)}{\nu-1}(n = 2\nu)$ .

Yu, et al. [24], proved that if G be a nonempty graph with n vertices, m edges, degree sequence  $d_1, d_2, \ldots, d_n$  and 2-degree sequence  $t_1, t_2, \ldots, t_n$ . Then

$$E(G) \le \sqrt{\frac{\sum_{i=1}^{n} t_i^2}{\sum_{i=1}^{n} d_i^2}} + \sqrt{(n-1)\left(2m - \frac{\sum_{i=1}^{n} t_i^2}{\sum_{i=1}^{n} d_i^2}\right)}.$$

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

- (1)  $G \cong \frac{n}{2}K_2$ ,
- (2)  $G \cong K_n$ ,

(3) G is a non-bipartite connected p-pseudo-regular graph with three distinct eigenvalues  $(p, \sqrt{\frac{2m-p^2}{n-1}}, -\sqrt{\frac{2m-p^2}{n-1}})$ , where  $p > \sqrt{\frac{2m}{n}}$ .

Yu, et al. [24], also proved that if G = (X, Y) be a nonempty bipartite graph with n > 2 vertices, m edges, degree sequence  $d_1, d_2, \ldots, d_n$  and 2-degree sequence  $t_1, t_2, \ldots, t_n$ . Then

$$E(G) \le 2\sqrt{\frac{\sum_{i=1}^{n} t_i^2}{\sum_{i=1}^{n} d_i^2}} + \sqrt{(n-2)\left(2m - 2\frac{\sum_{i=1}^{n} t_i^2}{\sum_{i=1}^{n} d_i^2}\right)}.$$

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

- (1)  $G \cong \frac{n}{2}K_2$ ,
- (2)  $G \cong K_{r_1,r_2}(n-r_1-r_2)K_1$ , where  $r_1r_2 = m$ ;

(3) G is a connected  $(p_x, p_y)$ -pseudo-semiregular bipartite graph with four distinct eigenvalues  $\left(\sqrt{p_x p_y}, \sqrt{\frac{2m-2p_x p_y}{n-2}}, -\sqrt{\frac{2m-2p_x p_y}{n-2}}, -\sqrt{p_x p_y}\right)$ , where  $\sqrt{p_x p_y} > \sqrt{\frac{2m}{n}}$ .

Zhou [25], proved that if G is a graph with n vertices, m edges and degree sequence  $d_1, d_2, \ldots, d_n$ , then

$$E(G) \le \sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}} + \sqrt{(n-1)\left(2m - \frac{\sum_{i=1}^{n} d_i^2}{n}\right)},\tag{4}$$

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

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value  $\sqrt{\frac{2m-(\frac{2m}{n})^2}{(n-1)}}$  or  $nK_1$ . Zhou [25], 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

$$E(G) \le 2\sqrt{\frac{\sum_{i=1}^{n} d_i^2}{n}} + \sqrt{(n-2)\left(2m - \frac{2\sum_{i=1}^{n} d_i^2}{n}\right)},\tag{5}$$

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 new upper bounds for the energy of graphs in terms of several graph invariants such as the number of vertices, number of edges, maximum degree and spread of the graph. The demonstration technique used in this paper for boundary the energy of a graph, in addition to considering the Koolen and Moulton technique, consists of making the difference between the spectral radius and the lower eigenvalue associated with a graph appear, that is, intrinsically consider the definition of the spread of the graph. With this, our results improve those already existing in the literature.

The organization of the paper is as follows. In the Section 2, we give a list of some previously known results. In Section 3, we present our main results about 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, bipartite graphs, connected graphs, triangle-free graphs, regular graphs. Finally, some computational experiments are presented.

## 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 eigenvalues of a graph.

**Lemma 1** [7] Let G be a graph with  $n \ge 2$  vertices and m edges. Then for  $1 \le r \le n$ , we have

$$\sqrt{\frac{2m(n-1)}{nr}} \ge \lambda_r \ge -\sqrt{\frac{2m(r-1)}{n(n-r+1)}}$$

**Lemma 2** [7] Let G be a triangle-free graph with  $n \ge 2$  vertices, m edges. Then for  $1 \le r \le n$ , we have

$$\sqrt{\frac{2m}{t+t^{\frac{2}{3}}}} \geqslant \lambda_r \geqslant -\sqrt{\frac{2m}{t+t^{\frac{2}{3}}}},$$

where t = n - r + 1.

**Theorem 3** [7] Let G be a graph with with n vertices, m edges and  $n_+$ ,  $n_-$  be the number of positive and negative eigenvalues, respectively. Then for  $1 \le r \le n$ , we have

$$\sqrt{\frac{2mn_-}{r(r+n_-)}} \geqslant \lambda_r \geqslant -\sqrt{\frac{2mn_+}{(n-r+1)(n-r+1+n_+)}}.$$

We next state some results on the spectral radius and the smallest eigenvalue of a graph.

**Theorem 4** [23] Let G be a simple graph with n vertices and degree sequence  $d_1 \ge d_2 \ge \dots \ge d_n$ . Then

$$\lambda_1 \geqslant \frac{(d_1 + d_2)}{\sqrt{2n}}.$$

**Theorem 5** [23] Let G be a bipartite graph with n vertices and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ . Then

$$\begin{split} 1) \ \lambda_1 &\ge \frac{1}{2} (\frac{(d_1+d_2)}{\sqrt{2n}} + \sqrt{d_1}), \\ 2) \ \lambda_1 &\ge \frac{1}{2} (\nu + \sqrt{d_1}) \\ where \ \nu &= \sqrt{\frac{\sum_{i=1}^n d_i^2}{n} - \left(\sum_{i=1}^n \frac{d_i}{n}\right)^2}. \end{split}$$

**Lemma 6** [6] Let G be a simple connected graph with n vertices, m edges and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ . Then

1) 
$$\lambda_1(G) \leq \sqrt{2m - (n-1)d_n + (d_n - 1)d_1},$$
  
2)  $\lambda_n(G) \geq -\sqrt{2m - (n-1)d_n + (d_n - 1)d_1}.$ 

**Lemma 7** [3] Let G be a simple connected graph with n vertices, then

$$\lambda_1 \leq n-1.$$

**Lemma 8** [4] Let G be a simple graph with n vertices, then

$$\lambda_n \geqslant -\sqrt{\frac{2m(n-1)}{n}}$$

**Lemma 9** [5] 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  $m_2 = m_1\mu_1$ .

**Theorem 10** [8] Let G be a graph with n vertices and m edges, then

$$S(G) \leq 2\sqrt{m}$$
.

**Lemma 11** [20] Let G be a k-regular graph with n vertices, m edges and  $\alpha$  independent set of vertices, then

$$S(G) \ge \frac{nk}{n-\alpha}$$

**Lemma 12** [8] Let G be a regular graph, then  $S(G) \leq n$  with equality if and only if  $\overline{G}$  is disconnected.

**Lemma 13** [8] Let G be a triangle-free graph with n vertices and m edges, then

$$S(G) \geqslant \frac{2m}{n} + \sqrt{d_1}$$

**Lemma 14** [20] Let G be a contains  $t(t \ge 1)$  independent vertices, the average degree of which is  $d_0$ , then

$$S(G) \ge 2d_0\sqrt{\frac{t}{n-t}}$$
.

**Theorem 15** [8] Let G be a graph with n vertices and m edges, then

$$S(G) \leqslant \frac{(1+\sqrt{2})n}{2}.$$

**Theorem 16** [23] Let G be a simple graph with n vertices and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ , then

$$S(G) \ge \left(\frac{(d_1+d_2)}{\sqrt{2n}} + \sqrt{d_1}\right).$$

**Corollary 17** [20] Let G be a graph with n vertices, independent set of vertices of cardinality  $\alpha(G)$  and the minimum vertex degree  $\delta$ , then

$$S(G) \ge 2\delta \sqrt{\frac{\alpha(G)}{n - \alpha(G)}}$$
.

If equality holds, then the graph is a semi-regular bipartite graph.

# 3 Upper Bounds for the Energy of Graphs

In this section, we present new upper bounds obtain for the energy of graphs. We deal with general graphs, bipartite graphs, connected graphs, triangle-free graphs and regular graphs. We divide this section into five subsections depending on the kind of graphs to studying.

### 3.1 Upper bound in general graphs

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

**Theorem 18** Let G be a non-empty graph with n vertices, m edges and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ . Then

$$E(G) \leqslant 2\sqrt{\frac{2m(n-1)}{n}}.$$
(6)

Equality holds if and only if  $G \cong K_n$ .

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

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

Hence

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

Note that the function  $F(x) = x + \sqrt{(n-1)(2m-x^2)}$  decreases for  $\sqrt{\frac{1}{2n}} \leq x \leq \sqrt{2m}$ . By Lemma 1, we have  $\lambda_1 \leq \sqrt{\frac{2m(n-1)}{n}}$ . Clearly,  $\sqrt{\frac{2m(n-1)}{n}} \leq \sqrt{2m}$ . Thereby,

$$\lambda_1 \leqslant \sqrt{\frac{2m(n-1)}{n}} \leqslant \sqrt{2m}$$
.

So  $F(\lambda_1(G)) \leq F(\sqrt{\frac{2m(n-1)}{n}})$ , which implies that

$$E(G) \le \sqrt{\frac{2m(n-1)}{n}} + \sqrt{(n-1)\left(2m - \left(\sqrt{\frac{2m(n-1)}{n}}\right)^2\right)}$$

If  $G \cong K_n$ , then it is easy to check that the equality in (6) holds. Conversely, if the equality in (6) holds, then according to the above argument, we have  $\lambda_1 = \sqrt{\frac{2m(n-1)}{n}}$ . Moreover,  $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$  ( $2 \le i \le n$ ). Since G is a non-empty graph, by Lemma 9, 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  $\lambda_1 = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}, (2 \leq i \leq n)$ , since G has at least two distinct eigenvalues. By Lemma 9,  $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1(2 \leq i \leq n)$ . Hence 2m = n(n-1) and also,  $|\lambda_2| = \ldots = |\lambda_n| = 1$ , then applying Lemma 9 again, we obtain that  $m_2 = m_1\lambda_1, \lambda_1 = n-1$ , and therefore  $m_1 = m_2$ . Then we obtain that  $\lambda_1 = n-1$  has multiplicity 1, and

 $\lambda_i = -1$  ( $2 \leq i \leq n$ ) has multiplicity n-1. Therefore G is the direct sum of  $m_1 = n-1$  complete graphs of order  $\lambda_1 + 1 = n$ . Thereby, G is  $K_n$ .

**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 9,  $|\lambda_i| = 1 (2 \le i \le n)$ . Since,  $\sum_{i=1}^{n} \lambda_i = 0$  and  $\lambda_2 = \lambda_3 = \ldots = \lambda_n = -1$ , we have,  $\lambda_1 = n - 1$ . Hence  $\lambda_1$  has multiplicity 1 and  $\lambda_i = -1$  has multiplicity n - 1. By Lemma 9, G is the direct sum of a complete graph of order  $\lambda_1 + 1 = n$ . Consequently, G is  $K_n$ .

**Theorem 19** Let G be a graph with  $n \ge 2$  vertices, m edges and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ , then

$$E(G) \leq 2\sqrt{m} + \sqrt{(n-2)\left[2m + 2\left(\left(\frac{d_1 + d_2}{\sqrt{2n}}\right)\sqrt{\frac{2m(n-1)}{n}}\right) - \left(\frac{(d_1 + d_2)}{\sqrt{2n}} + \sqrt{d_1}\right)^2\right]}.$$
(7)

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

**Proof.** Let  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$  be the eigenvalues of *G*. From Cauchy-Schwarz inequality, we have that

$$\sum_{i=1}^{n} |\lambda_i| = |\lambda_1| + |\lambda_n| + \sum_{i=2}^{n-1} |\lambda_i|$$

$$\leq \lambda_1 - \lambda_n + \sqrt{(n-2)\sum_{i=2}^{n-1} \lambda_i^2}$$

$$= \lambda_1 - \lambda_n + \sqrt{(n-2)\left(\sum_{i=1}^{n} \lambda_i^2 - \lambda_1^2 - \lambda_n^2\right)}$$

$$= \lambda_1 - \lambda_n + \sqrt{(n-2)\left(2m - \lambda_1^2 - \lambda_n^2\right)}$$

$$= \lambda_1 - \lambda_n + \sqrt{(n-2)\left(2m - (\lambda_1 - \lambda_n)^2 - 2\lambda_1\lambda_n\right)}$$

Then by Lemma 1, Theorems 4, 10 and 16 we have that

$$E(G) \leq 2\sqrt{m} + \sqrt{(n-2)\left[2m + 2\left((\frac{d_1+d_2}{\sqrt{2n}})\sqrt{\frac{2m(n-1)}{n}}\right) - \left(\frac{(d_1+d_2)}{\sqrt{2n}} + \sqrt{d_1}\right)^2\right]}.$$

If  $G \cong \frac{n}{2}K_2$ , then it is easy to check that the equality in (7) holds. Conversely, since G is a non-empty graph, by Lemma 9, 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  $\lambda_1 = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$   $(2 \leq i \leq n)$ , since *G* has at least two distinct eigenvalues. By Lemma 9,  $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1$   $(2 \leq i \leq n)$ . Hence 2m = n and also,  $\lambda_1 = |\lambda_2| = \ldots = |\lambda_n| = 1$ . By applying Lemma 9 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  $(2 \leq i \leq n)$  has multiplicity  $\frac{n}{2}$ . Thereby *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 9,  $|\lambda_i| = 1(2 \le i \le n)$ . Since,  $\sum_{i=1}^{n} \lambda_i = 0$  and  $\lambda_2 = \lambda_3 = \ldots = \lambda_n = -1$ , we have,  $\lambda_1 = n - 1$ . Hence  $\lambda_1$  has multiplicity 1 and  $\lambda_i = -1$  has multiplicity n - 1. By Lemma 9, G is the direct sum of a complete graph of order  $\lambda_1 + 1 = n$ . Therefore, G is  $K_n$ .

**Theorem 20** Let G be a graph with  $n \ge 2$  vertices, m edges and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n = \delta$ , then

$$E(G) < \frac{1}{2}(1+\sqrt{2})n + \sqrt{(n-2)\left[2m+2\left(\frac{2m(n-1)}{n}\right) - \left(4\delta^2\frac{\alpha(G)}{n-\alpha(G)}\right)\right]}.$$
 (8)

**Proof.** Let  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$  be the eigenvalues of *G*. From Cauchy-Schwarz inequality, we have that

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

Then by Lemma 1, Theorem 15 and Corollary 17 we have that

$$E(G) < \frac{1}{2}(1+\sqrt{2})n + \sqrt{(n-2)\left[2m+2\left(\frac{2m(n-1)}{n}\right) - \left(4\delta^2 \frac{\alpha(G)}{n-\alpha(G)}\right)\right]}$$

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**Theorem 21** Let G be a graph with  $n \ge 2$  vertices, m edges and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ , then

$$E(G) \leq 2\sqrt{m} + \sqrt{(n-2)\left[2m + 2\left(\frac{2m(n-1)}{n}\right) - \left(2\delta\sqrt{\frac{t}{n-t}}\right)^2\right]}$$
(9)

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

**Proof.** Let  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$  be the eigenvalues of *G*. From Cauchy-Schwarz inequality, we have that

$$\sum_{i=1}^{n} |\lambda_i| \leq \lambda_1 - \lambda_n + \sqrt{(n-2)\sum_{i=2}^{n-1} \lambda_i^2}$$
$$= \lambda_1 - \lambda_n + \sqrt{(n-2)\left(2m - (\lambda_1 - \lambda_n)^2 - 2\lambda_1\lambda_n\right)}.$$

Then by Lemmas 1, 14 and Theorem 10 we have that

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

If  $G \cong \frac{n}{2}K_2$ , then it is easy to check that the equality in (9) holds. Conversely, since G is a non-empty graph, by Lemma 9, 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  $\lambda_1 = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$   $(2 \leq i \leq n)$ , since *G* has at least two distinct eigenvalues. By Lemma 9,  $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1$   $(2 \leq i \leq n)$ . Hence 2m = n and also,  $\lambda_1 = |\lambda_2| = \ldots = |\lambda_n| = 1$ . By applying Lemma 9, 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  $\lambda_i = -1$   $(2 \leq i \leq n)$  has multiplicity  $\frac{n}{2}$ . Thereby *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 9,  $|\lambda_i| = 1 (2 \le i \le n)$ . Since,  $\sum_{i=1}^{n} \lambda_i = 0$  and  $\lambda_2 = \lambda_3 = \ldots = \lambda_n = -1$ , we have,  $\lambda_1 = n - 1$ . Hence  $\lambda_1$  has multiplicity 1 and  $\lambda_i = -1$  has multiplicity n - 1. By Lemma 9, *G* is the direct sum of a complete graph of order  $\lambda_1 + 1 = n$ . Therefore, *G* is  $K_n$ .

**Theorem 22** Let G be a graph with  $n \ge 2$  vertices, m edges, degree sequence  $d_1 \ge d_2 \ge$ ...  $\ge d_n$  and  $n_+$ ,  $n_-$  be the number of positive and negative eigenvalues, respectively. Then

$$E(G) \leq 2\sqrt{m} + \sqrt{(n-2)\left[2m + 2\left(\frac{2mn_+}{\sqrt{(1+n_+)(1+n_-)}}\right) - \left(\frac{(d_1+d_2)}{\sqrt{2n}} + \sqrt{d_1}\right)^2\right]}.$$
(10)

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

**Proof.** Let  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$  be the eigenvalues of *G*. From Cauchy-Schwarz inequality, we have that

$$\sum_{i=1}^{n} |\lambda_i| \leq \lambda_1 - \lambda_n + \sqrt{(n-2)\sum_{i=2}^{n-1} \lambda_i^2}$$
$$= \lambda_1 - \lambda_n + \sqrt{(n-2)\left(2m - (\lambda_1 - \lambda_n)^2 - 2\lambda_1\lambda_n\right)}.$$

Then by Theorems 3, 10 and 16 we have that

$$E(G) \leq 2\sqrt{m} + \sqrt{(n-2)\left[2m + 2\left(\frac{2mn_+}{\sqrt{(1+n_+)(1+n_-)}}\right) - \left(\frac{(d_1+d_2)}{\sqrt{2n}} + \sqrt{d_1}\right)^2\right]}.$$

If  $G \cong \frac{n}{2}K_2$ , then it is easy to check that the equality in (10) holds. Conversely, since G is a non-empty graph, by Lemma 9, 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  $\lambda_1 = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$   $(2 \le i \le n)$ , since *G* has at least two distinct eigenvalues. By Lemma 9,  $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1$   $(2 \le i \le n)$ . Hence 2m = n and also,  $\lambda_1 = |\lambda_2| = \ldots = |\lambda_n| = 1$ . By applying Lemma 9, we obtain that  $m_2 = m_1\lambda_1, \lambda_1 = 1$ , and then  $m_1 = m_2$ . So, we obtain that  $\lambda_1 = 1$  has multiplicity  $\frac{n}{2}$ , and  $\lambda_i = -1$   $(2 \le i \le n)$ has multiplicity  $\frac{n}{2}$ . Thereby *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 9,  $|\lambda_i| = 1(2 \le i \le n)$ . Since,  $\sum_{i=1}^{n} \lambda_i = 0$  and  $\lambda_2 = \lambda_3 = \ldots = \lambda_n = -1$ , we have,  $\lambda_1 = n - 1$ . Hence  $\lambda_1$  has multiplicity 1 and  $\lambda_i = -1$  has multiplicity n - 1. By Lemma 9, G is the direct sum of a complete graph of order  $\lambda_1 + 1 = n$ . Therefore, G is  $K_n$ .

### 3.2 Upper bounds for 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 and degree sequence. -508-

**Theorem 23** Let G be a non-empty bipartite graph with  $n \ge 2$  vertices, m edges and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ . Then

$$E(G) \le (\nu + \sqrt{d_1}) + \sqrt{(n-2)\left(2m - \frac{1}{2}\left(\frac{\sum_{i=1}^n d_i^2}{n} - \left(\sum_{i=1}^n \frac{d_i}{n}\right)^2 + d_1 + 2\nu\sqrt{d_1}\right)\right)}$$
(11)

where  $\nu^2 = \frac{\sum_{i=1}^n d_i^2}{n} - \left(\sum_{i=1}^n \frac{d_i}{n}\right)^2$ . Equality holds if and only if  $G \cong \frac{n}{2}K_2$ , (n = 2m).

**Proof.** Let  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$  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

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

It is not diffcult to see that  $H(x) = 2x + \sqrt{(n-2)(2m-2x^2)}$  decreases for  $\sqrt{\frac{1}{2n}} \leq x \leq \sqrt{2m}$ . By Theorem 5, we have  $\lambda_1 \geq \frac{1}{2}(\nu + \sqrt{d_1})$ , equality holds if and only if G is  $\frac{n}{2}K_2$ . Clearly,  $\frac{1}{2}(\nu + \sqrt{d_1}) \geq \frac{1}{\sqrt{2n}}$ . By Theorem 5, we have

$$\lambda_1 \geqslant \frac{1}{2}(\nu + \sqrt{d_1}) \geqslant \frac{1}{\sqrt{2n}}.$$

So  $H(\lambda_1(G)) \leq H(\frac{1}{2}(\nu + \sqrt{d_1}))$ , which implies that

$$E(G) \le (\nu + \sqrt{d_1}) + \sqrt{(n-2)\left(2m - \frac{1}{2}\left(\nu^2 + d_1 + 2\nu\sqrt{d_1}\right)\right)}.$$

If  $G \cong \frac{n}{2}K_2$  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  $\lambda_1 = -\lambda_n = \frac{1}{\sqrt{2n}}(d_1 + d_2)$ . Moreover,  $|\lambda_i| = \sqrt{\frac{2m - \lambda_1^2}{n-2}}$  ( $2 \le i \le n-1$ ). Since G is a non-empty graph, by Lemma 9, 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  $\lambda_1 = -\lambda_n = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-2}}$   $(2 \le i \le n-1)$ . By Lemma 9,  $\lambda_n = -\sqrt{\frac{2m-\lambda_1^2}{n-2}} = |\lambda_i| = -1$   $(2 \le i \le n-1)$ . Hence 2m = n and also,  $\lambda_1 = |\lambda_2| = \ldots = |\lambda_n| = 1$ . By Lemma 9,  $m_2 = m_1\lambda_1, \lambda_1 = 1$ , and therefore  $m_1 = m_2$ . Then we obtain that  $\lambda_1 = 1$  has multiplicity  $\frac{n}{2}$ , and  $\lambda_i = -1$   $(2 \le i \le n)$  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  $\frac{n}{2}K_2$ .

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**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 9,  $|\lambda_i| = -1(2 \leq i \leq n)$ . 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,  $\lambda_i = 0(2 \leq i \leq n-1)$ . Thus  $\mathcal{E}(G) = 2\lambda_1$ , and by Lemma 11, we have that  $2\lambda_1 \geq 2\sqrt{m}$ , and so  $2\lambda_1^2 \geq 2m$ . 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 11, G is a complete bipartite graph plus arbitrarily many isolated vertices. Thus, there exist integers  $r_1 \geq 1$  and  $r_2 \geq 2$  such that G is  $K_{r_1,r_2} \cup (n-r_1-r_2)K_1$ .

**Theorem 24** Let G be a non-empty bipartite graph with  $n \ge 2$  vertices, m edges and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ . Then

$$E(G) \le \left(\frac{1}{\sqrt{2n}}(d_1 + d_2) + \sqrt{d_1}\right) + \sqrt{(n-2)\left(2m - \frac{1}{2}\left(\frac{1}{\sqrt{2n}}(d_1 + d_2) + \sqrt{d_1}\right)^2\right)} \ . (12)$$

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

**Proof.** Let  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$  be the eigenvalues of *G*. 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

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

Note that the function  $N(x) = 2x + \sqrt{(n-1)(2m-x^2)}$  decreases for  $\frac{1}{2\sqrt{2n}} \leq x \leq \sqrt{2m}$ . By Theorem 5, we have  $\lambda_1 \geq \frac{1}{2} \left( \frac{1}{\sqrt{2n}} (d_1 + d_2) + \sqrt{d_1} \right)$ , equality holds if and only if *G* is  $\frac{n}{2}K_2$ . Clearly,  $\frac{1}{2} \left( \frac{1}{\sqrt{2n}} (d_1 + d_2) + \sqrt{d_1} \right) \geq \frac{1}{2\sqrt{2n}}$ . By Theorem 5, we have

$$\lambda_{1} \ge \frac{1}{2} \left( \frac{1}{\sqrt{2n}} (d_{1} + d_{2}) + \sqrt{d_{1}} \right) \ge \frac{1}{2\sqrt{2n}}.$$
  
So,  $N(\lambda_{1}(G)) \le N \left( \frac{1}{2} \left( \frac{1}{\sqrt{2n}} (d_{1} + d_{2}) + \sqrt{d_{1}} \right) \right)$ , which implies  
 $E(G) \le \left( \frac{1}{\sqrt{2n}} (d_{1} + d_{2}) + \sqrt{d_{1}} \right) + \sqrt{(n-2) \left( 2m - \frac{1}{2} \left( \left( \frac{1}{\sqrt{2n}} (d_{1} + d_{2}) + \sqrt{d_{1}} \right) \right)^{2} \right)}$ 

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If  $G \cong \frac{n}{2}K_2$  it is easy to check that the equality in (12) holds. Conversely, if the equality in (12) holds, according to the above argument, we have  $\lambda_1 = -\lambda_n = \frac{1}{2} \left( \frac{1}{\sqrt{2n}} (d_1 + d_2) + \sqrt{d_1} \right)$ . 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 9, 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 9,  $|\lambda_i| = -1(2 \leqslant i \leqslant n)$ . Noting that G is a bipartite graph, we have  $\lambda_1 = -\lambda_n$ , this is a contradiction. We consider the following case.

**Case 1.** The absolute value of all eigenvalues of G are equal. Note that  $\lambda_1 = -\lambda_n = |\lambda_i| = \sqrt{\frac{2m - \lambda_1^2}{n-2}}$   $(2 \leq i \leq n-1)$ . By Lemma 9,  $\lambda_n = -\sqrt{\frac{2m - \lambda_1^2}{n-2}} = |\lambda_i| = -1$   $(2 \leq i \leq n-1)$ . Hence 2m = n and also,  $\lambda_1 = |\lambda_2| = \ldots = |\lambda_n| = 1$ . By Lemma 9,  $m_2 = m_1\lambda_1, \lambda_1 = 1$ , and therefore  $m_1 = m_2$ . Then we obtain that  $\lambda_1 = 1$  has multiplicity  $\frac{n}{2}$ , and  $\lambda_i = -1$  ( $2 \leq i \leq n$ ) 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 9,  $|\lambda_i| = -1(2 \leq i \leq n)$ . 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,  $\lambda_i = 0(2 \leq i \leq n-1)$ . Thus  $\mathcal{E}(G) = 2\lambda_1$ , and by Lemma 11, we have that  $2\lambda_1 \geq 2\sqrt{m}$ , and so  $2\lambda_1^2 \geq 2m$ . 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 11, G is a complete bipartite graph plus arbitrarily many isolated vertices. Thus, there exist integers  $r_1 \geq 1$  and  $r_2 \geq 2$  such that G is  $K_{r_1,r_2} \cup (n - r_1 - r_2)K_1$ .

#### 3.3 Upper bound for connected graphs

In the following we consider connected graphs.

**Theorem 25** Let G be a connected graph with  $n \ge 2$  vertices, m edges and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ , then

$$E(G) \leq 2\sqrt{m} + \sqrt{(n-2)\left[2m+2(n-1)\sqrt{\frac{2m(n-1)}{n}} - \left(\frac{(d_1+d_2)}{\sqrt{2n}} + \sqrt{d_1}\right)^2\right]} \quad (13)$$

Equality holds if and only if  $G \cong K_2$ , (n = 2m).

**Proof.** Let  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$  be the eigenvalues of *G*. From Cauchy-Schwarz inequality, we have that

$$\sum_{i=1}^{n} |\lambda_i| \leq \lambda_1 - \lambda_n + \sqrt{(n-2)\sum_{i=2}^{n-1} \lambda_i^2}$$
$$= \lambda_1 - \lambda_n + \sqrt{(n-2)\left(2m - (\lambda_1 - \lambda_n)^2 - 2\lambda_1\lambda_n\right)}.$$

Then by Lemmas 7, 8 and Theorem 10 we have that

$$E(G) \leq 2\sqrt{m} + \sqrt{(n-2)\left[2m+2(n-1)\sqrt{\frac{2m(n-1)}{n}} - \left(\frac{(d_1+d_2)}{\sqrt{2n}} + \sqrt{d_1}\right)^2\right]}.$$

If  $G \cong K_2$ , then it is easy to check that the equality in (13) holds. Conversely, since G is a non-empty graph, by Lemma 9, 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  $\lambda_1 = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$   $(2 \leq i \leq n)$ , since *G* has at least two distinct eigenvalues. By Lemma 9,  $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1$   $(2 \leq i \leq n)$ . Hence 2m = n and also,  $\lambda_1 = |\lambda_2| = \ldots = |\lambda_n| = 1$ . By applying Lemma 9 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  $\lambda_i = -1$   $(2 \leq i \leq n)$  has multiplicity  $\frac{n}{2}$ . Therefore *G* is the direct sum of  $m_1 = \frac{n}{2}$  complete graphs of order  $\lambda_1 + 1 = 2$ . Thereby, *G* is  $\frac{n}{2}K_2$ . Since *G* is a connected graph, therefore, *G* is  $K_2$ .

**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 9,  $|\lambda_i| = 1(2 \le i \le n)$ . Since,  $\sum_{i=1}^{n} \lambda_i = 0$  and  $\lambda_2 = \lambda_3 = \ldots = \lambda_n = -1$ , we have,  $\lambda_1 = n - 1$ . Hence  $\lambda_1$  has multiplicity 1 and  $\lambda_i = -1$  has multiplicity n - 1. By Lemma 9, G is the direct sum of a complete graph of order  $\lambda_1 + 1 = n$ . Consequently, G is  $K_n(n > 2)$ .

**Theorem 26** Let G be a connected graph with  $n \ge 2$  vertices, m edges and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ , then

$$E(G) \leq 2\gamma + \sqrt{(n-2) \left[ 2m + 2\left(2m - (n-1)d_n + (d_n-1)d_1\right) - \left(\frac{(d_1+d_2)}{\sqrt{2n}} + \sqrt{d_1}\right)^2\right]}.$$
(14)

where  $\gamma = \sqrt{2m - (n-1)d_n + (d_n - 1)d_1}$ . Equality holds if and only if  $G \cong K_2$ , (n = 2m). **Proof.** Let  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$  be the eigenvalues of *G*. From Cauchy-Schwarz inequality, we have that

$$\sum_{i=1}^{n} |\lambda_i| = |\lambda_1| + |\lambda_n| + \sum_{i=2}^{n-1} |\lambda_i|$$
  
$$\leq \lambda_1 - \lambda_n + \sqrt{(n-2)\sum_{i=2}^{n-1} \lambda_i^2}$$
  
$$= \lambda_1 - \lambda_n + \sqrt{(n-2)\left(2m - (\lambda_1 - \lambda_n)^2 - 2\lambda_1\lambda_n\right)}.$$

Then by Lemma 6 and Theorems 10, 16 we have that

$$E(G) \leq 2\gamma + \sqrt{(n-2)\left[2m + 2\left(2m - (n-1)d_n + (d_n-1)d_1\right) - \left(\frac{(d_1+d_2)}{\sqrt{2n}} + \sqrt{d_1}\right)^2\right]}.$$

If  $G \cong K_2$ , then it is easy to check that the equality in (14) holds. Conversely, since G is a non-empty graph, by Lemma 9, 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  $\lambda_1 = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$   $(2 \leq i \leq n)$ , since *G* has at least two distinct eigenvalues. By Lemma 9,  $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1$   $(2 \leq i \leq n)$ . Hence 2m = n and also,  $\lambda_1 = |\lambda_2| = \ldots = |\lambda_n| = 1$ . By applying Lemma 9 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  $\lambda_i = -1$   $(2 \leq i \leq n)$  has multiplicity  $\frac{n}{2}$ . Therefore *G* is the direct sum of  $m_1 = \frac{n}{2}$  complete graphs of order  $\lambda_1 + 1 = 2$ . Thereby, *G* is  $\frac{n}{2}K_2$ . Since *G* is a connected graph, therefore, *G* is  $K_2$ .

**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 9,  $|\lambda_i| = 1(2 \le i \le n)$ . Since,  $\sum_{i=1}^n \lambda_i = 0$  and  $\lambda_2 = \lambda_3 = \ldots = \lambda_n = -1$ , we have,  $\lambda_1 = n - 1$ . Hence  $\lambda_1$  has multiplicity 1 and  $\lambda_i = -1$  has multiplicity n - 1. By Lemma 9, G is the direct sum of a complete graph of order  $\lambda_1 + 1 = n$ . Consequently, G is  $K_n(n > 2)$ .

### 3.4 Upper bound for triangle-free graphs

We next upper bounds is for the energy for triangle-free graphs.

**Theorem 27** Let G be a triangle-free graph with  $n \ge 2$  vertices, m edges and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ , then

$$E(G) \leq \sqrt{m} + \sqrt{\frac{2m}{n+n^{\frac{2}{3}}}} + \sqrt{(n-2)\left[4m - \left(\frac{2m}{n} + \sqrt{d_1}\right)^2\right]}$$
 (15)

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

**Proof.** Let  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$  be the eigenvalues of *G*. From Cauchy-Schwarz inequality, we have that

$$\sum_{i=1}^{n} |\lambda_i| \leq \lambda_1 - \lambda_n + \sqrt{(n-2)\sum_{i=2}^{n-1} \lambda_i^2}$$
$$= \lambda_1 - \lambda_n + \sqrt{(n-2)\left(2m - (\lambda_1 - \lambda_n)^2 - 2\lambda_1\lambda_n\right)}.$$

Then by Lemmas 2, 13 and Theorem 10 we have that

$$E(G) \leq \sqrt{m} + \sqrt{\frac{2m}{n+n^{\frac{2}{3}}}} + \sqrt{(n-2)\left[4m - \left(\frac{2m}{n} + \sqrt{d_1}\right)^2\right]}$$

If  $G \cong \frac{n}{2}K_2$ , then it is easy to check that the equality in (15) holds. Conversely, since G is a non-empty graph, by Lemma 9, 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  $\lambda_1 = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$   $(2 \leq i \leq n)$ , since *G* has at least two distinct eigenvalues. By Lemma 9,  $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1$   $(2 \leq i \leq n)$ . Hence 2m = n and also,  $\lambda_1 = |\lambda_2| = \ldots = |\lambda_n| = 1$ . By applying Lemma 9 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  $\lambda_i = -1$   $(2 \leq i \leq n)$  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 9,  $|\lambda_i| = 1(2 \le i \le n)$ . Since,  $\sum_{i=1}^{n} \lambda_i = 0$  and  $\lambda_2 = \lambda_3 = \ldots = \lambda_n = -1$ , we have,  $\lambda_1 = n - 1$ . Hence  $\lambda_1$  has multiplicity 1 and  $\lambda_i = -1$  has multiplicity n - 1. By Lemma 9, G is the direct sum of a complete graph of order  $\lambda_1 + 1 = n$ . Thereby, G is  $K_n$ .

**Theorem 28** Let G be a triangle-free graph with  $n \ge 2$  vertices, m edges and degree

sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ , then

$$E(G) \leqslant \sqrt{m} + \sqrt{\frac{2m}{n+n^{\frac{2}{3}}}} + \sqrt{(n-2)\left[4m - \left(\frac{1}{\sqrt{2n}}(d_1+d_2)\right)^2\right]}$$
 (16)

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

**Proof.** Let  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$  be the eigenvalues of *G*. From Cauchy-Schwarz inequality, we have that

$$\sum_{i=1}^{n} |\lambda_i| \leq \lambda_1 - \lambda_n + \sqrt{(n-2)\sum_{i=2}^{n-1} \lambda_i^2}$$
$$= \lambda_1 - \lambda_n + \sqrt{(n-2)\left(2m - (\lambda_1 - \lambda_n)^2 - 2\lambda_1\lambda_n\right)}.$$

Then by Lemma 2 and Theorems 10, 4; we have that

$$E(G) \leq \sqrt{m} + \sqrt{\frac{2m}{n+n^{\frac{2}{3}}}} + \sqrt{(n-2)\left[4m - \left(\frac{1}{\sqrt{2n}}(d_1+d_2)\right)^2\right]}.$$

If  $G \cong \frac{n}{2}K_2$ , then it is easy to check that the equality in (16) holds. Conversely, since G is a non-empty graph, by Lemma 9, 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  $\lambda_1 = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$   $(2 \leq i \leq n)$ , since *G* has at least two distinct eigenvalues. By Lemma 9,  $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1$   $(2 \leq i \leq n)$ . Hence 2m = n and also,  $\lambda_1 = |\lambda_2| = \ldots = |\lambda_n| = 1$ . By applying Lemma 9, 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  $\lambda_i = -1$   $(2 \leq i \leq n)$  has multiplicity  $\frac{n}{2}$ . Therefore *G* is the direct sum of  $m_1 = \frac{n}{2}$  complete graphs of order  $\lambda_1 + 1 = 2$ . Thereby, *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 9,  $|\lambda_i| = 1(2 \le i \le n)$ . Since,  $\sum_{i=1}^{n} \lambda_i = 0$  and  $\lambda_2 = \lambda_3 = \ldots = \lambda_n = -1$ , we have,  $\lambda_1 = n - 1$ . Hence  $\lambda_1$  has multiplicity 1 and  $\lambda_i = -1$  has multiplicity n - 1. By Lemma 9, G is the direct sum of a complete graph of order  $\lambda_1 + 1 = n$ . Consequently, G is  $K_n$ .

### 3.5 Upper bound for regular graphs

In this subsection, we present upper bounds for the energy of a regular graph. In the following result, we give an upper bounds in terms of order, size and degree sequence. **Theorem 29** Let G be a regular graph with  $n \ge 2$  vertices, m edges and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ , then

$$E(G) \leqslant n + \sqrt{(n-2)\left[2m+2\left(\frac{2m(n-1)}{n}\right) - \left(\frac{(d_1+d_2)}{\sqrt{2n}} + \sqrt{d_1}\right)^2\right]} .$$
(17)

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

**Proof.** Let  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$  be the eigenvalues of *G*. From Cauchy-Schwarz inequality, we have that

$$\sum_{i=1}^{n} |\lambda_i| \leq \lambda_1 - \lambda_n + \sqrt{(n-2)\sum_{i=2}^{n-1} \lambda_i^2}$$
$$= \lambda_1 - \lambda_n + \sqrt{(n-2)\left(2m - (\lambda_1 - \lambda_n)^2 - 2\lambda_1\lambda_n\right)}.$$

Then by Lemmas 1, 12 and Theorem 16 we have that

$$E(G) \leq n + \sqrt{(n-2)\left[2m+2\left(\frac{2m(n-1)}{n}\right) - \left(\frac{(d_1+d_2)}{\sqrt{2n}} + \sqrt{d_1}\right)^2\right]}$$

If  $G \cong \frac{n}{2}K_2$ , then it is easy to check that the equality in (17) holds. Conversely, since G is a non-empty graph, by Lemma 9, 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  $\lambda_1 = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$   $(2 \leq i \leq n)$ , since *G* has at least two distinct eigenvalues. By Lemma 9,  $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1$   $(2 \leq i \leq n)$ . Hence 2m = n and also,  $\lambda_1 = |\lambda_2| = \ldots = |\lambda_n| = 1$ . By applying Lemma 9 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  $\lambda_i = -1$   $(2 \leq i \leq n)$  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 9,  $|\lambda_i| = 1(2 \le i \le n)$ . Since,  $\sum_{i=1}^{n} \lambda_i = 0$  and  $\lambda_2 = \lambda_3 = \ldots = \lambda_n = -1$ , we have,  $\lambda_1 = n - 1$ . Hence  $\lambda_1$  has multiplicity 1 and  $\lambda_i = -1$  has multiplicity n - 1. By Lemma 9, G is the direct sum of a complete graph of order  $\lambda_1 + 1 = n$ . Thereby, G is  $K_n$ .

**Theorem 30** Let G be a k- regular graph with  $n \ge 2$  vertices, m edges, a coclique of order  $\alpha$  and degree sequence  $d_1 \ge d_2 \ge \ldots \ge d_n$ , then

$$E(G) \leq n + \sqrt{(n-2)\left[2m+2\left(\frac{2m(n-1)}{n}\right) - \left(\frac{nk}{n-\alpha}\right)^2\right]} .$$
(18)

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

**Proof.** Let  $\lambda_1 \ge \lambda_2 \ge \ldots \ge \lambda_{n-1} \ge \lambda_n$  be the eigenvalues of *G*. From Cauchy-Schwarz inequality, we have that

$$\sum_{i=1}^{n} |\lambda_i| = |\lambda_1| + |\lambda_n| + \sum_{i=2}^{n-1} |\lambda_i|$$
  
$$\leq \lambda_1 - \lambda_n + \sqrt{(n-2)\sum_{i=2}^{n-1} \lambda_i^2}$$
  
$$= \lambda_1 - \lambda_n + \sqrt{(n-2)\left(2m - (\lambda_1 - \lambda_n)^2 - 2\lambda_1\lambda_n\right)}.$$

Then by Lemmas 1, 12, 11 we have that

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

If  $G \cong \frac{n}{2}K_2$ , then it is easy to check that the equality in (18) holds. Conversely, since G is a non-empty graph, by Lemma 9, G has at least two distinct eigenvalues. We consider the following cases.

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

Then clearly  $\lambda_1 = |\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$   $(2 \leq i \leq n)$ , since *G* has at least two distinct eigenvalues. By Lemma 9,  $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1$   $(2 \leq i \leq n)$ . Hence 2m = n and also,  $\lambda_1 = |\lambda_2| = \ldots = |\lambda_n| = 1$ . By applying Lemma 9, 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  $\lambda_i = -1$   $(2 \leq i \leq n)$  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 9,  $|\lambda_i| = 1(2 \le i \le n)$ . Since,  $\sum_{i=1}^{n} \lambda_i = 0$  and  $\lambda_2 = \lambda_3 = \ldots = \lambda_n = -1$ , we have,  $\lambda_1 = n - 1$ . Hence  $\lambda_1$  has multiplicity 1 and  $\lambda_i = -1$  has multiplicity n - 1. By Lemma 9, G is the direct sum of a complete graph of order  $\lambda_1 + 1 = n$ . Consequently, G is  $K_n$ .

# 4 Comparing bounds and conclusions

In this section, we present some computational experiments to compare our new upper bounds to previously published upper bounds for certainly connected graphs. We compare the results obtained in Theorem 18 (Th.18), Theorem 19 (Th.19), Theorem 23 (Th.23), Theorem 24 (Th.24), Theorem 27 (Th.27) with the results obtained by McClelland (1), Koolen and Moulton (2) and (3), Zhou (4) and (5) with the original energy value for each given graph.

Graph (G)	E(G)	(1)	(2)	(4)	Th.18	Th.19	(3)	(5)	Th.23	Th.24	Th.27
$K_8$	14.0000	21.1660	14.0000	14.0000	14.0000	30.6673					
$K_{2,3}$	4.8990	7.7460	7.3960	7.3485	6.1968	10.5965	6.1856	4.8990	6.7689	7.7329	8.2384
$K_{4,3}$	6.9282	12.9615	12.0000	11.9494	9.0711	18.3272	8.5714	6.9282	11.2285	12.9561	14.5903
$S_4$	3.4641	4.8990	4.8541	4.7321	4.2426	5.5140	5.1213	3.4641	4.4352	4.5958	4.4542
$S_5$	4.0000	6.3246	6.2648	6.0000	5.0596	7.0865	6.5941	4.0000	5.4978	5.7636	6.0247
$S_6$	4.4821	7.7460	7.6759	7.2361	5.7735	8.5972	8.0474	4.4821	6.4142	6.8850	7.6404
$C_5$	6.4895	7.0711	6.8990	6.8990	6.6569	9.9433	6.8284	6.4895	6.6618	7.0647	8.3624
$C_6$	8.0000	8.4853	8.3246	8.3246	7.3246	12.0274	8.4721	8.0000	8.4695	8.4682	10.6119
C7	9.0000	9.8995	9.7460	9.7460	9.9282	14.0208	10.0000	9.4772	9.8784	9.8713	12.8315
$P_4$	4.4821	4.8990	4.8541	4.8215	4.5426	6.4221	5.1213	4.5765	4.4960	4.8987	5.3399
$P_5$	5.4689	6.3246	6.2648	6.2340	5.5596	8.6530	6.5941	6.0299	5.8030	6.3158	7.5593
$P_6$	7.0000	7.7460	7.6759	7.6481	7.7735	10.7333	8.0474	7.4641	7.1666	7.7209	9.7562
$P_7$	8.0611	9.1652	9.0877	9.0627	9.4143	12.7195	9.4895	8.8908	8.5413	9.1242	11.9404

• In almost all of our test cases, the upper bound in Th.18 and Th.23 were better than existing bounds.

• For bipartite graphs, the upper bound given by Th.23 is better than existing bounds for bipartite graph.

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