MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **79** (2018) 275-286

ISSN 0340 - 6253

Upper Bounds for the Energy of Graphs

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(Received March 9, 2017)

Abstract

Let G be a finite simple undirected graph with n vertices and m edges. The energy of a graph G, denoted by $\mathcal{E}(G)$, is defined as the sum of the absolute values of the eigenvalues of G. In this paper we present some new upper bounds for $\mathcal{E}(G)$ in terms of number of vertices, number of edges, chromatic number, diameter and Randić index. Also in section 3, improving upper bounds $\mathcal{E}(G)$ in inequalities (2) and (3).

1 Introduction

Let $G = (V, E)$ be a simple undirected graph with n vertices and m edges. For $v \in V$, the *degree* of v, denoted by $d(v)$, is the number of edges incident to v, let d_i be the *degree* of the vertex v_i. The *distance* between two vertices x and y, denoted by $d(x, y)$, is the number of edges of a *shortest path* between x and y, and its *maximum* value over all pair of vertices is called *diameter* of the graph G, in other words, $D = diam(G) = max\{d(x, y) : x, y \in V\}$. The *Randić index* of G, denoted by $R(G)$, is defined as $R = R(G) = \sum_{uv\in E} \frac{1}{\sqrt{d(v)d(u)}}$. The smallest number of colors needed to color a graph G is called its *chromatic number* of G, denoted by $\chi(G)$, when $\chi(G) = k$, G is called *k-chromatic*. If each pair of vertices in a graph is joined by a walk, the graph is said to be *connected* graph. A simple undirected graph in which every pair of distinct vertices is connected by a unique edge, is the *complete* graph and denoted by K_n. A simple graph $G = (X, Y)$ is called bipartite if its vertex set can be partitioned into two disjoint subsets $V = X_1 \cup X_2$ such that every edge has the form $e = (a, b)$ where $a \in X_1$ and $b \in X_1$. A complete bipartite graph is a special kind of bipartite graph where every vertex of the first set is connected to every vertex of the second set, denoted by $K_{m,n}$. The graph $K_{1,n-1}$ is also called the *star* of order n, denoted by S_n. The 2-*degree* of v_i [3] is the sum of the degrees of the vertices adjacent to v_i and denoted by t_i. We call $\frac{t_i}{d_i}$ the *average-degree* of v_i. A graph G is *regular* if there exists a constant r such that each vertex of G has degree r, such graphs are also called r-*regular*. A graph G is *pseudo-regular* if there exists a constant p such that each vertex of G has *average-degree* p, such graphs are also called p-*pseudo-regular*. A *bipartite graph* $G = (X, Y)$ is *pseudo-semiregular* if there exist two constants p_x and p_y such that each vertex in X has *average-degree* p_x and each vertex in Y has *average-degree* p_y, such *bipartite graphs* are also called $(p_x; p_y)$-*pseudo-semiregular*. The *adjacency matrix* $A(G)$ of 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 $A(G)$. The *spectral radius* of G, denoted by $\lambda_1(G)$, is the largest eigenvalue of $A(G)$. When more than one graphs are under consideration, then we write $\lambda_i(G)$ instead of λ_i. The *energy* of the graph G is defined as

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

This concept was introduced by I. *Gutman* and is intensively studied in *chemistry*, since it can be used to approximate the total π-*electron* energy of a *molecule* (see, e.g. [9,10]). In 1971, McClelland [17] 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. [1,8,9,11–17]).

Koolen and Moulton [13]: If $2m \geqslant n$ and G is a graph with n vertices, m edges, then

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

Equality holds 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 $\sqrt{\frac{(2m-(\frac{2m}{n})^2)}{(n-1)}}$.
Koolen and Moulton [14] : If $2m \geqslant n$ and G is a bipartite graph with $n > 2$ vertices, m edges, then

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

Equality holds 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 $\lambda = \frac{k(k-1)}{\nu-1}(n = 2\nu)$.

The paper is organized as follows. In Section 2, we give a list of some previously known results. In Section 3, we present two new upper bounds for the energy with Randić index of graphs and Improving upper bounds for energy in Inequalities (2) and (3). In Section 4, we present two new upper bounds for the energy with chromatic number of graphs. In Section 5, we present two new upper bounds for the energy with diameter of graphs.

2 Preliminaries

We list here some previously known results that will be needed in the sections.

Lemma 1. *[7] Let G be a non-empty graph with m edges and Randić R. Then*

$$\lambda_1 \geqslant \frac{m}{R} . \tag{4}$$

Lemma 2. *[2] Let G be a non-trivial graph with n vertices. Then*

$$R(G) \leqslant \frac{n}{2} . \tag{5}$$

Lemma 3. *[7] Let G be a connected graphs with chromatic number χ. Then*

$$\lambda_1 \geqslant \chi - 1 . \tag{6}$$

Lemma 4. *[6] If G is a graph with n vertices and chromatic number χ. Then*

$$\chi \geqslant \frac{n}{n-\lambda_1} . \tag{7}$$

Lemma 5. *[4] Let G be a graph with with m edges. Then*

$$\mathcal{E}(G) \geqslant 2\sqrt{m} . \tag{8}$$

Equality if and only if G is a complete bipartite graph plus arbitrarily many isolated vertices.

Lemma 6. *[5] G has only one distinct eigenvalue if and only if G is an empty 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 $m_2 = m_1\mu_1$.*

Lemma 7. *[7] Let G be a graph with with n vertices and m edges. Then*

$$\lambda_1 \geqslant \frac{2m}{n} . \tag{9}$$

Lemma 8. *[18] If G is a connected graph with n vertices and diameter D. Then*

$$\lambda_1 \geq \sqrt[D]{n-1} . \tag{10}$$

3 Upper bounds with Randić index of graphs

In this section present two new upper bounds for energy with *Randić index* of graphs and Improving upper bounds for energy in Inequalities (2) and (3).

Remark 1. *Suppose that* $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_{n-1} \geqslant \lambda_n$ *be the eigenvalues of* G. *By the Cauchy-Schwarz inequality,* $(\sum_{i=2}^{n}|\lambda_i|)^2 \leqslant (n-1)\sum_{i=2}^{n}|\lambda_i|^2)$ *which* $(\sum_{i=2}^{n}\lambda_i)^2 = 2m-\lambda_1^2$. *Therefore* $|\lambda_i| = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$.

Theorem 1. *Let* G *be a non-empty graph with* n *vertices,* m *edges and Randić* R. *Then*

$$\mathcal{E}(G) \leq \frac{m}{R} + \sqrt{(n-1)\left(2m - \left(\frac{m}{R}\right)^2\right)}\ . \tag{11}$$

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

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 $\frac{2m}{n} \leqslant x \leqslant \sqrt{2m}$. By Lemma 1 and Lemma 2,

$$\lambda_1 \geqslant \frac{m}{R} \geqslant \frac{2m}{n}.$$

So $F(\lambda_1(G)) \leqslant F(\frac{m}{R})$, which implies

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

If $G \cong K_n$ it is easy to check that the equality in (11) holds. Conversely, if the equality in (11) holds, according to the above argument, we have

$$\lambda_1 = \frac{m}{R}.$$

Note that G has only one distinct eigenvalue if and only if G is an empty graph.

G has two distinct eigenvalues.

If the two distinct eigenvalues of G have the same absolute value, then $\lambda_1 = |\ \lambda_i\ | = \sqrt{\frac{2m-\lambda_1^2}{n-1}}(2 \leqslant i \leqslant n)$. By Lemma 6, $|\ \lambda_i\ | = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1(2 \leqslant i \leqslant n)$, hence $2m = n$.

Therefore, $\lambda_1 =\mid \lambda_2 \mid= \cdots =\mid \lambda_n \mid= 1$. By Lemma 6, $m_2 = m_1\lambda_1, \lambda_1 = 1$, so $m_1 = m_2$, eigenvalues $\lambda_1 = 1$, with multiplicity $\frac{n}{2}$, also eigenvalues $\lambda_i = -1$, with multiplicity $\frac{n}{2}$. Hence G is the direct sum of $m_1 = \frac{n}{2}$ complete graphs of order $\lambda_1 + 1 = 2$. Namely, G is $\frac{n}{2}K_2$, that is contradiction with equality (11).

If the two eigenvalues of G have diferent absolute values, by Lemma 6, $\mid \lambda_i \mid= -1(2 \leqslant i \leqslant n)$. Since G is a simple graph, we have $\sum_{i=1}^{n} \lambda_i = 0$. Also $\lambda_2 = \lambda_3 = \cdots = \lambda_n = -1$. Hence eigenvalues λ_1, with multiplicity $n-1$, also eigenvalues $\lambda_i = -1$, with multiplicity 1. Therefore, by Lemma 6, G is the direct sum of 1 complete graph of order $\lambda_1 + 1 = n$. Namely, G is K_n. ∎

Theorem 2. *Let $G = (V, E)$ be a non-empty bipartite graph with $n \geqslant 2$ vertices, m edges and Randić R.Then*

$$\mathcal{E}(G) \leq 2\frac{m}{R} + \sqrt{(n-2)\left(2m - 2\left(\frac{m}{R}\right)^2\right)} . \tag{12}$$

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

(1) $G \cong K_{r_1,r_2}$; where $r_1r_2 = m$

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

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,

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

Hence

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

It is not diffcult to see that $H(x) = 2x + \sqrt{(n-2)(2m - 2x^2)}$ decreases for $\frac{2m}{n} \leqslant x \leqslant \sqrt{2m}$. By Lemma 1 and Lemma 2,

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

So $H(\lambda_1(G)) \leqslant H(\frac{m}{R})$, which implies

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

If G is one of the two graphs shown in the second part of the theorem, it is easy to check that the equality in (12) holds. Conversely, if the equality in (12) holds, according to the above argument,

$$\lambda_1 = -\lambda_n = \frac{m}{R}.$$

Moreover, $\mid \lambda_i \mid = \sqrt{\frac{2m-\lambda_1^2}{n-2}}$ $(2 \leqslant i \leqslant n-1)$. Note that G has only one distinct eigenvalue if and only if G is an empty graph. We are reduced to the following three possibilities:

(1) G has two distinct eigenvalues.

If the two distinct eigenvalues of G have the same absolute value, then $\lambda_1 = -\lambda_n = \mid \lambda_i \mid = \sqrt{\frac{2m-\lambda_1^2}{n-1}} (2 \leqslant i \leqslant n)$. By Lemma 6, $\lambda_n = -\sqrt{\frac{2m-\lambda_1^2}{n-1}} = -1 (2 \leqslant i \leqslant n)$, hence $2m = n$. Therefore, $\lambda_1 = \mid \lambda_2 \mid = \cdots = \mid \lambda_n \mid = 1$. By Lemma 6, $m_2 = m_1\lambda_1, \lambda_1 = 1$, so $m_1 = m_2$, eigenvalues $\lambda_1 = 1$, with multiplicity $\frac{n}{2}$, also eigenvalues $\lambda_i = -1$, with multiplicity $\frac{n}{2}$. Hence G is the direct sum of $m_1 = \frac{n}{2}$ complete graphs of order $\lambda_1 + 1 = 2$. Namely, G is $\frac{n}{2}K_2$, that is contradiction with equality (12).

If the two eigenvalues of G have diferent absolute values, by Lemma 6, $\mid \lambda_i \mid = -1 (2 \leqslant i \leqslant n)$. Noting that G is a bipartite graph, we have $\lambda_1 = -\lambda_n$, that is contradiction with two eigenvalues of G have diferent absolute values.

(2) G has three distinct eigenvalues.

In this case, noting that G is a bipartite graph, we have $\lambda_1 = -\lambda_n = \frac{m}{R}$ and $\lambda_i = \sqrt{\frac{2m-\lambda_1^2}{n-2}} = 0$ $(2 \leqslant i \leqslant n-1)$, which implies that $\mathcal{E}(G) = 2\lambda_1 = \frac{m}{R}$. By Lemma 5, we have $G \cong K_{r_1,r_2}$ where $r_1 r_2 = m$.

(3) G has four distinct eigenvalues.

In this case, noting that the multiplicity of λ_1 is one, we have 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 $\sqrt{p_x p_y} \geq \sqrt{\frac{2m}{n}}$. This completes the proof of theorem. ∎

Theorem 3. *For any graph Inequality (11) is better than (2).*

Proof. In order to show (11) is better than (2), we need to demonstrate that, $\frac{2m}{n} + \sqrt{(n-1)\left(2m - (\frac{2m}{n})^2\right)} \leqslant \frac{m}{R} + \sqrt{(n-1)(2m - (\frac{m}{R})^2)}$. Is sufficient to show

$$\frac{m}{R} \geqslant \frac{2m}{n}.$$

By Lemma 2, $R \leqslant \frac{n}{2}$ and by Lemma1, $\lambda_1 \geqslant \frac{m}{R}$, therefore

$$\frac{m}{R} \geqslant \frac{m}{\frac{n}{2}} = \frac{2m}{n}.$$

This completes the proof of Theorem. ■

Similarly it can be shown Inequality (12) is better than (3).

4 Upper bounds with chromatic number of graphs

In this section present two new upper bounds for energy with chromatic number of graphs.

Theorem 4. *Let G be a non-empty and connected graph with n vertices, m edges and chromatic number χ. Then*

$$\mathcal{E}(G) \leq (\chi - 1) + \sqrt{(n-1)(2m - (\chi - 1)^2)}\ . \tag{13}$$

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

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 $S(x) = x + \sqrt{(n-1)(2m - x^2)}$ decreases for $\frac{n^2}{n^2 - 2m} \leqslant x \leqslant \sqrt{2m}$. By Lemma 5 and Lemma 4,

$$\chi - 1 \geqslant \frac{n}{n - \lambda_1} \geqslant \frac{n}{n - \frac{2m}{n}} = \frac{n^2}{n^2 - 2m},$$

by Lemma 3

$$\lambda_1 \geqslant \chi - 1 \geqslant \frac{n^2}{n^2 - 2m}.$$

So $S(\lambda_1(G)) \leqslant S(\chi - 1)$, which implies

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

If $G \cong K_n$ 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

$$\lambda_1 = \chi - 1\ .$$

Note that G has only one distinct eigenvalue if and only if G is an empty graph.

G has two distinct eigenvalues.

If the two distinct eigenvalues of G have the same absolute value, then $\lambda_1 =\mid \lambda_i \mid = \sqrt{\frac{2m-\lambda_1^2}{n-1}}(2 \leqslant i \leqslant n)$. By Lemma 6, $\mid \lambda_i \mid = \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1(2 \leqslant i \leqslant n)$, hence $2m = n$. Therefore, $\lambda_1 =\mid \lambda_2 \mid = \cdots =\mid \lambda_n \mid = 1$. By Lemma 6, $m_2 = m_1\lambda_1, \lambda_1 = 1$, so $m_1 = m_2$, eigenvalues $\lambda_1 = 1$, with multiplicity $\frac{n}{2}$, also eigenvalues $\lambda_i = -1$, with multiplicity $\frac{n}{2}$. Hence G is the direct sum of $m_1 = \frac{n}{2}$ complete graphs of order $\lambda_1 + 1 = 2$. Namely, G is $\frac{n}{2}K_2$, that is contradiction with equality (13).

If the two eigenvalues of G have diferent absolute values, by Lemma 6, $\mid \lambda_i \mid = -1(2 \leqslant i \leqslant n)$. Since G is a simple graph, we have $\sum_{i=1}^{n} \lambda_i = 0$. Also $\lambda_2 = \lambda_3 = \cdots = \lambda_n = -1$. Hence eigenvalues λ_1, with multiplicity $n-1$, also eigenvalues $\lambda_i = -1$, with multiplicity 1. Therefore, by Lemma 6, G is the direct sum of 1 complete graph of order $\lambda_1 + 1 = n$. Namely, G is K_n. ■

Theorem 5. *Let G be a non-empty bipartite graph with $n \geqslant 2$ vertices, m edges chromatic number χ. Then*

$$\mathcal{E}(G) \leq 2(\chi - 1) + \sqrt{(n-2)(2m - 2(\chi-1)^2)} \ . \tag{14}$$

Equality holds if and only if $G \cong K_2$.

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 $N(x) = 2x + \sqrt{(n-1)(2m - x^2)}$ decreases for $\frac{n^2}{n^2-2m} \leqslant x \leqslant \sqrt{2m}$. By Lemma 3 and Lemma 4,

$$\lambda_1 \geqslant (\chi - 1) \geqslant \frac{n^2}{n^2 - 2m}.$$

So $N(\lambda_1(G)) \leqslant N(\chi - 1)$, which implies

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

If $G \cong K_2$ it is easy to check that the equality in (14) holds. Conversely, if the equality in (14) holds, according to the above argument,

$$\lambda_1 = -\lambda_2 = \chi - 1 \ .$$

Moreover, $|\lambda_2| = \sqrt{\frac{2m-\lambda_1^2}{n-2}}$. Note that G has only one distinct eigenvalue if and only if G is an empty graph. G has two distinct eigenvalues.

If the two distinct eigenvalues of G have the same absolute value, then $\lambda_1 = -\lambda_2 = \sqrt{\frac{2m-\lambda_1^2}{n-1}}$. By Lemma 6, $\lambda_2 = -\sqrt{\frac{2m-\lambda_1^2}{n-1}} = -1$, hence $2m = n$. Therefore, $\lambda_1 = |\lambda_2| = 1$, which implies $G \cong K_2$.

If the two eigenvalues of G have diferent absolute values, by Lemma 6, $|\lambda_2| = -1$. Noting that G is a bipartite graph, we have $\lambda_1 = -\lambda_2$, that is contradiction with two eigenvalues of G have diferent absolute values. ■

5 Upper bounds with diameter of graphs

In this section present two new upper bounds for energy with diameter of graphs.

Theorem 6. *Let G be a non-empty and connected graph with n vertices, m and diameter D. Then*

$$\mathcal{E}(G) \leq \sqrt[D]{n-1} + \sqrt{(n-1)\left(2m - \left(\sqrt[D]{n-1}\right)^2\right)} \,. \tag{15}$$

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

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 $\sqrt[D]{n-2} \leqslant x \leqslant \sqrt[D]{n}$. By Lemma 8, we have

$$\lambda_1 \geqslant \sqrt[D]{n-1},$$

we have

$$\lambda_1 \geqslant \sqrt[D]{n-1} \geqslant \sqrt[D]{n-2} \,.$$

So $G(\lambda_1(G)) \leqslant G(\sqrt[D]{n-1})$, which implies

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

If $G \cong K_n$ it is easy to check that the equality in (15) holds. Conversely, if the equality in (15) holds, according to the above argument, we have

$$\lambda_1 = \sqrt[D]{n-1} \,.$$

Note that G has only one distinct eigenvalue if and only if G is an empty graph.

G has two distinct eigenvalues.

If the two distinct eigenvalues of G have the same absolute value, then $\lambda_1 =\mid \lambda_i \mid= \sqrt{\frac{2m-\lambda_1^2}{n-1}}(2 \leqslant i \leqslant n)$. By Lemma 6, $\mid \lambda_i \mid= \sqrt{\frac{2m-\lambda_1^2}{n-1}} = 1(2 \leqslant i \leqslant n)$, hence $2m = n$. Therefore, $\lambda_1 =\mid \lambda_2 \mid= \cdots =\mid \lambda_n \mid= 1$. By Lemma 6, $m_2 = m_1\lambda_1, \lambda_1 = 1$, so $m_1 = m_2$, eigenvalues $\lambda_1 = 1$, with multiplicity $\frac{n}{2}$, also eigenvalues $\lambda_i = -1$, with multiplicity $\frac{n}{2}$. Hence G is the direct sum of $m_1 = \frac{n}{2}$ complete graphs of order $\lambda_1 + 1 = 2$. Namely, G is $\frac{n}{2}K_2$, that is contradiction with equality (15).

If the two eigenvalues of G have diferent absolute values, by Lemma 6, $\mid \lambda_i \mid= -1(2 \leqslant i \leqslant n)$. Since G is a simple graph, we have $\sum_{i=1}^{n} \lambda_i = 0$. Also $\lambda_2 = \lambda_3 = \cdots = \lambda_n = -1$. Hence eigenvalues λ_1, with multiplicity $n-1$, also eigenvalues $\lambda_i = -1$, with multiplicity 1. Therefore, by Lemma 6, G is the direct sum of 1 complete graph of order $\lambda_1 + 1 = n$. Namely, G is K_n. ■

Theorem 7. *Let G be a nonempty and connected bipartite graph graph with n vertices, m and diameter D. Then*

$$\mathcal{E}(G) \leqslant 2\sqrt[D]{n-1} + \sqrt{(n-2)(2m - 2(\sqrt[D]{n-1})^2)} \; . \tag{16}$$

Equality holds if and only $G \cong S_n(K_{1,n-1})$.

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 $Z(x) = 2x + \sqrt{(n-2)(2m - x^2)}$ decreases for $\sqrt[D]{n-2} \leqslant x \leqslant \sqrt[D]{n}$. By Lemma 8, we have

$$\lambda_1 \geqslant \sqrt[D]{n-1} \, ,$$

we have

$$\lambda_1 \geqslant \sqrt[D]{n-1} \geqslant \sqrt[D]{n-2} \; .$$

So $Z(\lambda_1(G)) \leqslant Z(\sqrt[D]{n-1})$, which implies

$$\mathcal{E}(G) \leq 2\sqrt[D]{n-1} + \sqrt{(n-2)(2m - 2(\sqrt[D]{n-1})^2)} \; .$$

If $G \cong K_{1,n-1}$, it is easy to check that the equality in (16)holds. Conversely, if the equality in (16) holds, according to the above argument,

$$\lambda_1 = -\lambda_n = \sqrt[D]{n-1}\ .$$

Moreover, $|\ \lambda_i\ | = \sqrt{\frac{2m-\lambda_1^2}{n-2}}$ $(2 \leqslant i \leqslant n-1)$. Note that G has only one distinct eigenvalue if and only if G is an empty graph. We are reduced to the following two possibilities:

(1)G has two distinct eigenvalues.

If G only two distinct eigenvalues which have the same absolute value, since G is a bipartite graph, we have $\lambda_1 = -\lambda_2 \neq 0$ also by Lemma 6, $\lambda_2 = -1$. Hence $\lambda_1 =|\ \lambda_2\ |=1$, which implies $G \cong K_2(S_2)$.

If the two distinct eigenvalues of G have the same absolute value, then $\lambda_1 = -\lambda_n =|\ \lambda_i\ |= \sqrt{\frac{2m-\lambda_1^2}{n-1}}(2 \leqslant i \leqslant n)$. By Lemma 6, $\lambda_n = -\sqrt{\frac{2m-\lambda_1^2}{n-1}} = -1(2 \leqslant i \leqslant n)$, hence $2m = n$. Therefore, $\lambda_1 =|\ \lambda_2\ |= \cdots =|\ \lambda_n\ |= 1$. By Lemma 6, $m_2 = m_1\lambda_1, \lambda_1 = 1$, so $m_1 = m_2$, eigenvalues $\lambda_1 = 1$, with multiplicity $\frac{n}{2}$, also eigenvalues $\lambda_i = -1$, with multiplicity $\frac{n}{2}$. Hence G is the direct sum of $m_1 = \frac{n}{2}$ complete graphs of order $\lambda_1 + 1 = 2$. Namely, G is $\frac{n}{2}K_2$, that is contradiction with equality (16).

If the two eigenvalues of G have diferent absolute values, by Lemma 6, $|\ \lambda_i\ |= -1(2 \leqslant i \leqslant n)$. Noting that G is a bipartite graph, we have $\lambda_1 = -\lambda_n$, that is contradiction with two eigenvalues of G have diferent absolute values.

(2) If G has three distinct eigenvalues.

noting that G is a bipartite graph, we have $\lambda_1 = -\lambda_n = \sqrt[D]{n-1}$ and $\lambda_i = \sqrt{\frac{2m-\lambda_1^2}{n-2}} = 0$ $(2 \leqslant i \leqslant n-1)$, which implies that $\mathcal{E}(G) = 2\lambda_1 = 2\sqrt{m}$ and hence $\lambda_1 = \sqrt{m}$ and $\mathcal{E}(G) = \sqrt[D]{n-1}$. By Lemma 5, we have $G \cong K_{1,n-1}$. ■

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