

# New Upper Bounds for the Energy and Spectral Radius of Graphs

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## Abstract

Let  $G$  be a finite simple undirected graph with  $n$  vertices and  $m$  edges. 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 we give some new upper bounds for  $E(G)$  in terms of  $n, m$ , the largest and the smallest eigenvalue, and the standard deviation of the squared eigenvalues of  $G$ . Moreover, we present an upper bound for the spectral radius of  $G$  in terms of  $n, m$  and  $E(G)$ . New upper bound for the energy of the reciprocal graphs is also obtained. A number of our results rely on the use of well-known inequalities which have not been applied in this area before.

## 1 Introduction

Let  $G = (V, E)$  be a simple undirected graph with vertex set  $V = V(G) = \{v_1, v_2, \dots, v_n\}$  and edge set  $E(G)$ ,  $|E(G)| = m$ . The *adjacency matrix*  $A = A(G)$  of the graph  $G$  is an  $n \times n$  matrix  $[a_{ij}]$  such that,  $a_{ij} = 1$  if  $v_i$  is adjacent to  $v_j$ , and 0 otherwise. The eigenvalues  $\lambda_1, \lambda_2, \dots, \lambda_n$  of the graph  $G$  are the eigenvalues of its adjacency matrix  $A$ . The set of eigenvalues of the graph including their multiplicities is the *spectrum* of the graph. Since  $A$  is a symmetric matrix with zero trace, these eigenvalues are real and their sum is equal to zero. Thus

$$\lambda_1 + \lambda_2 + \dots + \lambda_n = 0. \quad (1)$$

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We also have

$$\text{trace}(A^2) = \sum_{i=1}^n \lambda_i^2 = 2m. \tag{2}$$

The *mean* of the eigenvalues of  $G$  is trivially defined as  $\bar{\lambda} = \frac{\lambda_1 + \lambda_2 + \dots + \lambda_n}{n} = 0$ . The *standard deviation* of the eigenvalues of the graph  $G$  denoted by  $\sigma = \sigma(G)$  is

$$\sigma = \sqrt{\frac{(\lambda_1 - \bar{\lambda})^2 + (\lambda_2 - \bar{\lambda})^2 + \dots + (\lambda_n - \bar{\lambda})^2}{n}} = \sqrt{\frac{2m}{n}}. \tag{3}$$

The *energy* of  $G$ , denoted by  $E(G)$ , was first defined by I. Gutman as the sum of the absolute values of its eigenvalues. Hence,

$$E(G) = \sum_{i=1}^n |\lambda_i|. \tag{4}$$

This concept arose in theoretical chemistry, since it can be used to approximate the total  $\pi$ -electron energy of a molecule. For details see [4-7, 18]. The first upper bound for  $E(G)$  was obtained in 1971 by McClelland [18] who proved:

$$E(G) \leq \sqrt{2mn}. \tag{5}$$

Since then, numerous other bounds for  $E(G)$  were discovered, see [2, 8, 13, 17]. In [15] Koolen and Moulton improved the bound (5) as follows: If  $2m > n$  and  $G$  is a graph with  $n$  vertices and  $m$  edges, then

$$E(G) \leq \frac{2m}{n} + \sqrt{(n-1) \left( 2m - \left( \frac{2m}{n} \right)^2 \right)}. \tag{6}$$

Moreover, 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  $\sqrt{\frac{2m - (\frac{2m}{n})^2}{n-1}}$ . In [22] Zhou showed that if  $G$  is a graph with  $n$  vertices,  $m$  edges and degree sequence  $d_1, d_2, \dots, d_n$ , then

$$E(G) \leq \sqrt{\frac{\sum_{i=1}^n d_i^2}{n}} + \sqrt{(n-1) \left( 2m - \frac{\sum_{i=1}^n d_i^2}{n} \right)}. \tag{7}$$

Equality holds 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  $\sqrt{\frac{2m - (\frac{2m}{n})^2}{n-1}}$ ,  $nK_1$ .

A graph  $G$  is *reciprocal* if the reciprocal of each of its eigenvalues is also an eigenvalue of  $G$ . In [12] Indulal and Vijaykumar showed that if  $G$  is a reciprocal graph with  $n$  vertices and  $m$  edges, then

$$E(G) \leq \sqrt{\frac{n(2m+n)}{2}}. \tag{8}$$

This bound is the best possible for  $G = tK_2$  and  $tP_4$ .

The *spectral radius* of  $G$ , denoted by  $\rho(G)$ , is the largest eigenvalue of the adjacency matrix of  $G$ . In [10] Hong showed that if  $G$  is simple connected graph with  $n$  vertices and  $m$  edges then

$$\rho(G) \leq \sqrt{2m - n + 1}, \tag{9}$$

with equality if and only if  $G$  is isomorphic to the star  $K_{1,n-1}$  or to the complete graph  $K_n$ . More results concerning the upper bound for the spectral radius can be found in [3, 11, 21].

In this paper we give new upper bounds for the energy and spectral radius of graphs. In Theorem 2.1 we improve the bound  $\sqrt{2mn}$ . Unfortunately we are not able to compare this bound to the Koolen and Moulton bound (6). A new upper bound for the energy of graphs in terms of the largest and the smallest eigenvalue of  $G$  and the determinant of its adjacency matrix  $A$  is obtained in Theorem 2.5.

In this research we also address the energy of the reciprocal graphs. In Theorem 2.6 we give an upper bound for their energy in terms of  $n$  and  $\rho$ . We observe that our bound is better than (8) if  $\rho^2 + \frac{1}{\rho^2} < \frac{4m}{n}$ .

The last result in this paper presents an upper bound for the spectral radius of  $G$  in terms of  $n, m$  and  $E(G)$ , Theorem 2.7. This result also helps to estimate the energy of  $G$  in terms of  $n, m$  and  $\rho(G)$ .

## 2 Results

The first result in this paper presents an improvement for the upper bound on the energy of a graph given in (5)  $E(G) \leq \sqrt{2mn}$ . Our bound for  $E(G)$  uses the number of vertices, the number of edges, the largest and the smallest eigenvalue and the standard deviation of the eigenvalues of the matrix  $A^2$ . Similar parameters have been used in [1, 9, 19] which however focus on lower bounds for the energy of graphs.

**Theorem 2.1** *Let  $G$  be a graph with  $n$  vertices and  $m$  edges and let  $\lambda_1, \lambda_2, \dots, \lambda_n$  be the eigenvalues of the adjacency matrix  $A$  of the graph  $G$ . If  $\rho = \max_{1 \leq i \leq n} |\lambda_i|$ ,  $\mu =$*

$\min_{1 \leq i \leq n} |\lambda_i|$ , and  $\bar{\sigma}$  is the standard deviation of the eigenvalues of  $A^2$ , then

$$E(G) \leq \sqrt{2mn} - \frac{\mu n \bar{\sigma}^2}{4(\rho^4 + (\frac{2m}{n})^2)}. \tag{10}$$

*Proof.* First, we will prove that for each  $i \in \{1, \dots, n\}$

$$\frac{\lambda_i^2}{2m} + \frac{1}{n} \geq \left(2 + \frac{(n\lambda_i^2 - 2m)^2}{2(n^2\lambda_i^4 + 4m^2)}\right) \frac{|\lambda_i|}{\sqrt{2mn}}. \tag{11}$$

Setting  $a = \frac{\lambda_i^2}{2m}$  and  $b = \frac{1}{n}$ , we obtain the equivalent inequality

$$\sqrt{\frac{a}{b}} + \sqrt{\frac{b}{a} + \frac{ab}{a^2 + b^2}} \geq \frac{5}{2}. \tag{12}$$

Denoting  $x = \sqrt{\frac{a}{b}}$  in (12) we get

$$\sqrt{\frac{a}{b}} + \sqrt{\frac{b}{a} + \frac{ab}{a^2 + b^2}} \geq \frac{5}{2} \Leftrightarrow x + \frac{1}{x} + \frac{1}{x^2 + \frac{1}{x^2}} - \frac{5}{2} \geq 0 \Leftrightarrow \frac{(x-1)^4(2x^2 + 3x + 2)}{2x(x^4 + 1)} \geq 0.$$

Since  $x \geq 0$  it is clear that  $\frac{(x-1)^4(2x^2+3x+2)}{2x(x^4+1)} \geq 0$ . Therefore the inequality (11) is valid.

Now, using (11) we deduce

$$\frac{1}{2m} \sum_{i=1}^n \lambda_i^2 + \sum_{i=1}^n \frac{1}{n} \geq \frac{2}{\sqrt{2mn}} \sum_{i=1}^n |\lambda_i| + \sum_{i=1}^n \frac{(n\lambda_i^2 - 2m)^2}{2(n^2\lambda_i^4 + 4m^2)} \frac{|\lambda_i|}{\sqrt{2mn}}. \tag{13}$$

Since  $\sum_{i=1}^n \lambda_i^2 = 2m$ , the inequality in (13) becomes

$$2 \geq \frac{2E(G)}{\sqrt{2mn}} + \frac{1}{\sqrt{2mn}} \sum_{i=1}^n \frac{(n\lambda_i^2 - 2m)^2}{2(n^2\lambda_i^4 + 4m^2)} |\lambda_i|.$$

Hence

$$E(G) \leq \sqrt{2mn} - \frac{1}{4} \sum_{i=1}^n \frac{(n\lambda_i^2 - 2m)^2}{n^2\lambda_i^4 + 4m^2} |\lambda_i|. \tag{14}$$

Using  $\rho \geq |\lambda_i| \geq \mu$  we obtain

$$\sum_{i=1}^n \frac{(n\lambda_i^2 - 2m)^2}{n^2\lambda_i^4 + 4m^2} |\lambda_i| \geq \frac{\mu}{\rho^4 + (\frac{2m}{n})^2} \sum_{i=1}^n \left(\lambda_i^2 - \frac{2m}{n}\right)^2. \tag{15}$$

Observe that  $\lambda_1^2, \lambda_2^2, \dots, \lambda_n^2$  are the eigenvalues of  $A^2$ , and they satisfy  $\frac{\lambda_1^2 + \dots + \lambda_n^2}{n} = \frac{2m}{n}$ .

Thus, the standard deviation  $\bar{\sigma}$  of the spectrum of  $A^2$  is equal to  $\sqrt{\frac{\sum_{i=1}^n (\lambda_i^2 - \frac{2m}{n})^2}{n}}$ . Based on this observation and using (14) and (15) we obtain

$$E(G) \leq \sqrt{2mn} - \frac{\mu n \bar{\sigma}_1^2}{4(\rho^4 + (\frac{2m}{n})^2)}.$$

■

Let us note that the standard deviation of the eigenvalues of  $A^2$  is zero if and only if  $\lambda_i = \pm \lambda_j$  for each  $i, j \in \{1, \dots, n\}$ . In this case our bound matches the original bound  $\sqrt{2mn}$ . In the special case when the spectrum of  $G$  consists of integer eigenvalues, (in which case  $G$  is called an *integral graph*), we modify the bound  $\sqrt{2mn}$  as follows.

**Proposition 2.2** *Let  $G$  be a graph with  $n$  vertices and  $m$  edges and suppose that all eigenvalues of  $G$ ,  $\lambda_1, \lambda_2, \dots, \lambda_n$ , are non-zero integers. If  $\rho = \max_{1 \leq i \leq n} |\lambda_i|$  and  $\mu = \min_{1 \leq i \leq n} |\lambda_i|$ , then*

$$E(G) \leq (2m)^{\frac{\rho}{\rho+\mu}} \cdot n^{\frac{\mu}{\rho+\mu}}. \tag{16}$$

*Proof.* We use the inequality between the quadratic and the arithmetic mean for the positive integers  $|\lambda_1|, \dots, |\lambda_n|$ . Therefore

$$\frac{2m}{E(G)} = \frac{\lambda_1^2 + \dots + \lambda_n^2}{|\lambda_1| + \dots + |\lambda_n|} \geq \frac{|\lambda_1| + \dots + |\lambda_n|}{n}. \tag{17}$$

Since  $|\lambda_1|, |\lambda_2|, \dots, |\lambda_n|$  are positive integers, we get  $\frac{|\lambda_1| + \dots + |\lambda_n|}{n} \geq 1$ . Obviously,  $\frac{\rho}{\mu} \geq 1$ . From (17) it follows

$$\left(\frac{2m}{E(G)}\right)^\mu \geq \left(\frac{|\lambda_1| + \dots + |\lambda_n|}{n}\right)^\mu \geq \frac{|\lambda_1| + \dots + |\lambda_n|}{n} = \frac{E(G)}{n}. \tag{18}$$

The required bound (16) follows directly from (18). Note that if  $n > 2m$ , then  $(2m)^{\frac{\rho}{\rho+\mu}} \cdot n^{\frac{\mu}{\rho+\mu}} < \sqrt{2mn}$ . Moreover, if  $|\lambda_1| = \dots = |\lambda_n|$ , then  $(2m)^{\frac{\rho}{\rho+\mu}} \cdot n^{\frac{\mu}{\rho+\mu}} = \sqrt{2mn}$ . ■

It is not hard to see that if  $\lambda_i$  and  $\mu_i$  are eigenvalues of the graphs  $G$  and  $H$ , respectively, such that  $|\lambda_i| \leq |\mu_i|$ , then  $E(G) \leq E(H)$ . In the next result we extend this trivial comparison by using Karamata's inequality [14].

**Theorem 2.3** *Let  $G$  and  $H$  be two graphs with eigenvalues  $|\lambda_1| \geq |\lambda_2| \geq \dots \geq |\lambda_n|$  and  $|\mu_1| \geq |\mu_2| \geq \dots \geq |\mu_n|$ , respectively. If  $|\lambda_1| \leq |\mu_1|$ ,  $|\lambda_1 \lambda_2| \leq |\mu_1 \mu_2|, \dots, |\lambda_1 \cdot \dots \cdot \lambda_n| \leq |\mu_1 \cdot \dots \cdot \mu_n|$ , then*

$$E(G) \leq E(H).$$

*Proof.* Let  $|\lambda_i| = e^{x_i}$  and  $|\mu_i| = e^{y_i}$ . Then

$$x_1 \geq x_2 \geq \dots \geq x_n; \quad y_1 \geq y_2 \geq \dots \geq y_n.$$

Moreover, for each  $i \in \{1, \dots, n\}$  it holds  $y_1 + \dots + y_i \geq x_1 + \dots + x_i$ , that is,  $(y_1, y_2, \dots, y_n)$  majorizes  $(x_1, x_2, \dots, x_n)$ . Applying Karamata's inequality for the non-decreasing convex function  $f(x) = e^x$  we deduce

$$E(G) = \sum_{i=1}^n e^{x_i} = \sum_{i=1}^n f(x_i) \leq \sum_{i=1}^n f(y_i) = \sum_{i=1}^n e^{y_i} = E(H). \tag{19}$$

P. Schweitzer in a 1914 paper [20] proved the following inequality: ■

**Proposition 2.4** For  $0 < m < M$ , and  $x_i \in [m, M]$  for  $i \in \{1, \dots, n\}$ ,

$$\left(\frac{1}{n} \sum_{i=1}^n x_i\right) \left(\frac{1}{n} \sum_{i=1}^n \frac{1}{x_i}\right) \leq \frac{(m+M)^2}{4mM}. \quad (19)$$

Our next two results are based on Schweitzer's inequality. In order to be able to use Schweitzer's inequality, we will only consider graphs whose spectrum does not contain zero. In the following theorem, we give an upper bound for the energy of  $G$  in terms of the absolute value of the largest eigenvalue, the smallest eigenvalue, and the determinant of  $A$ .

**Theorem 2.5** Let  $G$  be a graph with  $n$  vertices,  $A$  be its adjacency matrix, and let  $\lambda_1, \lambda_2, \dots, \lambda_n$  be the eigenvalues of  $A$ . If  $\rho = \max_{1 \leq i \leq n} |\lambda_i|$  and  $\mu = \min_{1 \leq i \leq n} |\lambda_i| > 0$ , then

$$E(G) \leq \frac{n(\rho + \mu)^2}{4\rho\mu} \cdot |\det(A)|^{\frac{1}{n}}.$$

*Proof.* Substituting  $x_i = |\lambda_i|$  in (19) we obtain

$$(|\lambda_1| + \dots + |\lambda_n|) \left(\frac{1}{|\lambda_1|} + \dots + \frac{1}{|\lambda_n|}\right) \leq \frac{n^2(\rho + \mu)^2}{4\rho\mu}. \quad (20)$$

Now, applying the inequality between the arithmetic and the geometric mean to the positive numbers  $\frac{1}{|\lambda_1|}, \dots, \frac{1}{|\lambda_n|}$  we obtain

$$\frac{1}{|\lambda_1|} + \dots + \frac{1}{|\lambda_n|} \geq \frac{n}{|\lambda_1 \cdot \dots \cdot \lambda_n|^{\frac{1}{n}}} = \frac{n}{|\det(A)|^{\frac{1}{n}}}. \quad (21)$$

The inequalities (20) and (21) yield

$$E(G) \cdot \frac{n}{|\det(A)|^{\frac{1}{n}}} \leq \frac{n^2(\rho + \mu)^2}{4\rho\mu}, \quad (22)$$

that is,

$$E(G) \leq \frac{n(\rho + \mu)^2}{4\rho\mu} \cdot |\det(A)|^{\frac{1}{n}}. \quad \blacksquare$$

The next result addresses the upper bound for the energy of the reciprocal graphs. Thanks to Schweitzer's inequality we are in a position to estimate  $E(G)$  in terms of the number of vertices and the spectral radius of  $G$ .

**Theorem 2.6** Let  $G$  be a reciprocal graph with  $n$  vertices and let  $\lambda_1, \lambda_2, \dots, \lambda_n$  be the eigenvalues of  $G$ . If  $\rho = \max_{1 \leq i \leq n} |\lambda_i|$ , then

$$E(G) \leq \frac{n(\rho + \frac{1}{\rho})}{2}. \quad (23)$$

*Proof.* Since  $G$  is a reciprocal graph,  $\frac{1}{\rho} = \min_{1 \leq i \leq n} |\lambda_i|$ . Moreover, the energy of  $G$  satisfies

$$E(G) = |\lambda_1| + |\lambda_2| + \dots + |\lambda_n| = \frac{1}{|\lambda_1|} + \frac{1}{|\lambda_2|} + \dots + \frac{1}{|\lambda_n|}.$$

Substituting these identities into (20) yields the desired bound. ■

It is easy to check that if  $\rho^2 + \frac{1}{\rho^2} < \frac{4m}{n}$ , then our bound (23) is better than the bound (8).

In our final result we present an upper bound for the spectral radius of  $G$  in terms of  $n, m$  and  $E(G)$ .

**Theorem 2.7** *Let  $G$  be a graph with  $n$  vertices,  $m$  edges, and energy  $E(G)$ . The spectral radius of  $G$  satisfies the inequality*

$$\rho(G) \leq \frac{E(G)}{n} + \frac{n-1}{n} \sqrt{\frac{2mn - E(G)^2}{n-1}}. \tag{24}$$

*Proof.* Let  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$  be the eigenvalues of  $G$ . Then  $\rho(G) = \lambda_1$ . For any real number  $x$  it holds

$$\lambda_1 \leq x + \sqrt{(|\lambda_1| - x)^2 + \dots + (|\lambda_n| - x)^2} = f(x).$$

Since equality  $\lambda_1 = f(x)$  can be achieved when  $|\lambda_2| = |\lambda_3| = \dots = |\lambda_n| = x$ , we need to find the smallest value for  $f(x)$ . The identities  $\lambda_1^2 + \dots + \lambda_n^2 = 2m$  and  $E(G) = |\lambda_1| + \dots + |\lambda_n|$  yield

$$f(x) = x + \sqrt{nx^2 - 2E(G)x + 2m}.$$

Since  $f$  grows and tends to infinity, the minimum occurs when  $f' = 0$ . Calculating the derivative of  $f(x)$  we have

$$f'(x) = 1 + \frac{nx - E(G)}{\sqrt{nx^2 - 2E(G)x + 2m}}. \tag{25}$$

Solving the equation in (25) we get  $x = \frac{E(G)(n-1) \pm \sqrt{2mn(n-1) - E(G)^2(n-1)}}{n(n-1)}$ . The largest possible  $\lambda_1$  and greatest lower bound for  $f(x)$  is then

$$f\left(\frac{E(G)(n-1) - \sqrt{2mn(n-1) - E(G)^2(n-1)}}{n(n-1)}\right) = \frac{E(G)}{n} + \frac{n-1}{n} \sqrt{\frac{2mn - E(G)^2}{n-1}},$$

which occurs when  $|\lambda_2| = \dots = |\lambda_n| = \frac{E(G)(n-1) - \sqrt{2mn(n-1) - E(G)^2(n-1)}}{n(n-1)}$  and

$$\rho(G) = \lambda_1 = \frac{E(G)}{n} + \frac{n-1}{n} \sqrt{\frac{2mn - E(G)^2}{n-1}}.$$

■

In order to illustrate Theorem 2.7 we consider the complete graph  $K_n$ . It is well-known that  $m = \frac{n(n-1)}{2}$  and  $E(K_n) = 2n - 2$ . Applying the formula in (24) we obtain

$$\lambda_1 \leq \frac{2n-2}{n} + \frac{n-1}{n} \sqrt{\frac{(n-1)n^2 - 4(n-1)^2}{n-1}} = n-1.$$

This observation is in agreement with the fact that the spectrum of the complete graph  $K_n$  is  $\{(n-1)^1, (-1)^{n-1}\}$ .

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