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On Energy of Graphs

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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 *Math. Commun.* **5** (2010) 443–451, Fath-Tabar et al. gave a lower bound for the energy $E(G)$ of graph G. In *MATCH Commun. Math. Comput. Chem.* **72** (2014) 179–182, Milovanović et al. obtained sharper result than the lower bound on $E(G)$ given by Fath–Tabar et al. We found some error in these lower bounds and the characterization of extremal graphs. In this note we have corrected these results and obtain extremal graphs.

1 Introduction

Let G be a graph of order n with m edges. Let $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_{n-1}| \geq |\lambda_n|$ denote the absolute eigenvalues of G arranged in non-increasing order, respectively. The energy of graph G is defined as

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

For its basic properties and applications, including various lower and upper bounds, see the book [12], the surveys [8, 9], the recent papers [5, 6, 11] and the references cited there in. Throughout this paper we use $K_{a,\,b}$ $(a+b=n)$ and K_n to denote the complete bipartite graph and the complete graph on n vertices, respectively. The disjoint union of (vertex-disjoint) graphs G_1 and G_2 will be denoted with $G_1 \cup G_2$. When more than one graph is under consideration, then we write $\lambda_i(G)$ (or $\rho_i(G)$) instead of λ_i (or ρ_i).

In [7], Fath-Tabar et al. gave a lower bound for the energy $E(G)$ of graph G:

$$E(G) \geq \sqrt{2m\,n - \frac{n^2}{4}\,\left(|\lambda_1| - |\lambda_n|\right)^2}\,. \tag{1}$$

In [11], Milovanović et al. obtained the following lower bound on $E(G)$:

$$E(G) \geq \sqrt{2m\,n - \alpha(n)\;(|\lambda_1| - |\lambda_n|)^2}\,, \tag{2}$$

where $\alpha(n) = n\left[\frac{n}{2}\right]\left(1 - \frac{1}{n}\left[\frac{n}{2}\right]\right)$, while $[x]$ denotes integer part of a real number x. Moreover, the equality holds in (2) if and only if $G \cong \overline{K}_n$ or $G \cong C_4$.

Sometimes both of the lower bounds are imaginary. For example, $G \cong K_{a,b}$ ($a + b = n$, n is even, $n > 8$). Then we have $m = a\,b$, $|\lambda_1| = \sqrt{a\,b} = |\lambda_2|$, $|\lambda_3| = |\lambda_4| = \cdots = |\lambda_n| = 0$. Now,

$$\begin{aligned} 2m\,n - \alpha(n)\;(|\lambda_1| - |\lambda_n|)^2 &= 2m\,n - \frac{n^2}{4}\;(|\lambda_1| - |\lambda_n|)^2 \\ &= 2a\,b\,n - \frac{n^2}{4}\,a\,b = a\,b\left[2\,n - \frac{n^2}{4}\right] < 0, \qquad n > 8, \end{aligned}$$

the lower bounds in (1) and (2) are imaginary. Moreover, for $G \cong p\,K_2$ ($n = 2\,p$), the equality holds in (2). Hence the characterization of extremal graphs in (2) is not true. We now give some results that will be needed for our main results.

Lemma 1.1. *Let G be a connected graph of order n. Also let $\rho_1 \geq \rho_2 \geq \cdots \geq \rho_n$ be non-increasing eigenvalues of graph G. If G has diameter at least 3, then $\rho_1 > \rho_2 > 0$ and $\rho_n < 0$.*

Proof: By Perron-Frobenius theorem, we have $\rho_1 > \rho_2$. Since G has diameter at least 3, P_4 is an induced subgraph of G. Therefore we have $\rho_2(G) \geq \rho_2(P_4) \approx 0.618$ and $\rho_n(G) \leq \rho_2(K_2) = -1$. This proves the lemma. ∎

Lemma 1.2. [2] *Let G be a connected graph with the largest eigenvalue λ_1. Then G is bipartite if and only if $-\lambda_1$ is an eigenvalue of G.*

Lemma 1.3. *Let G be a graph of order $n\,(> 1)$ with m edges. Then $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_{k-1}| = |\lambda_k| > 0$ ($k \geq 2$) and the remaining eigenvalues are zero (if exists) if and only if $G \cong p\,K_1 \cup \cup_{i=1}^{q} K_{a_i,\,b_i}$, where $\sum\limits_{i=1}^{q}(a_i + b_i) + p = n$ with $a_i \cdot b_i = m/q$, $i = 1, 2, \ldots, q$ ($k = 2q$).*

Proof: If $G \cong p\,K_1 \cup \cup_{i=1}^{q} K_{a_i,\,b_i}$, where $\sum\limits_{i=1}^{q}(a_i + b_i) + p = n$ with $a_i \cdot b_i = m/q$, $i = 1, 2, \ldots, q$ ($k = 2q$), then $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_{k-1}| = |\lambda_k| > 0$ ($k \geq 2$) and the remaining eigenvalues are zero (if exists) hold. Conversely, let

$$|\lambda_1| = |\lambda_2| = \cdots = |\lambda_{k-1}| = |\lambda_k| > 0 \;(k \geq 2) \tag{3}$$

and the remaining eigenvalues are zero (if exists). Then each connected component contain at most three distinct eigenvalues (the magnitude of the non-zero eigenvalues are same) except isolated vertices. Let $G_1, G_2, \ldots, G_q$ be the $q\,(\geq 1)$ connected components in G except isolated vertices. Then by Lemma 1.2, from (3), G_i $(1 \leq i \leq q)$ is bipartite. If any one G_i $(1 \leq i \leq q)$ is not complete bipartite, then the diameter of G_i is at least 3. By Lemma 1.1, we can get a contradiction. Otherwise, each G_i $(1 \leq i \leq q)$ is complete bipartite K_{a_i, b_i}, $i = 1, 2, \ldots, q$. By (3), we conclude that $a_i \cdot b_i = m/q$, $i = 1, 2, \ldots, q$ with $k = 2q$. Therefore $G \cong p\,K_1 \cup \cup_{i=1}^{q} K_{a_i, b_i}$, where $\sum_{i=1}^{q} (a_i + b_i) + p = n$ with $a_i \cdot b_i = m/q$, $i = 1, 2, \ldots, q$ $(k = 2q)$. ■

Corollary 1.4. *Let G be a graph of order $n\,(> 1)$. Then $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_{n-1}| = |\lambda_n| > 0$ if and only if $G \cong \frac{n}{2}\,K_2$ (n is even).*

Proof: Setting $k = n$ in Lemma 1.3, we get the required result. ■

Lemma 1.5. [1] *Let $a_1, a_2, \ldots, a_n$ and $b_1, b_2, \ldots, b_n$ be real numbers for which there exist real constants a, b, A and B, so that for each i, $i = 1, 2, \ldots, n$, $0 < a \leq a_i \leq A$ and $0 < b \leq b_i \leq B$. Then the following inequality is valid:*

$$\left| n \sum_{i=1}^{n} a_i\, b_i - \sum_{i=1}^{n} a_i \sum_{i=1}^{n} b_i \right| \leq \alpha(n)\,(A - a)\,(B - b), \tag{4}$$

where $\alpha(n) = n \left[\frac{n}{2}\right] \left(1 - \frac{1}{n} \left[\frac{n}{2}\right]\right)$. Moreover, the equality holds in (4) if and only if $a_1 = a_2 = \cdots = a_n$ and $b_1 = b_2 = \cdots = b_n$.

Caporossi et al. [3] discovered the following simple lower bound:

Lemma 1.6. [3] *For a graph G with m edges.*

$$E(G) \geq 2\sqrt{m} \tag{5}$$

with equality holding if and only if G consists of a complete bipartite graph $K_{a,b}$ such that $a \cdot b = m$ and arbitrarily many isolated vertices.

Theorem 1.7. *Let G be a graph of order n with m edges. Also let $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_{k-1}| \geq |\lambda_k|$ $(k \leq n)$ be k non-zero eigenvalues of G. Then*

$$E(G) \geq \sqrt{\max\left\{4m,\, 2m\,k - \alpha(k)\,\left(|\lambda_1| - |\lambda_k|\right)^2\right\}}\,, \tag{6}$$

where $\alpha(k) = k \left[\frac{k}{2}\right] \left(1 - \frac{1}{k} \left[\frac{k}{2}\right]\right)$, while $[x]$ denotes integer part of a real number x. Moreover, the equality holds in (6) if and only if $G \cong p\,K_1 \cup \cup_{i=1}^{q} K_{a_i, b_i}$, where $\sum_{i=1}^{q} (a_i + b_i) + p = n$ with $a_i \cdot b_i = m/q$, $i = 1, 2, \ldots, q$ $(k = 2q)$.

Proof: If $G \cong n\,K_1$ (or $k=0$), then $m=0$ and $E(G)=0$. Hence the equality holds in (6). Otherwise, there is at least one edge in G, that is, $k \geq 2$. Let $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_{k-1}| \geq |\lambda_k|$ be the $k\,(2 \leq k \leq n)$ non-zero eigenvalues of G. Then we have

$$E(G) = \sum_{i=1}^{k} |\lambda_i| \quad \text{and} \quad \sum_{i=1}^{k} |\lambda_i|^2 = \sum_{i=1}^{n} |\lambda_i|^2 = \sum_{i=1}^{n} \lambda_i^2 = 2m. \tag{7}$$

By Cauchy-Schwarz inequality with the above result, we have

$$E(G)^2 = \left(\sum_{i=1}^{k} |\lambda_i|\right)^2 \leq 2m\,k. \tag{8}$$

Setting $a_i = |\lambda_i|$, $b_i = |\lambda_i|$, $a = b = |\lambda_k|$ and $A = B = |\lambda_1|$, $i = 1, 2, \ldots, k$, inequality (4) becomes

$$\left| k \sum_{i=1}^{k} |\lambda_i|^2 - \left(\sum_{i=1}^{k} |\lambda_i|\right)^2 \right| \leq \alpha(k)\,(|\lambda_1| - |\lambda_k|)^2\,.$$

By (7) and (8), from the above, we get

$$2m\,k - E(G)^2 \leq \alpha(k)\,(|\lambda_1| - |\lambda_k|)^2\,. \tag{9}$$

By (5) with the above result, we get the required result in (6). The first part of the proof is done.

By Lemma 1.5, the equality holds in (9) if and only if $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_{k-1}| = |\lambda_k| > 0$ $(k \geq 2)$ and the remaining eigenvalues are zero (if exists). By Lemma 1.6, we have $E(G) = 2\sqrt{m}$ if and only if G consists of a complete bipartite graph $K_{a,b}$ such that $a \cdot b = m$ and arbitrarily many isolated vertices. From these results with Lemma 1.3, we conclude that the equality holds in (6) if and only if $G \cong p\,K_1 \cup \cup_{i=1}^{q} K_{a_i, b_i}$, where $\sum_{i=1}^{q} (a_i + b_i) + p = n$ with $a_i \cdot b_i = m/q$, $i = 1, 2, \ldots, q$ $(k = 2q)$. ■

Already we have mentioned that sometimes the lower bounds on $E(G)$ in [7, 11] are imaginary. We now revise these lower bounds in the following:

Corollary 1.8. [7, 11] *Let G be a graph of order n with m edges. Let $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_{n-1}| \geq |\lambda_n|$ be non-increasing non-zero eigenvalues of G. Then*

$$\begin{aligned} E(G) &\geq \sqrt{\max\left\{4m,\, 2m\,n - \alpha(n)\,\left(|\lambda_1| - |\lambda_n|\right)^2\right\}} \\ &\geq \sqrt{\max\left\{4m,\, 2m\,n - \frac{n^2}{4}\,\left(|\lambda_1| - |\lambda_n|\right)^2\right\}}\,, \end{aligned} \tag{10}$$

where $\alpha(n) = n\left[\frac{n}{2}\right]\left(1 - \frac{1}{n}\left[\frac{n}{2}\right]\right)$, while $[x]$ denotes integer part of a real number x.

In [11], Milovanović et al. obtained another result on $E(G)$:

Lemma 1.9. [11] *Let G be a graph of order n with m edges. Also let $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_{n-1}| \geq |\lambda_n| > 0$ be a non-increasing arrangement of eigenvalues of G. Then*

$$E(G) \geq \frac{|\lambda_1|\,|\lambda_n| n + 2m}{|\lambda_1| + |\lambda_n|} \tag{11}$$

with equality holding if and only if $G \cong \overline{K}_n$.

The characterization of extremal graph is wrong. For $G \cong \overline{K}_n$, we have $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_{n-1}| = |\lambda_n| = 0$ and the right side of (11) does not exist. Moreover, it is mentioned in the statement that $|\lambda_1| = |\lambda_2| = \cdots = |\lambda_{n-1}| = |\lambda_n| > 0$, a contradiction.

We have corrected the above result:

Theorem 1.10. *Let G be a graph of order n with m edges. Let $|\lambda_1| \geq |\lambda_2| \geq \cdots \geq |\lambda_{n-1}| \geq |\lambda_n| > 0$ be a non-increasing arrangement of eigenvalues of G. Then*

$$E(G) \geq \frac{|\lambda_1|\,|\lambda_n| n + 2m}{|\lambda_1| + |\lambda_n|} \tag{12}$$

with equality holding if and only if $|\lambda_i| = |\lambda_n|$ or $|\lambda_i| = |\lambda_1|$ for any $i = 1, 2, \ldots, n$.

Proof: We have $|\lambda_n| \leq |\lambda_i| \leq |\lambda_1|$, for any $i = 1, 2, \ldots, n$, that is,

$$(|\lambda_i| - |\lambda_n|)\ (|\lambda_i| - |\lambda_1|) \leq 0. \tag{13}$$

From the above inequality, we get

$$\sum_{i=1}^{n} \Big(|\lambda_i|^2 - (|\lambda_1| + |\lambda_n|)\, |\lambda_i| + |\lambda_1|\, |\lambda_n| \Big) \leq 0,$$

that is,

$$2m - (|\lambda_1| + |\lambda_n|)\, E(G) + n\, |\lambda_1|\, |\lambda_n| \leq 0,$$

which gives the required result in (12). Moreover, the equality holds in (12) if and only if the equality holds in (13), that is, if and only if $|\lambda_i| = |\lambda_n|$ or $|\lambda_i| = |\lambda_1|$ for any $i = 1, 2, \ldots, n$. ■

Remark 1.11. *The equality holds in (12) if and only if $|\lambda_i| = |\lambda_n|$ or $|\lambda_i| = |\lambda_1|$ for any $i = 1, 2, \ldots, n$. Suppose that G has either $|\lambda_i| = |\lambda_n|$ or $|\lambda_i| = |\lambda_1|$ for any $i = 1, 2, \ldots, n$. Then G has at most four distinct eigenvalues. For two distinct eigenvalues of graph G, each connected component is complete graph K_p in G such that $p \cdot q = n$, where q $(q \geq 1)$ is the number of connected components. Cvetković et al. [4, p. 166] proved that a connected* *bipartite regular graph with four distinct eigenvalues must be the incidence graph of a symmetric* $2-(\nu, k, \lambda)$ *design (for definition of a* $2-(\nu, k, \lambda)$ *design, see [4, 10]). Moreover, its spectrum is*

$$\Big\{k, \underbrace{\sqrt{k-\nu}, \dots, \sqrt{k-\nu}}_{\nu-1}, \underbrace{-\sqrt{k-\nu}, \dots, -\sqrt{k-\nu}}_{\nu-1}, -k\Big\}.$$

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