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Some upper bounds for the energy of graphs

Huiqing Liu*
School of Mathematics and Computer Science, Hubei University, Wuhan 430062, China
E-mail: liuhuiqing@eyou.com

Mei Lu
Department of Mathematical Sciences, Tsinghua University, Beijing 100084, China
E-mail: mlu@math.tsinghua.edu.cn

Feng Tian
Institute of Systems Science, Academy of Mathematics and Systems Sciences, Chinese Academy of Sciences, Beijing 100080, China
E-mail: ftian@iss.ac.cn

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Let $G = (V, E)$ be a graph with n vertices and e edges. Denote $V(G) = \{v_1, v_2, \ldots, v_n\}$. The 2-degree of v_i, denoted by t_i, is the sum of degrees of the vertices adjacent to v_i, $1 \leqslant i \leqslant n$. Let σ_i be the sum of the 2-degree of vertices adjacent to v_i. In this paper, we present two sharp upper bounds for the energy of G in terms of n, e, t_i, and σ_i, from which we can get some known results. Also we give a sharp bound for the energy of a forest, from which we can improve some known results for trees.

KEY WORDS: graph, energy, bipartite graph, forest, tree

1. Introduction

Let $G = (V, E)$ be a simple undirected graph with n vertices and m edges. Denote $V(G) = \{v_1, v_2, \ldots, v_n\}$. For $v_i \in V(G)$, the degree of v_i, written by $d(v_i)$ or d_i, is the number of edges incident with v_i. The 2-degree of v_i [2] is the sum of degrees of the vertices adjacent to v_i and denoted by $t(v_i)$ or t_i. The *average 2-degree* of v_i, denoted by m_i, is the average of the degrees of the vertices adjacent to v_i. Then $t_i = d_i m_i$. Furthermore, denoted by σ_i the sum of the 2-degree of vertices adjacent to v_i. A bipartite graph $G = (X, Y; E)$ is (a, b)-*semiregular* if there exist two constants a and b such that each vertex in X has degree a and each vertex in Y has degree b. A bipartite graph $G = (X, Y; E)$ is (p_x, p_y)-*pseudo-semiregular* if there exist two constants p_x and p_y such that

*Corresponding author.

each vertex in X has average 2-degree p_x and each vertex in Y has average 2-degree p_y. The *incident graph of a* 2-(v,k,λ)-*design* is a (r,k)-semiregular bipartite graph with $v+b$ vertices and $vr(=bk)$ edges. The distance between v_i and v_j in G, denoted by $d(v_i,v_j)$, is the number of edges in a shortest path joining v_i and v_j. Moreover, if G is connected, then the eccentricity of v_i, denoted by $l(v_i)$, is defined by $l(v_i)=\max\{d(v_i,v_j):\ v_j\in V,\ i\neq j\}$.

The *energy* of G, denoted by $E(G)$, is defined as $E(G)=\sum_{i=1}^{n}|\lambda_i|$, where $\lambda_1\geqslant\lambda_2\geqslant\cdots\geqslant\lambda_n$ are the eigenvalues of the adjacency matrix of G. This concept was introduced by 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 [16] discovered the first upper bound for $E(G)$ as follows:

$$E(G)\leqslant\sqrt{2en}. \tag{1}$$

Since then, numerous other bounds for $E(G)$ were given (see, e.g., [1,6–9,11–16]).

Let us recall some upper bounds for $E(G)$ which were obtained recently.

(1) Koolen and Moulton [13]: Let G be a graph with n vertices and e edges. If $2e\geqslant n$, then

$$E(G)\leqslant\frac{2e}{n}+\sqrt{(n-1)\left[2e-\left(\frac{2e}{n}\right)^2\right]}. \tag{2}$$

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 $\sqrt{\frac{2e-(\frac{2e}{n})^2}{n-1}}$.

If $2e\leqslant n$, then

$$E(G)\leqslant 2e. \tag{3}$$

Equality holds if and only if G is disjoint union of edges and isolated vertices.

(1′) Koolen and Moulton [14]: Let G be a bipartite graph with $n>2$ vertices and e edges. If $2e\geqslant n$, then

$$E(G)\leqslant 2\left(\frac{2e}{n}\right)+\sqrt{(n-2)\left[2e-2\left(\frac{2e}{n}\right)^2\right]}. \tag{4}$$

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-(v,k,λ)-design with $k=\frac{2e}{n}$ and $\lambda=\frac{k(k-1)}{v-1}$ ($n=2v$, $2\sqrt{e}<n<2e$).

(2) Zhou [19]: If G is a graph with n vertices, e edges, and degree sequence $d_1, d_2, \ldots, d_n$, then

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

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 $\sqrt{(2e - (\frac{2e}{n})^2)/(n-1)}$ or nK_1.

(2′) Zhou [19]: If G is a bipartite graph with $n > 2$ vertices, e edges, and degree sequence $d_1, d_2, \ldots, d_n$, then

$$E(G) \leqslant 2\sqrt{\frac{\sum_{i=1}^n d_i^2}{n}} + \sqrt{(n-2)\left(2e - \frac{2\sum_{i=1}^n d_i^2}{n}\right)}. \tag{6}$$

Equality holds if and only if G is either $\frac{n}{2}K_2$, a complete bipartite graph, the incidence graph of a symmetric 2-(v, k, λ)-design with $k = \frac{2e}{n}$, and $\lambda = \frac{k(k-1)}{v-1}$ $(n = 2v)$ or nK_1.

(3) Yu, et al. [17]: Let G be a non-empty graph with n vertices, e edges, degree sequence $d_1, d_2, \ldots, d_n$, and 2-degree sequence $t_1, t_2, \ldots, t_n$. Then

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

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

(i) $G \cong \frac{n}{2}K_2$; (ii) $G \cong K_n$; (iii) G is a non-bipartite connected p-pseudo-regular graph with three distinct eigenvalues $\left(p,\ \sqrt{\frac{2m-p^2}{n-1}},\ -\sqrt{\frac{2m-p^2}{n-1}}\right)$, where $p > \sqrt{\frac{2m}{n}}$.

(3′) Yu et al. [17]: Let $G = (X, Y)$ be a non-empty bipartite graph with $n > 2$ vertices, e edges, degree sequence $d_1, d_2, \ldots, d_n$ and 2-degree sequence $t_1, t_2, \ldots, t_n$. Then

$$E(G) \leqslant 2\sqrt{\frac{\sum_{i=1}^n t_i^2}{\sum_{i=1}^n d_i^2}} + \sqrt{(n-2)\left(2e - \frac{2\sum_{i=1}^n t_i^2}{\sum_{i=1}^n d_i^2}\right)}. \tag{8}$$

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

(i) $G \cong \frac{n}{2}K_2$;

(ii) $G \cong K_{r_1,r_2} \cup (n - r_1 - r_2)K_1$, where $r_1r_2 = m$;

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

Note that inequality (2) and (4) can be obtained from inequality (5) and (6), and the inequality (5) and (6) can be obtained from inequality (7) and (8) (see [17]).

In this paper, we first present two new upper bounds for $E(G)$ in terms of n, e, t_i, and σ_i, from which we can improve some known results. We also obtain another upper bound for the energy of a forest T in terms of n, e, the degree d_i, and the average degree m_i of one vertex v_i, and give an example to illustrate that our result is, in some sense, best.

2. The energy of a graph

In order to obtain a sharp upper bound for the energy of a graph, we need the following lemmas.

In [18], for connected graph G, Hong and Zhang obtain an upper bound of $\lambda_1(G)$. In fact, it also holds for any non-empty graph.

Lemma 2.1 [18]. Let G be a non-empty simple graph of order n. Then

$$\lambda_1(G) \geqslant \sqrt{\frac{\sum_{i=1}^{n}\sigma_i^2}{\sum_{i=1}^{n}t_i^2}} \tag{9}$$

with equality if and only if

$$\frac{\sigma_1}{t_1} = \frac{\sigma_2}{t_2} = \cdots = \frac{\sigma_n}{t_n}$$

or G is a bipartite graph with $V = \{v_1, v_2, \ldots, v_s\} \cup \{v_{s+1}, v_{s+2}, \ldots, v_n\}$ such that $\sigma_1/t_1 = \sigma_2/t_2 = \cdots \sigma_s/t_s$ and $\sigma_{s+1}/t_{s+1} = \sigma_{s+2}/t_{s+2} = \cdots \sigma_n/t_n$.

Lemma 2.2 [4]. A graph G has only one distinct eigenvalue if and only if G is an empty graph. A graph G has two distinct eigenvalues $\mu_1 > \mu_2$ with multiplicities s_1 and s_2 if and only if G is the direct sum of s_1 complete graphs of order $\mu_1 + 1$. In this case, $\mu_2 = -1$ and $s_2 = s_1\mu_1$.

Lemma 2.3 [3]. Let G be a graph with e edges. Then

$$E(G) \geqslant 2\sqrt{e} \tag{10}$$

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

Lemma 2.4 [19]. Let

$$f(x) = 2x + \sqrt{(n-2)(2e-2x^2)}, \quad x \leqslant \sqrt{e},$$

and

$$g(x) = x + \sqrt{(n-2)(2e-x^2)}, \quad x \leqslant \sqrt{2e}.$$

Then $f(x)$ and $g(x)$ are monotonously decreasing in $x \geqslant \sqrt{\frac{2e}{n}}$.

First, we give an upper bound for $E(G)$ and characterize those graphs for which this bound is best possible.

Theorem 2.5. Let G be a non-empty simple graph with n vertices and e edges. Then

$$E(G) \leqslant \sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}} + \sqrt{(n-1)\left(2e - \frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}\right)}. \tag{11}$$

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 graph satisfying $\frac{\sigma_1}{t_1} = \cdots = \frac{\sigma_n}{t_n}$ and has three distinct eigenvalues $\left(p, \sqrt{\frac{2e-p^2}{n-1}}, -\sqrt{\frac{2e-p^2}{n-1}}\right)$, where $p = \frac{\sigma_1}{t_1} = \cdots = \frac{\sigma_n}{t_n} > \sqrt{\frac{2e}{n}}$.

Proof. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ be the eigenvalues of G. By the Cauchy–Schwartz inequality, we have

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

Hence

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

By lemma 2.1, we have

$$\lambda_1 \geqslant \sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}}$$

and equality holds if and only if $\sigma_1/t_1 = \sigma_2/t_2 = \cdots = \sigma_n/t_n$, or G is a bipartite graph with $V = \{v_1, \ldots, v_s\} \cup \{v_{s+1}, \ldots, v_n\}$ such that $\sigma_1/t_1 = \cdots \sigma_s/t_s$ and $\sigma_{s+1}/t_{s+1} = \cdots = \sigma_n/t_n$.

Noting that $d_1\sigma_1 + d_2\sigma_2 + \cdots + d_n\sigma_n = t_1^2 + t_2^2 + \cdots + t_n^2$ and $t_1 + t_2 + \cdots + t_n = d_1^2 + d_2^2 + \cdots + d_n^2$, we have

$$\lambda_1(G) \geqslant \sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}} \geqslant \sqrt{\frac{\left(\sum_{i=1}^n d_i\sigma_i\right)^2}{\sum_{i=1}^n t_i^2 \sum_{i=1}^n d_i^2}} = \sqrt{\frac{\sum_{i=1}^n t_i^2}{\sum_{i=1}^n d_i^2}} \geqslant \sqrt{\frac{\left(\sum_{i=1}^n t_i\right)^2}{n\sum_{i=1}^n d_i^2}}$$
$$= \sqrt{\frac{1}{n}\sum_{i=1}^n {d_i}^2} \geqslant \sqrt{\frac{2e}{n}}. \tag{12}$$

Hence, by lemma 2.4, $g(\lambda_1(G)) \leqslant g\left(\sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}}\right)$, which implies

$$E(G) \leqslant \sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}} + \sqrt{(n-1)\left(2e - \frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}\right)}.$$

If G is one of the three graphs shown in the second part of the theorem, it is easy to check that the equality (11) holds. Conversely, if the equality (11) holds, according to the above argument, we have

$$\lambda_1(G) = \sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}},$$

which implies that $\sigma_1/t_1 = \sigma_2/t_2 = \cdots = \sigma_n/t_n$, or G is a bipartite graph with $V = \{v_1, \ldots, v_s\} \cup \{v_{s+1}, \ldots, v_n\}$ such that $\sigma_1/t_1 = \cdots = \sigma_s/t_s$ and $\sigma_{s+1}/t_{s+1} = \cdots \sigma_n/t_n$. Moreover, $|\lambda_i| = \sqrt{\frac{2e-\lambda_1^2}{n-1}}$ $(2 \leqslant i \leqslant n)$. 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 the two distinct eigenvalues of G have the same absolute value, then $\lambda_1 = |\lambda_i| = \sqrt{\frac{2e-\lambda_1^2}{n-1}}$ $(2 \leqslant i \leqslant n)$. By lemma 2.2, $|\lambda_i| = \sqrt{\frac{2e-\lambda_1^2}{n-1}} = 1$ $(2 \leqslant i \leqslant n)$. Hence $2e = n$, which implies $G \cong \frac{n}{2}K_2$.
If the two eigenvalues of G have different absolute values, then by lemma 2.2, $\lambda_i = -1$ $(2 \leqslant i \leqslant n)$. Moreover, G is a complete graph of order n, i.e., $G \cong K_n$.

(2) G has three distinct eigenvalues.

In this case, $\lambda_1 = \sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}}$ and $|\lambda_i| = \sqrt{\frac{2e-\lambda_1^2}{n-1}}$ $(2 \leqslant i \leqslant n)$. Moreover, $\lambda_1 > \lambda_i$ and $\lambda_i \neq 0$. Combining the fact that

$$\frac{\sigma_1}{t_1} = \frac{\sigma_2}{t_2} = \cdots = \frac{\sigma_n}{t_n}$$

or G is a bipartite graph with $V = \{v_1, \ldots, v_s\} \cup \{v_{s+1}, \ldots, v_n\}$ such that $\sigma_1/t_1 = \cdots = \sigma_s/t_s$ and $\sigma_{s+1}/t_{s+1} = \cdots = \sigma_n/t_n$, we have G is a non-bipartite connected graph with $\frac{\sigma_1}{t_1} = \frac{\sigma_2}{t_2} = \cdots = \frac{\sigma_n}{t_n}$ and has three distinct eigenvalues $\left(p, \sqrt{\frac{2e-p^2}{n-1}}, -\sqrt{\frac{2e-p^2}{n-1}}\right)$, where $p = \sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}} = \frac{\sigma_i}{t_i} = \frac{t_i}{d_i} > \sqrt{\frac{2e}{n}}$ $(1 \leqslant i \leqslant n)$. This completes the proof theorem 2.5. □

Note 2.6. By (12), we have the bound (11) is better than (2), (5), and (7).

3. The energy of a bipartite graph

In this section, we give an upper bound for the energy of a bipartite graph and characterize those graphs for which this bound is best possible.

Theorem 3.1. Let $G = (X, Y)$ be a non-empty bipartite graph with $n > 2$ vertices and e edges. Then

$$E(G) \leqslant 2\sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}} + \sqrt{(n-2)\left(2e - \frac{2\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}\right)}. \tag{13}$$

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

(1) $G \cong \frac{n}{2} K_2$;

(2) $G \cong K_{r_1, r_2} \cup (n - r_1 - r_2) K_1$, where $r_1 r_2 = e$;

(3) G is a connected bipartite graph with $V = \{v_1, v_2, \ldots, v_s\} \cup \{v_{s+1}, v_{s+2}, \ldots, v_n\}$ such that $\sigma_1/t_1 = \sigma_2/t_2 = \cdots = \sigma_s/t_s$ and $\sigma_{s+1}/t_{s+1} = \sigma_{s+2}/t_{s+2} = \cdots = \sigma_n/t_n$, and has four distinct eigenvalues $\left(\sqrt{p_x p_y}, \sqrt{\frac{2e-2p_x p_y}{n-2}}, -\sqrt{\frac{2e-2p_x p_y}{n-2}}, -\sqrt{p_x p_y}\right)$, where $p_x = \sigma_1/t_1 = \cdots \sigma_s/t_s$, $p_y = \sigma_{s+1}/t_{s+1} = \cdots \sigma_n/t_n$ and $\sqrt{p_x p_y} > \sqrt{\frac{2e}{n}}$.

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

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

Hence

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

By lemma 2.1, we have

$$\lambda_1 \geqslant \sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}},$$

and equality holds if and only if $\sigma_1/t_1 = \sigma_2/t_2 = \cdots = \sigma_n/t_n$, or G is a bipartite graph with $V = \{v_1, \ldots, v_s\} \cup \{v_{s+1}, \ldots, v_n\}$ such that $\sigma_1/t_1 = \cdots = \sigma_s/t_s$ and $\sigma_{s+1}/t_{s+1} = \cdots = \sigma_n/t_n$.

Noting that $d_1\sigma_1 + d_2\sigma_2 + \cdots + d_n\sigma_n = t_1^2 + t_2^2 + \cdots + t_n^2$ and $t_1 + t_2 + \cdots + t_n = d_1^2 + d_2^2 + \cdots + d_n^2$, we have

$$\lambda_1(G) \geqslant \sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}} \geqslant \sqrt{\frac{\sum_{i=1}^n t_i^2}{\sum_{i=1}^n d_i^2}} \geqslant \sqrt{\frac{\left(\sum_{i=1}^n t_i\right)^2}{n\sum_{i=1}^n d_i^2}} = \sqrt{\frac{1}{n}\sum_{i=1}^n {d_i}^2} \geqslant \sqrt{\frac{2e}{n}}. \quad (14)$$

So $f(\lambda_1(G)) \leqslant f\left(\sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}}\right)$, which implies $E(G) \leqslant 2\sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}} + \sqrt{(n-2)\left(2e - \frac{2\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}\right)}$.

If G is one of the three graphs shown in the second part of the theorem, it is easy to check that the equality in (13) holds. Conversely, if the equality in (13) holds, according to the above argument, we have

$$\lambda_1 = -\lambda_n = \sqrt{\frac{\sum_{i=1}^n \sigma_i^2}{\sum_{i=1}^n t_i^2}},$$

which implies that G is a connected bipartite graph with $V = \{v_1, \ldots, v_s\} \cup \{v_{s+1}, \ldots, v_n\}$ such that $\sigma_1/t_1 = \cdots = \sigma_s/t_s$ and $\sigma_{s+1}/t_{s+1} = \cdots = \sigma_n/t_n$. Moreover, $|\lambda_i| = \sqrt{\frac{2e-2\lambda_1^2}{n-2}}$ $(2 \leqslant i \leqslant n-1)$. We are reduced to the following three possibilities:

(1) G has two distinct eigenvalues which have the same absolute value. $\lambda_1 = -\lambda_n = |\lambda_i| = \sqrt{\frac{2e-2\lambda_1^2}{n-2}}$ $(2 \leqslant i \leqslant n-1)$. By lemma 2.2, $\lambda_n = -\sqrt{\frac{2e-2\lambda_1^2}{n-2}} = -1$. Hence $2e = n$, which implies $G \cong \frac{n}{2}K_2$.

(2) G has three distinct eigenvalues.
In this case, noting that G is a bipartite graph, we have $\lambda_1 = -\lambda_n = \sqrt{\frac{\sum_{i=1}^{n}\sigma_i^2}{\sum_{i=1}^{n}t_i^2}}$ and $\lambda_i = \sqrt{\frac{2e-2\lambda_1^2}{n-2}} = 0$ $(2 \leqslant i \leqslant n-1)$, which implies that $E(G) = 2\lambda_1 = 2\sqrt{e}$. By lemma 2.3, we have $G \cong K_{r_1,r_2} \cup (n-r_1-r_2)K_1$, where $r_1 r_2 = e$.

(3) G has four distinct eigenvalues.

In this case, noting that the multiplicity of λ_1 is one, we have G is a connected bipartite graph with $V = \{v_1, v_2, \ldots, v_s\} \cup \{v_{s+1}, v_{s+2}, \ldots, v_n\}$ satisfying $\sigma_1/t_1 = \sigma_2/t_2 = \cdots = \sigma_s/t_s$ and $\sigma_{s+1}/t_{s+1} = \sigma_{s+2}/t_{s+2} = \cdots = \sigma_n/t_n$, and G has four distinct eigenvalues $\left(\sqrt{p_x p_y},\ \sqrt{\frac{2e-2p_x p_y}{n-2}},\ -\sqrt{\frac{2e-2p_x p_y}{n-2}},\ -\sqrt{p_x p_y}\right)$, where $p_x = \sqrt{\frac{\sigma_i}{t_i}}, 1 \leqslant i \leqslant s$, $p_y = \sqrt{\frac{\sigma_j}{t_j}}, s+1 \leqslant j \leqslant n$ and $\sqrt{p_x p_y} > \sqrt{\frac{2e}{n}}$. This completes the proof of theorem 3.1. □

Note 3.2. By (14), we have the bound (13) is better than (4), (6), and (8).

4. The energy of a forest

In order to investigate the energy of a forest, we need the following lemmas.

Lemma 4.1 [5]. Let T be a tree of order n $(n \geqslant 2)$ and suppose that there exists a vertex $v_i \in V(T)$ such that $l(v_i) \leqslant 2$, then

$$\lambda_1(T) \geqslant \sqrt{d+m-1}, \tag{15}$$

where $d = d(v_i)$ and $m = m_i$. Moreover, the equality holds in (15) if and only if the degree of the neighbors of v_i are equal.

Lemma 4.2 [4]. Let G be a graph and G' a subgraph of G. Then $\lambda_1(G') \leqslant \lambda_1(G)$ and equality holds if and only if $G' = G$.

Let $T_{d_i,d_j}(d_j \geqslant 2)$ be a tree obtained by joining the centers of d_i copies of K_{1,d_j-1} to a new vertex v_i. Then $T_{1,n-1} = K_{1,n-1}$.

In this section, the proof of our main result is carried out mainly by the following lemma (given in Das Thesis). We give the proof here for reference only.

Lemma 4.3. Let T be a tree with order n, degree sequence $d_1, d_2, \ldots, d_n$ and average 2-degree sequence $m_1, m_2, \ldots, m_n$. Then

$$\lambda_1(T) \geqslant \max\{\sqrt{d_i + m_i - 1}\ :\ 1 \leqslant i \leqslant n\}. \tag{16}$$

Moreover, the equality in (16) holds if and only if $T \cong T_{d_i,d_j}$.

Proof. We know that if H is a subgraph of G, then $\lambda_1(H) \leqslant \lambda_1(G)$. Thus by Lemma 4.1, we have

$$\lambda_1(T) \geqslant \sqrt{d_i + m_i - 1}, \quad 1 \leqslant i \leqslant n. \tag{17}$$

By (17) and (16) holds immediately.

Now suppose that the equality holds in (16). That is, for some $v_i \in V(T)$,

$$\lambda_1(T) = \sqrt{d_i + m_i - 1}.$$

Note that if $T' \subset T$, then $\lambda_1(T') < \lambda_1(T)$ by Lemma 4.2. Therefore $T = T_{d_i,d_j}$ by Lemma 4.1.

Conversely, let $T = T(d_i, d_j)$. It is easily to check that the equality holds in (16). □

Theorem 4.4. Let T be a forest with n vertices, e edges, degree sequence $d_1, d_2, \ldots, d_n$ and average 2-degree sequence $m_1, m_2, \ldots, m_n$. Then

$$E(T) \leqslant 2\sqrt{s} + \sqrt{(n-2)\,(2e-2s)}, \tag{18}$$

where $s = \max\{d_i + m_i - 1 \ : \ 1 \leqslant i \leqslant n\}$. Equality holds if and only if one of the following statements holds:

(i) $T \cong \frac{n}{2}K_2$;

(ii) $T \cong K_{1,e} \cup (n-1-e)K_1$;

(iii) $T \cong T_{d_i,d_j}(\ d_i \geqslant 2)$ with four distinct eigenvalues $\left(\sqrt{s},\ \sqrt{\frac{2e-2s}{n-2}},\ -\sqrt{\frac{2e-2s}{n-2}},\ -\sqrt{s}\right)$.

Proof. Let $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_n$ be the eigenvalues of T. Since T is a bipartite graph, we have $\lambda_1 = -\lambda_n$. By the Cauchy–Schwartz inequality,

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

Hence

$$E(T) \leqslant 2\lambda_1 + \sqrt{(n-2)(2e - 2\lambda_1^2)}.$$

By lemma 4.3, we have

$$\lambda_1 \geqslant \max\{\sqrt{d_i + m_i - 1},\ 1 \leqslant i \leqslant n\} = \sqrt{s}$$

and equality holds if and only if T has a component $T' \cong T_{d_i,d_j}$.

Noting that

$$\lambda_1 \geqslant \max\{\sqrt{d_i + m_i - 1},\ 1 \leqslant i \leqslant n\} = \sqrt{s} \geqslant \sqrt{2e/n}$$

and hence, by lemma 2.4, we have $f(\lambda_1) \leqslant f\left(\sqrt{s}\right)$, which implies

$$E(T) \leqslant 2\sqrt{s} + \sqrt{(n-2)\,(2e-2s)}.$$

If G is one of the three graphs shown in the second part of the theorem, it is easy to check that the equality in (18) holds.

Conversely, if the equality in (18) holds, according to the above argument, we have $\lambda_1 = -\lambda_n = \sqrt{s}$, which implies that T has a component $T' \cong T_{d_i,d_j}$. Moreover, $|\lambda_i| = \sqrt{\frac{2e-2\lambda_1^2}{n-2}}$ $(2 \leqslant i \leqslant n-1)$. We are reduced to the following three possibilities:

(1) T has two distinct eigenvalues which have the same absolute value.

$\lambda_1 = -\lambda_n = |\lambda_i| = \sqrt{\frac{2e-2\lambda_1^2}{n-2}}$ $(2 \leqslant i \leqslant n-1)$. By lemma 2.2, $\lambda_n = -\sqrt{\frac{2e-2\lambda_1^2}{n-2}} = -1$. Hence $2e = n$, which implies $T \cong \frac{n}{2}K_2$.

(2) T has three distinct eigenvalues.

In this case, noting that T is a bipartite graph, we have $\lambda_1 = -\lambda_n = \sqrt{s}$ and $\lambda_i = \sqrt{\frac{2e-2\lambda_1^2}{n-2}} = 0$ $(2 \leqslant i \leqslant n-1)$, which implies that $E(T) = 2\lambda_1 = 2\sqrt{e}$. By lemma 2.3, we have $T \cong K_{1,e} \cup (n-1-e)K_1$.

(3) T has four distinct eigenvalues.

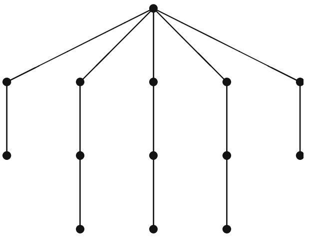
In this case, noting that the multiplicity of λ_1 is one, we have $T \cong T_{d_i,d_j}$ and T has four distinct eigenvalues $\left(\sqrt{s},\ \sqrt{\frac{2e-2s}{n-2}},\ -\sqrt{\frac{2e-2s}{n-2}},\ -\sqrt{s}\right)$.

This completes the proof of theorem 4.4. □

Let T be a tree with n vertices. Then $d_i \geqslant 1$ and $m_i \geqslant 1$ for $1 \leqslant i \leqslant n$. Note that $d_i + m_i = 2$ if and only if $T \cong K_2$, and if $d_i + m_i \geqslant 3$, then $d_i + m_i - 1 \geqslant 2 > 2(n-1)/n = 2e/n$. Thus

$$\sqrt{d_i + m_i - 1} \geqslant \sqrt{\frac{2e}{n}}, \quad 1 \leqslant i \leqslant n.$$

From the proof of theorem 4.4, we have the following result.



T^*

Figure 1.

Theorem 4.5. Let T be a tree with n vertices, degree sequence $d_1, d_2, \ldots, d_n$ and average 2-degree sequence $m_1, m_2, \ldots, m_n$. Then

$$E(T) \leqslant \min\left\{2\sqrt{d_i + m_i - 1} + \sqrt{(n-2)(2n - 2d_i - 2m_i)} \ : \ 1 \leqslant i \leqslant n\right\}. \quad (19)$$

Equality holds if and only if T is either K_2, a star $K_{1,n-1}$ or $T \cong T_{d_i,d_j},\ d_i \geqslant 2$ with four distinct eigenvalues $\left(\sqrt{d_i + m_i - 1},\ \sqrt{\frac{2n-2d_i-2m_i}{n-2}},\ -\sqrt{\frac{2n-2d_i-2m_i}{n-2}},\ -\sqrt{d_i + m_i - 1}\right)$.

Note 4.6. The bound (19) is always better than (4) for trees.

Note 4.7. It is easily to check that the bound (19) is better than (6) and (8) for T^*, where T^* is a graph shown in figure 1.

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