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On the Laplacian Energy of Trees with Perfect Matchings

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Abstract

Let $\mathcal{T}_n(d)$ be the set of all trees with n vertices, diameter d and perfect matchings. We show that the Laplacian energy of any tree in $\mathcal{T}_n(d)$, where $d = 4, 5$, is no less than the Laplacian energy of the path P_n. Thus, we partly show that a conjecture by Radenković and Gutman is true.

1 Introduction

Let A be adjacency matrix of a simple graph G with vertex set $V(G) = \{v_1, v_2, \ldots, v_n\}$. In chemistry, there is a closed relation between the molecular orbital energy levels of π-electrons in conjugated hydrocarbons and the eigenvalues of the corresponding molecular graph. In 1970s, Gutman [1] extended the concept of energy to simple graph G, and defined that

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

where λ_i , $(i = 1, 2, \ldots, n)$ are the eigenvalues of the adjacency matrix A of G. Let $\mu_1 \geq \mu_2 \geq \cdots \geq \mu_n = 0$ be eigenvalues of the Laplacian matrix $L = D - A$ of G, where D is the diagonal matrix of vertex degrees. Gutman and Zhou [2] define the Laplacian energy as follows:

$$LE(G) = \sum_{i=1}^{n} |\mu_i - \overline{d}|$$

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where $\overline{d}$ is average degree. When G is a tree, then $\overline{d} = 2 - 2/n$.

Many researchers established a lower and upper bounds of $LE(G)$ for some classes of graphs. For further details, we refer the readers to [3–8].

Besides these aspects, there were works aimed at finding the extremal values of $LE(G)$ over a class of graphs, and characterizing the elements of this class that achieve this extremal value. As an illustration, the connected graphs on n vertex with the smallest or highest Laplacian energy are not known for general n, not even when the class is restricted to trees. In [9], Radenković and Gutman found that the energy and the Laplacian energy behave very differently for trees, namely that the energy and the Laplacian energy of a tree are inversely proportional, and gave the following conjecture.

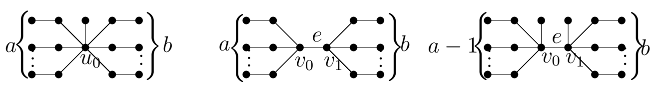
Conjecture 1. Let T be a tree on n vertices. Then

$$LE(P_n) \leq LE(T) \leq LE(S_n) \ .$$

In a recent paper [10] by Trevisan et al., it has been shown that the conjecture is true for trees of diameter 3. Furthermore, the authors of [11] proved the right–hand side of the conjecture.

Let a, b be two integers satisfying $a \geq b \geq 1$ and $a+b = \frac{n}{2}-1$. Denote by $T_n(4, a, b)$ the tree with n vertices, that is obtained by attaching $a+b$ paths of length 2 and one pendent edge to a vertex u_0 . $T_n(4, a, b)$ is shown in Fig. 1. It is obvious that $\mathcal{T}_n(4) = \{T_n(4, a, b)\}$.

Let $T_n^1(5, a, b)$ be the tree with n vertices obtained from an edge e by attaching a paths of length 2 to one end vertex v_0 of the edge e and b ones to the other end vertex v_1 of the edge e. Let $T_n^2(5, a-1, b)$ be the tree with n vertices which can be obtained from $T_n^1(5, a, b)$ by replacing a pendent path of length 2 connected with vertex v_0 with a pendent edge and attaching a pendent edge to vertex v_1. Two graphs $T_n^1(5, a, b)$ and $T_n^2(5, a-1, b)$ are shown in Fig. 1. Obviously, the set $\mathcal{T}_n(5)$ consists of only these two classes of trees.



$T_n(4, a, b)$ $\quad$ $T_n^1(5, a, b)$ $\quad$ $T_n^2(5, a-1, b)$

Fig.1 $T_n(4, a, b), T_n^1(5, a, b)$ and $T_n^2(5, a-1, b)$

In this paper, we show that the Laplacian energy of any tree in $\mathcal{T}_n(d)$, where $d = 4, 5$, is not less than the Laplacian energy of the path P_n, which partly confirms the validity of the above conjecture.

2 Preliminaries

First, using the algorithm described in [10], the characteristic polynomials of the Laplacian matrices of $T_n(4, a, b), T_n^1(5, a, b)$ and $T_n^2(5, a-1, b)$ are given by

$$\begin{aligned} p(T_n(4,a,b)) &= \lambda(\lambda-2)(\lambda^2-3\lambda+1)^{\frac{n}{2}-2}[\lambda^2-(3+a+b)\lambda+a+b+1] \quad (1)\\ p(T_n^1(5,a,b)) &= \lambda(\lambda-2)(\lambda^2-3\lambda+1)^{\frac{n}{2}-3}f(\lambda) \quad (2)\\ p(T_n^2(5,a-1,b)) &= \lambda(\lambda-2)(\lambda^2-3\lambda+1)^{\frac{n}{2}-4}f'(\lambda) \quad (3) \end{aligned}$$

where

$$\begin{aligned} f(\lambda) &= \lambda^4+(-a-b-6)\lambda^3+(ab+4b+4a+11)\lambda^2\\ &+ (-2ab-4b-4a-6)\lambda+a+b+1\\ f'(\lambda) &= \lambda^6+(-a-b-9)\lambda^5+(ab+6b+7a+30)\lambda^4\\ &+ (-4ab-13b-17a-45)\lambda^3+(5ab+12b+17a+30)\lambda^2\\ &+ (-2ab-5b-7a-9)\lambda+a+b+1\ . \end{aligned}$$

Next, we describe an algorithm [11] that can be used to estimate the Laplacian eigenvalues of a given tree. It counts the number of eigenvalues of the Laplacian matrix of a tree T lying in any real interval. The algorithm is based on the diagonalization of the matrix $L(T) + \alpha I$, where $L(T)$ is the Laplacian matrix of T and α is a real number. One of the main features of this algorithm is that it can be executed directly on the tree, so that the Laplacian matrix is not needed explicitly. Denote by $d(v)$ the degree of vertex v.

Input: tree T, scalar α
Output: diagonal matrix D congruent to $L(T) + \alpha I$

Algorithm Diagonalize(T, α)
  initialize $a(v) := d(v) + \alpha$, for all vertices v
  order vertices bottom up
  for $k = 1$ to n
    if v_k is a leaf then continue
    else if $a(c) \neq 0$ for all children c of v_k then
      $a(v_k) := d(v_k) - \sum \frac{1}{a(c)}$, summing over all children of v_k
    else

select one child v_j of v_k for which $a(v_j) = 0$
$a(v_k) := -\frac{1}{2}$
$a(v_j) := 2$
if v_k has a parent v_l, remove the edge $v_k v_l$.
end loop

Lemma 2.1 [11]. Let T be a tree and let D be the diagonal matrix produced by the algorithm Diagonalize $(T, -\alpha)$. The following assertions hold.

(a) The number of positive entries in D is the number of the Laplacian eigenvalues of T that are greater than α.

(b) The number of negative entries in D is the number of the Laplacian eigenvalues of T that are smaller than α.

(c) If there are j zero entries in D, then α is the Laplacian eigenvalue of T with multiplicity j.

Lemma 2.2 [12]. Let G be a connected graph on n vertices having at least one edge. Then $\mu_1(G) \geq \Delta(G) + 1$, with equality if and only if $\Delta(G) = n - 1$, where $\Delta(G)$ is maximum degree of G.

Lemma 2.3 [10]. Let P_n be the path on n vertices. Then

$$LE(P_n) = 2 + 4 \sum_{i=1}^{\lfloor n/2 \rfloor} \cos \frac{\pi i}{n} + \frac{1}{n}[(-1)^n - 1] \ .$$

Lemma 2.4 [11]. Let T be a tree on n vertices. Then $LE(T) \leq LE(S_n)$ and equality holds if and only if $T \cong S_n$.

3 Main results

In this section, we first use diagonalization algorithm to get some properties on the Laplacian eigenvalues of two classes of trees, and then prove our main results.

Lemma 3.1. The Laplacian eigenvalues of $T_n(4, a, b)$ satisfy the following properties:

(a) $T_n(4, a, b)$ has $\frac{n}{2}$ eigenvalues greater than 1 and $\frac{n}{2}$ eigenvalues smaller than 1.

(b) $T_n(4, a, b)$ has $\frac{n}{2} + 1$ eigenvalues greater than $\frac{3-\sqrt{5}}{2}$ and $\frac{n}{2} - 2$ eigenvalues with value equal to $\frac{3-\sqrt{5}}{2}$.

Proof. Apply the algorithm to the tree with $\alpha = -1$. The initialization step assigns 0 to all leaves and 1 to the vertices of degree 2, respectively, and lets $a(u_o) = \frac{n}{2} - 1$.

After processing, there are $\frac{n}{2}$ vertices with value 2, and $\frac{n}{2}$ vertices with value $-\frac{1}{2}$. By Lemma 2.1, then (a) follows. Fig. 2 and Fig. 3 show the two statuses of initialization and diagonalization, respectively.

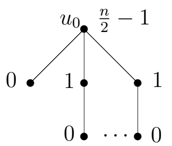


Fig. 2. Initialization

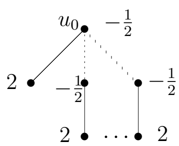


Fig. 3. Diagonalization

With the same as the above proof of (a), then (b) follows immediately. □

By Lemma 2.1, we have Lemma 3.2

Lemma 3.2. The number of the Laplacian eigenvalues in an interval $(\alpha_1,\ \alpha_2)$ is the number of positive entries in the diagonalization of $(T,\ -\alpha_1)$, minus the number of positive entries in the diagonalization of $(T,\ -\alpha_2)$.

Lemma 3.3. Let μ_1 and μ_{n-2} be the largest eigenvalue and the third smallest eigenvalue of $T_n(4,a,b)$, respectively. Then $\mu_1 > \frac{3+\sqrt{5}}{2}$ and $\frac{3-\sqrt{5}}{2} < \mu_{n-2} < 1$.

Proof. By Lemma 2.2, obviously, $\mu_1 > \frac{3+\sqrt{5}}{2}$. From the characteristic polynomial (1) of the Laplacian matrix of $T_n(4,a,b)$, it has one eigenvalue 0, one eigenvalue 2, $\frac{n}{2}-2$ eigenvalues with value $\frac{3+\sqrt{5}}{2}$ and $\frac{n}{2}-2$ eigenvalues with value $\frac{3-\sqrt{5}}{2}$. Then by (1) and $\mu_1 > \frac{3+\sqrt{5}}{2}$, μ_1 is the root of equation $\lambda^2-(3+a+b)\lambda+a+b+1=0$. From Lemma 3.1-(b) and (1), μ_{n-2} is the root of equation $\lambda^2-(3+a+b)\lambda+a+b+1=0$. By Lemma 3.1-(a), Lemma 3.1-(b) and Lemma 3.2, then $\frac{3-\sqrt{5}}{2} < \mu_{n-2} < 1$. □

Theorem 3.4. When $n \geq 6$, then $LE(P_n) < LE(T_n(4,a,b))$.

Proof. By (1), Lemma 3.3 and the definition of the Laplacian energy,

$$\begin{aligned} LE(T_n(4,a,b)) &= \overline{d}+\left(\frac{n}{2}-2\right)\left(\overline{d}-\frac{3-\sqrt{5}}{2}\right)+(\overline{d}-\mu_{n-2})+(2-\overline{d}) \\ &\quad +\left(\frac{n}{2}-2\right)\left(\frac{3+\sqrt{5}}{2}-\overline{d}\right)+(\mu_1-\overline{d}) \\ &= \left(\frac{n}{2}-2\right)\sqrt{5}+\mu_1-\mu_{n-2}+2\ . \end{aligned} \tag{4}$$

Hence, by Lemma 2.3,

$$\begin{aligned} LE(P_n) - LE(T_n(4,a,b)) &= 4\sum_{i=1}^{\lfloor n/2 \rfloor} \cos\frac{\pi i}{n} + \frac{1}{n}[(-1)^n - 1] - \frac{\sqrt{5}}{2}(n-4) \\ &+ \mu_{n-2} - \mu_1 \ . \end{aligned}$$

Since

$$\frac{\pi}{n}\sum_{j=1}^{[\frac{n}{2}]} \cos\frac{\pi j}{n} \leq \int_0^{\frac{\pi}{2}} \cos x dx = 1$$

then

$$LE(P_n) \leq 2 + \frac{4n}{\pi} \ . \tag{5}$$

According to (5)

$$\begin{aligned} LE(P_n) - LE(T_n(4,a,b)) &= 4\sum_{i=1}^{\lfloor n/2 \rfloor} \cos\frac{\pi i}{n} + \frac{1}{n}[(-1)^n - 1] - \frac{\sqrt{5}}{2}(n-4) \\ &- \frac{1}{2}\sqrt{(n-2)^2 + 4(n-2) + 20} \\ &\leq \frac{4n}{\pi} - \frac{\sqrt{5}}{2}(n-4) - \frac{1}{2}\sqrt{(n-2)^2 + 4(n-2) + 20} \ . \end{aligned}$$

Let

$$g(n) = \frac{4n}{\pi} - \frac{\sqrt{5}}{2}(n-4) - \frac{1}{2}\sqrt{(n-2)^2 + 4(n-2) + 20}.$$

When $g(n) = 0$, then we have

$$\left(1 + \frac{16}{\pi^2} - \frac{4\sqrt{5}}{\pi}\right)n^2 + \left(\frac{16\sqrt{5}}{\pi} - 10\right)n + 16 = 0 \ .$$

Let n_1, n_2 be two roots of the equation $g(n) = 0$, where $n_1 \leq n_2$. By direct computing, $n_1 \approx -5.880, n_2 \approx 12.056$. Thus, when $n > 12$, $LE(P_n) < LE(T_n(4,a,b)$. When $n = 6, 8, 10, 12$, we have

$$\begin{aligned} &n = 6,\ LE(P_6) = 7.4641,\ LE(T_n(4,a,b)) = 7.8417 \\ &n = 8,\ LE(P_8) = 10.0548,\ LE(T_n(4,a,b)) = 10.9443 \\ &n = 10,\ LE(P_{10}) = 12.6276,\ LE(T_n(4,a,b)) = 14.0935 \\ &n = 12,\ LE(P_{12}) = 15.1916,\ LE(T_n(4,a,b)) = 17.2690 \end{aligned}$$

Hence, the result follows. □

In an analogous manner as in the proof of Lemma 3.1, we have

Lemma 3.5. When $n \geq 8$, the Laplacian eigenvalues of $T_n^1(5,a,b)$ satisfy the following properties:

(a) $T_n^1(5,a,b)$ has $\frac{n}{2}+1$ eigenvalues greater than 1 and $\frac{n}{2}-1$ eigenvalues smaller than 1;

(b) $T_n^1(5,a,b)$ has two eigenvalues greater than $\frac{3+\sqrt{5}}{2}$ and $\frac{n}{2}-3$ eigenvalues with value $\frac{3+\sqrt{5}}{2}$;

(c) $T_n^1(5,a,b)$ has $\frac{n}{2}+1$ eigenvalues greater than $\frac{3-\sqrt{5}}{2}$ and $\frac{n}{2}-3$ eigenvalues with value $\frac{3-\sqrt{5}}{2}$;

(d) $T_n^1(5,a,b)$ has $\frac{n}{2}$ eigenvalues greater than $\overline{d}$ and $\frac{n}{2}$ eigenvalues smaller than $\overline{d}$.

Lemma 3.6. Let $\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \lambda_4$ be the roots of $f(\lambda)=0$, where $f(\lambda)$ is a factor of the characteristic polynomial (2) of the Laplacian matrix of $T_n^1(5,a,b)$. Then

$$\lambda_1 \geq \lambda_2 > \frac{3+\sqrt{5}}{2},\ 1 < \lambda_3 < \overline{d},\ 0 < \lambda_4 < \frac{3-\sqrt{5}}{2}\ .$$

Proof. By Lemma 3.5-(b) and (2), $\lambda_1 \geq \lambda_2 > \frac{3+\sqrt{5}}{2}$; From Lemma 3.5-(a), Lemma 3.5-(d) and Lemma 3.2 , we have $1 < \lambda_3 < \overline{d}$. Since $T_n^1(5,a,b)$ is connected, $\lambda_4 > 0$. And $\lambda_4 < \frac{3-\sqrt{5}}{2}$ follows by Lemma 3.5-(c) and (2). Thus, $0 < \lambda_4 < \frac{3-\sqrt{5}}{2}$. □

Theorem 3.7. When $n \geq 6$, then $LE(P_n) \leq LE(T_n^1(5,a,b))$.

Proof. When $n=6$, then $P_n \cong T_n^1(5,a,b)$, so that the result follows.

Next, we discuss the case of $n > 6$. By (2), Lemma 3.6 and the definition of the Laplacian energy,

$$LE(T_1(5,a,b)) = 2 + (\frac{n}{2}-3)\sqrt{5} + \lambda_1 + \lambda_2 - \lambda_3 - \lambda_4\ . \tag{6}$$

Since $\lambda_3 < 2, \lambda_4 < 1$, and $\sum_{i=1}^{4} \lambda_i = \frac{n}{2} + 5$,

$$\frac{n}{2} - 1 < \frac{n}{2} + 5 - 2(\lambda_3+\lambda_4) = \lambda_1 + \lambda_2 - \lambda_3 - \lambda_4\ .$$

Hence, by Lemma 2.3, (5) and (6),

$$\begin{aligned} LE(P_n) - LE(T_1(5,a,b)) &= 4\sum_{i=1}^{\lfloor n/2 \rfloor} \cos\frac{\pi i}{n} + \frac{1}{n}[(-1)^n - 1] - \left(\frac{n}{2}-3\right)\sqrt{5} \\ &- (\lambda_1+\lambda_2-\lambda_3-\lambda_4) \\ &\leq \frac{4n}{\pi} - \left(\frac{n}{2}-3\right)\sqrt{5} - (\lambda_1+\lambda_2-\lambda_3-\lambda_4) \\ &< \frac{4n}{\pi} - \frac{\sqrt{5}n}{2} - \frac{n}{2} + 3\sqrt{5} + 1\ . \end{aligned}$$

When $n > 22$, $\frac{4n}{\pi} - \frac{\sqrt{5}n}{2} - \frac{n}{2} + 3\sqrt{5} + 1 < 0$ and the result follows. For $8 \le n \le 22$, the result is checked from the table at the end of this section. □

With the analogous proof as of Lemma 3.1, we have

Lemma 3.8. The Laplacian eigenvalues of $T_n^2(5, a-1, b)$ satisfy the following properties:

(a) $T_n^2(5, a-1, b)$ has $\frac{n}{2} - 1$ eigenvalues greater than 2 and one eigenvalue 2;

(b) $T_n^2(5, a-1, b)$ has $\frac{n}{2}$ eigenvalues smaller than 1 and $\frac{n}{2}$ eigenvalues greater than 1.

Lemma 3.9. Let $\lambda_1' \ge \lambda_2' \ge \lambda_3' \ge \lambda_4' \ge \lambda_5' \ge \lambda_6'$ be the roots of the equation $f'(\lambda) = 0$, where $f'(\lambda)$ is a factor of the characteristic polynomial (3) of the Laplacian matrix of $T_n^2(5, a-1, b)$. Then

$$2 < \lambda_3' \le \lambda_2' \le \lambda_1', \; 0 < \lambda_6' \le \lambda_5' \le \lambda_4' < 1 \; .$$

Proof. By (3), $T_n^2(5, a-1, b)$ has one eigenvalue 0, one eigenvalue 2, $\frac{n}{2} - 4$ eigenvalues with value $\frac{3+\sqrt{5}}{2}$ and $\frac{n}{2} - 4$ eigenvalues with value $\frac{3-\sqrt{5}}{2}$. Then from Lemma 3.8-(a) and Lemma 3.8-(b), there are three eigenvalues larger than 2 and three eigenvalues smaller than 1, respectively. Since $T_n^2(5, a-1, b)$ is connected, $\lambda_6' > 0$. Thus, we have

$$2 < \lambda_3' \le \lambda_2' \le \lambda_1', \; 0 < \lambda_6' \le \lambda_5' \le \lambda_4' < 1 \; .$$

□

Theorem 3.10. When $n \ge 8$, then $LE(P_n) < LE(T_n^2(5, a-1, b))$.

Proof. By (3), Lemma 3.8 and the definition of the Laplacian energy,

$$LE(T_n^2(5, a-1, b)) = 2 + \left(\frac{n}{2} - 4\right)\sqrt{5} + \sum_{i=1,2,3} \lambda_i' - \sum_{i=4,5,6} \lambda_i' \; . \tag{7}$$

Since $\sum_{i=1}^{6} \lambda_i' = \frac{n}{2} + 8$ and $\sum_{i=4,5,6} \lambda_i' < 3$, by Lemma 3.9, then

$$\frac{n}{2} + 2 < \frac{n}{2} + 8 - 2\sum_{i=4,5,6} \lambda_i' = \sum_{i=1,2,3} \lambda_i' - \sum_{i=4,5,6} \lambda_i' \; .$$

Thus, by (5), (7) and Lemma 2.3,

$$\begin{aligned} LE(P_n) - LE(T_n^2(5, a-1, b)) &= 4\sum_{i=1}^{\lfloor n/2 \rfloor} \cos\frac{\pi i}{n} + \frac{1}{n}[(-1)^n - 1] \\ &- \left(\frac{n}{2} - 4\right)\sqrt{5} - \left(\sum_{i=1,2,3} \lambda_i' - \sum_{i=4,5,6} \lambda_i'\right) \\ &< \frac{4n}{\pi} - \frac{\sqrt{5}n}{2} - \frac{n}{2} + 4\sqrt{5} - 2\ . \end{aligned}$$

When $n > 20$, $\frac{4n}{\pi} - \frac{\sqrt{5}n}{2} - \frac{n}{2} + 4\sqrt{5} - 2 < 0$ and the result follows. For $8 \le n \le 20$, the result is checked from the table at the end of this section . $\square$

By Theorem 3.4, Theorem 3.7, Theorem 3.10 and Lemma 2.4, we have shown that, for $\forall\ T \in \{\mathcal{T}_n(d) | d = 4, 5\ \}$,

$$LE(P_n) \le LE(T) \le LE(S_n)\ .$$

The following table contains the Laplacian energies of $T_n(4, a, b)$, $T_n^1(5, a, b)$, $T_n^2(5, a-1, b)$, and P_n when $8 \le n \le 22$.

n	a	b	$LE(T_n(4,a,b))$	$LE(T_n^2(5,a,b))$	$LE(T_n^1(5,a,b))$	$LE(P_n)$
8	2	1	10.9443	10.8693	10.3898	10.0548
10	2	2	14.0935	13.9835	13.2908	12.6276
10	3	1	14.0935	13.9835	13.4548	12.6276
12	3	2	17.269	17.106	16.3556	15.1916
12	4	1	17.269	17.1413	16.5869	15.1916
14	3	3	20.4606	20.2696	19.4297	17.7504
14	4	2	20.4606	20.2696	19.4935	17.7504
14	5	1	20.4606	20.3232	19.7542	17.7504
16	4	3	23.6628	23.4372	22.5764	20.3064
16	5	2	23.6628	23.4558	22.6673	20.3064
16	6	1	23.6628	23.5199	22.9419	20.3064
18	4	4	26.8722	26.6263	25.7304	22.86
18	5	3	26.8722	26.6263	25.7574	22.86
18	6	2	26.8722	26.6557	25.8608	22.86
18	7	1	26.8722	26.726	26.1422	22.86
20	5	4	30.0868	29.8175	28.9167	25.4124
20	6	3	30.0868	29.8284	28.9566	25.4124
20	7	2	30.0868	29.8643	29.0661	25.4124
20	8	1	30.0868	29.9386	29.3508	25.4124
22	5	5	33.3052	33.0211	32.1069	27.9636
22	6	4	33.3052	33.0211	32.1199	27.9636
22	7	3	33.3052	33.0387	32.1665	27.9636
22	8	2	33.3052	33.0789	32.2791	27.9636
22	9	1	33.3052	33.1558	32.5652	27.9636

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