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Solutions to unsolved problems on the minimal energies of two classes of trees

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ABSTRACT

The energy of a graph is defined as the sum of the absolute values of all eigenvalues of the graph. Let $\mathbb{T}_{n,p}$, $\mathcal{T}_{n,d}$ be the set of all trees of order n with p pendent vertices, diameter d, respectively. In this paper, we completely characterize the trees with second-minimal and third-minimal energy in $\mathbb{T}_{n,p}$ ($\mathcal{T}_{n,d}$, respectively) for $4 \le p \le n-9$ ($10 \le d \le n-3$, respectively), which solves the problems left in Ma (2014).

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1. Introduction

Let G be a simple graph with n vertices, and $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of its adjacency matrix. Then the energy of G is defined as

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

Let G be an acyclic graph of order n. Then $E(G)$ can be expressed as the Coulson integral formula [11]

$$E(G) = \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2} \log\left[\sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G,k)x^{2k}\right]dx,$$

where $m(G, k)$ denotes the number of k-matchings in G and $m(G, 0) = 1$. Follow [15], denote

$$m^+(G,x) = \sum_{k=0}^{\lfloor \frac{n}{2} \rfloor} m(G,k)x^{2k}.$$

Then for a tree T with n vertices, we have

$$E(T) = \frac{2}{\pi}\int_0^{+\infty} \frac{1}{x^2} \log m^+(T,x)dx. \tag{1}$$

Since the energy of a graph can be used to approximate the total π-electron energy of the molecular, it has been intensively studied. For details on graph energy, we refer the readers to the book [18] and reviews [8,10]. One of the fundamental question that is encountered in the study of graph energy is which graphs (from a given class) have minimal and maximal

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energies. A large number of papers were published on such extremal problems, see Chapter 7 in [18] and some recent papers [9,12,13,15–17,19–30]. There are many other kinds of graph energies, such as matching energy [1–3], Laplacian energy [4], distance energy [5], Randić energy [6,14], incidence energy [6], etc.

For terminology and notation not defined here, we refer to [20]. A caterpillar is a tree in which a removal of all pendent vertices makes a path. Let $T(n, d; n_1, n_2, \ldots, n_{d-1})$ be a caterpillar obtained from a path $v_0v_1\ldots v_d$ by adding n_i $(n_i \geq 0)$ pendent edges to v_i $(i = 1, \ldots, d-1)$. For $1 \leq i \leq d-1$, denote $T_{n,d,i} = T(n, d; 0, \ldots, 0, n_i = n-d-1, 0, \ldots, 0)$.

Gutman [7] proved that the star S_n and the path P_n have minimal and maximal energy among all trees of order n, respectively. Let $\mathcal{T}_{n,d}$ be the set of all trees with n vertices and diameter d, where $2 \leq d \leq n-1$. The trees with minimal and second-minimal energies in $\mathcal{T}_{n,d}$ have been considered by Li and Li [16,17], Shan and Shao [24], Wang and Kang [26], Yan and Ye [27] and Zhou and Li [30]. Let $\mathbb{T}_{n,p}$ be the set of all trees of order n with p pendent vertices, where $2 \leq p \leq n-1$. The tree with minimal energy in $\mathbb{T}_{n,p}$ has been determined by Yu and Lv [29] and Ye and Yuan [28] independently. By the results in [27–29], the trees with minimal energy in $\mathcal{T}_{n,d}$ and $\mathbb{T}_{n,n-d+1}$ are the same for all $2 \leq d \leq n-1$. In [20], one of the present authors gave the further relations on the ordering of trees by minimal energies between $\mathcal{T}_{n,d}$ and $\mathbb{T}_{n,n-d+1}$, and completely characterized the trees with second-minimal and third-minimal energy in $\mathbb{T}_{n,p}$ ($\mathcal{T}_{n,d}$, respectively) except for the case $4 \leq p \leq n-9$ $(10 \leq d \leq n-3$, respectively). By Ma [20], the trees with second-minimal and third-minimal energy in $\mathbb{T}_{n,p}$ and $\mathcal{T}_{n,n-p+1}$ are the same, respectively, for $4 \leq p \leq n-9$, and the results on $\mathbb{T}_{n,p}$ are the following:

Theorem 1.1 ([20]). *Suppose that $4 \leq p \leq n-9$. Then the second-minimal energy tree in $\mathbb{T}_{n,p}$ is one of the two trees $T_{n,n-p+1,3}$ and $T(n, n-p+1; p-3, 0, \ldots, 0, 1)$.*

Theorem 1.2 ([20]). *Suppose that $4 \leq p \leq n-9$. If $E(T_{n,n-p+1,3}) > E(T(n, n-p+1; p-3, 0, \ldots, 0, 1))$, then $T_{n,n-p+1,3}$ is the unique tree with third-minimal energy in $\mathbb{T}_{n,p}$; If $E(T_{n,n-p+1,3}) < E(T(n, n-p+1; p-3, 0, \ldots, 0, 1))$, then the third-minimal energy tree in $\mathbb{T}_{n,p}$ is one of the two trees $T_{n,n-p+1,5}$ and $T(n, n-p+1; p-3, 0, \ldots, 0, 1)$.*

From Theorems 1.1 and 1.2, one can see that for $4 \leq p \leq n-9$, the author of [20] could not determine the unique extremal graph, respectively. In this paper, we will use the Coulson integral formula to solve the above unsolved problems. We only state our results on $\mathbb{T}_{n,p}$ instead of $\mathcal{T}_{n,d}$.

The rest of this paper is organized as follows. In Section 2, we give some preliminary results. In Section 3, we characterize the trees with second-minimal energy in $\mathbb{T}_{n,p}$ for $4 \leq p \leq n-9$. In Section 4, we determine the trees with third-minimal energy in $\mathbb{T}_{n,p}$ for $4 \leq p \leq n-9$.

2. Preliminaries

The following five results on properties of $m^+(G, x)$ appeared in [15].

Lemma 2.1. *Let v be a vertex of graph G and $N(v) = \{v_1, v_2, \ldots, v_j\}$ the set of all neighbors of v in G. Then*

$$m^+(G, x) = m^+(G - v, x) + x^2 \sum_{v_i \in N(v)} m^+(G - v - v_i, x).$$

Lemma 2.2. *Let P_t be the path on t vertices. Then*

(1) $m^+(P_t, x) = m^+(P_{t-1}, x) + x^2 m^+(P_{t-2}, x)$, for any $t \geq 1$,
(2) $m^+(P_t, x) = (1 + x^2)m^+(P_{t-2}, x) + x^2 m^+(P_{t-3}, x)$, for any $t \geq 2$.

The initials are $m^+(P_0, x) = m^+(P_1, x) = 1$, and we define $m^+(P_{-1}, x) = 0$.

Corollary 2.3. *Suppose $t \geq 1$. Then for any real number x,*

$$m^+(P_{t-1}, x) \leq m^+(P_t, x) \leq (1 + x^2)m^+(P_{t-1}, x).$$

Lemma 2.4. *For $t \geq -1$, the polynomial $m^+(P_t, x)$ has the following form*

$$m^+(P_t, x) = \frac{1}{\sqrt{1 + 4x^2}}(\lambda_1^{t+1} - \lambda_2^{t+1}),$$

where $\lambda_1 = \frac{1+\sqrt{1+4x^2}}{2}$ and $\lambda_2 = \frac{1-\sqrt{1+4x^2}}{2}$.

Lemma 2.5. *Suppose $t \geq 0$. If t is even, then*

$$\frac{2}{1 + \sqrt{1 + 4x^2}} \leq \frac{m^+(P_t, x)}{m^+(P_{t+1}, x)} \leq 1.$$

If t is odd, then

$$\frac{1}{1 + x^2} \leq \frac{m^+(P_t, x)}{m^+(P_{t+1}, x)} \leq \frac{2}{1 + \sqrt{1 + 4x^2}}.$$

The following result on real analysis is needed in the next sections.

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