MATCH
Communications in Mathematical and in Computer Chemistry

MATCH Commun. Math. Comput. Chem. **79** (2018) 263-274

ISSN 0340 - 6253

Minimal Energies of Trees with Three Branched Vertices*

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(Received May 16, 2017)

Abstract

The energy of a graph is defined as the sum of the absolute values of the eigenvalues of its adjacency matrix. Let $\Omega(n, 3)$ be the set of trees with n vertices and exactly three branched vertices. In this paper, we characterize the trees with the first to the fourth smallest energies in $\Omega(n, 3)$ for $n \geq 27$.

1 Introduction

Let G be a simple and undirected graph with n vertices and $A(G)$ be its adjacency matrix. Let $\lambda_1, \lambda_2, \ldots, \lambda_n$ be the eigenvalues of $A(G)$. Then the energy of G, denoted by $E(G)$, is defined as $E(G) = \sum_{i=1}^{n} |\lambda_i|$ (see [1, 2]). The theory of graph energy is well developed nowadays. Its details can be found in the recent book [3] and reviews [4], and references therein.

A fundamental problem encountered within the study of graph energy is the characterization of the graphs that belong to a given class of graphs having maximal or minimal

[1*] Research supported by the National Natural Science Foundation of China (No. 11501356), (No. 11426149) and (No. 71173145).

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energy. One of the graph classes that has been quite thoroughly studied is the class of all trees, i.e., connected graphs with no cycle. A remarkably large number of papers were published on such extremal problems: Trees with minimal energies [5–15]; Trees with maximal energies [16–22]; Unicyclic graphs [23–29]; Bicyclic graphs [30–32]; Tricyclic graphs [33–35].

The characteristic polynomial $det(xI - A(G))$ of the adjacency matrix $A(G)$ of a graph G is also called the characteristic polynomial of G, written as $\phi(G, x) = \sum_{i=0}^{n} a_i(G)x^{n-i}$.

If G is a bipartite graph, then it is well known that $\phi(G, x)$ has the form

$$\phi(G, x) = \sum_{i=0}^{\lfloor n/2 \rfloor} a_{2i}(G)x^{n-2i} = \sum_{i=0}^{\lfloor n/2 \rfloor} (-1)^i b_{2i}(G)x^{n-2i},$$

where $b_{2i}(G) = |a_{2i}(G)| = (-1)^i a_{2i}(G)$. In case G is a forest, then $b_{2i}(G) = m(G, i)$, the number of i-matchings of G.

In this paper, we assume that

$$\widetilde{\phi}(G, x) = \sum_{i=0}^{\lfloor n/2 \rfloor} b_{2i}(G)x^{n-2i}.$$

Using these coefficients of $\phi(G, x)$, the energy $E(G)$ of a bipartite graph G of order n can be expressed by the following Coulson integral formula [2]:

$$E(G) = \frac{2}{\pi} \int_0^{+\infty} \frac{1}{x^2} \ln \left(\sum_{i=0}^{\lfloor n/2 \rfloor} b_{2i}(G)x^{2i} \right) dx. \tag{1}$$

It follows that $E(G)$ is a strictly monotonically increasing function of those numbers $b_{2i}(G)(i = 0, 1, \dots, \lfloor n/2 \rfloor)$ for bipartite graphs. This in turn provides a way of comparing the energies of a pair of bipartite graphs as follows.

Definition 1.1. *Let G_1 and G_2 be two bipartite graphs of order n. If $b_{2i}(G_1) \le b_{2i}(G_2)$ for all i with $1 \le i \le \lfloor n/2 \rfloor$, then we write $G_1 \preceq G_2$.*

Furthermore, if $G_1 \preceq G_2$ and there exists at least one index j such that $b_{2j}(G_1) < b_{2j}(G_2)$, then we write that $G_1 \prec G_2$. If $b_{2i}(G_1) = b_{2i}(G_2)$ for all i, we write $G_1 \sim G_2$. According to the Coulson integral formula (1), we have for two biaprtite G_1 and G_2 of order n that

$$G_1 \preceq G_2 \Longrightarrow E(G_1) \le E(G_2)$$

$$G_1 \prec G_2 \Longrightarrow E(G_1) < E(G_2).$$

Trees with extremal energies are extensively studied in literature (see [3], Chapter 7). Gutman [5] determined the first four smallest energy trees of order n. Li and Li [7] determined the fifth and sixth smallest energy trees of order n. Wang and Kang [8] characterized the seventh to the ninth smallest energy trees of order n. Recently, Shan and Shao [9] further determined the tenth to the twelfth smallest energy tree of order n.

Because the first to the twelfth smallest energy trees of order n have one or two branched vertices, it is natural to consider determining the minimal energy trees over the set of trees of order n with few branched vertices. In [10], Marín et al. showed that the minimal energy tree of order n with exactly three branched vertices was $T(2,1,n-6)$ (see Figure 1). In this paper, we generalize the result and further characterize the trees with the second to the fourth smallest energies with exactly three branched vertices for $n \geq 27$.

Let $\Omega(n,3)$ be the set of trees with n vertices and exactly three branched vertices. The following theorem is the main result of this paper.

Theorem 1.1. *Let $T \in \Omega(n,3)$ and $n \geq 27$. If $T \neq T(2,1,n-6), T(2,n-7,2), T(3,1,n-7), T(2,2,n-7)$, then $E(T(2,1,n-6)) < E(T(2,n-7,2)) < E(T(3,1,n-7)) < E(T(2,2,n-7)) < E(T)$.*

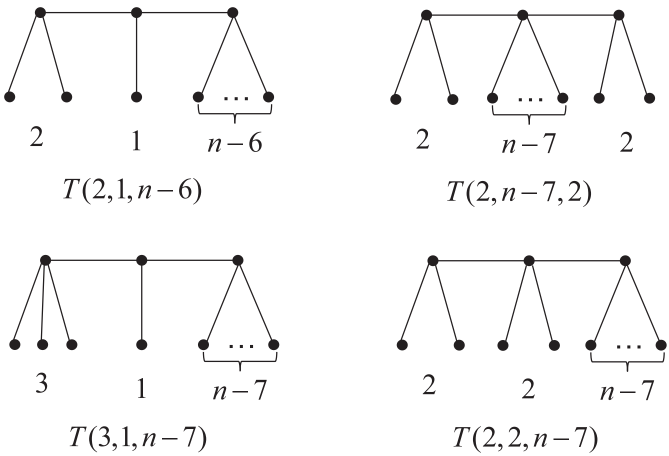

Figure 1. The trees $T(2,1,n-6)$, $T(2,n-7,2)$, $T(3,1,n-7)$ and $T(2,2,n-7)$.

2 The basic strategy of the proof of Theorem 1.1

In this section, we outline the basic strategy of the proof of Theorem 1.1. Let T be a tree with n vertices and exactly three branched vertices. Then T has the form of $T(a_1, \cdots, a_r|x|b_1, \cdots, b_s$
$|y|c_1, \cdots, c_t)$ as shown in Figure 2, where $a_1, \cdots, a_r, b_1, \cdots, b_s, c_1, \cdots, c_t, x, y$ are positive integers. When $a_1 = \cdots = a_r = b_1 = \cdots = b_s = c_1 = \cdots = c_t = 1$ and $x = y = 1$, we usually abbreviate $T(a_1, \cdots, a_r|x|b_1, \cdots, b_s|y|c_1, \cdots, c_t)$ by $T(r, s, t)$ which is depicted in Figure 2. Let $\Omega(n, 3)$ be the set of trees with n vertices and exactly three branched vertices. Let $A(n, 3) = \{T(r, s, t)|t \geq r \geq 2, s \geq 1, r+s+t = n-3\}$. Let $B(n, 3) = \Omega(n, 3)\setminus A(n, 3)$. Then we have $A(n, 3) \bigcup B(n, 3) = \Omega(n, 3)$.

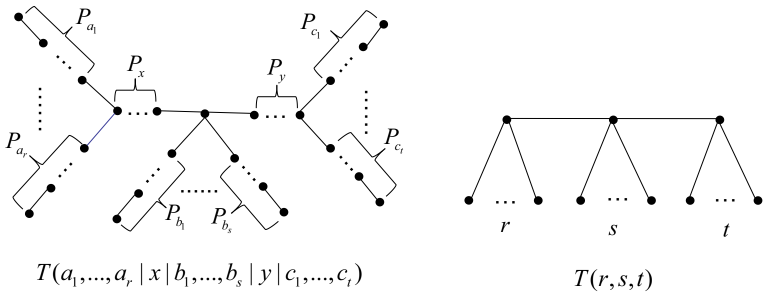

Figure 2. The trees $T(a_1, \cdots, a_r|x|b_1, \cdots, b_s|y|c_1, \cdots, c_t)$ and $T(r, s, t)$.

To conclude, for $n \geq 27$, our basic strategy of the proof of Theorem 1.1 is to prove the following results $(R_1) - (R_3)$:

(R_1). $E(T(2, 1, n-6)) < E(T(2, n-7, 2)) < E(T(3, 1, n-7)) < E(T(2, 2, n-7))$.

(R_2). Let $T \in A(n, 3)$. If $T \neq T(2, 1, n-6), T(2, n-7, 2), T(3, 1, n-7), T(2, 2, n-7)$, then $E(T) > E(T(2, 2, n-7))$;

(R_3). Let $T \in B(n, 3)$. Then $E(T) > E(T(2, 2, n-7))$;

It is easy to see that we can prove Theorem 1.1 by combining the above results $(R_1) - (R_3)$. Then we will prove the results $(R_1) - (R_3)$ in Sections 3 and 4, respectively.

3 The proof of (R_1)

Recently, Shan et al. [9] presented a new method of comparing the energies of two trees which are quasi-ordering incomparable. In this section, we will use the method to prove the result (R_1). First, we introduce some notations and lemmas.

Let u be a vertex of a graph G. A $k-$claw attaching graph of G at u, denoted by $G_u(k)$, is the graph obtained from G by attaching k new pendant edges to G at the vertex u.

For the sake of simplicity, the polynomials $\phi(G,x)$ and $\widetilde{\phi}(G,x)$ will be denoted by $\phi(G)$ and $\widetilde{\phi}(G)$. Let v be a vertex of a graph H. Let

$$\begin{aligned} D_1 &= \{x > 0 | \widetilde{\phi}(H)\widetilde{\phi}(G-u) - \widetilde{\phi}(G)\widetilde{\phi}(H-v) > 0\} \\ D_2 &= \{x > 0 | \widetilde{\phi}(H)\widetilde{\phi}(G-u) - \widetilde{\phi}(G)\widetilde{\phi}(H-v) < 0\}. \end{aligned}$$

Furthermore, we let

$$\begin{aligned} ED(k) &= E(H_v(k)) - E(G_u(k)) \\ ED &= E(H-v) - E(G-u). \end{aligned}$$

Lemma 3.1. *([9]) Let u be a vertex of a bipartite graph G and v be a vertex of a bipartite graph H. Let $D_1, D_2, ED(k), ED$ be defined as above. Then for $0 \le l < k$, we have*

(1) If $D_1 = \emptyset$ but $D_2 \neq \emptyset$, then $ED(l) < ED(k) < ED$;

(2) If $D_2 = \emptyset$ but $D_1 \neq \emptyset$, then $ED < ED(k) < ED(l)$;

(3) If $D_1 = D_2 = \emptyset$, then $ED = ED(k) = ED(l)$.

From Lemma 3.1, we can prove the following two lemmas.

Lemma 3.2. *If $n \ge 27$, then $E(T(2, n-7, 2)) < E(T(3, 1, n-7))$.*

Proof. Let $G = T(2, 20, 2)$ and $H = T(3, 1, 20)$. Let u be the vertex of G with degree 22 and v be the vertex of H with degree 21, respectively. Then $G_u(n-27) = T(2, n-7, 2)$ and $H_v(n-27) = T(3, 1, n-7)$, respectively. By some calculations, we can show that

$$\begin{aligned} \widetilde{\phi}(H) &= 60x^{21} + 106x^{23} + 26x^{25} + x^{27} \\ \widetilde{\phi}(G) &= 80x^{21} + 88x^{23} + 26x^{25} + x^{27} \\ \widetilde{\phi}(H-v) &= x^{20}(3x^2 + 5x^4 + x^6) \\ \widetilde{\phi}(G-u) &= x^{20}(4x^2 + 4x^4 + x^6), \end{aligned}$$

This implies that

$$\widetilde{\phi}(H)\widetilde{\phi}(G-u)-\widetilde{\phi}(G)\widetilde{\phi}(H-v)=-x^{27}(x^2+2)(x^2+5).$$

Then $D_1=\emptyset$. Using Lemma 3.1, we have

$$ED(n-27)\geq ED(0)=E(H)-E(G)\doteq 9.8567\times 10^{-4}>0.$$

Thus $E(T(2,n-7,2))<E(T(3,1,n-7))$. ■

Lemma 3.3. *If* $n\geq 16$, *then* $E(T(2,2,n-7))<E(T(4,1,n-8))$.

Proof. Let $G=T(2,2,9)$ and $H=T(4,1,8)$. Let u be the vertex of G with degree 10 and v be the vertex of H with degree 9, respectively. Then $G_u(n-16)=T(2,2,n-7)$ and $H_v(n-16)=T(4,1,n-8)$, respectively. By some direct calculations, we can get

$$\begin{aligned}\widetilde{\phi}(H) &= 32x^{10}+56x^{12}+15x^{14}+x^{16}\\ \widetilde{\phi}(G) &= 36x^{10}+51x^{12}+15x^{14}+x^{16}\\ \widetilde{\phi}(H-v) &= x^8(4x^3+6x^5+x^7)\\ \widetilde{\phi}(G-u) &= x^8(4x^3+5x^5+x^7).\end{aligned}$$

It follows that

$$\widetilde{\phi}(H)\widetilde{\phi}(G-u)-\widetilde{\phi}(G)\widetilde{\phi}(H-v)=-x^{13}(x^2+2)(x^6+8x^4+14x^2+8).$$

Thus $D_1=\emptyset$. According to Lemma 3.1, we have

$$ED(n-16)\geq ED(0)=E(H)-E(G)\doteq 0.0129>0.$$

Then $E(T(2,2,n-7))<E(T(4,1,n-8))$. ■

According to Lemmas 3.2 and 3.3, we can prove the following result.

Lemma 3.4. *If* $n\geq 27$, *then* $E(T(2,1,n-6))<E(T(2,n-7,2))<E(T(3,1,n-7))<E(T(2,2,n-7))$.

Proof. By some direct, calculations, we can show that

$$\begin{aligned}\widetilde{\phi}(T(2,1,n-6)) &= 2(n-6)x^{n-6}+4(n-5)x^{n-4}+(n-1)x^{n-2}+x^n\\ \widetilde{\phi}(T(2,n-7,2)) &= 4(n-7)x^{n-6}+4(n-5)x^{n-4}+(n-1)x^{n-2}+x^n\\ \widetilde{\phi}(T(3,1,n-7)) &= 3(n-7)x^{n-6}+(5n-29)x^{n-4}+(n-1)x^{n-2}+x^n\\ \widetilde{\phi}(T(2,2,n-7)) &= 4(n-7)x^{n-6}+(5n-29)x^{n-4}+(n-1)x^{n-2}+x^n.\end{aligned}$$

It follows that $T(2,1,n-6)\prec T(2,n-7,2)$ and $T(3,1,n-7)\prec T(2,2,n-7)$. By Lemma 3.2, we can have $E(T(2,1,n-6))<E(T(2,n-7,2))<E(T(3,1,n-7))<E(T(2,2,n-7))$. ■

The proof of (R_1):

Proof. The result can follow from Lemma 3.4 immediately. ■

4 The proofs of (R_2) and (R_3)

In this section, we will prove the results (R_2) and (R_3). The following two lemmas were obtained by MArín et al. in [10].

Lemma 4.1. *([10]) Let $T(r,s,t)$ be the tree depicted in Figure 2. If $t \geq r \geq 2$, then $T(r-1,s,t+1) \prec T(r,s,t)$.*

Lemma 4.2. *([10]) Let $T(2,s,t)$ be the tree depicted in Figure 2. We have the followings.*

(1) If $2 \leq s \leq t$, then $T(2,s-1,t+1) \prec T(2,s,t)$;

(2) If $2 \leq t < s$, then $T(2,s+1,t-1) \prec T(2,s,t)$;

The following lemma will be used in Lemma 4.4.

Lemma 4.3. *If $n \geq 11$, then $T(2,2,n-7) \prec T(2,n-8,3)$.*

Proof. By some direct calculations, we can have

$$\begin{aligned} \widetilde{\phi}(T(2,2,n-7)) &= 4(n-7)x^{n-6} + (5n-29)x^{n-4} + (n-1)x^{n-2} + x^n \\ \widetilde{\phi}(T(2,n-8,3)) &= 6(n-8)x^{n-6} + (5n-29)x^{n-4} + (n-1)x^{n-2} + x^n. \end{aligned}$$

It follows that $T(2,2,n-7) \prec T(2,n-8,3)$. We have completed the proof. ■

Now we prove the result (R_2) in the following lemma.

Lemma 4.4. *Let $T \in A(n,3)$ and $n \geq 16$. If $T \neq T(2,1,n-6), T(2,n-7,2), T(3,1,n-7), T(2,2,n-7)$, then $E(T) > E(T(2,2,n-7))$.*

Proof. Since $T \in A(n,3)$, we have that T has the form of $T(r,s,t)$ shown in Figure 2. Because $T \neq T(2,n-7,2)$, we have $1 \leq s \leq n-8$. We consider the following three cases.

Case 1: $s = 1$

Then $T = T(r,1,t)$ with $r+t = n-4$. Since $T \neq T(2,1,n-6), T(3,1,n-7)$, we have $r \geq 4$. By Lemma 4.1, we can show that $T \succeq T(4,1,n-8)$. Furthermore, using Lemma 3.3 we have $E(T) > E(T(2,2,n-7))$.

Case 2: $s = 2$

So $T = T(r,2,t)$ with $r+t = n-4$. Since $T \neq T(2,2,n-7)$, we have $r \geq 3$. According to Lemma 4.1, we can get $T \succeq T(3,2,n-8) \succ T(2,2,n-7)$.

Case 3: $3 \leq s \leq n-8$

By Lemma 4.1, we have $T \succeq T(2,s,n-s-5)$.

If $s \le n-s-5$, then by Lemma 4.2 we have $T \succeq T(2,3,n-8) \succ T(2,2,n-7)$.

If $s > n-s-5$, then using Lemma 4.2 we have $T \succeq T(2,n-8,3)$. Moreover, according to Lemma 4.3, we can show that $T \succ T(2,2,n-7)$. Then we complete the proof. ■

The proof of (R_2):

Proof. The result can follow from Lemma 4.4 immediately. ■

Let T be a tree of order $n \ge 4$ and uv be a nonpendent edge. Assume that $T - uv = T_1 \cup T_2$ with $u \in V(T_1)$ and $v \in V(T_2)$. Now we construct a new tree T_0 obtained by identifying vertex u with vertex v and attaching a pendent vertex to vertex $u(=v)$ (see Figure 3). Then we say that T_0 is obtained by running edge-growing transformation of T on edge uv, or e.g.t. of T on edge uv for short.

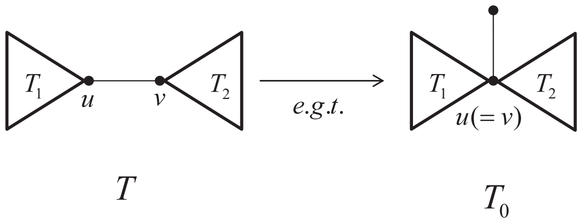

Figure 3. Two trees for e.g.t. in Lemma 4.5

Lemma 4.5. *([10]) Let T be a tree of order $n \ge 4$ and uv be nonpendent edge of T. If T_0 is a tree obtained from T by running one step of e.g.t. on edge uv, then $T_0 \prec T$.*

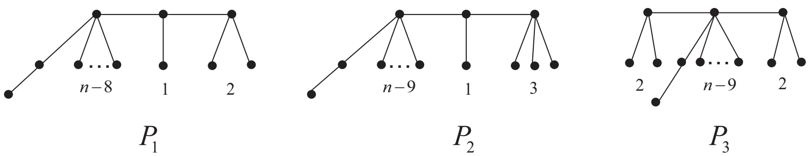

Figure 4. Three trees used in Lemma 4.7

Let G be a graph. Denote by $m(G,k)$ the $k-$matching numbers of G. The following lemma will be used in the proof of Lemma 4.7.

Lemma 4.6. *Let P_1, P_2, P_3 be the trees as shown in Figure 4. If $n \ge 27$, then $P_i \succ T(2,2,n-7)$ for $i = 1,2,3$.*

Proof. By some calculations we have

$$\begin{aligned}
m(P_1,3) &\geq 4(n-8)+2(n-6)=6n-44\\
m(P_1,2) &\geq n-2+4(n-7)+4=5n-26\\
m(P_2,3) &\geq 5(n-9)+3(n-8)=8n-69\\
m(P_2,2) &\geq n-2+5(n-8)+4=6n-42\\
m(P_3,3) &\geq 4(n-7)+4(n-9)=8n-64\\
m(P_3,2) &\geq 4(n-4)+n-9=5n-25.
\end{aligned}$$

Moreover, $\widetilde{\phi}(T(2,2,n-7)) = 4(n-7)x^{n-6} + (5n-29)x^{n-4} + (n-1)x^{n-2} + x^n$. Then we have $P_i \succ T(2,2,n-7)$ for $i = 1,2,3$. ■

The result (R_3) will be proved in the following lemma.

Lemma 4.7. *Let $T \in B(n,3)$. If $n \geq 27$, then $E(T) > E(T(2,2,n-7))$.*

Proof. Let $T \in B(n,3)$. Then T have the form of $T(a_1,\cdots,a_r|x|b_1,\cdots,b_s|y|c_1,\cdots,c_t)$ where a_i, b_i, c_i, x, y are positive integers. For simplicity, when $a_1 = \cdots = a_r = b_1 = \cdots = b_s = c_1 = \cdots = c_t = 1$, we abbreviate $T(a_1,\cdots,a_r|x|b_1,\cdots,b_s|y|c_1,\cdots,c_t)$ by $T(r|x|s|y|t)$. We consider the following five cases.

Case 1: $x \geq 2$

According to Lemma 4.5, we have $T \succeq T(r|2|s|1|t)$ where $r+s+t = n-4$. If $s = 1$, then by Lemmas 4.1 and 4.5 we have $T \succ T(2,2,n-7)$. If $s = n-8$, then $T \succ T(2,n-8,3)$ by Lemmas 4.1 and 4.5. If $2 \leq s \leq n-9$, using Lemma 4.5 we have $T \succ T(r,s+1,t)$. By Lemma 4.4, we can show that $T \succ T(2,2,n-7)$.

Case 2: $y \geq 2$

The proof is similar to Case 1.

Case 3: there at least exists one index i satisfying that $a_i \geq 2$.

If $x \geq 2$ or $y \geq 2$, then we can prove the result by Case 1 or Case 2. Then we can assume $x = y = 1$ in the followings. By Lemma 4.5, we have $T \succeq T(1,\cdots,1,2|1|s|1|t)$. If $s \geq 2$, then by Lemma 4.1 we have $T \succ T(2,2,n-7)$. Then we assume that $s = 1$ in what follows. If $t = 2$, then we can show that $T \succeq P_1$. Using Lemma 4.6, we can obtain that $T \succ T(2,2,n-7)$. If $t = 3$, then we have $T \succeq P_2$. According to Lemma 4.6, we can show that $T \succ T(2,2,n-7)$. If $t \geq 4$, then by Lemmas 4.4 and 4.5, we can have $T \succ T(2,2,n-7)$.

Case 4: there at least exists one index i satisfying that $c_i \geq 2$.

The proof is similar to Case 3.

Case 5: there at least exists one index i satisfying that $b_i \geq 2$.

According to the above results, we can assume that $x = y = a_1 = \cdots = a_r = c_1 = \cdots = c_t = 1$. By Lemma 4.5, we have $T \succeq T(r|1|1, \cdots, 1, 2|1|t)$. If $r = t = 2$, then $T \succeq P_3$. Using Lemma 4.6, we can show that $T \succ T(2, 2, n-7)$. If $r \geq 3$, then by Lemma 4.5 we have $T \succ T(r, s, t)$ where $r \geq 3$ and $s \geq 2$. According to Lemma 4.4, we have $T \succ T(2, 2, n-7)$. If $t \geq 3$, then we prove the result similarly.

To conclude, we have completed the proof. ■

The proof of (R_3):

Proof. The result can follow from Lemma 4.7 immediately. ■

Acknowledgments: This work was completed while the first author was visiting the School of Business of East China University of Science and Technology.

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