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Chemical Indices, Mean Distance, and Radius

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Abstract

A chemical index of a molecular graph G is the sum of weights $w(u,v)$ over all pairs of vertices u and v in G. It is the Wiener index $W(G)$ if $w(u,v)$ is the distance of u and v, the Randić index $R(G)$ if $w(u,v) = [d(u)d(v)]^{-1/2}$ for u adjacent to v and 0 otherwise, and the harmonic index $H(G)$ if $w(u,v) = 2/[d(u)+d(v)]$ for u adjacent to v and 0 otherwise, where $d(v)$ denotes the degree of v. In 1988, Fajtlowicz conjectured that $W(G) \leq \binom{n}{2}R(G)$ for all connected graphs G of order n. Strengthening another conjecture of Fajtlowicz as well as Caporossi and Hansen, Deng, Tang and Zhang conjectured that $H(G) \geq r(G)$ for all connected graphs G except paths of even order, where $r(G)$ denotes the radius of G. In this paper, we prove these conjectures for dense triangle-free graphs, and also prove that $W(T) \leq \binom{n}{2}H(T)$ for all trees T of order n with equality if and only if T is a star. As a consequence, the Fajtlowicz conjecture holds for trees which was recently proven by Cygan, Pilipczuk and Škrekovski.

1 Introduction

All graphs in this paper are simple, i.e., without loops and multiple edges. Let $G = (V, E)$ be a connected graph of order $n = |V|$. The *size* of G is $|E|$. For a vertex v of G, the *degree* of v denoted by $d(v)$ is the number of its neighbors. A graph is called *regular* if its vertices are all of the same degree, and called *bi-regular* if its vertices have degrees among two values. For a pair of vertices u and v of G, the *distance* between u and v in G, denoted by $d(u,v)$, is the length of a shortest path between u and v. The *radius* of G,

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denoted by $r(G)$, is defined as

$$r(G) := \min_{u\in V} \max_{v\in V} d(u,v).$$

A chemical index is a topological molecular descriptor on the molecular graph of a chemical compound. More precisely, a *chemical index* of G is the sum of weights $w(u,v)$ over all pairs of vertices u and v in G. Different weights lead to different chemical indices. In 1947, Wiener [19] introduced the first chemical index denoted by $W(G)$, now called the *Wiener index* as follows,

$$W(G) := \sum_{\{u,v\}\in V_2} d(u,v),$$

where V_2 denotes the set of all 2-element subsets of V. In 1975, Randić [17] introduced another chemical index denoted by $R(G)$, called the *Randić index* as follows,

$$R(G) := \sum_{uv\in E} [d(u)d(v)]^{-1/2}.$$

As a variance of the Randić index, in 1987 Fajtlowicz [11] introduced the *harmonic index* denoted by $H(G)$ as follows,

$$H(G) := \sum_{uv\in E} \frac{2}{d(u)+d(v)}.$$

Since the geometric mean of $d(u)$ and $d(v)$ cannot exceed their arithmetic mean, we have $H(G) \leq R(G)$ with equality if and only if G is regular. The *mean distance* $\mu(G)$ of G is defined by $\mu(G) := W(G)/\binom{n}{2}$. It was introduced by Doyle and Graver [7] as a measure of the "compactness" of the graph. These indices of graphs have some important applications in mathematical chemistry and are well studied by many mathematical or chemical researchers. Their relationships were studied in [12,25]. The Randić index were investigated for graphs with cyclomatic number at most 3 [4,8]. In 1988, Fajtlowicz [10] posed the following conjectures based on the computer program Graffiti.

Conjecture 1.1 [10] *For all connected graphs G, $\mu(G) \leq R(G)$.*

Conjecture 1.2 [10] *For all connected graphs G, $r(G) \leq 1 + R(G)$.*

Conjecture 1.2 was strengthened by Caporossi and Hansen [1] as follows.

Conjecture 1.3 [1] *For all connected graphs G except paths of even order, $r(G) \leq R(G)$.*

Conjecture 1.3 was further strengthened by Deng, Tang and Zhang [6] as follows.

Conjecture 1.4 [6] *For all connected graphs G except paths of even order, $r(G) \leq H(G)$.*

Conjecture 1.1 was proven for trees by Cygan, Pilipczuk and Škrekovski [2] and for unicyclic graphs by You and Liu [21]. Li and Shi [15] found that the Delorme-Favaron-Rautenbach conjecture [5] implies Conjecture 1.1 for dense graphs of order $n \geq 15$ with minimum degree at least $n/5$. Strengthening the result of Cygan et al. we obtain the following result.

Theorem 1.1 *For all trees T, $\mu(T) \leq H(T)$ with equality if and only if T is a star.*

Conjectrue 1.2 was proven for graphs with cyclomatic number at most 3 [1, 16, 22]. Conjecture 1.3 was proven for trees by Caporossi and Hansen [1] and for bi-regular graphs by You and Liu [22]. Conjecture 1.4 was proven for trees and unicyclic graphs by Deng, Tang and Zhang [6]. In this paper, we also prove these conjectures for dense triangle-free graphs.

Theorem 1.2 *Let G be a connected triangle-free graph of order n with minimum degree δ. Then for sufficiently large n, the following statements hold.*

1. *$r(G) \leq R(G)$ if $\delta \geq n^{1/3} + 25n^{-1/3}$.*
2. *$\mu(G) \leq R(G)$ if $\delta \geq (n/2)^{1/3}$.*
3. *$r(G) \leq H(G)$ if $\delta \geq \sqrt{n/2} + 7$.*
4. *$\mu(G) \leq H(G)$ if $\delta \geq \sqrt{n/3} + 5$.*

The proofs of Theorems 1.1 and 1.2 will be presented in the following two sections respectively.

2 Trees

The proof of Theorem 1.1 is based on an upper bound on $\mu(T)$ by Cygan et al. [2] and a sharp estimate on $H(T)$ where T is a tree with given number of leaves. We will give the sharp bounds on $H(T)$ in the following subsection and finish the proof afterwards.

2.1 Trees with given number of leaves

Let T be a tree. For a vertex v of T, denote the neighborhood of v by $N(v)$ and thus the degree $d(v) = |N(v)|$. We use $T - v$ to denote the graph that arises from T by deleting the vertex v of T. A *leaf* of T is a vertex of degree one and a *pendent edge* is incident to a leaf. Let $P_s = v_0v_1 \cdots v_s$ be a path of T with $d(v_1) = d(v_2) = \cdots = d(v_{s-1}) = 2$ (unless $s = 1$). If the vertex v_0 is a leaf and $d(v_s) \geq 3$, then we call P_s a *pendent path* of T and also call that s the *length* of the pendent path P_s. Let $\mathcal{T}_{n,k} := \{T : T \text{ is a tree of order } n \text{ with } k \text{ leaves}\}$. For $T \in \mathcal{T}_{n,k}$, denote

$$V_i(T) := \{v \mid v \in V(T),\ d(v) = i\}, \text{ and } n_i(T) := |V_i(T)|.$$

Denote the neighborhood of leaves by $N(V_1) := \cup_{v \in V_1(T)} N(v)$. Set $E_2(T) := \{uv \in E(T) \mid d(u) = d(v) = 2\}$ and $\mathcal{P}(T) := \{P : P \text{ is a pendent path of length at least 2 in } T\}$. Let S_k^n denote a tree of order n created from a star $K_{1,k}$ by attaching a path of length $n - k - 1$ to a leaf of $K_{1,k}$. We call T a $(k, 3)$-*regular* tree if T is a tree with k leaves and for each vertex $v \in V(T) \setminus V_1(T)$, $d(v) = 3$ and it is clear that $|V(T)| = 2k - 2$. Denote by $\mathcal{T}_{n,k}^*$ the set of $T_{n,k}^*$, where $T_{n,k}^*$ is a tree of order n created from a $(k, 3)$-regular tree by adding at least one new vertex on each pendent edge, and thus the total number of new vertices is $n - 2k + 2$.

Our main results in this section are the following sharp estimates on $H(T)$ for all trees T of order n with k leaves. Note that T is just a path if $k = 2$ and is a star if $k = n - 1$. Therefore we may always assume that $3 \leq k \leq n - 2$.

Theorem 2.1 *Let k and n be two integers with $3 \leq k \leq n - 2$ and $T \in \mathcal{T}_{n,k}$, then*

$$H(T) \geq \frac{n-k}{2} + \frac{5}{3} + \frac{2}{k+2} - \frac{4}{k+1}$$

with equality if and only if $T \cong S_k^n$.

Theorem 2.2 *For every $T \in \mathcal{T}_{n,k}$ with $n \geq 3k - 2$ and $k \geq 3$, we have $H(T) \leq \frac{n}{2} - \frac{k}{10}$ with equality if and only if $T \in \mathcal{T}_{n,k}^*$.*

Theorem 2.2 will not be used in the proof of Theorem 1.1, but it is interesting itself, so we include it here for completeness.

Proof of Theorem 2.1. Let $f(n, k) := \frac{n-k}{2} + \frac{5}{3} + \frac{2}{k+2} - \frac{4}{k+1}$. Note that if $T \cong S_k^n$, then $H(T) = f(n, k)$ by a direct calculation. We use induction on k. First consider $k = 3$.

Since $n \geq 5$ and $T \in \mathcal{T}_{n,3}$, $\mathcal{P}(T) \neq \emptyset$. Let $P := v_0 v_1 \cdots v_s$ $(s \geq 2)$ be a pendent path in T with $v_0 \in V_1(T)$ and $d(v_s) = 3$. Let $N(v_s) = \{v_{s-1}, u_1, u_2\}$ and $d_i := d(u_i)$, $i = 1, 2$. Then it is clear that $1 \leq d_i \leq 2$ for $i = 1, 2$. Let $T' := T - \{v_0, v_1, ..., v_{s-1}\}$, then T' is a path of order $n - s$. Thus $H(T') = (n - s - 3)/2 + 4/3$ and

$$\begin{aligned} H(T) &= H(T') + \frac{2}{3} + \frac{2}{5} + \frac{s-2}{2} + \sum_{i=1}^{2} \left(\frac{2}{3 + d_i} - \frac{2}{2 + d_i} \right) \\ &= f(n, 3) + 1/3 - 2 \sum_{i=1}^{2} [(3 + d_i)(2 + d_i)]^{-1} \geq f(n, 3), \end{aligned}$$

where the equality holds if and only if $d_1 = d_2 = 1$ and thus $T \cong S_k^n$.

Next we assume that $k \geq 4$ and the result holds for smaller values k. Let $T \in \mathcal{T}_{n,k}$ such that $H(T)$ is as small as possible.

Claim. $|\mathcal{P}(T)| \leq 1$.

Assume to the contrary that $P = v_0 v_1 \cdots v_s$ and $Q = u_0 u_1 \cdots u_l$ $(s, l \geq 2)$ are two distinct pendent paths of T with $u_0, v_0 \in V_1(T)$ and $d(v_s), d(v_l) \geq 3$. Let $T_0 := T - v_{s-1}v_{s-2} + u_0 v_0$. Then $T_0 \in \mathcal{T}_{n,k}$, but

$$\begin{aligned} H(T_0) - H(T) &= \frac{2}{1 + d(v_s)} - \frac{2}{2 + d(v_s)} + \frac{1}{2} - \frac{2}{3} \\ &= \frac{2}{[1 + d(v_s)][2 + d(v_s)]} - \frac{1}{6} \leq \frac{1}{10} - \frac{1}{6} < 0, \end{aligned}$$

contradicting the choice of T. This completes the proof of the claim.

By the claim and $k \geq 4$, there exists a vertex $u \in N(V_1)$ such that $3 \leq t := d(u) \leq k$. Let $N(u) \cap V_1(T) = \{v_1, v_2, ..., v_r\}$ $(r \geq 1)$ and $N(u) \setminus V_1(T) = \{u_1, u_2, ..., u_{t-r}\}$. Then $t - r \geq 1$ (as $T \ncong K_{1,n-1}$) and all $d_i := d(u_i) \geq 2$ for $1 \leq i \leq t - r$. Let $T' := T - v_1$. Since $k \geq 4$, we have $T' \in \mathcal{T}_{n-1,k-1}$ and thus

$$\begin{aligned} H(T) &= H(T') + \frac{2r}{t+1} - \frac{2(r-1)}{t} + \sum_{i=1}^{t-r} \left(\frac{2}{t + d_i} - \frac{2}{t + d_i - 1} \right) \\ &\geq f(n-1, k-1) + \frac{2(t - r + 1)}{t(t+1)} - 2 \sum_{i=1}^{t-r} [(t + d_i)(t + d_i - 1)]^{-1} \\ &\geq f(n-1, k-1) + \frac{2(t - r + 1)}{t(t+1)} - \frac{2(t - r)}{(t+2)(t+1)} \\ &= f(n-1, k-1) + \frac{4(t-r)}{t(t+1)(t+2)} + \frac{2}{t(t+1)} \\ &\geq f(n-1, k-1) + \frac{4}{k(k+1)(k+2)} + \frac{2}{k(k+1)} = f(n, k), \end{aligned}$$

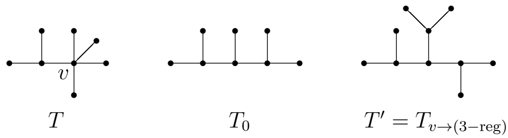

Figure 1: The tree T' is obtained from T by blowing up the vertex v.

where the equality holds if and only if $H(T') = f(n-1, k-1)$, $k = t$, $t - r = 1$ and $d_1 = 2$. By the induction hypothesis, $H(T') = f(n-1, k-1)$ if and only if $T' \cong S_{k-1}^{n-1}$. Note that S_{k-1}^{n-1} has a unique vertex of degree greater than 2, and hence the equality holds if and only if $T \cong S_k^n$. $\square$

In order to prove Theorem 2.2, we need three kinds of operations on a tree T introduced by Zhang, Lu and Tian [23].

1. If uv is an edge of T and T' is obtained from T by contracting uv, i.e., identifying the two vertices u and v in $T - uv$, we say that T' is obtained from T by *contraction* and denote $T' = T_{uv}$. Clearly T_{uv} is still a tree with one vertex less than T.

2. Let $N(v) = X \cup Y$ such that $X \cap Y = \emptyset$, $|X| = x \geq 1$ and $|Y| = y \geq 1$, where $v \in V(T)$. If T' is obtained from T by splitting the vertex v into two new vertices u and w, linking u and w, and linking u to all vertices in X and w to all vertices in Y, we say that T' is obtained from T by *splitting* and denote $T' = T_{v\to(x,y)}$. Thus $T_{v\to(x,y)})$ is still a tree with one more vertex than T.

3. If $v \in V(T)$ with $d(v) = s > 3$ and T' is obtained from T by replacing the vertex v by a $(s, 3)$-regular tree T_0 such that each vertex in $N(v)$ and each leaf of T_0 are identified one by one, we say that T' is obtained from T by *blow-up* and denote $T' = T_{v\to(3-\mathrm{reg})}$, see Fig. 1 for example. Thus $T_{v\to(3-\mathrm{reg})}$ is still a tree on $|V(T)|+s-3$ vertices with $|E(T)| + s - 3$ edges.

Lemma 2.1 [23] *Let $T \in \mathcal{T}_{n,k}$ with maximum degree $\Delta \geq 4$. If $n \geq 3k - 2$ and $E_2(T) \subset E(\mathcal{P}(T))$, then $|E_2(T)| \geq n_4(T) + 2n_5(T) + \cdots + (\Delta - 3)n_\Delta(T)$.*

Lemma 2.2 *Let $T \in \mathcal{T}_{n,k}$. If there is a vertex $v \in V(T)$ with $d(v) = 2$ and the degrees of the vertices adjacent to v are both at least 2, then there is a tree $T' \in \mathcal{T}_{n,k}$ such that $H(T') \geq H(T)$.*

Proof. Suppose $N(v) = \{u, w\}$, where $v \in V(T)$ with $d(v) = 2$ and $d(u), d(w) \geq 2$. Let x be a leaf of T and y its neighbor. Let T' be obtained from T_{uv} by adding an edge to the vertex x. Then $T' \in \mathcal{T}_{n,k}$ and

$$\begin{aligned} H(T) - H(T') &= \frac{2}{2+d(u)} + \frac{2}{2+d(w)} + \frac{2}{1+d(y)} - \frac{2}{d(u)+d(w)} - \frac{2}{2+d(y)} - \frac{2}{3} \\ &= \frac{2[d(w)-2]}{[2+d(u)][d(u)+d(w)]} + \frac{2}{2+d(w)} + \frac{2}{[1+d(y)][2+d(y)]} - \frac{2}{3} \\ &\leq \frac{d(w)/2-1}{2+d(w)} + \frac{2}{2+d(w)} + \frac{1}{6} - \frac{2}{3} = 0. \end{aligned}$$

Therefore, $H(T') \geq H(T)$. □

Lemma 2.3 *Suppose $T \in \mathcal{T}_{n,k}$, and $v \in V(T)$ with $d(v) = s > 3$, $N(v) = \{u_1, u_2, ..., u_s\}$ and $d(u_1) \leq d(u_2) \leq \cdots \leq d(u_s)$. If $|E_2(T)| \geq s-3$, then there is a tree $T' \in \mathcal{T}_{n,k}$ such that the following statements hold.*

1. *If $s = 4$, $d(u_3) \leq 3$ and $d(u_4) \leq 5$, then $H(T) < H(T')$.*
2. *If $s \geq 5$ and $d(u_{s-1}) \leq 3$, then $H(T) < H(T')$.*
3. *If $s \geq 8$ and $d(u_{s-1}) \leq 4$, then $H(T) < H(T')$.*

Proof. Let T^* be obtained from T by contracting $s-3$ edges in $E_2(T)$ and $T' := T^*_{v\to(3-\mathrm{reg})}$. It is clear that $T' \in \mathcal{T}_{n,k}$. Let $r := d(u_{s-1})$, then we have

$$\begin{aligned} H(T) - H(T') &= \frac{s-3}{6} + \sum_{i=1}^{s} \left(\frac{2}{s+d(u_i)} - \frac{2}{3+d(u_i)} \right) \\ &= \frac{s-3}{6} + \sum_{i=1}^{s} \frac{2(3-s)}{[s+d(u_i)][3+d(u_i)]} \\ &\leq \frac{s-3}{6} + \frac{2(s-1)(3-s)}{(s+r)(3+r)} + \frac{2(3-s)}{[s+d(u_s)][3+d(u_s)]}. \end{aligned}$$

If $s = 4$, $r \leq 3$ and $d(u_4) \leq 5$, then $H(T) - H(T') \leq \frac{1}{6} - \frac{1}{7} - \frac{1}{36} < 0$. Let

$$f(r, s) := \frac{s-3}{6} + \frac{2(s-1)(3-s)}{(s+r)(3+r)}.$$

Taking partial derivatives, we have

$$\begin{aligned} \frac{\partial f(r,s)}{\partial s} &= \frac{1}{6} - \frac{2}{r+3} + \frac{2(r+1)}{(s+r)^2}, \\ \frac{\partial^2 f(r,s)}{\partial s^2} &= -\frac{4(r+1)}{(s+r)^3} < 0. \end{aligned}$$

Thus $\frac{\partial f(r,s)}{\partial s}$ is monotonously decreasing in s. Since $\left.\frac{\partial f(3,s)}{\partial s}\right|_{s=5} < 0$ and $\left.\frac{\partial f(4,s)}{\partial s}\right|_{s=8} < 0$, the following statements hold.

- If $s \geq 5$ and $d(u_{s-1}) \leq 3$, then $H(T) - H(T') < f(3,s) \leq f(3,5) = 0$.
- If $s \geq 8$ and $d(u_{s-1}) \leq 4$, then $H(T) - H(T') < f(4,s) \leq f(4,8) = 0$.

In either case, we have $H(T) < H(T')$. $\square$

Lemma 2.4 *Let $T \in \mathcal{T}_{n,k}$ with $E_2(T) \neq \emptyset$ and a vertex $u \in V(T)$ be adjacnet to a leaf $v \in V(T)$ with $d(u) \geq 3$. If $T' \in \mathcal{T}_{n,k}$ is obtained from T by contracting an edge in $E_2(T)$ and adding an edge to the leaf v, then $H(T') > H(T)$.*

Proof. Let $r := d(u) \geq 3$. It is easy to see that

$$H(T) - H(T') = \frac{1}{2} + \frac{2}{r+1} - \frac{2}{3} - \frac{2}{r+2} = \frac{2}{(r+1)(r+2)} - \frac{1}{6} \leq \frac{1}{10} - \frac{1}{6} < 0.$$

Therefore, $H(T') > H(T)$. $\square$

Now we are ready to prove Theorem 2.2.

Proof of Theorem 2.2. It is easy to see that if $T \in \mathcal{T}^*_{n,k}$, then $H(T) = \frac{n}{2} - \frac{k}{10}$. Thus it suffices to show that if $T \in \mathcal{T}_{n,k}$ with $n \geq 3k-2$ and $k \geq 3$ such that $H(T)$ is as large as possible, then $T \in \mathcal{T}^*_{n,k}$.

Let $T \in \mathcal{T}_{n,k}$ be such a tree that maximizes $H(T)$. By the proof of Lemma 2.2, we can assume, without loss of generality, that all vertices of T with degree 2 are on pendent paths, thus $E_2(T) \subset E(\mathcal{P}(T))$. Let $\Delta(T)$ denote the maximum degree of T. Note that $\Delta(T) \geq 3$ since $k \geq 3$. We first show that $\Delta(T) = 3$. Assume to the contrary that $\Delta(T) \geq 4$. By Lemma 2.1, we have

$$|E_2(T)| \geq n_4(T) + 2n_5(T) + \cdots + (\Delta - 3)n_\Delta(T) \geq \Delta - 3 \geq 1.$$

Let $u_0 \in V(T)$ with $d(u_0) = \Delta \geq 4$ and let

$$\mathcal{Q} := \{P \mid P = u_0 u_1 \cdots u_t \text{ with } d(u_t) \geq 4\}.$$

Choose P in $\mathcal{Q}$ such that the length of P is as large as possible. By Lemma 2.3 (1) and (2), we have that $t \geq 1$. Let $N'(u_{t-1}) := N(u_{t-1}) \setminus \{u_{t-2}\}$ if $t \geq 2$, otherwise $N'(u_{t-1}) := N(u_{t-1})$. Then $u_t \in N'(u_{t-1})$.

Claim. For each $v \in N'(u_{t-1})$, we have $d(v) \leq 4$ and $|\{w \mid w \in N'(u_{t-1}) \text{ and } d(w) = 4\}| \geq 1$.

Let $v \in N'(u_{t-1})$ and write $N(v) = \{v_1, v_2, ..., v_s\}$ with $d(v_1) \leq d(v_2) \leq \cdots \leq d(v_s)$. By the choice of P, we have $d(v_{s-1}) \leq 3$ and $v_s = u_{t-1}$. By lemma 2.3 (2), we have $d(v) \leq 4$. Since $d(u_t) \geq 4$ and $u_t \in N'(u_{t-1})$, we have $d(u_t) = 4$, which completes the proof of the claim.

By the claim and Lemma 2.3 (1) and (3), we have $6 \leq d(u_{t-1}) \leq 7$. Let $r := d(u_{t-1})$ and $N(u_{t-1}) = \{w_1, w_2, ..., w_r\}$. Let T^* be obtained by contracting one edge in $E_2(T)$ and $T' := T^*_{u_{t-1}\to(3,r-3)}$. Then $T' \in \mathcal{T}_{n,k}$, and

$$\begin{aligned}
H(T) - H(T') &= \frac{1}{2} - \frac{2}{r+2} + \sum_{i=1}^{3}\left(\frac{2}{r+d(w_i)} - \frac{2}{4+d(w_i)}\right) \\
&+ \sum_{j=4}^{r}\left(\frac{2}{r+d(w_j)} - \frac{2}{r-2+d(w_j)}\right) \\
&= \frac{1}{2} - \frac{2}{r+2} + \sum_{i=1}^{3}\frac{2(4-r)}{[r+d(w_i)][4+d(w_i)]} \\
&- \sum_{j=4}^{r}\frac{4}{[r+d(w_j)][r-2+d(w_j)]} \\
&< \frac{1}{2} - \frac{2}{r+2} + \frac{3(4-r)}{4(r+4)} - \frac{4(r-4)}{(r+4)(r+2)} \leq 0
\end{aligned}$$

for $r = 6, 7$, which contradicts the maximality of $H(T)$. Thus we have $\Delta(T) = 3$.

Let $n_i := n_i(T)$ for $i = 1, 2, 3$. By the Handshake Theorem, we have $n_1 + 2n_2 + 3n_3 = 2(n-1) = 2(n_1 + n_2 + n_3 - 1)$. Since $n_1 = k$ and $n \geq 3k-2$, we have $n_3 = k-2$ and $n_2 \geq k$. By Lemma 2.4, all pendent paths of T are of length at least 2 and hence $T \in \mathcal{T}^*_{n,k}$. $\square$

2.2 Proof of Theorem 1.1

Let a, b and n be three integers such that $a, b \geq 1$ and $n \geq a+b+2$. A *double comet* $DC(n, a, b)$ is a tree composed of a path of order $n-a-b$ with a leaves attached to one end of the path and b leaves attached to the other end of the path. Thus, $DC(n, a, b) \in \mathcal{T}_{n,a+b}$.

Lemma 2.5 [2, 18] *Let k and n be two integers with $3 \leq k \leq n-2$ and $T \in \mathcal{T}_{n,k}$. There exists a double comet $T' = DC(n, a, b)$ for some $a, b \geq 1$, $a + b = k$ such that*

$$\mu(T) \leq \mu(T') \leq \binom{n}{2}^{-1}\left[\frac{k^2(n-k)}{4} + \frac{3k^2}{4} + \frac{k(n-k)^2}{2} + \frac{k(n-k)}{2} + \frac{(n-k)^3}{6}\right].$$

Proof of Theorem 1.1. The inequality holds trivially for $n \leq 6$, thus we assume that $n \geq 7$ and $k \geq 2$. If $k = 2$, then T is a path and $\mu(T) = \frac{n+1}{3} \leq \frac{4}{3} + \frac{n-3}{2} = H(T)$. If

$k = n-1$, then T is a star and $\mu(T) = 2-2/n = H(T)$. Therefore, we can further assume that $3 \le k \le n-2$ and thus Theorem 2.1 is applicable.

By Theorem 2.1 and Lemma 2.5, it suffices to show that

$$k^2(n-k)+3k^2+2k(n-k)^2+2k(n-k)+2(n-k)^3/3 < 4\binom{n}{2}\left(\frac{n-k}{2}+\frac{5}{3}+\frac{2}{k+2}-\frac{4}{k+1}\right)$$

for $3 \le k \le n-2$ and $n \ge 7$. In order to prove this inequality, we put $l := n-k \ge 2$ and view the difference as a function of k and l as follows,

$$\begin{aligned} f(k,l) &:= 4\binom{k+l}{2}\left(\frac{l}{2}+\frac{5}{3}+\frac{2}{k+2}-\frac{4}{k+1}\right)-(k^2l+3k^2+2kl^2+2kl+2l^3/3) \\ &= 4(k^2+l^2+2kl-k-l)\left(\frac{5}{6}+\frac{1}{k+2}-\frac{2}{k+1}\right)+l^3/3-3kl-l^2-3k^2. \end{aligned}$$

Let

$$g(k) := \frac{1}{k+2}-\frac{2}{k+1}.$$

Then

$$\frac{\mathrm{d}g}{\mathrm{d}k} = \frac{2}{(k+1)^2}-\frac{1}{(k+2)^2} > 0 \text{ for } k \ge 0,$$

which implies that $g(k) \ge g(3) = -3/10$ for $k \ge 3$. Taking partial derivative of f, we get

$$\frac{\partial f(k,l)}{\partial l} = l^2+\left(\frac{14}{3}+\frac{8}{k+2}-\frac{16}{k+1}\right)l+4\left(\frac{5}{6}+\frac{1}{k+2}-\frac{2}{k+1}\right)(2k-1)-3k.$$

For fixed $k \ge 3$, the graph of $\frac{\partial f}{\partial l}$ is a parabolic curve in l, and it is symmetric to the line

$$l = -\frac{1}{2}\left(\frac{14}{3}+\frac{8}{k+2}-\frac{16}{k+1}\right) = -\frac{7}{3}-4g(k) \le -\frac{7}{3}-4g(3) = -\frac{17}{15}.$$

Thus $\frac{\partial f}{\partial l}$ is monotonously increasing in $l \ge 0$, and thus for $k \ge 3$,

$$\begin{aligned} \frac{\partial f(k,l)}{\partial l} &\ge \left.\frac{\partial f(k,l)}{\partial l}\right|_{l=0} = 4\left(\frac{5}{6}+\frac{1}{k+2}-\frac{2}{k+1}\right)(2k-1)-3k \\ &\ge 4\left(\frac{5}{6}-\frac{3}{10}\right)(2k-1)-3k = \frac{19k-32}{15} > 0. \end{aligned}$$

This implies that f is also monotonously increasing in $l > 0$. Since $f(3,3) = 10$, $f(4,3) = 84/5$ and $f(k,2) = (k^2-20)/3 \ge f(5,2) = 5/3$ for $k \ge 5$, we have $f(k,l) > 0$ for $3 \le k \le n-2$ and $n \ge 7$. This completes the proof. $\square$

3 Triangle-free graphs

The proof of Theorem 1.2 splits into the following two sections and is based on the following lemma due to Erdős et al. [9] and Dankelmann and Entringer [3] respectively.

Lemma 3.1 [3, 9] *Let G be a connected triangle-free graph of order n with minimum degree δ. Then $r(G) \le \frac{n-2}{\delta}+12$ and $\mu(G) \le \frac{2n}{3\delta}+\frac{25}{3}$.*

3.1 The Randić index

Lemma 3.2 [14] *For each connected triangle-free graph G of order n and minimum degree δ, we have $R(G) \geq \sqrt{\delta(n-\delta)}$ with equality if and only if G is isomorphic to the complete bipartite graph $K_{\delta,n-\delta}$.*

Proof of Theorem 1.2 (1) and (2). Note that $\delta \leq n/2$ since G is triangle-free. If $\delta \geq n^{1/3} + 25n^{-1/3}$ and n is large enough, then by Lemmas 3.1 and 3.2 we have

$$\begin{aligned} R(G) &\geq \sqrt{\delta(n-\delta)} \geq \sqrt{(n^{1/3}+25n^{-1/3})\,(n-n^{1/3}-25n^{-1/3})} \\ &= \sqrt{n^{4/3}+24n^{2/3}-50-625n^{-2/3}} \\ &\geq n^{3/2} - n^{-1/3} + 12 \geq r(G). \end{aligned}$$

If $\delta \geq (n/2)^{1/3}$ and n is large enough, then we also have

$$R(G) \geq \sqrt{\delta(n-\delta)} \geq \sqrt{(n/2)^{1/3}\,[n-(n/2)^{1/3}]} = 2^{-1/6}n^{2/3} + O(1) \geq \mu(G).$$

3.2 The harmonic index

In this section, we will complete the proof of Theorem 1.2. Zhong [24] found the minimum and maximum values of the harmonic index for simple connected graphs and trees, and characterized the corresponding extremal graphs.

Theorem 3.1 [24] *Let T be a tree of order $n > 2$, then*

$$2 - \frac{2}{n} \leq H(T) \leq \frac{n}{2} - \frac{1}{6},$$

where the first equality holds if and only if T is a star and the second equality holds if and only if T is a path.

Recently, Ilić [13] gave a simplified proof of Theorem 3.1 based on the following result for triangle-free graphs.

Theorem 3.2 [13] *Let G be a triangle-free graph of order n and size m, then $H(G) \geq 2m/n$ with equality if and only if G is a complete bipartite graph.*

Wu, Tang and Deng [20] also obtained a best possible lower bound for the harmonic index of triangle-free graphs with minimum degree two. For our purpose, we establish the following identity for the harmonic index and apply it to extend Lemma 3.2 and the result of Wu et al. [20] to the harmonic index of all triangle-free graphs with any given minimum degree.

Theorem 3.3 *Let $G = (V, E)$ be a connected graph of order n, then*

$$H(G) = \frac{n}{2} - \frac{1}{2} \sum_{uv \in E} \frac{[d(u) - d(v)]^2}{d(u)d(v)[d(u) + d(v)]}.$$

Proof. This follows readily from the observation:

$$\sum_{uv \in E} \left[\frac{1}{d(u)} + \frac{1}{d(v)} \right] = n.$$

□

The following lemma is an easy exercise of calculus and its proof is omitted.

Lemma 3.3 *Let $f(x, y) := \frac{1}{x} + \frac{1}{y} - \frac{2}{x+y}$, then $0 \leq f(x, y) \leq f(\delta, \Delta)$ for all $0 < \delta \leq x, y \leq \Delta$, where $f(x, y) = 0$ if and only if $x = y$, and $f(x, y) = f(\delta, \Delta)$ if and only if $(x, y) = (\delta, \Delta)$ or (Δ, δ).*

Since $f(x, y) = \frac{(x-y)^2}{xy(x+y)}$, Theorem 3.3 and Lemma 3.3 easily imply the following consequence.

Corollary 3.1 *Let G be a connected graph of order n and size m with maximum degree Δ and minimum degree δ, then*

$$\frac{n}{2} - \frac{m(\Delta - \delta)^2}{2\Delta\delta(\Delta + \delta)} \leq H(G) \leq \frac{n}{2},$$

where the first equality holds if and only if G is bi-regular and the second equality holds if and only if G is regular.

Theorem 3.3 and Corollary 3.1 produce a very short proof of Theorem 3.1 as follows.

Proof of Theorem 3.1. The lower bound of $H(T)$ follows readily from Corollary 3.1 and Lemma 3.3:

$$H(T) \geq \frac{n}{2} - \frac{(n-1)(\Delta - \delta)^2}{2\Delta\delta(\Delta + \delta)} = \frac{n}{2} - \frac{n-1}{2} f(\delta, \Delta) \geq \frac{n}{2} - \frac{n-1}{2} f(1, n-1) = 2 - \frac{2}{n}$$

with equality if and only if $d(v) = 1$ or $n - 1$ for all v of T, i.e., T is a star.

For the upper bound of $H(T)$, we view the value $f(d(u), d(v))$ as the *weight* of the edge uv in T, and call it a *symmetric edge* if $f(d(u), d(v)) = 0$, and *asymmetric* otherwise. Theorem 3.3 and Corollary 3.1 imply that a tree has maximum harmonic index if it simultaneously satisfies the following conditions:

- it has no asymmetric edges other than pendent edges,

- it has a minimum number of leaves (i.e. 2),
- the weights of these pendent edges are as small as possible, i.e. equal to $f(1,2)$.

It is easily checked that these three conditions are obeyed by and only by a path. $\square$

Theorem 3.4 *Let G be a connected triangle-free graph of order n with minimum degree δ, then $H(G) \geq 2\delta - 2\delta^2/n$ with equality if and only if G is isomorphic to the complete bipartite graph $K_{\delta,n-\delta}$.*

Proof. Let m and Δ denote the size and maximum degree of G respectively. If $m \geq \delta(n-\delta)$, then the result follows from Theorem 3.2. Hence we may assume that $m < \delta(n-\delta)$. Since G is triangle-free, adjacent vertices have disjoint neighborhoods, which implies that $\Delta \leq n - \delta$. Then Corollary 3.1 and Lemma 3.3 imply

$$H(G) \geq \frac{n}{2} - \frac{m(\Delta-\delta)^2}{2\Delta\delta(\Delta+\delta)} > \frac{n}{2} - \frac{\delta(n-\delta)}{2} f(\delta, n-\delta) = 2\delta - 2\delta^2/n.$$

This completes the proof. $\square$

Now we are ready to complete the proof of Theorem 1.2.

Proof of Theorem 1.2 (3) and (4). Recall that $\delta \leq n/2$ since G is triangle-free. If $\delta \geq \sqrt{n/2} + 7$ and n is large enough, then by Lemma 3.1 and Theorem 3.4 we have

$$H(G) \geq 2\delta - 2\delta^2/n \geq \sqrt{2n} + 14 - 2\left(\sqrt{n/2}+7\right)^2/n \geq \sqrt{2n} + 13 + o(1) \geq r(G).$$

If $\delta \geq \sqrt{n/3} + 5$ and n is large enough, then we also have

$$H(G) \geq 2\delta - 2\delta^2/n \geq 2\sqrt{n/3} + 10 - 2\left(\sqrt{n/3}+5\right)^2/n \geq 2\sqrt{n/3} + 28/3 + o(1) \geq \mu(G).$$

This completes the proof. $\square$

References

[1] G. Caporossi, P. Hansen, Variable neighborhood search for extremal graphs 1: The AutographiX system, *Discr. Math.* **212** (2000) 29–44.

[2] M. Cygan, M. Pilipczuk, R. Škrekovski, Relation between Randić index and average distance of trees, *MATCH Commun. Math. Comput. Chem.* **66** (2011) 605–612.

[3] P. Dankelmann, R. Entringer, Average distance, minimum degree, and spanning trees, *J. Graph Theory* **33** (2000) 1–13.

[4] T. Dehghan-Zadeh, A. R. Ashrafi, N. Habibi, Maximum and second maximum of Randić index in the class of tricyclic graphs, *MATCH Commun. Math. Comput. Chem.* **74** (2015) 137–144.

[5] C. Delorme, O. Favaron, D. Rautenbach, On the Randić index, *Discr. Math.* **257** (2002) 29–38.

[6] H. Deng, Z. Tang, J, Zhang, On a conjecture of Randić index and graph radius, arXiv:1210.2543 [math.CO] 9 Oct 2012.

[7] J. K. Doyle, J. E. Graver, Mean distance in a graph, *Discr. Math.* **17** (1977) 147–154.

[8] Z. Du, B. Zhou, On Randić indices of trees, unicyclic graphs, and bicyclic graphs, *Int. J. Quantum Chem.* **111** (2011) 2760–2770.

[9] P. Erdős, J. Pach, R. Pollack, Z. Tuza, Radius, diameter, and minimum degree, *J. Comb. Theory Ser. B* **47** (1989) 73–79.

[10] S. Fajtlowicz, On conjectures of Graffiti, *Discr. Math.* **72** (1988) 113–118.

[11] S. Fajtlowicz, On conjectures of Graffiti-II, *Congr. Numer.* **60** (1987) 187–197.

[12] I. Gutman, L. Zhong, K. Xu, Relating the ABC and harmonic indices, *J. Serb. Chem. Soc.* **79** (2014) 557–563.

[13] A. Ilić, Note on the harmonic index of a graph, arXiv:1204.3313, 2012.

[14] X. Li, J. Liu, Complete solution to a conjecture on the Randić index of triangle-free graphs, *Discr. Math.* **309** (2009) 6322–6324.

[15] X. Li, Y. Shi, Randić index, diameter and average distance, *MATCH Commun. Math. Comput. Chem.* **64** (2010) 425–431.

[16] B. Liu, I. Gutman, On a conjecture in Randić indices, *MATCH Commun. Math. Comput. Chem.* **62** (2009) 143–154.

[17] M. Randić, On characterization of molecular branching, *J. Am. Chem. Soc.* **97** (1975) 6609–6615.

[18] R. Shi, The average distance of trees, *Systems Sci. Math. Sci.* **6** (1993) 18–24.

[19] H. Wiener, Correlation of heats of isomerization and differences in heats of vaporization of isomers among the paraffin hydrocarbons, *J. Am. Chem. Soc.* **69** (1947) 2636–2638.

[20] R. Wu, Z. Tang, H. Deng, A lower bound for the harmonic index of a graph with minimum degree at least two, *Filomat* **27** (2013) 51–55.

[21] Z. You, B. Liu, On a conjecture between Randić index and average distance of unicyclic graphs, *Filomat* **28** (2014) 767–773.

[22] Z. You, B. Liu, On a conjecture of the Randić index, *Discr. Appl. Math.* **157** (2009) 1766–1772.

[23] L. Zhang, M. Lu, F. Tian, Maximum Randić index on trees with k-pendent vertices, *J. Math. Chem.* **41** (2007) 161–171.

[24] L. Zhong, The harmonic index for graphs, *Appl. Math. Lett.* **25** (2012) 561–566.

[25] L. Zhong, K. Xu, Inequalities between vertex-degree-based topological indices, *MATCH Commun. Math. Comput. Chem.* **71** (2014) 627–642.