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On the Sum of a Topological Index and Its Reciprocal Index for Unicyclic Graphs

Abeer M. Albalahi[a], **Zhibin Du**[b], **Akbar Ali**[a,*], **Muhammad Javaid**[c], **Amjad E. Hamza**[a]

[a] *Department of Mathematics, College of Science, University of Ha'il, Ha'il, Saudi Arabia*

[b] *School of Artificial Intelligence, South China Normal University, Foshan, Guangdong, China*

[c] *Department of Mathematics, School of Science, University of Management and Technology, Lahore, Pakistan*

a.albalahi@uoh.edu.sa, zhibindu@126.com, akbarali.maths@gmail.com, javaidmath@gmail.com, boaljod2@hotmail.com

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Abstract

This paper gives the optimal values of the sum of a topological index and its reciprocal version of fixed-order unicyclic graphs for the cases of the first Zagreb index, second Zagreb index, forgotten topological index, and Sombor index. For each of the aforementioned four topological indices, the cycle graph uniquely attains the minimum value of the mentioned sum and the graph formed by inserting one edge in the star graph uniquely attains the maximum value of this sum in the considered class of graphs. These findings extend the results of the recent paper [W. Gao, MATCH Commun. Math. Comput. Chem. 93 (2025) 535–547] from trees to unicyclic graphs. The results about the minimum values remain valid for fixed-order molecular unicyclic graphs.

*Corresponding author.

1 Introduction

Topological indices play a particular role in predicting physicochemical properties of molecules based solely on their structural features [7, 18]. According to [8], "Topological indices are mathematical entities encoding the structure of molecules which are depicted as graphs. In these graphs, the vertices correspond to the atoms and the edges represent the bonds between these atoms". More precisely, real-valued graph invariants are commonly referred to as topological indices in chemical graph theory [20, 21], where a graph invariant is a property of graphs that remains the same under graph isomorphisms [12]. The graph-theoretical terms (chemical-graph-theoretical terms, respectively) used here but not defined in this paper can be found in the books [4, 6] ([20, 21], respectively).

We consider the following topological indices of a graph G:

$$TI(G) = \sum_{uv\in E(G)} \Phi(u,v) \quad \text{and} \quad RTI(G) = \sum_{uv\in E(G)} \frac{1}{\Phi(u,v)},$$

where Φ is a positive-valued function defined on the Cartesian square of the vertex set $V(G)$ of G. Following [14], we call the index $RTI(G)$ as the reciprocal version of $TI(G)$ and vice versa. Let $d_G(w)$ denote the degree of a vertex $w \in V(G)$. If we take $\Phi(u,v) = d_G(u) + d_G(v)$, or $\Phi(u,v) = d_G(u)d_G(v)$, or $\Phi(u,v) = (d_G(u))^2 + (d_G(v))^2$ or $\Phi(u,v) = \sqrt{(d_G(u))^2 + (d_G(v))^2}$ in the above definitions of $TI(G)$ and $RTI(G)$, we obtain $(TI, RTI) = (\mathcal{Z}_1, \mathcal{RZ}_1)$, or $(TI, RTI) = (\mathcal{Z}_2, {}^m\mathcal{Z}_2)$, or $(TI, RTI) = (\mathcal{F}, \mathcal{RF})$, or $(TI, RTI) = (\mathcal{SO}, {}^m\mathcal{SO})$, respectively; where $\mathcal{Z}_1$ is the first Zagreb index [5, 16], $2\mathcal{RZ}_1$ is the harmonic index [3, 9], $\mathcal{Z}_2$ is the second Zagreb index [5, 15], ${}^m\mathcal{Z}_2$ is the modified second Zagreb index [19], $\mathcal{F}$ is the forgotten (topological) index [10], $\mathcal{RF}$ is the reciprocal forgotten (topological) index, $\mathcal{SO}$ is the Sombor index [13], and ${}^m\mathcal{SO}$ is the modified Sombor index [17].

Recently, Gao [11] characterized the graphs attaining the minimum and maximum values of the following topological indices from the class of all fixed-order trees: $\mathcal{Z}_1 + \mathcal{RZ}_1$, $\mathcal{Z}_2 + {}^m\mathcal{Z}_2$, $\mathcal{F} + \mathcal{RF}$. The primary goal of the present study is to extend the results of Gao [11] to unicyclic graphs not only for the aforementioned three sums but also for the sum $\mathcal{SO}+{}^{m}\mathcal{SO}$, where a unicyclic graph is a connected graph of the same order and size. The obtained results concerning minimum values are valid also for molecular graphs, which are the graphs of maximum degree at most 4.

2 Preliminary lemmas

In this section, we provide several preliminary results, which are used in the subsequent section. By an n-order graph, we mean a graph of order n.

Lemma 1. [2] *Let G be an n-order connected graph of size $m \geq 2$. Let $\hbar$ be a function defined on the Cartesian square of the set of real numbers greater than or equal to 1 such that $\hbar(x_1, x_2) = \hbar(x_2, x_1) \geq 0$ for all x_1 and x_2 belonging to the domain of $\hbar$ and $\hbar(x_1, x_2) > 0$ for $x_1 \neq x_2$. Define the function Φ on the Cartesian square of the set of positive integers as*

$$\Phi(r_1, r_2) := \hbar(r_1, r_2) + \frac{2\hbar(1,2)(r_1 r_2 - r_1 - r_2)}{r_1 r_2} + \frac{\hbar(2,2)(2r_1 + 2r_2 - 3r_1 r_2)}{r_1 r_2},$$

such that $n-1 \geq r_2 \geq r_1 \geq 1$ and $(r_1, r_2) \notin \{(1,2),(2,2)\}$. If $\Phi(r_1, r_2) > 0$ then

$$\sum_{uv \in E(G)} \hbar(d_G(u), d_G(v)) \geq 2[\hbar(1,2) - \hbar(2,2)]n + [3\hbar(2,2) - 2\hbar(1,2)]m,$$

with equality if and only if G is either path graph P_n or cycle graph C_n.

By a k-cyclic n-order graph, we mean a connected n-order graph of size $n + k - 1$. Particularly, for $k = 0$ and $k = 1$, such graphs are called n-order trees and n-order unicyclic graphs, respectively.

Lemma 2. [1] *Let $\hbar$ be a strictly increasing function defined on the Cartesian square of the set of real numbers greater than or equal to 1 such that $\hbar(x_1, x_2) = \hbar(x_2, x_1) \geq 0$ for all x_1 and x_2 belonging to the domain of $\hbar$, and the following inequalities hold for $2 \leq x_4 + 1 \leq x_3 \leq x_1$ and $1 \leq x_2 \leq x_1$:*

$$\hbar(x_1 + x_4, x_2) - \hbar(x_1, x_2) + \hbar(x_3 - x_4, x_2) - \hbar(x_3, x_2) \geq 0,$$

$$\hbar(x_1 + x_4, x_3 - x_4) - \hbar(x_1, x_3) \geq 0.$$

If G is a graph having the maximum value of $\sum_{uv\in E(G)} \hbar(d_G(u), d_G(v))$ among all n-order k-cyclic graphs, then the maximum degree of G is $n-1$.

Lemma 3. *The function f defined as*

$$f(x_1, x_2) = \sqrt{x_1^2 + x_2^2} + \frac{1}{\sqrt{x_1^2 + x_2^2}}, \quad \text{with } x_1 \geq 1 \text{ and } x_2 \geq 1,$$

is strictly increasing (in both variables).

Proof. For $i = 1, 2$, we have $\frac{\partial f}{\partial x_i}(x_1, x_2) = \frac{x_i(x_1^2+x_2^2-1)}{(x_1^2+x_2^2)^{3/2}}$. ■

Lemma 4. *For the function f defined in Lemma 3, the inequality*

$$f(x_1 + t, c - t) - f(x_1, c) > 0$$

holds for $2 \leq t + 1 \leq c \leq x_1$.

Proof. Take $g(x_1, c, t) = f(x_1 + t, c - t) - f(x_1, c)$. Since

$$\frac{\partial g}{\partial t}(x_1, c, t) = \frac{(x_1 + 2t - c)\left((x_1 + t)^2 + (c - t)^2 - 1\right)}{\left((x_1 + t)^2 + (c - t)^2\right)^{3/2}} > 0,$$

we have $g(x_1, c, t) \geq f(x_1+1, c-1) - f(x_1, c) > 0$ for $2 \leq t+1 \leq c \leq x_1$. ■

Lemma 5. *For the function f defined in Lemma 3, the inequality*

$$f(x_1 + x_4, x_2) - f(x_1, x_2) + f(x_3 - x_4, x_2) - f(x_3, x_2) > 0$$

holds for $2 \leq x_4 + 1 \leq x_3 \leq x_1$ and $1 \leq x_2 \leq x_1$.

Proof. We take

$$\Phi(x_1, x_2, x_3, x_4) = f(x_1 + x_4, x_2) - f(x_1, x_2) + f(x_3 - x_4, x_2) - f(x_3, x_2).$$

Since the function h defined as

$$h(y_1, y_2) = -\frac{y_2(y_1^2 + y_2^2 - 1)}{(y_1^2 + y_2^2)^{3/2}} \quad \text{with } y_1 \geq 1 \text{ and } y_2 \geq 1,$$

is strictly decreasing in y_2, we have

$$\frac{\partial \Phi}{\partial x_3}(x_1, x_2, x_3, x_4) = h(x_2, x_3) - h(x_2, x_3 - x_4) < 0$$

and

$$\frac{\partial \Phi}{\partial x_4}(x_1, x_2, x_3, x_4) = h(x_2, x_3 - x_4) - h(x_2, x_1 + x_4) > 0.$$

Hence, $\Phi(x_1, x_2, x_3, x_4) \geq \Phi(x_1, x_2, x_1, 1) > 0$. ■

Lemma 6. *The function ψ defined as*

$$\psi(x_1, x_2) = j(x_1, x_2) + \frac{1}{j(x_1, x_2)},$$

with $x_1 \geq 1$ and $x_2 \geq 1$, is strictly increasing (in both variables), where $j(x_1, x_2) \in \left\{x_1 + x_2, x_1^2 + x_2^2\right\}$. Also, the inequality

$$\psi(x_1 + x_4, x_2) - \psi(x_1, x_2) + \psi(x_3 - x_4, x_2) - \psi(x_3, x_2) > 0 \qquad (1)$$

holds for $2 \leq x_4 + 1 \leq x_3 \leq x_1$ and $1 \leq x_2 \leq x_1$.

Proof. We only prove (1). If $j(x_1, x_2) = x_1 + x_2$, then

$$\begin{aligned}&\psi(x_1 + x_4, x_2) - \psi(x_1, x_2) + \psi(x_3 - x_4, x_2) - \psi(x_3, x_2)\\ &= \frac{x_4^2 x_1 + 2x_2 x_4^2 + x_3 x_4^2 + x_4(x_1^2 - x_3^2) + 2x_2 x_4(x_1 - x_3)}{(x_1 + x_2)(x_2 + x_3)(x_2 + x_3 - x_4)(x_1 + x_2 + x_4)} > 0.\end{aligned}$$

In what follows, we assume that $j(x_1, x_2) = x_1^2 + x_2^2$ and we take

$$\psi_F(x_1, x_2, x_3, x_4) = \psi(x_1 + x_4, x_2) - \psi(x_1, x_2) + \psi(x_3 - x_4, x_2) - \psi(x_3, x_2).$$

Then, $\frac{\partial \psi_F}{\partial x_3}(x_1, x_2, x_3, x_4)$ is equal to

$$2\left(\frac{x_3}{(x_2^2 + x_3^2)^2} - \frac{x_3}{(x_2^2 + (x_3 - x_4)^2)^2} - x_4 + \frac{x_4}{(x_2^2 + (x_3 - x_4)^2)^2}\right),$$

which is negative under the given constraints. Hence,

$$\psi_F(x_1, x_2, x_3, x_4) \geq \psi_F(x_1, x_2, x_1, x_4).$$

Now,

$$\frac{\partial \psi_F}{\partial x_4}(x_1, x_2, x_1, x_4) = 4x_4 + \frac{2\,(x_1 - x_4)}{(x_2^2 + (x_1 - x_4)\,^2)\,^2} - \frac{2\,(x_1 + x_4)}{(x_2^2 + (x_1 + x_4)\,^2)\,^2},$$

which is positive because of the given conditions. Hence,

$$\begin{aligned}\psi_F(x_1, x_2, x_3, x_4) &\geq \psi_F(x_1, x_2, x_1, x_4) \geq \psi_F(x_1, x_2, x_1, 1)\\ &= \frac{2\left(x_1^6 + 3x_2^4x_1^2 + 4x_1^2 + x_2^6 + 2x_2^4 + x_1^4(3x_2^2 - 2) - 1\right)}{(x_1^2 + x_2^2)\,(x_1^2 - 2x_1 + x_2^2 + 1)\,(x_1^2 + 2x_1 + x_2^2 + 1)} > 0,\end{aligned}$$

as $x_1 \geq 2$ and $x_2 \geq 1$. ■

Lemma 7. *For the function ψ defined in Lemma 6, the inequality*

$$\psi(x_1 + t, c - t) - \psi(x_1, c) \geq 0$$

holds for $2 \leq t + 1 \leq c \leq x_1$.

Proof. If $j(x_1, x_2) = x_1 + x_2$, then $\psi(x_1 + t, c - t) - \psi(x_1, c) = 0$. Next, assume that $j(x_1, x_2) = x_1^2 + x_2^2$. Then, $\psi(x_1 + t, c - t) - \psi(x_1, c)$ equals

$$\frac{2c^2t(x_1 - c) + 2c^2t^2 + 2t^2x_1^2 + 2tx_1^2(x_1 - c) - 1}{c^2 + x_1^2} + \frac{1}{(c - t)^2 + (x_1 + t)^2},$$

which is positive for $2 \leq t + 1 \leq c \leq x_1$. ■

3 Results

For a vertex x of a graph G, let $N_G(x)$ be the set of neighbors of x in G.

First, we study the sum $\mathcal{Z}_2 + {}^m\mathcal{Z}_2$ of the second Zagreb index and its modified version. For finding the maximum value of this sum over the class of fixed-order unicyclic graphs, we need the following two lemmas:

Lemma 8. *Let G be an n-order unicyclic graph of maximum degree at most $n-2$. Let $x, y, y_1 \in V(G)$ provided that $xy, yy_1 \in E(G)$, $xy_1 \notin E(G)$, x has the maximum degree in G, and $|N_G(x) \cap N_G(y)| = 1$. Also, let $N_G(y) \backslash N_G(x) := \{x, y_1, \ldots, y_r\}$ with $r \geq 1$. If G' is a new graph such that*

$V(G') := V(G)$ and $E(G') := (E(G) \setminus \{yy_i : 1 \leq i \leq r\}) \cup \{xy_i : 1 \leq i \leq r\}$ (see Figure 1), then $\mathcal{Z}_2(G) + {}^m\mathcal{Z}_2(G) < \mathcal{Z}_2(G') + {}^m\mathcal{Z}_2(G')$.

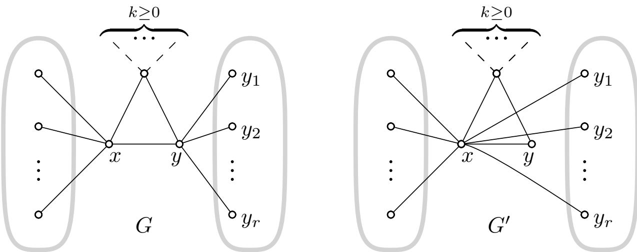

Figure 1. The unicyclic graphs G and G' used in Lemma 8.

Proof. For any $s \in V(G) = V(G')$, we assume that $d_s = d_G(s)$. We define $\Theta := \mathcal{Z}_2(G) + {}^m\mathcal{Z}_2(G) - \mathcal{Z}_2(G') - {}^m\mathcal{Z}_2(G')$. We note here that $d_y = r + 2$. If $N_G(x) \cap N_G(y)| = \{w\}$, then we have

$$\begin{aligned}\Theta = &\sum_{u \in N_G(x) \setminus \{w,y\}} \left(\frac{(d_x d_u)^2 + 1}{d_x d_u} - \frac{(d_x + r)^2 d_u^2 + 1}{(d_x + r) d_u} \right) \\ &+ \sum_{i=1}^{r} \left(\frac{(r+2)^2 d_{y_i}^2 + 1}{(r+2) d_{y_i}} - \frac{(d_x + r)^2 d_{y_i}^2 + 1}{(d_x + r) d_{y_i}} \right) \\ &+ \frac{(d_x(r+2))^2 + 1}{d_x(r+2)} - \frac{4(d_x + r)^2 + 1}{2(d_x + r)} \\ &- \frac{r(d_x - 2)(d_x + r + 2)}{2 d_x d_w (r+2)(d_x + r)}. \end{aligned} \tag{2}$$

Since the functions ϕ and ψ defined as

$$\phi(t_1, t_2, t_3) = \frac{(t_1 t_2)^2 + 1}{t_1 t_2} - \frac{(t_1 + t_3)^2 t_2^2 + 1}{(t_1 + t_3) t_2},$$

$$\psi(t_1, t_2, t_3) = \frac{((t_3 + 2) t_2)^2 + 1}{(t_3 + 2) t_2} - \frac{(t_1 + t_3)^2 t_2^2 + 1}{(t_1 + t_3) t_2},$$

with $t_1 \geq t_i \geq 1$, $i = 2, 3$, and $t_1 \geq 3$, are strictly decreasing in t_2, Equation

(2) yields

$$\begin{aligned}\Theta \le (d_x-2)\left(\frac{d_x^2+1}{d_x}-\frac{(d_x+r)^2+1}{(d_x+r)}\right)\\ +r\left(\frac{(r+2)^2+1}{r+2}-\frac{(d_x+r)^2+1}{(d_x+r)}\right)\\ +\frac{(d_x(r+2))^2+1}{d_x(r+2)}-\frac{4(d_x+r)^2+1}{2(d_x+r)}\\ -\frac{r(d_x-2)(d_x+r+2)}{2d_xd_w(r+2)(d_x+r)}\\ =-\frac{\Psi(d_x,d_w,r)}{2(r+2)(d_x+r)d_xd_w},\end{aligned} \tag{3}$$

where $\Psi(d_x,d_w,r)$ is equal to

$$r(d_x-2)\Big(2(r^2+2r-1)d_wd_x+d_w\big((2r+4)d_x^2-(2r+3)\big)+d_x+r+2\Big),$$

which is positive because $d_x \ge 3$, $d_w \ge 2$, and $r \ge 1$. Therefore, the right-hand side of (3) is negative and hence $\Theta < 0$, as desired. ■

Lemma 9. *Let G be an n-order unicyclic graph of maximum degree at most $n-2$. Let $x, y, y_1 \in V(G)$ such that $xy, yy_1 \in E(G)$, $xy_1 \notin E(G)$, x has the maximum degree in G and $|N_G(x) \cap N_G(y)| = 0$. Moreover, let $N_G(y) := \{x, y_1, y_2, \dots, y_r\}$ with $r \ge 1$. If G' is a new graph such that $V(G') := V(G)$ and $E(G') := (E(G)\backslash\{yy_i : 1 \le i \le r\}) \cup \{xy_i : 1 \le i \le r\}$, then $\mathcal{Z}_2(G) + {}^m\mathcal{Z}_2(G) < \mathcal{Z}_2(G') + {}^m\mathcal{Z}_2(G')$.*

Proof. With the same notations as used in the proof of Lemma 8, we have

$$\begin{aligned}\Theta \le& (d_x-1)\left(\frac{d_x^2+1}{d_x}-\frac{(d_x+r)^2+1}{d_x+r}\right)\\ &+r\left(\frac{(r+1)^2+1}{r+1}-\frac{(d_x+r)^2+1}{d_x+r}\right)\\ &+\frac{(d_x(r+1))^2+1}{d_x(r+1)}-\frac{(d_x+r)^2+1}{d_x+r}\\ =&-\frac{r(d_x-1)(rd_x+d_x-1)}{(r+1)d_x}<0,\end{aligned} \tag{4}$$

because $r \geq 1$ and $d_x \geq 3$. Therefore, (4) yields $\Theta < 0$, as desired. ■

For $n \geq 3$, let S_n^+ denote the graph formed by adding an edge (between any two vertices of degree 1) in the n-order star graph S_n.

Theorem 1. *If G is an n-order unicyclic graph, then*

$$\mathcal{Z}_2(G) + {}^m\mathcal{Z}_2(G) \leq \frac{4n^3 - 4n^2 + 17n - 21}{4(n-1)},$$

with equality if and only if $G = S_n^+$.

Proof. Among all n-order unicyclic graphs, let G^* be a graph such that $\mathcal{Z}_2(G^*) + {}^m\mathcal{Z}_2(G^*)$ is maximum. Then

$$\mathcal{Z}_2(G) + {}^m\mathcal{Z}_2(G) \leq \mathcal{Z}_2(G^*) + {}^m\mathcal{Z}_2(G^*). \tag{5}$$

We claim that the maximum degree of G^* is $n-1$. Contrarily, suppose that the maximum degree of G^* is less than $n-1$. Let $x, y, y_1 \in V(G^*)$ such that $xy, yy_1 \in E(G^*)$, $xy_1 \notin E(G^*)$, x has the maximum degree in G^* and $|N_{G^*}(x) \cap N_{G^*}(y)| \leq 1$. Moreover, let $N_{G^*}(y) \backslash N_{G^*}(x) := \{x, y_1, y_2, \ldots, y_r\}$ with $r \geq 1$. If G' is a new graph such that $V(G') := V(G^*)$ and $E(G') := (E(G^*) \setminus \{yy_i : 1 \leq i \leq r\}) \cup \{xy_i : 1 \leq i \leq r\}$, then by Lemmas 8 and 9 we have $\mathcal{Z}_2(G^*) + {}^m\mathcal{Z}_2(G^*) < \mathcal{Z}_2(G') + {}^m\mathcal{Z}_2(G')$, a contradiction. Hence, the maximum degree of G^* is $n-1$ and so it is isomorphic to S_n^+. Thus,

$$\mathcal{Z}_2(G^*) + {}^m\mathcal{Z}_2(G^*) = \frac{4n^3 - 4n^2 + 17n - 21}{4(n-1)}. \tag{6}$$

Now, the desired inequality follows from (5) and (6). ■

Theorem 2. *Let G be an n-order connected graph of size $|E(G)| \geq 2$. Then*

$$\mathcal{Z}_2(G) + {}^m\mathcal{Z}_2(G) \geq \frac{31}{4}|E(G)| - \frac{7}{2}n,$$

with equality if and only if G is either the path P_n or the cycle graph C_n.

Proof. We take $\hbar(x_1, x_2) = x_1x_2 + \frac{1}{x_1x_2}$. Then, the function Φ defined in

Lemma 1 becomes

$$\Phi(r_1, r_2) = \frac{1}{r_1}\left(\frac{1}{r_2} + \frac{7}{2}\right) + r_1 r_2 + \frac{7}{2r_2} - \frac{31}{4}.$$

If $r_2 \geq r_1 > 2$, then we have

$$\Phi(r_1, r_2) \geq \Phi(r_1, r_1) = \frac{(r_1 - 2)(4r_1^3 + 8r_1^2 - 15r_1 - 2)}{4r_1^2} > 0.$$

If $r_1 \in \{1, 2\}$ and $r_2 \geq 3$, then

$$\Phi(r_1, r_2) \geq \Phi(r_1, 3) = \frac{36r_1^2 - 79r_1 + 46}{12r_1} > 0.$$

Hence, by Lemma 1, we have

$$\mathcal{Z}_2(G) + {}^{m}\mathcal{Z}_2(G) \geq \frac{31}{4}|E(G)| - \frac{7}{2}n,$$

with equality if and only if G is either the path graph P_n or the cycle graph C_n. ■

Remark. For $|E(G)| = n$ ($|E(G)| = n - 1$, respectively) Theorem 2 gives the best possible lower bound, in terms of only n, on $\mathcal{Z}_2 + {}^{m}\mathcal{Z}_2$ for n-order unicyclic graphs (n-order trees of size at least 2, respectively); remarks similar to this one, hold for (forthcoming) Theorems 3, 4, and 5.

Theorem 3. *Let G be an n-order connected graph of size $|E(G)| \geq 2$. Then*

$$\mathcal{SO}(G) + {}^{m}\mathcal{SO}(G) \geq \frac{3}{20}\left[(45\sqrt{2} - 16\sqrt{5})|E(G)| + (16\sqrt{5} - 30\sqrt{2})n\right],$$

with equality if and only if G is either the path P_n or the cycle graph C_n.

Proof. We take $\hbar(x_1, x_2) = \sqrt{x_1^2 + x_2^2} + \frac{1}{\sqrt{x_1^2 + x_2^2}}$. Then the function Φ

defined in Lemma 1 becomes

$$\Phi(r_1,r_2)=\frac{1}{20}\left(24\sqrt{5}\left(-\frac{2}{r_2}-\frac{2}{r_1}+2\right)+45\sqrt{2}\left(\frac{2}{r_2}+\frac{2}{r_1}-3\right)\right.$$
$$\left.+20\sqrt{r_1^2+r_2^2}+\frac{20}{\sqrt{r_1^2+r_2^2}}\right).$$

If $r_2 \geq r_1 > 2$, then we have

$$\Phi(r_1,r_2)\geq\Phi(r_1,r_1)=\frac{(r_1-2)\left(20\sqrt{2}r_1+48\sqrt{5}-95\sqrt{2}\right)}{20r_1}>0.$$

If $r_1 \in \{1,2\}$ and $r_2 \geq 3$, then $\Phi(r_1,r_2) \geq \Phi(r_1,3) > 0$. Hence, by Lemma 1, we have the required inequality. ■

Corollary 1. *If G is an n-order unicyclic graph, then*

$$\mathcal{SO}(G)+{}^{m}\mathcal{SO}(G)\geq\frac{9}{2\sqrt{2}}\,n,$$

with equality if and only if G is the cycle graph C_n.

Theorem 4. *Let G be an n-order connected graph of size $m \geq 2$. Then*

$$\mathcal{F}(G)+\mathcal{RF}(G)\geq\frac{13}{40}\Big(43m-18n\Big),$$

with equality if and only if G is either the path P_n or the cycle graph C_n.

Proof. We take $\hbar(x_1,x_2)=x_1^2+x_2^2+\frac{1}{x_1^2+x_2^2}$. Then the function Φ defined in Lemma 1 becomes

$$\Phi(r_1,r_2)=r_1^2+r_2^2+\frac{117}{20r_2}+\frac{1}{r_1^2+r_2^2}+\frac{117}{20r_1}-\frac{559}{40}.$$

If $r_2 \geq r_1 > 2$, then

$$\Phi(r_1,r_2)\geq\Phi(r_1,r_1)=\frac{(r_1-2)(80r_1^3+160r_1^2-239r_1-10)}{40r_1^2}>0.$$

If $r_1 \in \{1,2\}$ and $r_2 \geq 3$, then $\Phi(r_1,r_2) \geq \Phi(r_1,3) > 0$. Hence, by Lemma 1, we have the desired conclusion. ■

Corollary 2. *If G is an n-order unicyclic graph, then*

$$\mathcal{F}(G) + \mathcal{RF}(G) \geq \frac{65}{8}\,n,$$

with equality if and only if G is the cycle graph C_n.

Since the proof of the next result is similar to that of Theorem 4, we omit it.

Theorem 5. *Let G be an n-order connected graph of size $m \geq 2$. Then*

$$\mathcal{Z}_1(G) + \mathcal{RZ}_1(G) \geq \frac{1}{12}\Big(73m - 22n\Big),$$

with equality if and only if G is either the path P_n or the cycle graph C_n.

Corollary 3. *If G is an n-order unicyclic graph, then*

$$\mathcal{Z}_1(G) + \mathcal{RZ}_1(G) \geq \frac{17}{4}n,$$

with equality if and only if G is the cycle graph C_n.

Theorem 6. *If G is a graph having the maximum value of any of the following indices over the class of all n-order k-cyclic graphs, then the maximum degree of G is $n-1$: $\mathcal{SO} + {}^{m}\mathcal{SO}$, $\mathcal{Z}_1 + \mathcal{RZ}_1$, $\mathcal{F} + \mathcal{RF}$.*

Proof. The result follows from Lemmas 2, 3, 4, 5, 6, and 7. ■

The next result follows immediately from Theorem 6.

Corollary 4. *In the class of all n-order unicyclic graphs (n-order trees, respectively), the graph S_n^+ (S_n, respectively) uniquely attains the maximum value of any of the following indices: $\mathcal{SO} + {}^{m}\mathcal{SO}$, $\mathcal{Z}_1 + \mathcal{RZ}_1$, $\mathcal{F} + \mathcal{RF}$.*

We end this paper with the remark that Theorems 2, 3, 4, and 5 remain valid if we consider molecular graphs in these results.

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