# Graphs with maximal Hosoya index and minimal Merrifield-Simmons index

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**Abstract.** For a graph $G$, the Hosoya index and the Merrifield-Simmons index are defined as the total number of its matchings and the total number of its independent sets, respectively. In this paper, we characterize the structure of those graphs that minimize the Merrifield-Simmons index and those that maximize the Hosoya index in two classes of simple connected graphs with $n$ vertices: graphs with fixed matching number and graphs with fixed connectivity.

**Keywords**: matching number; vertex connectivity; Merrifield-Simmons index; Hosoya index

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## 1. Introduction

Throughout this paper, we consider finite, undirected simple graphs. For graph-theoretical terms that are not defined here, we refer to Bollobás's book [2].

Two vertices of $G$ are said to be independent if they are not adjacent in $G$. The *Merrifield-Simmons index* [13], denoted by $i(G)$, is defined to be the total number of independent sets of $G$, including the empty set.

Likewise, two edges of $G$ are said to be independent if they are not adjacent in $G$. A set of pairwise independent edges in $G$ is called a matching in $G$. The maximum cardinality of a matching in $G$ is called the *matching number* of $G$, denoted by $\beta(G)$. The *Hosoya index* [11], denoted by $z(G)$, is defined to be the total number of matchings, where the empty set of edges counts as a matching as well.

The Merrifield-Simmons index and the Hosoya index of a graph $G$ are two prominent examples of topological indices which are of interest in combinatorial chemistry. The Hosoya index was introduced by Hosoya [11] in 1971, and it turned out to be applicable to several questions of molecular chemistry. For example, the connections with physico-chemical properties such as boiling point, entropy or heat of vaporization are well studied. Similar connections are known for the Merrifield-Simmons index that was introduced in 1982 in a paper of Prodinger and Tichy [15], where it is called the Fibonacci number of a graph. For detailed information on the chemical applications, we refer to [10, 11] and the references therein.

In recent years, many researchers have investigated these graph invariants. An important direction in this area is to determine the graphs with maximal or minimal indices in a given class of graphs. It is easy to see that the complete graph has largest Hosoya index and smallest Merrifield-Simmons index among all graphs of given order $n$. Generally, it is clear that removing edges decreases the Hosoya index and increases the Merrifield-Simmons index (see the inequalities (2.1) and (2.2) later).

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Things become more interesting, but also more difficult if one imposes further restrictions. For instance, it is known that the path has maximal Hosoya index and the star has minimal Hosoya index [10] among trees of given order. Treelike graphs have also been investigated extensively: for example, Deng and Chen [7] determined a sharp lower bound for the Hosoya index of unicyclic graphs, and Ou [14] an upper bound. The Merrifield-Simmons index of unicyclic graphs was studied in [18]. Bicyclic graphs have been the object of study of a series of articles by Deng and coauthors [4–6, 8]. For further results and references, we refer the reader to the survey paper [17].

In [19], Yu and Tian characterized the graphs with minimum Hosoya index and maximum Merrifield-Simmons index, respectively, among connected graphs of given order and matching number. Here, we will study a closely related question: we determine the graphs with minimum Merrifield-Simmons index and maximum Hosoya index in the class of graphs with given order $n$ and matching number $\beta$. We remark that the analogous question for the independence number (given the order of a graph and the maximum size of an independent set, determine minimum and maximum of the Merrifield-Simmons index) was recently considered by Bruyère and Mélot [3].

Using similar methods, we also characterize the graphs with given order $n$ and connectivity $s$ (the minimum number of vertices that needs to be removed to make the graph disconnected) that maximize the Hosoya index and minimize the Merrifield-Simmons index.

## 2. Preliminaries

Let us first introduce some notation and terminology. $V = V(G)$ will always denote the vertex subset and $E = E(G)$ the edge subset of a graph $G$. For a subset $W$ of $V(G)$, we denote by $G-W$ the subgraph of $G$ obtained by deleting the vertices of $W$ and the edges incident with them. Similarly, for a subset $F$ of $E(G)$, we denote by $G-F$ the subgraph of $G$ obtained by deleting the edges of $F$. If $W = \{v\}$ and $F = \{xy\}$ consist of a single element, we use the abbreviations $G-v$ and $G-xy$ instead of $G-\{v\}$ and $G-\{xy\}$, respectively.

We denote by $K_n$ and $\overline{K}_n$ the complete graph and the empty graph (with no edges) on $n$ vertices, respectively. For two graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, the union $G_1 \cup G_2$ is defined to be $G_1 \cup G_2 = (V_1 \cup V_2, E_1 \cup E_2)$. We will write $kG$ for the union of $k$ copies of $G$. The join $G_1 \bigvee G_2$ of $G_1$ and $G_2$ is obtained from $G_1 \cup G_2$ by connecting each vertex of $G_1$ with each vertex of $G_2$ by an edge.

We will frequently make use of the following formulas that can be used to compute the Merrifield-Simmons index and the Hosoya index recursively. We write $N(v) = \{u|uv \in E(G)\}$ and $N[v] = N(v) \cup \{v\}$ for the open and closed neighborhood of a vertex $v$ in a graph $G$.

**Lemma 2.1** ( [10]). *Let $G$ be a graph.*

(i) *If $uv \in E(G)$, then $i(G) = i(G-uv) - i(G - \{N[u] \cup N[v]\})$;*
(ii) *If $v \in V(G)$, then $i(G) = i(G-v) + i(G - N[v])$;*
(iii) *If $G_1, G_2, \ldots, G_t$ are the connected components of $G$, then $i(G) = \prod_{j=1}^{t} i(G_j)$.*

**Lemma 2.2** ( [10]). *Let $G$ be a graph.*

(i) *If $uv \in E(G)$, then $z(G) = z(G-uv) + z(G - \{u, v\})$;*
(ii) *If $v \in V(G)$, then $z(G) = z(G-v) + \sum_{u \in N(v)} z(G - \{u, v\})$;*
(iii) *If $G_1, G_2, \ldots, G_t$ are the components of the graph $G$, then $z(G) = \prod_{j=1}^{t} z(G_j)$.*

We write $G + uv$ for the graph obtained from $G$ by adding the edge $uv$, provided that $uv \notin E(G)$. The two lemmas immediately yield the following inequalities:

$$i(G + uv) < i(G), \tag{2.1}$$

$$z(G + uv) > z(G). \tag{2.2}$$

The following lemma, known as the Tutte-Berge formula, is an important tool to characterize the matching number.

**Lemma 2.3** ( [1,12,16]). *Suppose $G$ is a graph on $n$ vertices with matching number $\beta$. Let $o(H)$ denote the number of odd components (i.e., components of odd cardinality) of a graph $H$. Then*

$$n - 2\beta = \max\{o(G - S) - |S| : S \subset V(G)\},$$

*and in particular this means that there exists a subset $S_0 \subset V(G)$ such that $n - 2\beta = o(G - S_0) - |S_0|$.*

The next lemma already provides us with important information on the structure of extremal graphs with given matching number.

**Lemma 2.4.** *Suppose that $G$ has minimum Merrifield-Simmons index or maximum Hosoya index among connected graphs of order $n$ and matching number $\beta$. If $\beta = \lfloor n/2 \rfloor$, then $G = K_n$; otherwise, there exist a nonnegative integer $s \le \beta$ and positive odd numbers $n_1, n_2, \ldots, n_q$ such that $G \cong K_s \bigvee (\bigcup_{j=1}^{q} K_{n_j})$ with $s = q + 2\beta - n$ and $\sum_{j=1}^{q} n_j = n - s$.*

*Proof.* Let $G$ be a connected graph of order $n$ with matching number $\beta$ that minimizes the Merrifield-Simmons index. Moreover, let $M$ be a maximum matching in $G$, so that $|M| = \beta$. By Lemma 2.3, there exists a subset $S_0 \subset V(G)$ of vertices in $G$ such that

$$n - 2\beta = \max\{o(G - S) - |S| : S \subset V(G)\} = o(G - S_0) - |S_0|.$$

Set $s = |S_0|$ and $q = o(G - S_0)$, and let $G_1, G_2, \ldots, G_q$ be the odd components of $G - S_0$ with $|V(G_j)| = n_j \ge 1$ for $j = 1, 2, \ldots, q$. Clearly, $n \ge s + q = n + 2s - 2\beta$. Thus $s \le \beta$.

**Case 1** If $s = 0$, then $G - S_0 = G$ and $n + s - 2\beta = n - 2\beta = q \le 1$ since $G$ is connected. If $q = 0$, then $n = 2\beta$; if $q = 1$, then $n = 2\beta + 1$, so $\beta = \lfloor n/2 \rfloor$ in either case. It is clear (by (2.1)) that $K_n$ maximizes the Hosoya index and minimizes the Merrifield-Simmons index among *all* graphs of order $n$, so we must have $G \cong K_n$ in this case.

**Case 2** If $s \ge 1$, then $q = n + s - 2\beta \ge 1$ since $n \ge 2\beta$. We claim that $G - S_0$ contains no even component. Otherwise, let $W$ be a even component of $G - S_0$. Then by adding an edge to $G$ between a vertex $w$ of $W$ and a vertex $v$ of an odd component of $G - S_0$, we obtain a graph $G'$ for which

$$n - 2\beta(G') \ge o(G' - S_0) - |S_0| = o(G - S_0) - |S_0| = n - 2\beta(G),$$

so that $\beta(G) \ge \beta(G')$. Moreover, $\beta(G) \le \beta(G')$ since $G$ is a proper subgraph of $G'$, which means that $\beta(G) = \beta(G')$. By (2.1), we have $i(G') < i(G)$, a contradiction.

Next we claim that each component $G_j$ is a complete graph. If not, we can add an edge to the component to obtain a graph $G'$ with $\beta(G') = \beta(G)$ and $i(G') < i(G)$ as before.

Similarly, we find that the subgraph induced by $S_0$ has to be complete, and every vertex of $G_j$ $(1 \le j \le q)$ is adjacent to every vertex in $S_0$. So finally, $G \cong K_s \bigvee (\bigcup_{j=1}^{q} K_{n_j})$, which is what we wanted to prove. The proof for the Hosoya index is analogous. □

## 3. Graphs with minimum Merrifield-Simmons index

In this section, we determine the maximum Merrifield-Simmons index of graphs with given order $n$ and either given matching number $\beta$ or given connectivity $s$. Lemma 2.4 already gives us some rough information on the shape of the extremal graphs, given the order and matching number. It remains to determine the values of $n_1, n_2, \ldots, n_q$. We first derive a formula for the Merrifield-Simmons index.

**Lemma 3.1.** *If $G = K_s \bigvee (\bigcup_{j=1}^{q} K_{n_j})$, then $i(G) = (n_1 + 1)(n_2 + 1) \cdots (n_q + 1) + s$.*

*Proof.* An independent set of $G$ either consists of one of the vertices of the $K_s$-part (which are adjacent to all other vertices), or they consist of a collection of independent sets in $K_{n_1}, K_{n_2}, \ldots, K_{n_q}$. Since a complete graph has only independent sets of cardinality 0 or 1, we have $i(K_n) = n + 1$ and thus

$$i(G) = s + \prod_{j=1}^{q} i(K_{n_j}) = s + (n_1 + 1)(n_2 + 1) \cdots (n_q + 1),$$

which proves the lemma. □

**Theorem 3.2.** *Let $G$ be a graph with $n$ vertices and matching number $\beta$.*

(i) *If $\beta = \lfloor \frac{n}{2} \rfloor$, then $i(G) \geq n + 1$ with equality if and only if $G \cong K_n$.*
(ii) *If $1 \leq \beta \leq \lfloor \frac{n}{2} \rfloor - 1$, then $i(G) \geq \beta \cdot 2^{n+1-2\beta} + 1$, with equality if and only if $G \cong K_1 \bigvee ((n - 2\beta)K_1 \cup K_{2\beta-1})$.*

*Proof.* (i) As it was mentioned in the proof of Lemma 2.4, it is clear that $i(G) \geq i(K_n) = n + 1$ for any graph of order $n$ (in view of (2.1)), with equality only if $G \cong K_n$. This settles the case that $\beta = \lfloor \frac{n}{2} \rfloor$.

(ii) If $n \geq 2\beta + 2$, let $G^*$ be a graph with minimum Merrifield-Simmons index among graphs with $n$ vertices and matching number $\beta$. By Lemma 2.4, there exist positive odd numbers $n_1, n_2, \ldots, n_q$ and a positive integer $s \leq \beta$ such that $G^* = K_s \bigvee (\bigcup_{j=1}^{q} K_{n_j})$ with $s = q + 2\beta - n$ and $\sum_{j=1}^{q} n_j = n - s$. Since $n \geq 2\beta + 2$ we have $q = n - 2\beta + s \geq 2$.

Now we show that there is at most one number in the set $\{n_1, n_2, \ldots, n_q\}$ that is greater than 1. If not, assume without loss of generality that $n_2 \geq n_1 \geq 3$. Let $G' = K_s \bigvee (K_{n_1-2} \cup K_{n_2+2} \cup \cdots \cup K_{n_{q-1}} \cup K_{n_q})$. By Lemma 3.1, we have

$$\begin{aligned} i(G^*) - i(G') &= (n_3 + 1) \cdots (n_q + 1)[(n_1 + 1)(n_2 + 1) - (n_1 - 1)(n_2 + 3)] \\ &= (n_3 + 1) \cdots (n_q + 1)[2(n_2 - n_1) + 4] > 0, \end{aligned}$$

which contradicts the choice of $G^*$. Hence we have $G^* \cong K_s \bigvee ((q-1)K_1 \cup K_{n_q})$. Note that $n = s + n_q + q - 1$ and $q = n + s - 2\beta$, so $n_q = 2\beta - 2s + 1$. It follows that $G^* \cong K_s \bigvee ((n + s - 2\beta - 1)K_1 \cup K_{2\beta-2s+1})$.

By Lemma 3.1, we have

$$\begin{aligned} i(G^*) &= i\left(K_s \bigvee ((n + s - 2\beta - 1)K_1 \cup K_{2\beta-2s+1})\right) = (2\beta - 2s + 2)2^{n+s-2\beta-1} + s \\ &= (\beta - s + 1)2^{n+s-2\beta} + s. \end{aligned}$$

Let $f(s) = (\beta - s + 1)2^{n+s-2\beta} + s$. If $1 \leq s < \beta$, then

$$f(s + 1) - f(s) = (\beta - s - 1)2^{n+s-2\beta} + 1 > 0$$

and thus $f(s + 1) > f(s)$. Therefore, the minimum of $f(s)$ is obtained for $s = 1$. This means that the graph that minimizes the Merrifield-Simmons index is $G^* \cong K_1 \bigvee ((n - 2\beta)K_1 \cup K_{2\beta-1})$, and $i(G^*) = f(1) = \beta \cdot 2^{n+1-2\beta} + 1$. □

For graphs with given connectivity, the result and its proof are very similar.

**Theorem 3.3.** *Let $G$ be a graph of order $n$ with connectivity $s$. We have $i(G) \geq 2n - s$, with equality if and only if $G \cong (K_s \bigvee K_1 \cup K_{n-s-1})$.*

*Proof.* Let $G^*$ be a graph that minimizes the Merrifield-Simmons index among all graphs of order $n$ whose connectivity is $s$. Let $S$ be a set of cardinality $s$ such that $G^* - S$ is disconnected. In view of (2.1), the graph induced by $S$ has to be complete, the vertices in $S$ have to be connected to all vertices of $G^*$, and $G^* - S$ has to be the union of two complete graphs. Otherwise, it would be possible to add edges to $G^*$ without increasing the connectivity, thereby decreasing the Merrifield-Simmons index. Thus $G^* \cong K_s \bigvee (K_{n_1} \cup K_{n_2})$ for some positive integers $n_1, n_2$ with $n_1 + n_2 = n - s$. By Lemma 3.1, we have

$$i(G^*) = s + (n_1 + 1)(n_2 + 1) = s + (n_1 + 1)(n - s - n_1 + 1).$$

This is minimized for $n_1 = 1$ or $n_1 = n - s - 1$, so that $G^* \cong K_s \bigvee (K_1 \cup K_{n-s-1})$ and thus $i(G^*) = s + 2(n - s) = 2n - s$. □

## 4. Graphs with maximum Hosoya index

In this section, we focus on the Hosoya index, for which we obtain similar results as in the previous section. Once again, Lemma 2.4 provides information on the rough shape of the extremal graphs. The following lemma will help us to reduce the possibilities for the numbers $s$ and $n_1, n_2, \dots, n_q$.

**Lemma 4.1.** *Let $G$ be the graph $K_s \bigvee (\bigcup_{j=1}^{q} K_{n_j})$, where $n_1, n_2, \dots, n_q$ are all positive integers and $n_1 \le n_2 \le \dots \le n_q$. If there exists an index $i \in \{1, 2, \dots, q-1\}$ such that $n_i \ge 2$, let $G'$ be the graph $K_s \bigvee (K_{n_1} \cup \dots \cup K_{n_{i-1}} \cup K_{n_i - 1} \cup K_{n_{i+1}} \cup \dots \cup K_{n_q+1})$. The inequality $z(G) < z(G')$ holds.*

*Proof.* In the following, we use the abbreviation $H = K_{n_1} \cup \dots \cup K_{n_{i-1}} \cup K_{n_{i+1}} \cup \dots \cup K_{n_{q-1}}$. We prove the statement by induction on $n_i$. If $n_i = 2$, then by part (ii) of Lemma 2.2, applied to one of the vertices of the part $K_{n_i}$ of $G$, we have

$$\begin{aligned} z(G) &= z\left(K_s \bigvee (H \cup K_2 \cup K_{n_q})\right) \\ &= z\left(K_s \bigvee (H \cup K_1 \cup K_{n_q})\right) + z\left(K_s \bigvee (H \cup K_{n_q})\right) + sz\left(K_{s-1} \bigvee (H \cup K_1 \cup K_{n_q})\right). \end{aligned}$$

Likewise, if we apply part (ii) of Lemma 2.2 to one of the vertices of the part $K_{n_q+1}$ of $G'$, we get

$$\begin{aligned} z(G') &= z\left(K_s \bigvee (H \cup K_1 \cup K_{n_q+1})\right) \\ &= z\left(K_s \bigvee (H \cup K_1 \cup K_{n_q})\right) + n_q z\left(K_s \bigvee (H \cup K_1 \cup K_{n_q-1})\right) + sz\left(K_{s-1} \bigvee (H \cup K_1 \cup K_{n_q})\right). \end{aligned}$$

It follows that

$$\begin{aligned} z(G') - z(G) &= n_q z\left(K_s \bigvee (H \cup K_1 \cup K_{n_q-1})\right) - z\left(K_s \bigvee (H \cup K_{n_q})\right) \\ &= (n_q - 1)\left[z\left(K_s \bigvee (H \cup K_{n_q-1})\right) - z\left(K_s \bigvee (H \cup K_{n_q-2})\right)\right] \\ &\quad + s(n_q - 1) z\left(K_{s-1} \bigvee (H \cup K_{n_q-1})\right) \\ &\ge s(n_q - 1) z\left(K_{s-1} \bigvee (H \cup K_{n_q-1})\right) > 0. \end{aligned}$$

The first inequality holds because $K_s \bigvee (H \cup K_{n_q-2})$ is a proper subgraph of $K_s \bigvee (H \cup K_{n_q-1})$ and $n_q \ge 2$.

Now assume that the result holds for all positive integers less than $n_i \ge 3$. By Lemma 2.2(ii), we have

$$\begin{aligned} z(G) &= z\left(K_s \bigvee (H \cup K_{n_i} \cup K_{n_q})\right) \\ &= z\left(K_s \bigvee (H \cup K_{n_i-1} \cup K_{n_q})\right) + (n_i - 1) z\left(K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q})\right) \\ &\quad + sz\left(K_{s-1} \bigvee (H \cup K_{n_i-1} \cup K_{n_q})\right), \end{aligned}$$

and

$$\begin{aligned} z(G') &= z\left(K_s \bigvee (H \cup K_{n_i-1} \cup K_{n_q+1})\right) \\ &= z\left(K_s \bigvee (H \cup K_{n_i-1} \cup K_{n_q})\right) + n_q z\left(K_s \bigvee (H \cup K_{n_i-1} \cup K_{n_q-1})\right) \\ &\quad + sz\left(K_{s-1} \bigvee (H \cup K_{n_i-1} \cup K_{n_q})\right). \end{aligned}$$

It follows that

$$z(G') - z(G) = n_q z\left(K_s \bigvee (H \cup K_{n_i-1} \cup K_{n_q-1})\right) - (n_i - 1) z\left(K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q})\right)$$

$$
\begin{aligned}
&= n_q \Big[ z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) + (n_i-2) z \Big( K_s \bigvee (H \cup K_{n_i-3} \cup K_{n_q-1}) \Big) \\
&\quad + sz \Big( K_{s-1} \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) \Big] - (n_i-1) \Big[ z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) \\
&\quad + (n_q-1) z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-2}) \Big) + sz \Big( K_{s-1} \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) \Big] \\
&= (n_q - n_i + 1) z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) \\
&\quad + s(n_q - n_i + 1) z \Big( K_{s-1} \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) \\
&\quad + n_q(n_i-2) z \Big( K_s \bigvee (H \cup K_{n_i-3} \cup K_{n_q-1}) \Big) \\
&\quad - (n_i-1)(n_q-1) z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-2}) \Big) \\
&= (n_q - n_i + 1) z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) \\
&\quad + s(n_q - n_i + 1) z \Big( K_{s-1} \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) \\
&\quad + n_q(n_i-1) \Big[ z \Big( K_s \bigvee (H \cup K_{n_i-3} \cup K_{n_q-1}) \Big) - z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-2}) \Big) \Big] \\
&\quad - n_q z \Big( K_s \bigvee (H \cup K_{n_i-3} \cup K_{n_q-1}) \Big) + (n_i-1) z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-2}) \Big) \\
&= (n_q - n_i + 1) z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) \\
&\quad + s(n_q - n_i + 1) z \Big( K_{s-1} \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) \\
&\quad + n_q(n_i-1) \Big[ z \Big( K_s \bigvee (H \cup K_{n_i-3} \cup K_{n_q-1}) \Big) - z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-2}) \Big) \Big] \\
&\quad - n_q z \Big( K_s \bigvee (H \cup K_{n_i-3} \cup K_{n_q-1}) \Big) + n_q z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-2}) \Big) \\
&\quad - n_q z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-2}) \Big) + (n_i-1) z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-2}) \Big) \\
&= (n_q - n_i + 1) \Big[ z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) - z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-2}) \Big) \Big] \\
&\quad + s(n_q - n_i + 1) z \Big( K_{s-1} \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) \\
&\quad + n_q(n_i-2) \Big[ z \Big( K_s \bigvee (H \cup K_{n_i-3} \cup K_{n_q-1}) \Big) - z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-2}) \Big) \Big] \\
&\geq s(n_q - n_i + 1) z \Big( K_{s-1} \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) \\
&\quad + n_q(n_i-2) \Big[ z \Big( K_s \bigvee (H \cup K_{n_i-3} \cup K_{n_q-1}) \Big) - z \Big( K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-2}) \Big) \Big] \\
&\geq s(n_q - n_i + 1) z \Big( K_{s-1} \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1}) \Big) > 0.
\end{aligned}
$$

Here, the first inequality holds because $K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-2})$ is a proper subgraph of $K_s \bigvee (H \cup K_{n_i-2} \cup K_{n_q-1})$; the second one holds by the induction hypothesis. This completes the proof. □

For the class of graphs with given connectivity, we immediately obtain the following result now:

**Theorem 4.2.** *Let $G$ be a graph with $n$ vertices and connectivity $s$. We have $z(G) \leq z\left(K_s \bigvee (K_1 \cup K_{n-s-1})\right)$, with equality if and only if $G \cong K_s \bigvee (K_1 \cup K_{n-s-1})$.*

*Proof.* By the same argument as in the proof of Theorem 3.3, the graph $G^*$ that maximizes the Hosoya index under the given conditions must be of the form $G^* \cong K_s \bigvee (K_{n_1} \cup K_{n_2})$. By Lemma 4.1, we must have $n_1 = 1$ or $n_2 = 1$. This completes the proof. □

Now we direct our attention to graphs with fixed matching number. We will prove a result analogous to Theorem 3.2, which however will be somewhat more complicated. In the following, we will denote the graph $K_s \bigvee(n+s-2\beta-1)K_1 \cup K_{2\beta-2s+1})$ by $G(n,s,\beta)$. It consists of a complete graph $K_s$, which is joined to an empty graph $\overline{K}_{n-2\beta+s-1}$ by all possible $s(n-2\beta+s-1)$ edges and to a complete graph $K_{2\beta-2s+1}$ by all possible $s(2\beta-2s+1)$ edges, see Figure 1.

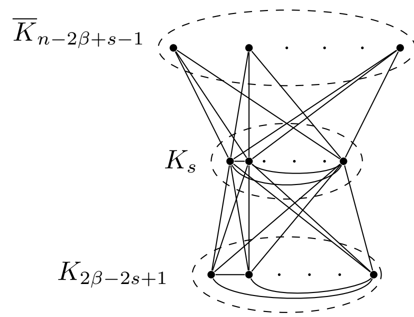


Figure 1: $G(n,s,\beta)$.

**Theorem 4.3.** *Let $G$ be a graph with $n$ vertices and matching number $\beta$.*

(i) *If $\beta = \lfloor \frac{n}{2} \rfloor$, then $z(G) \le z(K_n)$ with equality if and only if $G \cong K_n$.*
(ii) *If $n \ge 2\beta+2$, then $z(G) \le \max(z(G(n,1,\beta), G(n,\beta,\beta))$, with equality if and only if $G \cong G(n,1,\beta)$ or $G \cong G(n,\beta,\beta)$, whichever has greater Hosoya index.*

*Proof.* (i) Once again, it is clear that $z(G) \le z(K_n)$ for any graph of order $n$ (in view of (2.2)), with equality only if $G \cong K_n$. This settles the case that $\beta = \lfloor \frac{n}{2} \rfloor$.

(ii) Suppose that $n \ge 2\beta+2$, and let $G^*$ be a graph with $n$ vertices and matching number $\beta$ whose Hosoya index is maximal among all such graphs. By Lemma 2.4, there exist positive odd numbers $n_1, n_2, \ldots, n_q$ such that $G^* \cong K_s \bigvee(\bigcup_{j=1}^q K_{n_j})$ with $s = q+2\beta-n$ (so $q = n-2\beta+s \ge 2$) and $\sum_{j=1}^q n_j = n-s$.

First, we show that at most one of the numbers $n_1, n_2, \ldots, n_q$ is greater than one. Otherwise, assume that $n_2 \ge n_1 \ge 3$. Set $H = \bigcup_{j=3}^q K_{n_j}$, $G' = K_s \bigvee(K_{n_1-1} \cup K_{n_2+1} \cup H)$ and $G'' = K_s \bigvee(K_{n_1-2} \cup K_{n_2+2} \cup H)$. By Lemma 4.1, we have $z(G^*) < z(G') < z(G'')$. Moreover, it is easy to see that $G''$ has order $n$ and matching number $\beta$, which gives us a contradiction to the choice of $G^*$. Hence we must have $G^* \cong K_s \bigvee((q-1)K_1 \cup K_{n_q})$. Note also that $n = s+n_q+q-1$ and $q = n+s-2\beta$, so $n_q = 2\beta-2s+1$. It follows that $G^* \cong K_s \bigvee((n+s-2\beta-1)K_1 \cup K_{2\beta-2s+1}) = G(n,s,\beta)$.

Now we have to study the behavior of $z(G(n,s,\beta))$ as a function of $s$ for fixed $n$ and $\beta$. Transforming $G(n,s,\beta)$ to $G(n,s-1,\beta)$ amounts to increasing the $K_{2\beta-2s+1}$-part by two vertices (denoted by $u$ and $v$ in Figure 2) and then reducing the $\overline{K}_{n-2\beta+s-1}$-part and the $K_s$-part by one vertex each.

Let us compare $z(G(n,s,\beta))$ and $z(G(n,s-1,\beta))$, considering the graphical representations in Figure 2. We only have to compare the numbers $z_s$ and $z_{s-1}$ of matchings containing edges (thick in Figure 2) joining $u$ and any vertex in the $\overline{K}_{n-2\beta+s-2}$-part of $G(n,s,\beta)$, and joining $v$ to any vertex in the $K_{2\beta-2s+1}$-part of $G(n,s-1,\beta)$, respectively, since if all these edges are removed, the remaining graphs are isomorphic.

It is easy to check that removing the end vertices of a thick edge from $G(n,s,\beta)$ or $G(n,s-1,\beta)$ leads to a graph isomorphic to $G(n-2,s-1,\beta)$. Thus we have

$$z_s = (n-2\beta+s-2)z(G(n-2,s-1,\beta)),$$
$$z_{s-1} = (2\beta-2s+1)z(G(n-2,s-1,\beta)).$$

It follows that

$$z(G(n,s,\beta)) - z(G(n,s-1,\beta)) = z_s - z_{s-1} = \big((n-2\beta+s-2)-(2\beta-2s+1)\big)z(G(n-2,s-1,\beta))$$
$$= (n-4\beta+3s-3)z(G(n-2,s-1,\beta)).$$

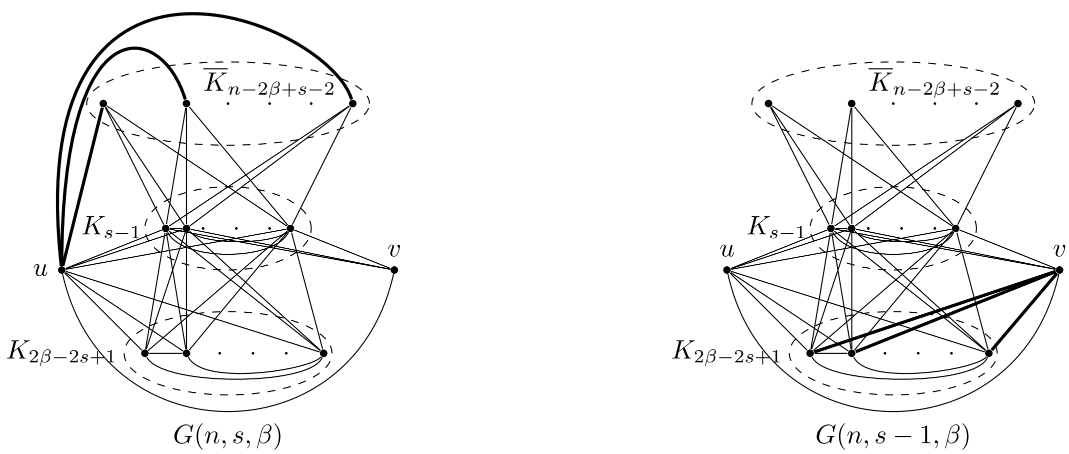


Figure 2: $G(n,s,\beta)$ and $G(n,s-1,\beta)$; the thick edges are those that are only present in one of the two.

Hence if $s \leq (4\beta-n)/3+1$, we have $z(G(n,s,\beta)) \leq z(G(n,s-1,\beta))$, while $z(G(n,s,\beta)) > z(G(n,s-1,\beta))$ if $s > (4\beta-n)/3+1$. This means that $z(G(n,s,\beta))$, regarded as a function of $s$, is a unimodular function whose maximum must occur at one of the two ends. This means that $G^* = G(n,1,\beta)$ or $G^* = G(n,\beta,\beta)$, which completes the proof. □

Theorem 4.3 still leaves us with two possibilities: the maximum can be obtained for either $G(n,1,\beta)$ or for $G(n,\beta,\beta)$. For $\beta = 1$, we are done of course, but in general we would like to know which of the two applies to a given choice of $n$ and $\beta$. It is not hard to see that for $\beta > 1$, $G(2\beta,1,\beta) = K_{2\beta} \neq G(2\beta,\beta,\beta)$, which means that $z(G(2\beta,1,\beta)) > z(G(2\beta,\beta,\beta))$. We will see in the next lemma that if $n$ is large enough then the inequality is reversed.

**Theorem 4.4.** *For any fixed $\beta > 1$, there exists a unique integer $n_0(\beta) \geq 2\beta$ such that*

$$z(G(n_0(\beta),1,\beta)) \geq z(G(n_0(\beta),\beta,\beta))$$

*and*

$$z(G(n_0(\beta)+1,1,\beta)) < z(G(n_0(\beta)+1,\beta,\beta)).$$

*Proof.* We study how much $z(G(n,1,\beta))$ and $z(G(n,\beta,\beta))$ increase when $n$ is increased by 1. The

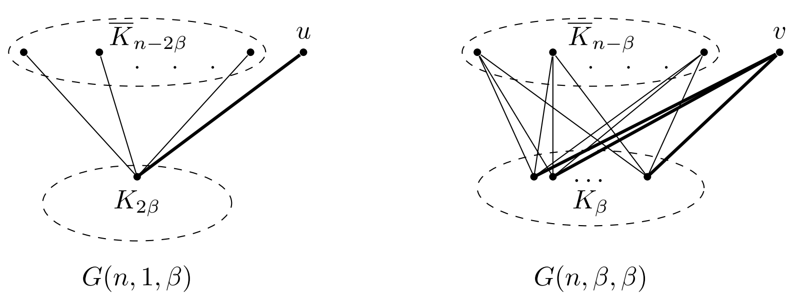


Figure 3: How $G(n+1,1,\beta)$ and $G(n+1,\beta,\beta)$ are obtained from $G(n,1,\beta)$ and $G(n,\beta,\beta)$.

difference

$$z(G(n+1,1,\beta)) - z(G(n,1,\beta)) = z(K_{2\beta-1})$$

comes from matchings that contain vertex $u$ in Figure 3, and it does not depend on $n$, while

$$z(G(n+1,\beta,\beta)) - z(G(n,\beta,\beta)) = \beta z(G(n-2,\beta-1,\beta-1)) \text{ (for } n \geq 2\beta \text{ and } \beta \geq 2),$$

the number of matchings that cover vertex $v$ in Figure 3, is a strictly increasing function of $n$. Thus

$$D(n) = z(G(n,\beta,\beta)) - z(G(n,1,\beta))$$

is a strictly convex function of $n \geq 2\beta$, since

$$D(n+1) - D(n) = \beta z(G(n-2,\beta-1,\beta-1)) - z(K_{2\beta-1})$$

is increasing. Since $D(2\beta) < 0$, there must be a unique $n_0(\beta)$ such that $D(n_0(\beta)+1) > 0$ and $D(n_0(\beta)) \leq 0$. □

# 5. Asymptotic considerations

Let $n_0 = n_0(\beta)$ be as in Theorem 4.4. In the following, we derive information on the value of $n_0(\beta)$. To this end, we need formulas for both $z(G(n,\beta,\beta))$ and $z(G(n,1,\beta))$. First of all, we have

$$z(G(n,1,\beta)) = z(K_{2\beta}) + (n-2\beta)z(K_{2\beta-1}),$$

since $G(n,1,\beta)$ consists of a $K_{2\beta}$ (which accounts for the first term) and $n-2\beta$ additional pendant vertices attached to one of its $2\beta$ vertices (so each of them is part of $z(K_{2\beta-1})$ matchings, and there are no matchings containing more than one of them). It is well-known that $z(K_n)$, which also counts involutions (permutations that are equal to their own inverse) of a set of cardinality $n$, has exponential generating function

$$F(x) = \sum_{n\geq 0} \frac{z(K_n)}{n!} x^n = e^{x+x^2/2},$$

where we set $z(K_0) = 1$. Moreover, it is known [9, Proposition VIII.2] that

$$z(K_n) \sim \frac{1}{\sqrt{2}} \cdot n^{n/2} \cdot e^{-n/2+\sqrt{n}-1/4} \tag{5.3}$$

as $n \to \infty$. For our purposes, a simple upper bound will be useful as well. One has the trivial bound (see [9, Proposition IV.1])

$$z(K_n) = n![x^n]F(x) \leq n! \cdot u^{-n} F(u)$$

for any positive real $u$. Setting $u = \sqrt{n}$ and $u = \sqrt{n+1}$ respectively, we get

$$z(K_n) \leq n! \cdot n^{-n/2} \cdot e^{n/2+\sqrt{n}} \tag{5.4}$$

and

$$z(K_n) \leq n! \cdot (n+1)^{-n/2} \cdot e^{(n+1)/2+\sqrt{n+1}}. \tag{5.5}$$

We also have a generating function for $z(G(n,\beta,\beta))$: write $n = 2\beta + m$, and note that $G(n,\beta,\beta)$ consists of a complete graph $K_\beta$ and an empty graph $\overline{K}_{\beta+m}$, connected by all possible $\beta(\beta+m)$ edges. We have

$$z(G(n,\beta,\beta)) = \sum_{k=0}^{\beta} \binom{\beta}{k}\binom{\beta+m}{k} k! z(K_{\beta-k}),$$

which can be argued as follows: the $k$-th term counts matchings with precisely $k$ edges containing one of the vertices of the empty graph $\overline{K}_{\beta+m}$. $\binom{\beta}{k}\binom{\beta+m}{k}k!$ counts the number of ways to pick $k$ vertices in $K_\beta$ and $\overline{K}_{\beta+m}$ respectively and connect them by a perfect matching. This leaves a complete graph $K_{\beta-k}$ in the $K_\beta$-part of $G(n,\beta,\beta)$, which explains the factor $z(K_{\beta-k})$.

Now we obtain the following exponential generating function:

$$\begin{aligned}
G_m(x) &= \sum_{\beta\geq 0} \frac{z(G(2\beta+m,\beta,\beta))}{\beta!}x^\beta = \sum_{\beta\geq 0}\frac{x^\beta}{\beta!}\sum_{k=0}^{\beta}\binom{\beta}{k}\binom{\beta+m}{k}k!z(K_{\beta-k}) \\
&= \sum_{\beta\geq 0}\frac{x^\beta}{\beta!}\sum_{k=0}^{\beta}\binom{\beta+m}{\beta-k}\binom{\beta}{\beta-k}(\beta-k)!z(K_k) = \sum_{k\geq 0}\sum_{\ell\geq 0}\frac{x^{k+\ell}}{(k+\ell)!}\binom{k+\ell+m}{\ell}\binom{k+\ell}{\ell}\ell!z(K_k) \\
&= \sum_{k\geq 0}\frac{z(K_k)x^k}{k!}\sum_{\ell\geq 0}\binom{k+\ell+m}{\ell}x^\ell = \sum_{k\geq 0}\frac{z(K_k)x^k}{k!}(1-x)^{-k-m-1} \\
&= (1-x)^{-m-1}\sum_{k\geq 0}\frac{z(K_k)}{k!}\left(\frac{x}{1-x}\right)^k = (1-x)^{-m-1}\exp\left(\frac{x}{1-x}+\frac{x^2}{2(1-x)^2}\right).
\end{aligned}$$

Since the second factor has a power series expansion with positive coefficients only and constant coefficient 1, it is clear that the coefficient of $x^\beta$ in $G_m(x)$ is greater or equal to the coefficient of $x^\beta$ in $(1-x)^{-m-1}$, which is $\binom{m+\beta}{m}$, hence

$$z(G(n,\beta,\beta)) = \beta![x^\beta]G_m(x) \geq \beta!\binom{m+\beta}{m}. \tag{5.6}$$

Now we have all the necessary ingredients for the following theorem.

**Theorem 5.1.** *For all $\beta > 1$, $n_0(\beta) \leq 3\beta$. Moreover, as $\beta \to \infty$, we have*

$$\lim_{\beta\to\infty}\frac{n_0(\beta)}{\beta} = A \approx 2.2938153733404154,$$

*which is the unique positive real solution of the equation $(A-1)^{A-1} = 2(A-2)^{A-2}$.*

*Proof.* To prove the first statement for some value of $\beta$, we simply need to show that $z(G(3\beta,1,\beta)) < z(G(3\beta,\beta,\beta))$. In view of our estimate (5.6), we have

$$z(G(3\beta,\beta,\beta)) \geq \beta!\binom{2\beta}{\beta} = \frac{(2\beta)!}{\beta!}.$$

On the other hand, (5.4) and (5.5) yield

$$\begin{aligned}
z(G(3\beta,1,\beta)) &= z(K_{2\beta}) + \beta z(K_{2\beta-1}) \leq (2\beta)!\cdot(2\beta)^{-\beta}\cdot e^{\beta+\sqrt{2\beta}} + \frac{(2\beta)!}{2}\cdot(2\beta)^{-\beta+1/2}\cdot e^{\beta+\sqrt{2\beta}} \\
&= \left(1+\sqrt{\beta/2}\right)\cdot(2\beta)!\cdot(2\beta)^{-\beta}\cdot e^{\beta+2\sqrt{\beta}}.
\end{aligned}$$

Thus we are done if

$$\left(1+\sqrt{\beta/2}\right)\cdot(2\beta)^{-\beta}\cdot e^{\beta+2\sqrt{\beta}}\cdot\beta! < 1.$$

To this end, we use the following well-known inequality, which is a form of Stirling's approximation:

$$\beta! \leq \beta^{\beta+1/2}e^{1-\beta}.$$

It remains to show that

$$\left(1+\sqrt{\beta/2}\right)\sqrt{\beta}\cdot 2^{-\beta}\cdot e^{1+2\sqrt{\beta}} < 1.$$

| $\beta$ | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 | 13 | 14 | 15 | 16 | 17 | 18 | 19 | 20 |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $n_0(\beta)$ | 6 | 8 | 10 | 13 | 15 | 18 | 20 | 22 | 25 | 27 | 30 | 32 | 34 | 37 | 39 | 41 | 44 | 46 | 49 |

Table 1: Values of $n_0(\beta)$.

However, it is straightforward to prove that

$$\left(1+\sqrt{\beta/2}\right)\cdot e\sqrt{\beta} \le 2\sqrt{\beta/2}\cdot e\sqrt{\beta} = \sqrt{2}e\beta < 4\beta < 2^{\beta/2}$$

for $\beta \ge 11$, and that $e^{2\sqrt{\beta}} \le 2^{\beta/2}$ for $\beta \ge 17$. Thus we can conclude that $n_0(\beta) \le 3\beta$ for $\beta \ge 17$. For smaller values of $\beta$, this can be checked directly (see Table 1).

For the second statement of the theorem, we also need an upper bound for $z(G(n,\beta,\beta))$. Set

$$H(x) = \sum_{k=0}^{\infty} h_k x^k = \exp\left(\frac{x}{1-x} + \frac{x^2}{2(1-x)^2}\right).$$

Using the same idea that gave us (5.4) and (5.5), we get, with $u = 1 - k^{-1/3}$,

$$h_k = [x^k]H(x) \le u^{-k}H(u) = \left(1-k^{-1/3}\right)^{-k} \exp\left(\frac{k^{2/3}-1}{2}\right) = \exp\left(\frac{3k^{2/3}}{2} + O(k^{1/3})\right).$$

Thus there exists an absolute positive constant $C$ such that $h_k \le \exp(Ck^{2/3})$ for all $k \ge 0$ (this even holds for $h_0 = 1$). Now we have

$$\begin{aligned} z(G(n,\beta,\beta)) &= \beta![x^\beta](1-x)^{-n+2\beta-1}H(x) = \beta!\sum_{r=0}^{\beta}\binom{n-2\beta+r}{r}h_{\beta-r} \\ &\le \beta!\sum_{r=0}^{\beta}\binom{n-2\beta+r}{r}\exp(C\beta^{2/3}) = \beta!\binom{n-\beta+1}{\beta}\exp(C\beta^{2/3}) \\ &= \frac{(n-\beta+1)!}{(n-2\beta+1)!}\exp(C\beta^{2/3}). \end{aligned}$$

Combining this with (5.6), we get

$$\frac{(n-\beta)!}{(n-2\beta)!} \le z(G(n,\beta,\beta)) \le \frac{(n-\beta+1)!}{(n-2\beta+1)!}\exp(C\beta^{2/3}),$$

from which it follows that

$$\log z(G(n,\beta,\beta)) = \log(n-\beta)! - \log(n-2\beta)! + O(\beta^{2/3}).$$

Write $n = A\beta$ and use Stirling's approximation to obtain

$$\log z(G(n,\beta,\beta)) = \beta\log\beta + ((A-1)\log(A-1) - (A-2)\log(A-2) - 1)\beta + O(\beta^{2/3}). \tag{5.7}$$

On the other hand, for $n < 3\beta$, we have

$$z(K_{2\beta}) \le z(G(n,1,\beta)) \le \beta z(K_{2\beta}),$$

thus in view of (5.3)

$$\log z(G(n,1,\beta)) = \log z(K_{2\beta}) + O(\log\beta) = \beta\log(2\beta) - \beta + O(\sqrt{\beta}). \tag{5.8}$$

Comparing (5.7) and (5.8) shows that we have

$$z(G(n,\beta,\beta)) < z(G(n,1,\beta))$$

for sufficiently large $\beta$ if $(A-1)\log(A-1)-(A-2)\log(A-2) < \log 2$, and

$$z(G(n,\beta,\beta)) > z(G(n,1,\beta))$$

for sufficiently large $\beta$ if $(A-1)\log(A-1)-(A-2)\log(A-2) > \log 2$. Now the second statement of the theorem follows immediately. □

Table 1 shows values of $n_0(\beta)$ which are increasing with $\beta$. We use the inequality $2\beta \le n_0(\beta) \le 3\beta$, to show in the next theorem that $n_0(\beta)$ is indeed a non-decreasing function of $\beta$.

**Theorem 5.2.** *For any $\beta > 1$ we have $n_0(\beta+1) \ge n_0(\beta)$.*

*Proof.* To prove the theorem, we show that $z(G(n_0(\beta+1),1,\beta)) < z(G(n_0(\beta+1),\beta,\beta))$. If $n_0(\beta) \le n_0(\beta+1)-2$, then we are immediately done. If $n_0(\beta+1) \ge 3\beta$, then combined with $n_0(\beta) \le 3\beta$, we get $n_0(\beta+1) \ge n_0(\beta)$, so for the rest of this proof, we assume that $n_0(\beta+1) \le 3\beta-1$ and $n_0(\beta) > n_0(\beta+1)-2$. The latter implies that

$$z(G(n_0(\beta+1)-2,1,\beta)) \ge z(G(n_0(\beta+1)-2,\beta,\beta)). \tag{5.9}$$

For simplicity, we use the abbreviation $N = n_0(\beta+1)$. There are $N-\beta-1$ edges in $G(n,\beta+1,\beta+1)$

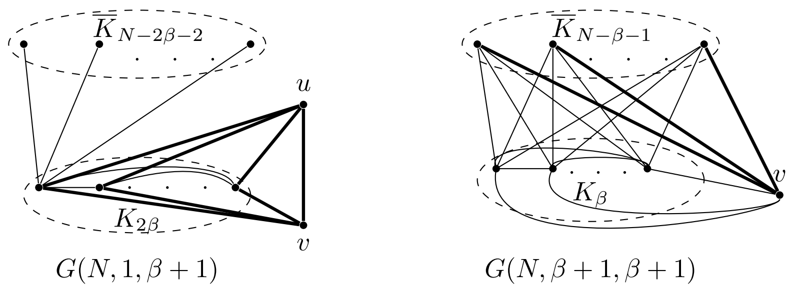


Figure 4: $G(N,1,\beta+1)$ and $G(N,\beta+1,\beta+1)$.

that are not present in $G(n,\beta,\beta)$ (thick edges in Figure 4). They all have an end in common, and removing one of them yields a graph that is isomorphic to $G(N-2,\beta,\beta)$. Therefore,

$$\begin{aligned} z(G(N,\beta+1,\beta+1)) &= z(G(N,\beta,\beta)) + (N-\beta-1)z(G(N-2,\beta,\beta)) \\ &\le z(G(N,\beta,\beta)) + (2\beta-2)z(G(N-2,\beta,\beta)), \end{aligned}$$

using the assumption that $N \le 3\beta-1$. Let $H$ be the graph obtained by attaching $N-2\beta-1$ pendant vertices to one vertex of $K_{2\beta+1}$. Note that one can get $G(N,1,\beta+1)$ from $H$ by connecting one of those pendant vertices to the remaining $2\beta$ vertices of the complete graph $K_{2\beta+1}$. Likewise, it is easy to see that $G(N,1,\beta)$ is a subgraph of $H$, so

$$z(G(N,1,\beta+1)) = z(H) + 2\beta z(G(N-2,1,\beta)) \ge z(G(N,1,\beta)) + 2\beta z(G(N-2,1,\beta)).$$

Together with (5.9) and the fact that $z(G(N,1,\beta+1)) < z(G(N,\beta+1,\beta+1))$ by definition of $N = n_0(\beta+1)$, it follows that

$$\begin{aligned} z(G(N,1,\beta)) &\le z(G(N,1,\beta+1)) - 2\beta z(G(N-2,1,\beta)) \\ &< z(G(N,\beta+1,\beta+1)) - 2\beta z(G(N-2,\beta,\beta)) \\ &\le z(G(N,\beta+1,\beta+1)) - (2\beta-2)z(G(N-2,\beta,\beta)) \le z(G(N,\beta,\beta)), \end{aligned}$$

as desired. □

We deduce as corollary of Theorem 5.2 the following reversed version of Theorem 4.4:

**Corollary 5.3.** *For every $n \geq 6$, there is a unique positive integer $\beta_0 = \beta_0(n)$ such that $z(G(n, \beta, \beta)) > z(G(n, 1, \beta))$ for $1 < \beta < \beta_0$, and $z(G(n, \beta, \beta)) \leq z(G(n, 1, \beta))$ for $\lfloor n/2 \rfloor \geq \beta \geq \beta_0$.*

*Proof.* Since $n_0(2) = 6$ and $n_0(\beta)$ is an unbounded function of $\beta$, for any integer $n \geq 6$ there exists a $\beta_1$ such that $n \leq n_0(\beta_1)$. We choose $\beta_1$ to be as small as possible. This means that for any $\beta < \beta_1$ we have $n_0(\beta) < n$ and hence $z(G(n, 1, \beta)) < z(G(n, \beta, \beta))$, while for all $\beta \geq \beta_1$ we have $n_0(\beta) \geq n_0(\beta_1) \geq n$ and thus $z(G(n, \beta, \beta)) \leq z(G(n, 1, \beta))$. Hence we can take $\beta_0(n) = \beta_1$. The uniqueness of $\beta_0(n)$ follows from the necessity of choosing $\beta_1$ to be minimal. □

We remark that Theorem 5.1 also implies

$$\lim_{n \to \infty} \frac{\beta_0(n)}{n} = A^{-1} \approx 0.4359548774597885.$$

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