Matchings in graphs with a given number of cuts

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Abstract

Let $m(G,k)$ denote the number of matchings of cardinality k in a graph G. A quasi-order $\preceq$ is defined by writing $G \preceq H$ whenever $m(G,k) \leq m(H,k)$ holds for all k. We consider the set $\mathcal{G}_1(n,\gamma)$ of connected graphs with n vertices and γ cut vertices as well as the set $\mathcal{G}_2(n,\gamma)$ of connected graphs with n vertices and γ cut edges. We determine the greatest and least elements with respect to this quasi-order in $\mathcal{G}_1(n,\gamma)$ and the greatest element in $\mathcal{G}_2(n,\gamma)$ for all values of n and γ. As corollaries, we find that these graphs maximize (resp. minimize) the Hosoya index and the matching energy within the respective sets.

Keywords: matchings; matching energy; quasi-order; cut vertex; cut edge

1 Introduction

There is a rich history of research on the number of matchings in graphs. The idea of defining a quasi-order based on the number of matchings goes back to the work of

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Gutman [9, 10]. Let G be a graph (finite, undirected and simple, as all graphs in the following) with n vertices, and let $m(G,k)$ be the number of k-matchings in G, i.e., the number of sets of k pairwise nonadjacent edges. In particular, $m(G,0)=1$ (the empty matching), and $m(G,1)$ is the number of edges of G. We also clearly have $m(G,k)=0$ if $k<0$ or $k>\frac{n}{2}$. A quasi-order $\preceq$ is defined as follows:

$$G \preceq H \quad \Longleftrightarrow \quad m(G,k) \leq m(H,k) \text{ for all } k.$$

If at least one of the inequalities is strict, we write $G \prec H$.

The *Hosoya index* [15], a classical graph invariant in chemical graph theory that has been widely studied, is the total number of matchings in a graph G, i.e.,

$$Z(G) = \sum_{k \geq 0} m(G,k).$$

Clearly, we have $Z(G) \leq Z(H)$ if $G \preceq H$, and $Z(G) < Z(H)$ if $G \prec H$. Another graph invariant whose analysis typically relies on the quasi-order $\preceq$ is the *matching energy* $ME(G)$, which was introduced much more recently [14]. It has two equivalent definitions: it can either be defined as the sum of the absolute values of the zeros of the *matching polynomial* [7, 8, 11]

$$\sum_{k \geq 0} (-1)^k m(G,k) x^{n-2k}, \tag{1.1}$$

or equivalently by means of the so-called *Coulson integral formula*

$$ME(G) = \frac{2}{\pi} \int_0^\infty \frac{1}{x^2} \ln \left[\sum_{k \geq 0} m(G,k) x^{2k} \right] dx. \tag{1.2}$$

From the second representation, it is clear that $ME(G)$ is an increasing function of each of the coefficients $m(G,k)$, so $G \preceq H$ implies $ME(G) \leq ME(H)$, and $G \prec H$ implies $ME(G) < ME(H)$.

An important feature of the matching energy is that it coincides with the *graph energy*, which is the sum of the absolute values of the eigenvalues (see [20] for a comprehensive treatise) if the graph is acyclic, i.e., a forest. This is due to the well-known fact that the characteristic polynomial of a forest is precisely its matching polynomial.

There is a great amount of literature on finding the graphs in a given set for which the Hosoya index attains its minimum or maximum value; see [21] for a recent survey. The quasi-order $\preceq$ often plays a role in this context. The same applies to the matching energy, which has been studied quite thoroughly over the past couple of years, with many results on maximum and minimum values and the associated extremal graphs.

Results on trees and unicyclic graphs were already given in the first paper on the matching energy [14]. Ji, Li and Shi [17] followed by characterizing the graphs with the extremal matching energy among all bicyclic graphs. The graphs that maximize or minimize the matching energy have also been determined among unicyclic and bicyclic graphs with a given diameter [4], tricyclic graphs [6], graphs with given connectivity or chromatic number [19], and many more [2, 3, 5, 16, 18, 22, 23]. See [12] for a survey on the topic. The quasi-order $\preceq$ generally plays a very prominent role.

In this paper, we will be concerned with a new class: graphs for which the number of cut vertices or the number of cut edges is prescribed along with the number of vertices. Recall that a vertex is called a *cut vertex* of a graph if its removal increases the number of components. In particular, if the graph is connected, then removing a cut vertex renders the graph disconnected. Likewise, an edge is called a *cut edge* if its removal increases the number of components.

We define the set $\mathcal{G}_1(n,\gamma)$ to be the set of all connected graphs with n vertices and γ cut vertices. In Section 3.1, we will show that there are unique greatest and least elements with respect to $\preceq$ in $\mathcal{G}_1(n,\gamma)$ for every possible combination of n and γ, and characterize the shape of these elements. As an immediate corollary, we find that these graphs simultaneously maximize (minimize, respectively) the Hosoya index and the matching energy.

The extremal graphs can be defined as follows. Denote, as usual, by P_n, S_n and K_n the path, star and complete graph on n vertices, respectively. The graph $KP_{n,\gamma}$ (sometimes called a "lollipop graph") is obtained by attaching a path of γ vertices to a vertex of the complete graph $K_{n-\gamma}$, see Figure 1.1. It will be shown that this graph is the greatest element in $\mathcal{G}_1(n,\gamma)$ with respect to $\preceq$ for all values of n and γ.

Likewise, the graph $SP_{n,\gamma}$ (which is called a "broom") is obtained by attaching a path of γ vertices to the center of a star $S_{n-\gamma}$, as shown in Figure 1.2. This graph turns out to be the least element with respect to $\preceq$ in $\mathcal{G}_1(n,\gamma)$.

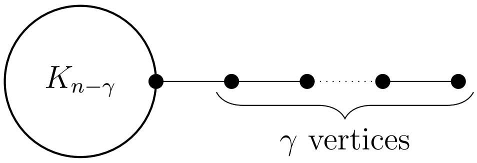

Figure 1.1. The graph $KP_{n,\gamma}$

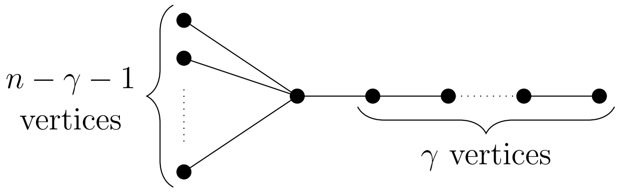

Figure 1.2. The graph $SP_{n,\gamma}$

In Section 3.2, we obtain an analogous result for the set $\mathcal{G}_2(n,\gamma)$ of connected graphs with n vertices and γ cut edges. The unique greatest element with respect to $\preceq$ turns out to be the same as in $\mathcal{G}_1(n,\gamma)$ (namely $KP_{n,\gamma}$), with the same immediate consequences. However, there is generally no least element in this case.

2 Preliminaries

Let us first recall some important definitions and notation. For standard graph-theoretical terminology, we refer the reader to [1]. We will need a number of auxiliary results on matchings and the quasi-order $\preceq$. First of all, the following standard lemma provides us with a way to calculate the number of k-matchings in a graph recursively. For a subset X of the vertex set of G, we let $G-X$ be the subgraph of G obtained by deleting the vertices of X together with their incident edges. For a subset Y of the edge set of G, we denote by $G-Y$ the subgraph of G obtained by deleting the edges of Y. For the sake of brevity, we shall write $G-v$ instead of $G-\{v\}$, and $G-e$ instead of $G-\{e\}$.

Lemma 2.1 ([7, 11]) *Let G be a graph. For every edge $e = uv$, we have the following identity:*

$$m(G, k) = m(G - uv, k) + m(G - u - v, k - 1). \tag{2.1}$$

Moreover, if u is an arbitrary vertex of G, and $v_1, v_2, \ldots, v_t$ its neighbors, then we have

$$m(G, k) = m(G - u, k) + \sum_{i=1}^{t} m(G - u - v_i, k - 1). \tag{2.2}$$

A vertex without neighbors is called an *isolated vertex*, while a vertex with precisely one neighbor will be called a *pendant vertex* in the following. For an isolated vertex u, we get $m(G, k) = m(G - u, k)$ for every k, and for a pendant vertex u whose only neighbor is v, we get

$$m(G, k) = m(G - u, k) + m(G - u - v, k - 1) \tag{2.3}$$

as a special case of (2.2).

A graph H is called a *subgraph* of a graph G if the vertex set of H is a subset of the vertex set of G, and the edge set of H is a subset of the edge set of G. If H is a subgraph of G and $H \ncong G$, we call H a *proper subgraph* of G. If H is a subgraph of G and all the edges between two vertices of H that are present in G are also present in H, then we call H an *induced subgraph.* If S is a set of edges, the *edge-induced subgraph* $G[S]$ is the subgraph of G whose edge set is S and whose vertex set consists of all ends of edges of S. Our next lemma is immediate from the definition, noting that every matching in a subgraph H of G is also a matching in G itself.

Lemma 2.2 ([10]) *Let G be a graph and H a subgraph of G. Then $H \preceq G$. If the edge set of H is a proper subset of the edge set of G, then we even have $H \prec G$.*

If we take the disjoint union $G \uplus H$ of two graphs G and H, every matching of $G \uplus H$ decomposes uniquely into matchings of G and H, respectively. Thus we have

$$m(G \uplus H, k) = \sum_{j=0}^{k} m(G, j)m(H, k - j). \tag{2.4}$$

In particular, if H is a single vertex or only consists of isolated vertices, then $m(G \uplus H, k) = m(G, k)$ for all k, since the empty matching is the only matching in H (compare the remark after Lemma 2.1). The following well-known lemma is also an immediate consequence of the identity (2.4).

Lemma 2.3 ([13]) *Let H_1 and H_2 be two graphs with $H_1 \prec H_2$, and let G be an arbitrary graph. Then we have $H_1 \uplus G \prec H_2 \uplus G$.*

The following lemmas characterize the greatest and least elements with respect to the quasi-order $\preceq$ among trees.

Lemma 2.4 ([9]) *For every tree T with n vertices, we have $T \preceq P_n$. If T is not a path, we even have $T \prec P_n$.*

Lemma 2.5 ([9]) *For every tree T with n vertices that is not isomorphic to S_n or $SP_{n,2}$, we have $S_n \prec SP_{n,2} \prec T$.*

Lemma 2.6 ([24]) *For every tree T with β pendant vertices and n vertices in total, we have $SP_{n,n-\beta} \preceq T$. If T is not isomorphic to $SP_{n,n-\beta}$, we even have $SP_{n,n-\beta} \prec T$.*

Let us remark that while Lemma 2.6 is not stated in this way in [24], it is implicit in the proofs. Finally, we recall an important lemma that describes the change in the number of matchings under an operation that replaces an arbitrary tree by a star.

Lemma 2.7 ([14]) *Suppose that G is a connected graph and T an induced subgraph of G such that T is a tree and T is connected to the rest of G only by a cut vertex v. Let G' be obtained from G by replacing T with a star of the same order, centered at v. Then we have $G' \prec G$, unless G and G' are isomorphic.*

3 The extremal graphs in $\mathcal{G}_1(n,\gamma)$ and $\mathcal{G}_2(n,\gamma)$

3.1 Fixed number of cut vertices

We first consider the set $\mathcal{G}_1(n,\gamma)$ of graphs with n vertices, of which γ are cut vertices. We will characterize the greatest and least elements with respect to the quasi-order $\preceq$ for all values of n and γ.

A *block* of a simple graph G is a subgraph of G that is connected and has no cut vertex, and is maximal with respect to this property (see [1]). The notion of terminal blocks will be useful in the following. Recall that one can associate a *block-cut tree* with every connected graph G: its vertices are the blocks and the cut vertices of G. There is an edge in the block-cut tree between a block and a cut vertex if and only if the cut vertex lies in the block, and there are no further edges. Suppose that v is a cut vertex of G that is contained in a block B. If B contains no other cut vertices of G, then we call B a *terminal block*. Terminal blocks correspond precisely to the leaves of the block-cut tree.

Let us now formulate the first main theorem.

Theorem 3.1 *Let n,γ be integers with $0 \le \gamma \le n-2$. For every graph G in $\mathcal{G}_1(n,\gamma)$ that is not isomorphic to $KP_{n,\gamma}$, we have $G \prec KP_{n,\gamma}$. In particular, $KP_{n,\gamma}$ is the unique graph in $\mathcal{G}_1(n,\gamma)$ that attains the maximum Hosoya index, and the unique graph that attains the maximum matching energy.*

Proof. For $\gamma = n-2$, the result follows trivially since $\mathcal{G}_1(n,n-2) = \{P_n\}$ and $P_n \cong KP_{n,n-2}$, while for $\gamma = 0$ we trivially have $G \prec K_n$ unless $G \cong K_n$. Hence, we only need to consider the case that $1 \le \gamma \le n-3$.

We prove the statement of the theorem by induction on n. Before we get to the actual induction proof, let us remark that we can assume without loss of generality that all of the blocks of G are single edges or complete graphs. Otherwise, we can add edges to all non-complete blocks to make them complete, which yields a graph G' with the same number of vertices and cut vertices for which $G \prec G'$ by Lemma 2.2.

Moreover, we may assume that G does not contain an induced claw $K_{1,3}$ (thus also no larger induced star). If there was one, then its center would have to be a cut vertex of G (since all blocks are complete), and its neighbors would lie in distinct blocks. Adding an edge between any two of these neighbors would yield a new graph G' with the same number of vertices and cut vertices, but again $G \prec G'$. Therefore, we can rule out this possibility and assume in the following that every cut vertex belongs to exactly two blocks of G.

Finally, it is useful to observe that

$$KP_{n,\gamma+1} \prec KP_{n,\gamma}, \tag{3.1}$$

since the former can be seen as a proper subgraph of the latter.

Now we proceed with the induction. The statement is easily verified for small values of n ($n \leq 4$), so we suppose that the statement holds for graphs on less than n vertices. Consider a graph G with n vertices and γ cut vertices that is not isomorphic to $KP_{n,\gamma}$. We consider the following cases based on the sizes of terminal blocks.

Case 1: There exists a pendant vertex v in G, or equivalently a terminal block of two vertices. Let its unique neighbor be w, and note that $G - v$ has $n - 1$ vertices and $\gamma - 1$ cut vertices (w is no longer a cut vertex in $G - v$, since we were assuming that no cut vertex belongs to more than two blocks). By the induction hypothesis, $G - v \preceq KP_{n-1,\gamma-1}$.

Since w belongs to only two blocks by assumption, we know that $G - v - w$ is connected. Note also that $G - v - w$ has $n - 2$ vertices and at least $\gamma - 2$ cut vertices: all cut vertices of G remain cut vertices, except for w and potentially one more vertex if the other block that w belongs to also only contains two vertices. It follows from the induction hypothesis and (3.1) that $G - v - w \preceq KP_{n-2,\gamma-2}$.

So for every k, we have

$$\begin{aligned} m(G,k) &= m(G-v,k) + m(G-v-w,k-1) \\ &\leq m(KP_{n-1,\gamma-1},k) + m(KP_{n-2,\gamma-2},k-1) \\ &= m(KP_{n,\gamma},k). \end{aligned}$$

Strict inequality holds for at least one value of k unless $G - v \cong KP_{n-1,\gamma-1}$ and $G - v - w \cong KP_{n-2,\gamma-2}$. However, it is easy to see that this would imply $G \cong KP_{n,\gamma}$.

Case 2: There is no pendant vertex, but a terminal block consisting of three vertices. Let w be its cut vertex, and v_1, v_2 the two other vertices. Note that $G - v_1$ has $n-1$ vertices and γ cut vertices, so $G - v_1 \preceq KP_{n-1,\gamma}$ by the induction hypothesis. Second, $G - v_1 - v_2$ has $n-2$ vertices and $\gamma - 1$ cut vertices (all cut vertices of G, except for w), so $G - v_1 - v_2 \preceq KP_{n-2,\gamma-1}$ by the induction hypothesis. Finally, $G - v_1 - w$ consists of an isolated vertex and a graph with $n-3$ vertices and at least $\gamma - 2$ cut vertices (similar to the first case). Thus by the induction hypothesis and (3.1), we have $G - v_1 - w \preceq KP_{n-3,\gamma-2}$. We combine all inequalities to obtain

$$\begin{aligned} m(G,k) &= m(G - v_1, k) + m(G - v_1 - v_2, k-1) + m(G - v_1 - w, k-1) \\ &\leq m(KP_{n-1,\gamma}, k) + m(KP_{n-2,\gamma-1}, k-1) + m(KP_{n-3,\gamma-2}, k-1) \end{aligned}$$

for all k if $\gamma \geq 2$, and

$$m(G,k) \leq m(KP_{n-1,1}, k) + m(KP_{n-2,0}, k-1) + m(KP_{n-3,0}, k-1)$$

if $\gamma = 1$.

We further note that $n \geq \gamma + 4$: there must be at least two terminal blocks with at least two non-cut vertices each, since we are assuming that there is no pendant vertex. Combined with the γ cut vertices, this gives us at least $\gamma + 4$ vertices.

So in order to complete the proof in Case 2, we have to show that

$$m(KP_{n-1,\gamma}, k) + m(KP_{n-2,\gamma-1}, k-1) + m(KP_{n-3,\gamma-2}, k-1) \leq m(KP_{n,\gamma}, k) \quad (3.2)$$

for all values of n, γ, k such that $\gamma \geq 2$ and $n \geq \gamma + 4$, with at least one strict inequality for some k, and

$$m(KP_{n-1,1}, k) + m(KP_{n-2,0}, k-1) + m(KP_{n-3,0}, k-1) \leq m(KP_{n,1}, k)$$

for all values of n, k such that $n \geq 5$, with at least one strict inequality for some k. Let us first consider the latter: applying (2.3) to the pendant vertices of $KP_{n,1}$ and $KP_{n-1,1}$, we obtain

$$m(KP_{n,1}, k) - \big(m(KP_{n-1,1}, k) + m(KP_{n-2,0}, k-1) + m(KP_{n-3,0}, k-1)\big)$$

$$
\begin{aligned}
&= m(K_{n-1},k) + m(K_{n-2},k-1) - m(K_{n-2},k) \\
&\quad - m(K_{n-3},k-1) - m(K_{n-2},k-1) - m(K_{n-3},k-1) \\
&= m(K_{n-1},k) - m(K_{n-2},k) - 2m(K_{n-3},k-1).
\end{aligned}
$$

Applying (2.2) to any vertex of a complete graph yields the recursion $m(K_n,k) = m(K_{n-1},k) + (n-1)m(K_{n-2},k-1)$. Thus we get

$$
\begin{aligned}
m(KP_{n,1},k) &- \big(m(KP_{n-1,1},k) + m(KP_{n-2,0},k-1) + m(KP_{n-3,0},k-1)\big) \\
&= (n-4)m(K_{n-3},k-1),
\end{aligned}
$$

which is indeed nonnegative for all k and strictly positive for some values of k (e.g. $k=1$).

Finally, we prove (3.2) by induction on γ, starting with $\gamma = 2$. Using similar manipulations as in the case $\gamma = 1$, we find that

$$
\begin{aligned}
m(KP_{n,2},k) &- \big(m(KP_{n-1,2},k) + m(KP_{n-2,1},k-1) + m(KP_{n-3,0},k-1)\big) \\
&= m(K_{n-2},k) + m(K_{n-2},k-1) + m(K_{n-3},k-1) \\
&\quad - \big(m(K_{n-3},k) + 3m(K_{n-3},k-1) + m(K_{n-4},k-1) + m(K_{n-4},k-2)\big) \\
&= (n-5)m(K_{n-4},k-1) + (n-4)\big(m(K_{n-4},k-2) - m(K_{n-5},k-2)\big).
\end{aligned}
$$

Clearly, this is nonnegative for all $n \geq 6$ and all values of k, and strictly positive for at least one value of k (e.g. $k = 1$).

Next, for $\gamma = 3$, we have

$$
\begin{aligned}
m(KP_{n,3},k) &- \big(m(KP_{n-1,3},k) + m(KP_{n-2,2},k-1) + m(KP_{n-3,1},k-1)\big) \\
&= m(K_{n-3},k) + 2m(K_{n-3},k-1) + m(K_{n-4},k-1) + m(K_{n-4},k-2) \\
&\quad - \big(m(K_{n-4},k) + 4m(K_{n-4},k-1) + m(K_{n-4},k-2) \\
&\qquad + m(K_{n-5},k-1) + 3m(K_{n-5},k-2)\big) \\
&= (n-6)m(K_{n-5},k-1) + (2n-11)m(K_{n-5},k-2) - (n-5)m(K_{n-6},k-2).
\end{aligned}
$$

Again, we easily see that the expression is nonnegative for all $n \geq 7$ (note in particular that $2n - 11 > n - 5$), and strictly positive for at least one value of k (e.g. $k = 1$).

For the induction step, all we need is the identity

$$m(KP_{n,\gamma},k) = m(KP_{n-1,\gamma-1},k) + m(KP_{n-2,\gamma-2},k-1),$$

which follows from (2.3). This allows us to write the difference of the two sides in (3.2) as

$$\begin{aligned}
m(KP_{n,\gamma},k) &- \big(m(KP_{n-1,\gamma},k) + m(KP_{n-2,\gamma-1},k-1) + m(KP_{n-3,\gamma-2},k-1)\big) \\
&= m(KP_{n-1,\gamma-1},k) + m(KP_{n-2,\gamma-2},k-1) \\
&\quad - \big(m(KP_{n-2,\gamma-1},k) + m(KP_{n-3,\gamma-2},k-1) + m(KP_{n-4,\gamma-3},k-1)\big) \\
&\quad - \big(m(KP_{n-3,\gamma-2},k-1) + m(KP_{n-4,\gamma-3},k-2) + m(KP_{n-5,\gamma-4},k-2)\big)
\end{aligned}$$

and apply the induction hypothesis for $n-1,\gamma-1$ and $n-2,\gamma-2$ respectively. This completes the proof of the auxiliary inequality (3.2) and thus the statement in Case 2.

Case 3: Every terminal block in G has more than three vertices. Pick a terminal block B and let v be one of its vertices that is not a cut vertex. As explained earlier, we can assume without loss of generality that this block is complete. Let b be the number of vertices of B. If $b \geq n-\gamma$, then there are at most γ vertices outside of B, $\gamma - 1$ of which have to be cut vertices. So a terminal block other than B cannot contain more than one vertex that is not a cut vertex, which means that such a terminal block cannot contain more than two vertices in total. This contradicts the assumption of this case. Thus $3 < b < n - \gamma$.

Now let w be the unique neighbor of v that is a cut vertex of G, and let $x_1, x_2, \ldots, x_{b-2}$ be the other neighbors. Note that $G - v$ has $n-1$ vertices and γ cut vertices, so by the induction hypothesis $G - v \preceq KP_{n-1,\gamma}$. The graphs $G - v - x_j$ ($1 \leq j \leq b-2$) are all isomorphic and have $n-2$ vertices and γ cut vertices, so $G - v - x_j \preceq KP_{n-2,\gamma}$. Finally, since $G - v - w$ is isomorphic to a proper subgraph of $G - v - x_1$, we have $G - v - w \prec G - v - x_1$. Hence for every k, we obtain

$$\begin{aligned}
m(G,k) &= m(G-v,k) + (b-2)m(G-v-x_1,k-1) + m(G-v-w,k-1) \\
&\leq m(G-v,k) + (b-1)m(G-v-x_1,k-1) \\
&\leq m(KP_{n-1,\gamma},k) + (b-1)m(KP_{n-2,\gamma},k-1)
\end{aligned}$$

$$\leq m(KP_{n-1,\gamma}, k) + (n - \gamma - 2)m(KP_{n-2,\gamma}, k - 1)$$
$$\leq m(KP_{n-1,\gamma}, k) + (n - \gamma - 2)m(KP_{n-2,\gamma}, k - 1) + m(K_{n-\gamma-2} \uplus P_\gamma, k - 1)$$
$$= m(KP_{n,\gamma}, k).$$

Moreover, we have $m(G - v - w, 1) < m(G - v - x_1, 1)$ since $G - v - w$ is a proper subgraph of $G - v - x_1$. Thus we get $m(G, 2) < m(KP_{n,\gamma}, 2)$, which finally implies that $G \prec KP_{n,\gamma}$.

So in each of the cases, we obtain the desired statement $G \prec KP_{n,\gamma}$, completing the induction. ∎

We now turn our attention to the minimization problem for the set $\mathcal{G}_1(n, \gamma)$. We first need the following lemma involving a typical graph transformation.

Lemma 3.2 *Suppose that the connected graph H_1 can be decomposed into a graph G_0 and a graph H_0 sharing only a cut vertex u, as in Figure 3.3. Moreover, let H_2 be a graph consisting of G_0 and $|H_0|-1$ pendant vertices attached to u (see again Figure 3.3). Then we have $H_2 \prec H_1$, unless H_1 and H_2 are isomorphic.*

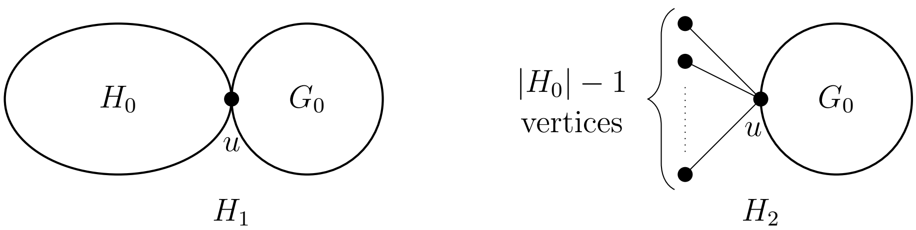

Figure 3.3. Lemma 3.2: H_1 to H_2

Proof. Let $\widetilde{H}$ be a graph obtained from H_1 by replacing H_0 with a spanning tree of H_0. Clearly, $\widetilde{H}$ is a subgraph of H_1. So by Lemma 2.2, we have $\widetilde{H} \preceq H_1$. Moreover, in view of Lemma 2.7, we have $H_2 \preceq \widetilde{H}$. So we can conclude that $H_2 \prec H_1$, unless $H_1 \cong \widetilde{H} \cong H_2$. ∎

Next, we can use Lemma 2.5 (due to Gutman) to settle the cases $\gamma = 1$ and $\gamma = 2$, which will serve as the base of an induction.

Lemma 3.3 *1. Let $n > 2$ be an integer. For every graph $G \in \mathcal{G}_1(n, 1)$ that is not isomorphic to the star S_n, we have $S_n \prec G$.*

2. Let $n > 3$ be an integer. For every graph $G \in \mathcal{G}_1(n, 2)$ that is not isomorphic to $SP_{n,2}$, we have $SP_{n,2} \prec G$.

Proof. The first statement holds for arbitrary connected graphs: let T be any spanning tree of G. By Lemma 2.2 and Lemma 2.5, we have $S_n \preceq T \preceq G$, and $S_n \prec G$ holds unless $S_n \cong T \cong G$.

The second statement is obtained in a similar fashion, and is even true for every connected graph G other than the star S_n. Since G is not isomorphic to a star or the complete graph K_3, there are two non-adjacent edges. These two edges can be extended to a spanning tree T that cannot be a star. Therefore, we have $SP_{n,2} \preceq T \preceq G$ by Lemma 2.2 and Lemma 2.5, and again we have $SP_{n,2} \prec G$ unless $SP_{n,2} \cong T \cong G$. ∎

We need one more auxiliary result before we can get to the proof of the main minimization theorem.

Lemma 3.4 *Let n, γ be integers with $1 \leq \gamma \leq n - 3$. We have $SP_{n,\gamma} \prec SP_{n,\gamma+1}$.*

Proof. In $SP_{n,\gamma+1}$, let u be the vertex that is adjacent to precisely one pendant vertex v (at the right end in Figure 1.2). In $SP_{n,\gamma}$, let x be the vertex of degree $n - \gamma$, and let y be one of the pendant vertices adjacent to it (at the left end in Figure 1.2). We observe that $SP_{n,\gamma+1} - v$ and $SP_{n,\gamma} - y$ are isomorphic. Moreover, $SP_{n,\gamma} - x - y$ consists of $n - \gamma - 2$ isolated vertices and a path P_γ, which is easily seen to be isomorphic to a proper subgraph of $SP_{n,\gamma+1} - u - v$. By Lemma 2.2, $SP_{n,\gamma} - x - y \prec SP_{n,\gamma+1} - u - v$. So for every k, we have

$$\begin{aligned} m(SP_{n,\gamma}, k) &= m(SP_{n,\gamma} - y, k) + m(SP_{n,\gamma} - x - y, k - 1) \\ &\leq m(SP_{n,\gamma+1} - v, k) + m(SP_{n,\gamma+1} - u - v, k - 1) \\ &= m(SP_{n,\gamma+1}, k). \end{aligned}$$

Strict inequality holds for at least one value of k, since $SP_{n,\gamma} - x - y \prec SP_{n,\gamma+1} - u - v$. Hence, we have $SP_{n,\gamma} \prec SP_{n,\gamma+1}$. ∎

Theorem 3.5 *Let n, γ be integers with $1 \leq \gamma \leq n-2$. For every graph G in $\mathcal{G}_1(n,\gamma)$ that is not isomorphic to $SP_{n,\gamma}$, we have $SP_{n,\gamma} \prec G$. In particular, $SP_{n,\gamma}$ is the unique graph in $\mathcal{G}_1(n,\gamma)$ that attains the minimum Hosoya index, and the unique graph that attains the minimum matching energy.*

Proof. We prove by induction on n that for every connected graph G with n vertices and γ cut vertices, we have $SP_{n,\gamma} \prec G$ unless $G \cong SP_{n,\gamma}$.

Before we get to the actual induction proof, let us remark that we can assume without loss of generality that all of the terminal blocks of G are single edges. Otherwise, we can apply the operation of Lemma 3.2 to obtain a graph G' with the same number of vertices and cut vertices for which $G' \prec G$.

We have already proven the statement for $\gamma = 1$ and $\gamma = 2$ in Lemma 3.3. For $\gamma = n-2$, we must have $G \cong P_n \cong SP_{n,n-2}$, since there are no other graphs with $n-2$ cut vertices. Also, the statement clearly holds for small values of n ($n \leq 3$) since there are no possible graphs except for $SP_{n,\gamma}$.

Consider a graph G with n vertices and γ cut vertices ($3 \leq \gamma \leq n-2$) that is not isomorphic to $SP_{n,\gamma}$. Let $B(G)$ be the block-cut tree of G. Choose an arbitrary vertex r of $B(G)$, and a cut vertex w of G whose distance from r in $B(G)$ is greatest. In view of this choice of w, we know that w is contained in at least one terminal block of G and exactly one non-terminal block of G. As explained earlier, we can assume without loss of generality that the terminal blocks of G are single edges. Hence the terminal blocks containing w in G are single edges. Let v be a pendant vertex that is adjacent to w. We distinguish two cases.

Case 1: There exists only one pendant vertex, say v, adjacent to w in G. Then $G-v$ is a connected graph with $n-1$ vertices and $\gamma-1$ cut vertices (w is no longer a cut vertex in $G-v$, since w belongs to exactly one non-terminal block). By the induction hypothesis, $SP_{n-1,\gamma-1} \preceq G-v$. Moreover, $G-v-w$ is a connected graph with $n-2$ vertices and at least $\gamma-2$ cut vertices: all cut vertices of G remain cut vertices, except for w and potentially one more vertex if the non-terminal block that w belongs to only contains two vertices. Thus by the induction hypothesis and Lemma 3.4, we have

$SP_{n-2,\gamma-2} \preceq G - v - w$.

So for every k, we have

$$\begin{aligned} m(G,k) &= m(G-v,k) + m(G-v-w,k-1) \\ &\geq m(SP_{n-1,\gamma-1},k) + m(SP_{n-2,\gamma-2},k-1) \\ &= m(SP_{n,\gamma},k). \end{aligned}$$

Strict inequality holds for at least one value of k unless $G - v \cong SP_{n-1,\gamma-1}$ and $G - v - w \cong SP_{n-2,\gamma-2}$. However, it is easy to see that this would imply $G \cong SP_{n,\gamma}$.

Case 2: There are t pendant vertices adjacent to w in G, where $t > 1$. If $t \geq n-\gamma-1$, then there are only $n-t \leq \gamma+1$ vertices left, γ of which have to be cut vertices in G. It is easy to see that this implies $G \cong SP_{n,\gamma}$. Thus we can assume that $1 < t < n-\gamma-1$.

Let v be a pendant vertex that is adjacent to w. Then $G - v$ is a connected graph with $n-1$ vertices and γ cut vertices (all cut vertices of G remain cut vertices). Thus by the induction hypothesis, $SP_{n-1,\gamma} \preceq G-v$. Moreover, $G-v-w$ consists of $t-1$ isolated vertices and a connected graph with $n-t-1$ vertices and at least $\gamma-2$ cut vertices (as in Case 1). Thus by the induction hypothesis and Lemma 3.4, $SP_{n-t-1,\gamma-2} \preceq G-v-w$. Since $t < n-\gamma-1$, we must have $\gamma < n-t-1$. Consequently, P_γ is a proper subgraph of $SP_{n-t-1,\gamma-2}$, which shows that $P_\gamma \prec SP_{n-t-1,\gamma-2} \preceq G - v - w$ by Lemma 2.2.

Again, we get

$$\begin{aligned} m(G,k) &= m(G-v,k) + m(G-v-w,k-1) \\ &\geq m(SP_{n-1,\gamma},k) + m(P_\gamma,k-1) \\ &= m(SP_{n,\gamma},k) \end{aligned}$$

for every k.

Since $P_\gamma \prec G - v - w$, we have strict inequality for at least one value of k.

In each of the two cases, we obtain the desired statement $G \prec SP_{n,\gamma}$, completing the induction. ∎

We remark that the situation is different for $\gamma = 0$. Note that $\mathcal{G}_1(n,0)$ is precisely the set of 2-connected graphs on n vertices. In this case, there is generally no graph G_0 such that $G_0 \preceq G$ for all $G \in \mathcal{G}_1(n,0)$. For example, there are three minimal elements with respect to $\preceq$ in $\mathcal{G}_1(7,0)$, which are pairwise incomparable. They are shown in Figure 3.4. We have

$$m(G_1,0) = 1,\ m(G_1,1) = 7,\ m(G_1,2) = 14,\ m(G_1,3) = 7,$$
$$m(G_2,0) = 1,\ m(G_2,1) = 9,\ m(G_2,2) = 19,\ m(G_2,3) = 6,$$
$$m(G_3,0) = 1,\ m(G_3,1) = 10,\ m(G_3,2) = 20,\ m(G_3,3) = 0,$$

and none of the three graphs has a matching of cardinality greater than 3. The minimum Hosoya index in this case is $Z(G_1) = 29$, while the minimum matching energy is $ME(G_3) = 2\sqrt{10 + 4\sqrt{5}}$.

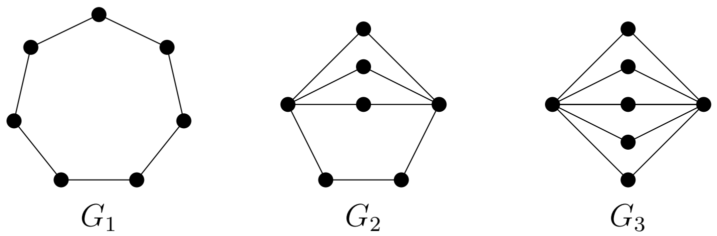

Figure 3.4. The three minimal graphs for $n = 7$, $\gamma = 0$.

3.2 Fixed number of cut edges

Now we turn our attention to graphs with a given number of cut edges. Recall that $\mathcal{G}_2(n,\gamma)$ is the set of graphs with n vertices and γ cut edges. It is worth pointing out the elementary facts that a graph with n vertices is a tree if and only if it has $n-1$ cut edges, and that there are no graphs with n vertices and $n-2$ or more than $n-1$ cut edges for any n.

The main result of this section is very similar to Theorem 3.1.

Theorem 3.6 *Let n and γ be integers with $0 \le \gamma \le n-1$, $\gamma \ne n-2$. For every graph G in $\mathcal{G}_2(n,\gamma)$ that is not isomorphic to $KP_{n,\gamma}$, we have $G \prec KP_{n,\gamma}$. In particular, $KP_{n,\gamma}$ is the unique graph in $\mathcal{G}_2(n,\gamma)$ that attains the maximum Hosoya index, and the unique graph that attains the maximum matching energy.*

Proof. If $\gamma = n-1$, then the graph G must be a tree, so the statement is equivalent to Lemma 2.4. For $\gamma = 0$ we trivially have $G \prec K_n$ unless $G \cong K_n$. Thus we can assume that $1 \le \gamma \le n-3$. We prove the statement of the theorem by induction on n.

For a graph $G \in \mathcal{G}_2(n,\gamma)$, let B be the set of cut-edges of G. Let $\mathcal{C}$ denote the set of connected components of $G' = G - B$. There are two types of elements in $\mathcal{C}$, singletons and connected bridgeless subgraphs of G. Let $\mathcal{S} \subseteq \mathcal{C}$ denote the singletons and let $\mathcal{D} = \mathcal{C} \setminus \mathcal{S}$. Each element of $\mathcal{S}$ is, therefore, a vertex, and each element of $\mathcal{D}$ is a connected bridgeless subgraph of G. Similar to the proof of Theorem 3.1, we can assume without loss of generality that all the elements in $\mathcal{D}$ are complete.

We then proceed with the induction. The statement we aim to prove is easily verified for small values of n ($n \le 4$). We suppose that the statement holds for graphs on less than n vertices. Consider a graph G with n vertices and γ cut edges that is not isomorphic to $KP_{n,\gamma}$. We distinguish two cases.

Case 1: There exists a pendant vertex in G. Let v be such a pendant vertex, let its unique neighbor be w, and note that $G - v$ has $n-1$ vertices and $\gamma - 1$ cut edges. By the induction hypothesis, $G - v \preceq KP_{n-1,\gamma-1}$.

Suppose that $G - v - w$ has t connected components (possibly $t = 1$). For each of these components, there is at most one cut edge in G connecting it to w (if there are several edges connecting such a component to w, they cannot be cut edges). Thus $G - v - w$ still has at least $\gamma - t - 1$ cut edges left. Add $t - 1$ edges between the components of $G - v - w$ so that the resulting graph G' is connected. Then G' is a connected graph with $n-2$ vertices and at least $\gamma - 2$ cut edges. It follows from the induction hypothesis and (3.1) that $G - v - w \preceq G' \preceq KP_{n-2,\gamma-2}$.

So for every k, we have

$$\begin{aligned} m(G,k) &= m(G-v,k) + m(G-v-w,k-1) \\ &\le m(KP_{n-1,\gamma-1},k) + m(KP_{n-2,\gamma-2},k-1) \\ &= m(KP_{n,\gamma},k). \end{aligned}$$

Strict inequality holds for at least one value of k unless $G - v \cong KP_{n-1,\gamma-1}$ and

$G - v - w \cong KP_{n-2,\gamma-2}$. However, it is easy to see that this would imply $G \cong KP_{n,\gamma}$.

Case 2: There exists no pendant vertex in G. Let S be the set of cut edges of G. Then the edge-induced subgraph $G[S]$ is a forest with γ edges, which implies that $G[S]$ has $\gamma + c(G[S])$ vertices, where $c(G[S])$ is the number of components of $G[S]$.

Since all the cut edges of G are not pendant edges, all vertices of $G[S]$ are cut vertices of G. Thus we obtain that G has $\gamma + c(G[S])$ cut vertices. From Theorem 3.1 and Eq. (3.1), we know that $G \preceq KP_{n,\gamma+c(G[S])} \preceq KP_{n,\gamma+1} \prec KP_{n,\gamma}$.

In each of the two cases, we obtain the desired statement that $G \prec KP_{n,\gamma}$, completing the induction. ∎

Let us finally remark that the situation is much more involved for the analogous minimizing problem in $\mathcal{G}_2(n,\gamma)$ in that there is generally no least element with respect to the quasi-order $\preceq$. For example, when $n = 6$ and $\gamma = 1$, then there are three different minimal elements that are mutually incomparable. They are shown in Figure 3.5. We have

$$m(G_1,0) = 1,\ m(G_1,1) = 6,\ m(G_1,2) = 8,\ m(G_1,3) = 1,$$
$$m(G_2,0) = 1,\ m(G_2,1) = 7,\ m(G_2,2) = 7,\ m(G_2,3) = 1,$$
$$m(G_3,0) = 1,\ m(G_3,1) = 7,\ m(G_3,2) = 9,\ m(G_3,3) = 0,$$

and none of the three graphs has a matching of cardinality greater than 3. The minimum Hosoya index in this case is $Z(G_1) = Z(G_2) = 16$, while the minimum matching energy is $ME(G_3) = 2\sqrt{13}$.

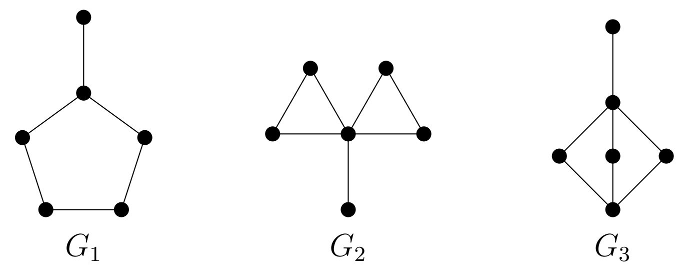

Figure 3.5. The three minimal graphs for $n = 6$, $\gamma = 1$.

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