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On graphs whose Hosoya indices are primitive Pythagorean triples

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Abstract: We discuss families of triples of graphs whose Hosoya indices are primitive Pythagorean triples. Hosoya gave a method to construct such families of caterpillars, i.e., trees whose vertices are within distance 1 of a central path. He also pointed out a common structure to the families. In this paper, we show the uniqueness of the common structure.

Keywords: Caterpillar trees, continuants, Z-indices, reduced Pythagorean triples, continued fractions.
AMS Classification: 05C30, 05C70, 05C05, 05C50, 11A05, 11A55.

1 Introduction

In this paper, we consider *a primitive Pythagorean triple*, i.e., a triple (a, b, c) of positive integers satisfying the following conditions:

- $a^2 + b^2 = c^2$,
- a, b and c are relatively prime, and
- a and c are odd, b is even.

We discuss a way to realize a primitive Pythagorean triple as the Hosoya indices of graphs. For a graph G, a matching in G is a subset of the edge set of G such that any two distinct edges do not share any vertices. The *Hosoya index* $Z(G)$, or the Z*-index*, introduced in Hosoya [1] is the number of matchings in a graph G. He introduced the graph invariant for his chemical studies, and developed mathematical theory. Recently he studies a family of triples (A, B, C) of graphs such that $(Z(A), Z(B), Z(C))$ is a Pythagorean triple. In [3, 4], Hosoya studied primitive Pythagorean triples with consecutive legs. He gave a family of triples of caterpillars which realizes them. (See Definition 2.1 for the definition of a graph called a caterpillar.) In [5], he showed that a triple of graphs obtained by gluing copies of a graph in some manner realize a Pythagorean triple. He also introduced a method to construct a triple of caterpillars which realizes a primitive Pythagorean triple in [6]. His method is based on the Euclidean algorithm. First we run the Euclidean algorithm for some integers. Next we construct a caterpillar from the information of the Euclidean algorithm. The number of leaves of the caterpillar obtained by the second procedure corresponds to the quotient of each step of the Euclidean algorithm. In this sense, the caterpillar is a visualization of the Euclidean algorithm. Finally we construct a triple of caterpillars by gluing copies of the caterpillar obtained by the second procedure to a certain triple of caterpillars, called a symmetric kernel. Then the triple of the caterpillars realizes a primitive Pythagorean triple. Hosoya gave two candidates of symmetric kernels. From one of them, we can constract a triple of caterpillars for each primitive Pythagorean triples (a, b, c) satisfying $a/b < 3/4$. From the other symmetric kernel, we can constract triples for the other primitive Pythagorean triples. Hosoya conjectured the uniquness of such symmetric kernels.

In this paper, we discuss the following problem: We construct a triple of graphs by gluing copies of a graph to a symmetric kernel. We do not assume that the graphs are caterpillars. We obtain a family of triples of graphs from a family of graphs and a common symmetric kernel by this construction. Characterize a common symmetric kernel such that we can obtain a family of triples of graphs which realizes a family of primitive Pythagorean triples. In this paper, we divide primitive Pythagorean triples (a, b, c) into two families by the ratio a/b, and show the uniqueness of the common symmetric kernel for each family (Theorems 3.4 and 3.5).

This paper is organized as follows: In Section 2, we define notation and give examples. We show main results in Section 3. In the proof, we use some technical lemmas shown in Section 4.

2 Definition

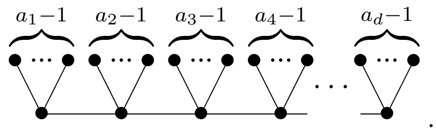
First we define some typical graphs in our discussion. In this paper we consider a non-directed simple graph $G = (V, E)$, i.e., a graph whose set of vertices is V and whose set of non-directed edges is E which contains no multiple edges and no self loops. We can regard E as a subset of $\{\, \{v, w\} \subset V \mid v \neq w \,\}$.

Definition 2.1. For positive integers $a_1, \ldots, a_d$, we define the *caterpillar* $C(a_1, \ldots, a_d)$ to be the following graph (V, E):

$$V_i = \{\, (i, j) \mid j = 1, \ldots, a_i \,\},$$
$$V = \bigcup_{i=1}^{d} V_i,$$
$$E_i = \{\, \{(i, 1), (i, j)\} \mid 1 < j \leq a_i \,\},$$

$$H = \{ \{(i,1),(i+1,1)\} \mid i = 1,\dots,d-1 \},$$
$$E = H \cup \bigcup_{i=1}^{d} E_i.$$

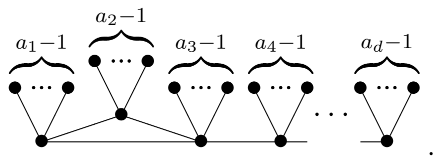
The graph (V_i, E_i) is the star graph or the complete bipartite graph K_{1,a_i-1}. The edges in H connects the central vertices $(i,1)$ and $(i+1,1)$ of (V_i, E_i) and (V_{i+1}, E_{i+1}). Hence $C(a_1,\dots,a_d)$ is



Note that the caterpillar $C(a_1,\dots,a_{d-1},a_d,1)$ is isomorphic to the caterpillar $C(a_1,\dots,a_{d-1},a_d+1)$ as graphs.

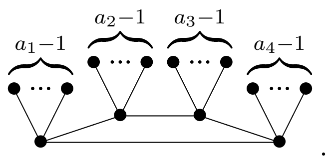
Definition 2.2. For positive integers $a_1,\dots,a_d$ and s, we define the graph $Q_s(a_1,\dots,a_d)$ to be the graph obtained from the caterpillar $C(a_1,\dots,a_d)$ by adding the edge $\{(1,1),(s,1)\}$.

Example 2.3. Since the caterpillar $C(a_1,\dots,a_d)$ is a tree, the graph $Q_3(a_1,\dots,a_d)$ has a unique cycle of length 3. The graph $Q_3(a_1,\dots,a_d)$ is



Note that the graph $Q_3(a_1,a_2,a_3,\dots,a_d)$ is isomorphic to the graph $Q_3(a_2,a_1,a_3,\dots,a_d)$ as graphs.

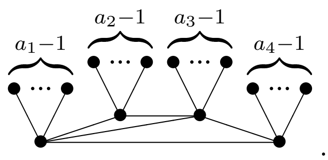
Example 2.4. The graph $Q_4(a_1,a_2,a_3,a_4)$ has a unique cycle of length 4. The graph $Q_4(a_1,a_2,a_3,a_4)$ is



Note that $Q_4(a_1,a_2,a_3,a_4)$, $Q_4(a_2,a_3,a_4,a_1)$ and $Q_4(a_4,a_3,a_2,a_1)$ are isomorphic to one another as graphs.

Definition 2.5. For positive integers $a_1,\dots,a_d$ and s, we define the graph $\Theta_s(a_1,\dots,a_d)$ to be the graph obtained from the caterpillar $C(a_1,\dots,a_d)$ by adding the edge $\{(1,1),(s,1)\}$ and $\{(1,1),(d,1)\}$.

Example 2.6. For the positive integers a_1, a_2, a_3 and a_4, the graph $\Theta_3(a_1,a_2,a_3,a_4)$ is



In this paper, we discuss a common structure to a family of graphs. To formulate such structures, we define an operation to make a new graph from two graphs.

Definition 2.7. Let G and H be graphs. For a vertex v in G and a vertex h in H, we define a *one-point union* $G \underset{g,h}{\vee} H$ *at base points* g *and* h to be the graph obtained from the disjoint union of G and H by contracting the vertices g and h.

If the context makes base points clear, then we will omit base points as $G \vee H$.

Definition 2.8. For $i = 1, \dots, d$, we write $C(a_1, \dots, \dot{a}_i, \dots, a_d)$ to denote the caterpillar $C(a_1, \dots, a_d)$ with the base point $(i, 1)$ to make a one-point union. Similarly, for l and r satisfying $l \le r$, we write $C(a_1, \dots, \dot{a}_l, \dots, \dot{a}_r, \dots, a_d)$ to denote the caterpillar $C(a_1, \dots, a_d)$ with the base point $(l, 1)$ to make a one-point union from the left and with the base point $(r, 1)$ to make a one-point union from the right. If $l = r$, then we write $C(a_1, \dots, \ddot{a}_l, \dots, a_d)$. We also define this notation for Q in the same manner.

Example 2.9. Let

$$G = C(\dot{a}_1, a_2, \dots, a_{d-1}, \dot{a}_d),$$
$$H = C(\dot{b}_1, b_2, \dots, b_{e-1}, \dot{b}_e).$$

In this case, we have

$$G \vee H = C(\dot{a}_1, a_2, \dots, a_{d-1}, a_d + b_1 - 1, b_2, \dots, b_{e-1}, \dot{b}_e).$$

Definition 2.10. Let S_i be a graph with the base point l_i to make a one-point union from the left and with the base point r_i to make a one-point union from the right. We say that (S_1, S_2, S_3) is a *symmetric kernel* of a triple (G_1, G_2, G_3) of graphs if there exist a graph G and a vertex g of G such that

$$G_i = G \underset{g,l_i}{\vee} S_i \underset{r_i,g}{\vee} G \quad (i = 1, 2, 3).$$

Next we recall the Hosoya index for a graph. The Hosoya index is defined as follows.

Definition 2.11. For a graph G, we call a set M of edges a *matching* in G if no pair of edges in M share a vertex. Define $p(G, k)$ to be the number of matchings with k edges in G. We also define the *Hosoya index* $Z(G)$ by $Z(G) = \sum_k p(G, k)$.

Remark 2.12. If G' is a subgraph of G, then a matching in G' is a matching in G. Hence we have $p(G', k) \le p(G, k)$, which implies $Z(G') \le Z(G)$. Since $p(G, k)$ is the number of edges in G, the Hosoya index $Z(G)$ is greater than the number of edges in G.

The following formulas for $Z(G)$ are known.

Lemma 2.13. *If the graph G is the disjoint union of graphs G_1 and G_2, then the graphs G, G_1 and G_2 satisfy the equation*

$$Z(G) = Z(G_1) \cdot Z(G_2).$$

Lemma 2.14. *Fix an edge $\{u, v\}$ of the graph G. Let $G_{\{u,v\}}$ be the graph obtained from G by removing the edge $\{u, v\}$, and $G_{u,v}$ the restriction of G to vertices other than u and v. The graphs G, G' and G'' satisfy the equation*

$$Z(G) = Z(G_{\{u,v\}}) + Z(G_{u,v}).$$

Thanks to these two formulas, we can calculate the Hosoya index recursively.

Example 2.15. The following are the complete list of connected graphs with at most three edges:

$$Z(C(1)) = 1, \qquad Z(C(2)) = 2, \qquad Z(C(3)) = 3,$$
$$Z(C(2,2)) = 5, \qquad Z(C(4)) = 4, \qquad Z(Q_3(1,1,1)) = 4.$$

The following are the complete list of connected graphs with four edges:

$$Z(C(2,1,2)) = 8, \qquad Z(C(2,3)) = 7, \qquad Z(C(5)) = 5,$$
$$Z(Q_3(1,1,2)) = 6, \qquad Z(Q_4(1,1,1,1)) = 7.$$

The following are the complete list of caterpillar graphs with five edges:

$$Z(C(2,1,1,2)) = 13, \qquad Z(C(2,1,3)) = 11, \qquad Z(C(2,2,2)) = 12,$$
$$Z(C(2,4)) = 9, \qquad Z(C(3,3)) = 10, \qquad Z(C(6)) = 6.$$

The following are the complete list of connected graphs with five edges containing $Q_3(1,1,1)$ as a subgraph:

$$Z(Q_3(1,1,1;2)) = 10, \qquad Z(Q_3(1,1,3)) = 8, \qquad Z(Q_3(2,1,2)) = 9,$$
$$Z(\Theta_3(1,1,1,1)) = 8.$$

The following are the complete list of the other connected graphs with five edges:

$$Z(Q_4(1,1,1,2)) = 10, \qquad Z(Q_5(1,1,1,1,1)) = 11.$$

See also Section 4.1.

Finally we define notation for continued fractions and continuants.

Definition 2.16. For positive integers $a_1, \ldots, a_d$, we define a rational number $[a_1, \ldots, a_d]$ by

$$[a_1, \ldots, a_d] = a_1 + \cfrac{1}{a_2 + \cfrac{1}{\ddots \, \cfrac{\ddots}{a_{d-1} + \cfrac{1}{a_d}}}}.$$

Note that $[a_1, \ldots, a_{d-1}, a_d, 1] = [a_1, \ldots, a_{d-1}, a_d + 1]$.

Definition 2.17. We define the polynomials K_d in variables $x_1, x_2, \ldots$ by

$$\begin{aligned} K_0 &= 1, \\ K_1 &= x_1, \\ K_d &= x_d K_{d-1} + K_{d-2}. \end{aligned}$$

The polynomial K_d is called the *continuant*. For positive integers $a_1, \ldots, a_d$, we write $K(a_1, \ldots, a_d)$ to denote the integer obtained by substituting a_i for x_i in K_d.

It is known that $K(a_1, \ldots, a_d)$ and $K(a_2, \ldots, a_d)$ are relatively prime integers satisfying

$$[a_1, \ldots, a_d] = \frac{K(a_1, \ldots, a_d)}{K(a_2, \ldots, a_d)}$$

for positive integers $a_1, \ldots, a_d$. In [2], Hosoya showed that

$$K(a_1, \ldots, a_d) = Z(C(a_1, \ldots, a_d)).$$

Since $K(a_1, \ldots, a_d) = K(a_d, \ldots, a_1)$, it also follows that

$$K(a_1, a_2, \ldots, a_d) = a_1 K(a_2, \ldots, a_d) + K(a_3, \ldots, a_d).$$

Lemma 2.18. *If positive integers* $a_1, \ldots, a_d$, $b_1, \ldots, b_e$ *satisfy*

$$\begin{aligned} K(a_1, \ldots, a_d) &= K(b_1, \ldots, b_e), \\ K(a_2, \ldots, a_d) &= K(b_2, \ldots, b_e), \\ a_d, b_e &> 1, \end{aligned}$$

then $d = e$ *and* $(a_1, \ldots, a_d) = (b_1, \ldots, b_e)$.

Proof. First consider the case where $e = 1$. In this case, $K(b_1, \ldots, b_e) = K(b_1) = b_1$ and $K(b_2, \ldots, b_e) = K_0 = 1$. If $d \geq 2$, then we have

$$K(a_2, \ldots, a_d) \geq K(a_d) = a_d > 1,$$

which contradicts the condition. If $d = 1$, then we have $K(a_1) = a_1$, which implies $a_1 = b_1$.

We consider the case where $d \geq e \geq 2$. Let

$$\begin{aligned} m &= K(a_1, \ldots, a_d) = K(b_1, \ldots, b_e), \\ n &= K(a_2, \ldots, a_d) = K(b_2, \ldots, b_e). \end{aligned}$$

It follows by the definition of continuants that

$$\begin{aligned} m &= K(a_1, \ldots, a_d) = a_1 K(a_2, \ldots, a_d) + K(a_3, \ldots, a_d) \\ &= a_1 n + K(a_3, \ldots, a_d), \\ m &= K(b_1, \ldots, b_e) = b_1 K(b_2, \ldots, b_e) + K(b_3, \ldots, b_e) \\ &= b_1 n + K(b_3, \ldots, b_e). \end{aligned}$$

Hence we have

$$(b_1 - a_1)n = K(a_3, \dots, a_d) - K(b_3, \dots, b_e).$$

Since both $K(a_3, \dots, a_d)$ and $K(b_3, \dots, b_e)$ are less than

$$n = K(a_2, \dots, a_d) = K(b_2, \dots, b_e),$$

we have the inequality

$$-n < K(a_3, \dots, a_d) - K(b_3, \dots, b_e) < n.$$

Hence $b_1 - a_1 = 0$. It also follows that

$$K(a_3, \dots, a_d) - K(b_3, \dots, b_e) = 0.$$

Hence we have the lemma by induction. □

Lemma 2.18 implies the following lemma.

Lemma 2.19. *Let $G = C(a_1, \dots, a_d)$ and $G' = C(b_1, \dots, b_e)$. Assume that $d \geq e \geq 2$. If*

$$Z(C(a_1, \dots, a_d)) = Z(C(b_1, \dots, b_e)),$$
$$Z(C(a_2, \dots, a_d)) = Z(C(b_2, \dots, b_e)),$$

then the caterpillar G is isomorphic to the caterpillar G' as graphs, and $a_i = b_i$ for each $i = 1, \dots, e-1$.

Proof. If a_d and b_e are greater than 1, then it follows from Lemma 2.18 that G is isomorphic to G' as graphs. Consider the case where $b_e = 1$. If $e > 2$, then we have

$$C(b_1, \dots, b_{e-1}, 1) = C(b_1, \dots, b_{d-1} + 1),$$
$$C(b_2, \dots, b_{e-1}, 1) = C(b_2, \dots, b_{d-1} + 1).$$

Hence we may assume that $b_e > 1$. Similarly we may assume that $a_d > 1$. Hence it follows from Lemma 2.18 that G is isomorphic to G' as graphs. If $e = 2$, then $Z(C(a_2, \dots, a_d)) = Z(C(b_2)) = 1$. Hence the graph G is the caterpillar $C(a_1, 1)$. Since $Z(C(a_1, 1)) = Z(C(b_1, 1))$, we have $a_1 + 1 = b_1 + 1$, which implies $a_1 = b_1$. □

3 Main results

We consider a family of triples $(A_{m,n}, B_{m,n}, C_{m,n})$ of graphs which gives primitive Pythagorean triples as $(Z(A_{m,n}), Z(B_{m,n}), Z(C_{m,n}))$, and the common symmetric kernel to the family. In other words, we consider the triple (A, B, C) of graphs with base points and the family of graphs $G_{m,n}$ with base points satisfying

$$A_{m,n} = G_{m,n} \vee A \vee G_{m,n},$$
$$B_{m,n} = G_{m,n} \vee B \vee G_{m,n},$$
$$C_{m,n} = G_{m,n} \vee C \vee G_{m,n}.$$

Let $\mathcal{P}$ be the set of the pair (m, n) of positive integers satisfying the following:

- m and n are relatively prime,
- m and n have opposite parity,
- $m > n$.

It is known that there exists a bijection φ from $\mathcal{P}$ to the set of primitive Pythagorean triples defined by $\varphi(m,n) = (m^2 - n^2, 2mn, m^2 + n^2)$.

Define $\mathcal{P}_1$ and $\mathcal{P}_2$ by

$$\mathcal{P}_1 = \left\{ (m,n) \in \mathcal{P} \;\middle|\; \frac{m}{n} \geq 2 \right\}$$
$$\mathcal{P}_2 = \left\{ (m,n) \in \mathcal{P} \;\middle|\; 1 < \frac{m}{n} < 2 \right\}.$$

Remark 3.1. For $(m,n) \in \mathcal{P}$, the primitive Pythagorean triple corresponding (m,n) is $(m^2 - n^2, 2mn, m^2 + n^2)$. Hence the pair in $\mathcal{P}_1$ corresponds to the primitive Pythagorean triple (a,b,c) such that $a/b \geq 3/4$. the pair in $\mathcal{P}_2$ corresponds to the primitive Pythagorean triple (a,b,c) such that $0 < a/b < 3/4$.

In [6], Hosoya developed a method, based on Euclidean algorithm, to construct a triple of caterpillars whose Hosoya indices are primitive Pythagorean triples corresponding to $\mathcal{P}_1$. He also gave one for $\mathcal{P}_2$. Here we show essentially the same propositions as his methods.

Proposition 3.2. *Let $(m,n) \in \mathcal{P}_1$ and positive integers $a_1, \ldots, a_d$ satisfy $m/n = [a_1, \ldots, a_d]$. Note that $a_1 \geq 2$. Define $G^{(1)}_{m,n}$, $A_{m,n}$, $B_{m,n}$, $C_{m,n}$ by*

$$\begin{aligned} G^{(1)}_{m,n} &= C(a_1 \dot{-} 1, a_2, \ldots, a_d), \\ A_{m,n} &= G^{(1)}_{m,n} \vee C(\dot{1}, 1, \dot{1}) \vee G^{(1)}_{m,n}, \\ B_{m,n} &= G^{(1)}_{m,n} \vee C(\ddot{4}) \vee G^{(1)}_{m,n}, \\ C_{m,n} &= G^{(1)}_{m,n} \vee C(\dot{2}, \dot{2}) \vee G^{(1)}_{m,n}. \end{aligned}$$

The triple $(Z(A_{m,n}), Z(B_{m,n}), Z(C_{m,n}))$ of Hosoya indices is the primitive Pythagorean triple $(m^2 - n^2, 2mn, m^2 + n^2)$.

Proof. Since m and n are relatively prime, we have

$$\begin{aligned} Z(C(a_1, \ldots, a_d))) &= K(a_1, \ldots, a_d) = m, \\ Z(C(a_2, \ldots, a_d))) &= K(a_2, \ldots, a_d) = n. \end{aligned}$$

Since $G^{(1)}_{m,n} = C(a_1 \dot{-} 1, a_2, \ldots, a_d)$, we obtain

$$\begin{aligned} A_{m,n} &= G^{(1)}_{m,n} \vee C(\dot{1}, 1, \dot{1}) \vee G^{(1)}_{m,n} \\ &= C(a_d, a_{d-1}, \ldots, a_2, a_1 - 1, 1, a_1 - 1, a_2, \ldots, a_{d-1}, a_d), \\ B_{m,n} &= G^{(1)}_{m,n} \vee C(\ddot{4}) \vee G^{(1)}_{m,n} \\ &= C(a_d, a_{d-1}, \ldots, a_3, a_2, 2a_1, a_2, a_3, \ldots, a_{d-1}, a_d), \\ C_{m,n} &= G^{(1)}_{m,n} \vee C(\dot{2}, \dot{2}) \vee G^{(1)}_{m,n} \\ &= C(a_d, a_{d-1}, \ldots, a_3, a_2, a_1, a_1, a_2, a_3, \ldots, a_{d-1}, a_d). \end{aligned}$$

Applying Lemma 2.14 to the central edge $\{(d,1),(d+1,1)\}$ of $C_{m,n}$, we obtain

$$\begin{aligned}
&Z(C_{m,n})\\
=&Z(C(a_d,a_{d-1},\dots,a_3,a_2,a_1,a_1,a_2,a_3,\dots,a_{d-1},a_d))\\
=&Z(C(a_d,a_{d-1},\dots,a_3,a_2,a_1)\cdot Z(C(a_1,a_2,a_3,\dots,a_{d-1},a_d)\\
&+Z(C(a_d,a_{d-1},\dots,a_3,a_2))\cdot Z(C(a_2,a_3,\dots,a_{d-1},a_d)\\
=&m^2+n^2.
\end{aligned}$$

Similarly, since

$$\begin{aligned}
&Z(C(2a_1,a_2,a_3,\dots,a_d))+Z(C(a_3,\dots,a_d))\\
&=2a_1Z(C(a_2,a_3,\dots,a_d))+Z(C(a_3,\dots,a_d))+Z(C(a_3,\dots,a_d))\\
&=2(a_1Z(C(a_2,a_3,\dots,a_d))+Z(C(a_3,\dots,a_d)))\\
&=2Z(C(a_1,a_3,\dots,a_d))=2m,
\end{aligned}$$

we obtain

$$\begin{aligned}
&Z(B_{m,n})\\
=&Z(C(a_d,a_{d-1},\dots,a_3,a_2,2a_1,a_2,a_3,\dots,a_{d-1},a_d))\\
=&Z(C(a_d,a_{d-1},\dots,a_3,a_2,2a_1))\cdot Z(C(a_2,a_3,\dots,a_{d-1},a_d))\\
&+Z(C(a_d,a_{d-1},\dots,a_3,a_2))\cdot Z(C(a_3,\dots,a_{d-1},a_d))\\
=&Z(C(2a_1,a_2,\dots,a_d))\cdot n+n\cdot Z(C(a_3,\dots,a_d))\\
=&n(Z(C(2a_1,a_2,\dots,a_d))+Z(C(a_3,\dots,a_d)))\\
=&2mn.
\end{aligned}$$

Since $K(a_1,\dots,a_d)=a_1K(a_2,\dots,a_d)+K(a_3,\dots,a_d)$, we have

$$\begin{aligned}
K(a_1-1,\dots,a_d)&=(a_1-1)K(a_2,\dots,a_d)+K(a_3,\dots,a_d)\\
&=a_1K(a_2,\dots,a_d)+K(a_3,\dots,a_d)-K(a_2,\dots,a_d)\\
&=K(a_1,\dots,a_d)-K(a_2,\dots,a_d)\\
&=m-n.
\end{aligned}$$

Hence it follows that

$$\begin{aligned}
&Z(A_{m,n})\\
=&Z(C(a_d,a_{d-1},\dots,a_2,a_1-1,1,a_1-1,a_2,\dots,a_{d-1},a_d))\\
=&Z(C(a_d,a_{d-1},\dots,a_2,a_1-1))\cdot Z(C(1,a_1-1,a_2,\dots,a_{d-1},a_d))\\
&+Z(C(a_d,a_{d-1},\dots,a_2))\cdot Z(C(a_1-1,a_2,\dots,a_{d-1},a_d))\\
=&(m-n)\cdot Z(C(1,a_1-1,a_2,\dots,a_d))+Z(C(a_2,\dots,a_d))\cdot(m-n)\\
=&(m-n)(Z(C(a_1,a_2,\dots,a_d))+Z(C(a_2,\dots,a_d)))\\
=&(m-n)(m+n)=m^2+n^2.
\end{aligned}$$

□

Proposition 3.3. *Let* $(m,n) \in \mathcal{P}_2$ *and positive integers* $a_1, \dots, a_d$ *satisfy* $m/n = [a_1, \dots, a_d]$. *Define* $G^{(2)}_{m,n}$, $A_{m,n}$, $B_{m,n}$, $C_{m,n}$ *by*

$$\begin{aligned} G^{(2)}_{m,n} &= C(\dot{a}_2, a_3, \dots, a_d), \\ A_{m,n} &= G^{(2)}_{m,n} \vee C(\ddot{3}) \vee G^{(2)}_{m,n}, \\ B_{m,n} &= G^{(2)}_{m,n} \vee C(\dot{1}, 2, \dot{1}) \vee G^{(2)}_{m,n}, \\ C_{m,n} &= G^{(2)}_{m,n} \vee C(\dot{1}, 1, 1, \dot{1}) \vee G^{(2)}_{m,n}. \end{aligned}$$

The triple $(Z(A_{m,n}), Z(B_{m,n}), Z(C_{m,n}))$ *of Hosoya indices is the primitive Pythagorean triple* $(m^2 - n^2, 2mn, m^2 + n^2)$.

Proof. Similarly to the case where $(m,n) \in \mathcal{P}_1$, we have

$$\begin{aligned} Z(C(a_1, \dots, a_d))) &= m, \\ Z(C(a_2, \dots, a_d))) &= n. \end{aligned}$$

Since $G^{(2)}_{m,n} = C(\dot{a}_2, a_3, \dots, a_d)$ and $a_1 = 1$, we have

$$\begin{aligned} A_{m,n} &= G^{(2)}_{m,n} \vee C(\ddot{3}) \vee G^{(2)}_{m,n} \\ &= C(a_d, a_{d-1}, \dots, a_3, 2a_2 + 1, a_3, \dots, a_{d-1}, a_d), \\ B_{m,n} &= G^{(2)}_{m,n} \vee C(\dot{1}, 2, \dot{1}) \vee G^{(2)}_{m,n} \\ &= C(a_d, a_{d-1}, \dots, a_3, a_2, 2, a_2, a_3, \dots, a_{d-1}, a_d) \\ &= C(a_d, a_{d-1}, \dots, a_3, a_2, 2a_1, a_2, a_3, \dots, a_{d-1}, a_d), \\ C_{m,n} &= G^{(2)}_{m,n} \vee C(\dot{1}, 1, 1, \dot{1}) \vee G^{(2)}_{m,n} \\ &= C(a_d, a_{d-1}, \dots, a_3, a_2, 1, 1, a_2, a_3, \dots, a_{d-1}, a_d) \\ &= C(a_d, a_{d-1}, \dots, a_3, a_2, a_1, a_1, a_2, a_3, \dots, a_{d-1}, a_d). \end{aligned}$$

Hence, similarly to the case where $(m,n) \in \mathcal{P}_1$, we obtain $Z(B_{m,n}) = 2mn$ and $Z(C_{m,n}) = m^2 + n^2$. Since

$$\begin{aligned} Z(C(a_1, \dots, a_d)) &= a_1 Z(C(a_2, \dots, a_d)) + Z(C(a_3, \dots, a_d)) \\ &= Z(C(a_2, \dots, a_d)) + Z(C(a_3, \dots, a_d)), \end{aligned}$$

we have

$$\begin{aligned} Z(C(a_3, \dots, a_d)) &= Z(C(a_1, \dots, a_d)) - Z(C(a_2, \dots, a_d)) \\ &= m - n. \end{aligned}$$

Applying Lemma 2.14 to central edges $\{(d-1, 1), (d-1, j)\}$ in $A_{m,n}$ for $j = 2, 3, \dots, 2a_2 + 1$, we obtain

$$\begin{aligned} & Z(A_{m,n}) \\ =& Z(C(a_d, a_{d-1}, \dots, a_3, 2a_2 + 1, a_3, \dots, a_{d-1}, a_d)) \\ =& Z(C(a_d, a_{d-1}, \dots, a_3, 1, a_3, \dots, a_{d-1}, a_d)) + 2a_2 Z(C(a_3, \dots, a_{d-1}, a_d))^2 \\ =& Z(C(a_d, a_{d-1}, \dots, a_3, 1, a_3, \dots, a_{d-1}, a_d)) + 2a_2(m-n)^2. \end{aligned}$$

Since

$$\begin{aligned}
&Z(C(a_d, a_{d-1}, \ldots, a_3, 1, a_3, \ldots, a_{d-1}, a_d)) \\
=&Z(C(a_d, a_{d-1}, \ldots, a_3, 1)) \cdot Z(C(a_3, \ldots, a_{d-1}, a_d)) \\
&+ Z(C(a_d, a_{d-1}, \ldots, a_3)) \cdot Z(C(a_4, \ldots, a_{d-1}, a_d)) \\
=&Z(C(1, a_3, \ldots, a_d)) \cdot (m-n) + (m-n) \cdot Z(C(a_4, \ldots, a_d)) \\
=&(m-n)(Z(C(a_d, a_{d-1}, \ldots, a_3, 1)) + Z(C(a_4, \ldots, a_{d-1}, a_d)),
\end{aligned}$$

we obtain

$$\begin{aligned}
&Z(A_{m,n}) \\
=&Z(C(a_d, a_{d-1}, \ldots, a_3, 1, a_3, \ldots, a_{d-1}, a_d)) + 2a_2(m-n)^2 \\
=&(m-n)(Z(C(1, a_3, \ldots, a_d)) + Z(C(a_4, \ldots, a_{d-1}, a_d)) + 2a_2(m-n)).
\end{aligned}$$

Since $Z(C(1, a_3, \ldots, a_d)) = Z(C(a_3, \ldots, a_d)) + Z(C(a_4, \ldots, a_d))$, we have

$$\begin{aligned}
&Z(C(1, a_3, \ldots, a_d)) + Z(C(a_4, \ldots, a_d)) + 2a_2(m-n) \\
=&Z(C(a_3, \ldots, a_d)) + 2(Z(C(a_4, \ldots, a_d) + a_2(m-n)).
\end{aligned}$$

Since $Z(C(a_3, \ldots, a_d)) = m - n$, we have $Z(C(a_4, \ldots, a_d) + a_2(m-n)) = Z(C(a_2, \ldots, a_d))$. Hence we obtain

$$\begin{aligned}
Z(A_{m,n}) &= (m-n)(Z(C(a_3, \ldots, a_d)) + 2Z(C(a_2, \ldots, a_d))) \\
&= (m-n)(Z(C(a_1, \ldots, a_d)) + Z(C(a_2, \ldots, a_d))) \\
&= (m-n)(m+n) = m^2 - n^2.
\end{aligned}$$

□

These families for $\mathcal{P}_1$ and $\mathcal{P}_2$ have common symmetric kernels

$$(C(\dot{1}, 1, \dot{1}), C(\ddot{4}), C(\dot{2}, \dot{2}))$$

and

$$(C(\ddot{3}), C(\dot{1}, 2, \dot{1}), C(\dot{1}, 1, 1, \dot{1})),$$

respectively. Hosoya also conjectured the uniqueness of such structure. Main results gives an answer to his conjecture. First we show our main result for $\mathcal{P}_1$.

Theorem 3.4. *Let* $\{ (A_{m,n}, B_{m,n}, C_{m,n}) \}_{(m,n)\in\mathcal{P}_1}$ *be a family of triples of connected graphs satisfying*

$$\begin{aligned}
Z(A_{m,n}) &= m^2 - n^2, \\
Z(B_{m,n}) &= 2mn, \\
Z(C_{m,n}) &= m^2 + n^2.
\end{aligned}$$

If the family $\{ (A_{m,n}, B_{m,n}, C_{m,n}) \}_{(m,n)\in\mathcal{P}_1}$ *has the common symmetric kernel* $(A^{(1)}, B^{(1)}, C^{(1)})$*, then*

$$(A^{(1)}, B^{(1)}, C^{(1)}) = (C(\dot{1}, 1, \dot{1}), C(\ddot{4}), C(\dot{2}, \dot{2})).$$

Proof. We find the graphs $A^{(1)}$, $B^{(1)}$, $C^{(1)}$ and $G_{m,n}$ so that

$$Z(G_{m,n} \vee A^{(1)} \vee G_{m,n}) = m^2 - n^2,$$
$$Z(G_{m,n} \vee B^{(1)} \vee G_{m,n}) = 2mn,$$
$$Z(G_{m,n} \vee C^{(1)} \vee G_{m,n}) = m^2 + n^2$$

for $(m,n) \in \{ (2,1), (4,1), (5,2) \}$. Since $Z(G_{2,1} \vee A^{(1)} \vee G_{2,1}) = 3$, the graph $G_{2,1} \vee A^{(1)} \vee G_{2,1}$ is the caterpillar $C(3)$. By Lemma 4.2, the graph $G_{2,1} \vee B^{(1)} \vee G_{2,1}$ is the caterpillar $C(4)$. Hence the graph $G_{2,1}$ is either $C(\dot{1})$ or $C(\dot{2})$.

If $G_{2,1} = C(\dot{2})$, then the graphs $A^{(1)}$ and $B^{(1)}$ are $C(\ddot{1})$ and $C(\ddot{2})$, respectively. Since $Z(G_{4,1} \vee B^{(1)} \vee G_{4,1}) = 8$, it follow from the table in Lemma 4.1 that the graph $G_{4,1}$ is the caterpillar $C(\dot{4})$. Hence we obtain $Z(G_{4,1} \vee A^{(1)} \vee G_{4,1}) = Z(7) = 7$, which contradicts $Z(G_{4,1} \vee A^{(1)} \vee G_{4,1}) = 15$.

If $G_{2,1} = C(\dot{1})$, then the graphs $A^{(1)}$ and $B^{(1)}$ are $C(3)$ and $C(4)$, respectively. Since $Z(G_{4,1} \vee B^{(1)} \vee G_{4,1}) = 8$, the graph $G_{4,1} \vee B^{(1)} \vee G_{4,1}$ is the caterpillar $C(8)$. Hence the graphs $B^{(1)}$ and $G_{4,1}$ are $C(\ddot{4})$ and $C(\dot{3})$, respectively. It follows from direct calculation that

$$Z(G_{4,1} \vee A^{(1)} \vee G_{4,1}) = \begin{cases} Z(C(3,4)) = 13 & (A^{(1)} = C(\dot{1}, \dot{2})) \\ Z(C(5,2)) = 14 & (A^{(1)} = C(\ddot{1}, 2)) \\ Z(C(7)) = 7 & (A^{(1)} = C(\ddot{3})). \end{cases}$$

Hence the graph $A^{(1)}$ is $C(\dot{1}, 1, \dot{1})$. Since $Z(C^{(1)}) = Z(G_{2,1} \vee C^{(1)} \vee G_{2,1}) = 5$, the graph $C^{(1)}$ is either $C(2,2)$ or $C(5)$. By Lemmas 4.3 and 4.4, candidates of $C^{(1)}$ are $C(\dot{2}, \dot{2})$ and $C(\ddot{1}, 1, 2)$. By Lemma 4.5, if $C^{(1)} = C(\ddot{1}, 1, 2)$, then we can not construct $G_{5,2}$. Hence the graph $C^{(1)}$ is $C(\dot{2}, \dot{2})$. Therefore $(A^{(1)}, B^{(1)}, C^{(1)}) = (C(\dot{1}, 1, \dot{1}), C(\ddot{4}), C(\dot{2}, \dot{2}))$. □

Next we show our main result for $\mathcal{P}_2$.

Theorem 3.5. *Let* $\{ (A_{m,n}, B_{m,n}, C_{m,n}) \}_{(m,n) \in \mathcal{P}_2}$ *be a family of triples of connected graphs satisfying*

$$Z(A_{m,n}) = m^2 - n^2,$$
$$Z(B_{m,n}) = 2mn,$$
$$Z(C_{m,n}) = m^2 + n^2.$$

If the family $\{ (A_{m,n}, B_{m,n}, C_{m,n}) \}_{(m,n) \in \mathcal{P}_2}$ *has the common symmetric kernel* $(A^{(2)}, B^{(2)}, C^{(2)})$, *then*

$$(A^{(2)}, B^{(2)}, C^{(2)}) = (C(\ddot{3}), C(\dot{1}, 3, \dot{1}), C(\dot{1}, 1, 1, \dot{1})).$$

Proof. We find the graphs $A^{(2)}$, $B^{(2)}$, $C^{(2)}$ and $G_{m,n}$ so that

$$Z(G_{m,n} \vee A^{(2)} \vee G_{m,n}) = m^2 - n^2,$$
$$Z(G_{m,n} \vee B^{(2)} \vee G_{m,n}) = 2mn,$$
$$Z(G_{m,n} \vee C^{(2)} \vee G_{m,n}) = m^2 + n^2$$

for $(m,n) \in \{ (3,2),(4,3),(7,4) \}$. It follows from Lemma 4.6 that the graph $G_{4,3} \vee A^{(2)} \vee G_{4,3}$ is the caterpillar $C(7)$, which implies

$$(A^{(2)}, G_{3,2}, G_{4,3}) \in \left\{ \begin{array}{c} (C(\dddot{5}), C(\dot{1}), C(\dot{2})), \\ (C(\ddot{3}), C(\dot{2}), C(\dot{3})), \\ (C(\ddot{1}), C(\dot{3}), C(\dot{4})) \end{array} \right\}.$$

If $(A^{(2)}, G_{3,2}, G_{4,3}) = (C(\dddot{5}), C(\dot{1}), C(\dot{2}))$, then we have

$$Z(B^{(2)}) = Z(G_{3,2} \vee B^{(2)} \vee G_{3,2}) = 12.$$

By Lemma 4.7, we have $Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) \neq 56$ for any $(G_{7,4}, B^{(2)})$ such that

$$Z(G_{7,4} \vee A^{(2)} \vee G_{7,4}) = 33$$
$$Z(G_{4,3} \vee B^{(2)} \vee G_{4,3}) = 24.$$

Hence $(A^{(2)}, G_{3,2}, G_{4,3}) = (C(5), C(1), C(2))$ does not satisfy the condition. By Lemma 4.8, for $(A^{(2)}, G_{3,2}, G_{4,3}) = (C(\ddot{1}), C(\dot{3}), C(\dot{4}))$, we have $Z(G_{4,3} \vee B^{(2)} \vee G_{4,3}) \neq 24$. Hence $(A^{(2)}, G_{3,2}, G_{4,3}) = (C(\ddot{1}), C(\dot{3}), C(\dot{4}))$ does not satisfy the condition. By Lemma 4.9, if $(A^{(2)}, G_{3,2}, G_{4,3}) = (C(\ddot{3}), C(\dot{2}), C(\dot{3}))$ and $B^{(2)} \neq C(\dot{1}, 2, \dot{1})$, then

$$Z(G_{4,3} \vee B^{(2)} \vee G_{4,3}) \neq 24.$$

Hence we may consider only the case where

$$(A^{(2)}, B^{(2)}, G_{3,2}, G_{4,3}) = (C(\ddot{3}), C(\dot{1}, 2, \dot{1}), C(\dot{2}), C(\dot{3})).$$

In this case, it follows from Lemma 4.10 that $G_{7,4} = C(\dot{1}, 3)$. We also obtain $C^{(2)} = C(\dot{1}, 1, 1, \dot{1})$ by Lemma 4.11. Therefore we have

$$(A^{(2)}, B^{(2)}, C^{(2)}) = (C(\ddot{3}), C(\dot{1}, 2, \dot{1}), C(\dot{1}, 1, 1, \dot{1})). \qquad \square$$

Theorems 3.4 and 3.5 imply the uniqueness of the symmetric kernels $(A^{(1)}, B^{(1)}, C^{(1)})$ and $(A^{(2)}, B^{(2)}, C^{(2)})$. However $G_{m,n}$ are not unique.

Example 3.6. Let $G = C(\dot{2}, 3)$ and $G' = Q_4(\dot{1}, 1, 1, 1)$. In this case, the Hosoya indices of G and G' are equal to each other. Moreover the Hosoya indices of the restrictions G and G' to vertices other than the base points are also equal to each other. Hence we have $Z(A) = Z(A')$, $Z(B) = Z(B')$ and $Z(C) = Z(C')$, where

$$\begin{aligned} A &= G \vee C(\ddot{3}) \vee G, & A' &= G' \vee C(\ddot{3}) \vee G', \\ B &= G \vee C(\dot{1}, 2, \dot{1}) \vee G, & B' &= G' \vee C(\dot{1}, 2, \dot{1}) \vee G', \\ C &= G \vee C(\dot{1}, 1, 1, \dot{1}) \vee G, & C' &= G' \vee C(\dot{1}, 1, 1, \dot{1}) \vee G'. \end{aligned}$$

Since $[1, 2, 3]$ is equal to $10/7$, the both triples $(Z(A), Z(B), Z(C))$ and $(Z(A'), Z(B'), Z(C'))$ are equal to the primitive Pythagorean triple for $(10, 7) \in \mathcal{P}_2$.

If we consider only caterpillars, then we have the uniqueness of $G_{m,n}$. First we show the theorem for $(m,n) \in \mathcal{P}_1$.

Theorem 3.7. *Define the caterpillars G, A, B and C by*

$$\begin{aligned} G &= C(\dot{\alpha}_1, \alpha_2, \ldots, \alpha_\delta), \\ A &= G \vee C(\dot{1}, 1, \dot{1}) \vee G, \\ B &= G \vee C(\ddot{4}) \vee G, \\ C &= G \vee C(\dot{2}, \dot{2}) \vee G). \end{aligned}$$

If the triple $(Z(A), Z(B), Z(C))$ is the primitive Pythagorean triple $(m^2 - n^2, 2mn, m^2 + n^2)$ for $(m,n) \in \mathcal{P}_1$, then we have

$$\frac{m}{n} = [\alpha_1 + 1, \alpha_2 \ldots, \alpha_d].$$

Proof. Let $\mu = Z(C(\alpha_1, \alpha_2, \ldots, \alpha_\delta))$, $\nu = Z(C(\alpha_2, \ldots, \alpha_\delta))$. Similarly to the proof of Proposition 3.2, we obtain $Z(A) = \mu^2 - \nu^2$, $Z(B) = 2\mu\nu$ and $Z(C) = \mu^2 + \nu^2$. If both μ and ν are odd or both are even, then it follows that $Z(A)$ and $Z(C)$ are even, which contradicts the assumption that the triple $(Z(A), Z(B), Z(C))$ is the primitive Pythagorean triple. Moreover, since $\mu = K(\alpha_1, \ldots, \alpha_\delta)$ and $\nu = K(\alpha_2, \ldots, \alpha_d)$, the positive integers μ and ν are relatively prime and satisfy $\mu > \nu$. Hence $(\mu, \nu) \in \mathcal{P}$. It follows from the bijectivity of φ that $\mu = m$ and that $\nu = n$. Let $C(a_1 - 1, a_2, \ldots, a_d)$ be the caterpillar $G^{(1)}_{m,n}$ in Proposition 3.2. Both caterpillars $C(a_1 - 1, a_2, \ldots, a_d)$ and $C(\alpha_1, \ldots, \alpha_\delta)$ satisfy the equations

$$\begin{aligned} Z(C(a_1 - 1, a_2, \ldots, a_d)) = C(\alpha_1, \ldots, \alpha_\delta) = m, \\ Z(C(a_2, \ldots, a_d)) = C(\alpha_2, \ldots, \alpha_\delta) = n. \end{aligned}$$

Therefore it follows from Lemma 2.19 that

$$\frac{m}{n} = [a_1, a_2, \ldots, a_d] = [\alpha_1 + 1, \alpha_2, \ldots, \alpha_\delta]. \qquad \square$$

Similarly we can show the theorem for $(m,n) \in \mathcal{P}_2$.

Theorem 3.8. *Define the caterpillars G, A, B and C by*

$$\begin{aligned} G &= C(\dot{\alpha}_1, \alpha_2, \ldots, \alpha_\delta), \\ A &= G \vee C(\ddot{3}) \vee G, \\ B &= G \vee C(\dot{1}, 2, \dot{1}) \vee G, \\ C &= G \vee C(\dot{1}, 1, 1, \dot{1}) \vee G. \end{aligned}$$

If the triple $(Z(A), Z(B), Z(C))$ is the primitive Pythagorean triple $(m^2 - n^2, 2mn, m^2 + n^2)$ for $(m,n) \in \mathcal{P}_2$, then

$$\frac{m}{n} = [1, \alpha_1, \ldots, \alpha_\delta].$$

4 Technical lemmas

In this section, we show lemmas on the Hosoya indices, which is used in the proof of main results.

4.1 Tables of Hosoya indices

Here we calculate Hosoya indices for small graphs. Hosoya indices for all graphs with at most five edges are in Example 2.15. The following are the complete list of caterpillars G with six edges such that $Z(G) \leq 13$:

$$Z(C(7)) = 7, \qquad Z(C(2,5)) = 11, \qquad Z(C(3,4)) = 13.$$

The following are the complete list of the other connected graphs G with six edges such that $Z(G) \leq 13$:

$$\begin{aligned} Z(Q_3(1,1,4)) &= 10, & Z(Q_3(1,2,3)) &= 12, \\ Z(\Theta_3(1,1,2,1)) &= 11, & Z(\Theta_3(1,2,1,1)) &= 12, \\ Z(\Theta_3(1,1,1,1,1)) &= 13, & Z(Q_4(1,1,1,3)) &= 13, \\ Z(K_4) &= 10, & Z(K_{2,3}) &= 13, \\ Z(Q_3(1,1,\dot{1}) \vee Q_3(1,1,\dot{1})) &= 12, \end{aligned}$$

where K_4 stands for the complete graph and $K_{2,3}$ stands for the complete bipartite graph. The following are the complete list of the connected graphs G with seven edges such that $Z(G) \leq 13$:

$$Z(C(8)) = 8, \qquad Z(C(2,6)) = 13, \qquad Z(Q_3(1,1,5)) = 12.$$

The Hosoya index of a graph with at least eight edges except $C(k)$ is greater than 13. Hence we have the following.

Lemma 4.1. *Let $\mathfrak{Z}_n$ be the set of connected graphs G such that $Z(G) = n$. We have*

$$\begin{aligned} \mathfrak{Z}_1 &= \{\, C(1) \,\}, \\ \mathfrak{Z}_2 &= \{\, C(2) \,\}, \\ \mathfrak{Z}_3 &= \{\, C(3) \,\}, \\ \mathfrak{Z}_4 &= \{\, C(4),\ Q_3(1,1,1) \,\}, \\ \mathfrak{Z}_5 &= \{\, C(2,2),\ C(5) \,\}, \\ \mathfrak{Z}_6 &= \{\, C(6),\ Q_3(1,1,2) \,\}, \\ \mathfrak{Z}_7 &= \{\, C(7),\ C(2,2,1),\ Q_4(1,1,1,1) \,\}, \\ \mathfrak{Z}_8 &= \{\, C(8),\ C(2,1,2),\ Q_3(1,1,3),\ \Theta_3(1,1,1,1) \,\}, \\ \mathfrak{Z}_9 &= \{\, C(9),\ C(2,4),\ Q_3(1,2,2) \,\}, \\ \mathfrak{Z}_{10} &= \left\{ \begin{array}{c} C(10),\ C(3,3),\ Q_3(1,1,1;2), \\ Q_3(1,1,4),\ Q_4(1,1,1,2),\ K_4 \end{array} \right\}, \end{aligned}$$

$$\mathfrak{Z}_{11} = \left\{ \begin{array}{c} C(11),\ C(2,1,3),\ C(2,5), \\ Q_5(1,1,1,1,1),\ \Theta_3(1,1,2,1) \end{array} \right\},$$

$$\mathfrak{Z}_{12} = \left\{ \begin{array}{c} C(12),\ C(2,2,2),\ Q_3(1,2,3),\ Q_3(1,1,5), \\ Q_3(1,1,\dot{1}) \vee Q_3(\dot{1},1,1),\ \Theta_3(1,2,1,1) \end{array} \right\},$$

$$\mathfrak{Z}_{13} = \left\{ \begin{array}{c} C(13),\ C(2,6),\ C(3,4),\ C(2,1,1,2), \\ \Theta_3(1,1,1,1,1),\ Q_4(1,1,1,3),\ K_{2,3} \end{array} \right\}.$$

4.2 Lemmas for the case where $(m,n) \in \mathcal{P}_1$

Here we show lemmas to prove Theorem 3.4. First we show the following lemma to determine the shape of $B^{(1)}$.

Lemma 4.2. *Let $A^{(1)}$, $B^{(1)}$, $G_{2,1}$ and $G_{4,1}$ be connected graphs satisfying*

$$G_{2,1} \vee A^{(1)} \vee G_{2,1} = C(3)$$
$$Z(G_{2,1} \vee B^{(1)} \vee G_{2,1}) = 4,$$
$$Z(G_{4,1} \vee A^{(1)} \vee G_{4,1}) = 15.$$

If $G_{2,1} \vee B^{(1)} \vee G_{2,1} \neq C(4)$, then $Z(G_{4,1} \vee B^{(1)} \vee G_{4,1})$ does not equal 8.

Proof. Since $Z(G_{2,1} \vee B^{(1)} \vee G_{2,1}) = 4$, the graph $G_{2,1} \vee B^{(1)} \vee G_{2,1}$ is either $Q_3(1,1,1)$ or $C(4)$. In this case where $G_{2,1} \vee B^{(1)} \vee G_{2,1} = Q_3(1,1,1)$, the graphs $G_{2,1}$ and $B^{(1)}$ are $C(\dot{1})$ and $Q_3(1,1,1)$, respectively. Since the graph $G_{2,1} \vee A^{(1)} \vee G_{2,1}$ is the caterpillar $C(3)$, the graph $A^{(1)}$ is the caterpillar $C(3)$. Since $Z(C(\dot{2}) \vee C(3) \vee C(\dot{2})) \leq 8 < 15$ for any base points, the graph $G_{4,1}$ is not $C(\dot{2})$. Since $G_{4,1} \neq C(\dot{2})$, it follows that $Z(G_{4,1} \vee Q_3(1,1,1) \vee G_{4,1}) \neq 8$. □

Next we show three lemmas to determine $C^{(1)}$.

Lemma 4.3. *For $C^{(1)} = C(5)$ and $G_{4,1} = C(\dot{3})$, the Hosoya index $Z(G_{4,1} \vee C^{(1)} \vee G_{4,1})$ does not equal* 17 *for any base points.*

Proof. It follows from direct calculation that

$$Z(G_{4,1} \vee C^{(1)} \vee G_{4,1}) = \begin{cases} Z(C(9)) = 9 & (C^{(1)} = C(\ddot{5})) \\ Z(C(3,6)) = 19 & (C^{(1)} = C(\dot{1},\dot{4})) \\ Z(C(3,3,3)) = 33 & (C^{(1)} = C(\dot{1},3,\dot{1})) \\ Z(C(5,4)) = 21 & (C^{(1)} = C(\ddot{1},4)). \end{cases}$$

□

Lemma 4.4. *Let $C^{(1)} = C(2,2)$ and $G_{4,1} = C(\dot{3})$. If $C^{(1)} \neq C(\dot{2},\dot{2})$ and $C^{(1)} \neq C(\ddot{1},1,2)$, then the Hosoya index $Z(G_{4,1} \vee C^{(1)} \vee G_{4,1})$ does not equal* 17.

Proof. It follows from direct calculation that

$$Z(G_{4,1} \vee C^{(1)} \vee G_{4,1}) = \begin{cases} Z(C(3,3,2)) = 23 & (C^{(1)} = C(\dot{1},\dot{1},2)) \\ Z(C(3,1,4)) = 19 & (C^{(1)} = C(\dot{1},1,\dot{2})) \\ Z(C(3,1,1,3)) = 25 & (C^{(1)} = C(\dot{1},1,1,\dot{1})) \\ Z(C(6,2)) = 13 & (C^{(1)} = C(\ddot{2},2)). \end{cases}$$

□

Lemma 4.5. *If* $B^{(1)} = C(\ddot{4})$ *and* $C^{(1)} = C(\ddot{1},1,2)$*, then there does not exist a connected graph* $G_{5,2}$ *such that* $Z(G_{5,2} \vee B^{(1)} \vee G_{5,2}) = 20$ *and* $Z(G_{5,2} \vee C^{(1)} \vee G_{5,2}) = 29$*.*

Proof. Let G be a graph with a base point v, and G_v the restriction of G to vertices other than the vertex v. Since $B^{(1)} = C(\ddot{4})$, we have

$$Z(G \vee B^{(1)} \vee G) = 3Z(G_v)^2 + Z(G \vee C(\ddot{1}) \vee G).$$

Since $C^{(1)} = C(\dot{1},1,2)$, we have

$$Z(G \vee C^{(1)} \vee G) = 2Z(G_v)^2 + 3Z(G \vee C(\ddot{1}) \vee G).$$

The following system of equation, however, has no integer solution:

$$\begin{pmatrix} 3 & 1 \\ 2 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 20 \\ 29 \end{pmatrix}.$$

□

4.3 Lemmas for the case where $(m,n) \in \mathcal{P}_2$

Here we show lemmas to prove Theorem 3.5. First we show the following lemma to determine the shape of $A^{(2)}$.

Lemma 4.6. *Let* $A^{(2)}$*,* $G_{3,2}$ *and* $G_{4,3}$ *be connected graphs. Assume that* $Z(G_{4,3} \vee A^{(2)} \vee G_{4,3}) = 7$*. If* $G_{4,3} \vee A^{(2)} \vee G_{4,3} \neq C(7)$*, then* $Z(G_{3,2} \vee A^{(2)} \vee G_{3,2})$ *does not equal* 5*.*

Proof. Since $Z(G_{4,3} \vee A^{(2)} \vee G_{4,3}) = 7$, the graph $G_{4,3} \vee A^{(2)} \vee G_{4,3}$ is $C(2,3)$, $C(7)$ or $Q_4(1,1,1,1)$.

Consider the case where $G_{4,3} \vee A^{(2)} \vee G_{4,3} = Q_4(1,1,1,1)$. In this case, the graphs $A^{(2)}$ and $G_{4,3}$ are $Q_4(1,1,1,1)$ and $C(\dot{1})$, respectively. Hence we have

$$Z(G_{3,2} \vee A^{(2)} \vee G_{3,2}) \geq Z(A^{(2)}) = 7.$$

Consider the case where $G_{4,3} \vee A^{(2)} \vee G_{4,3} = C(2,3)$. In this case, candidates of $(A^{(2)}, G_{4,3})$ are the following:

$$(C(2,3), C(\dot{1})), \qquad (C(2,\ddot{1}), C(\dot{2})), \qquad (C(\dot{1},\dot{2}), C(\dot{2})).$$

Since the difference of the numbers of edges of the graphs $G_{4,3} \vee A^{(2)} \vee G_{4,3}$ and $G_{3,2} \vee A^{(2)} \vee G_{3,2}$ is even, the graph $G_{3,2} \vee A^{(2)} \vee G_{3,2}$ has even edges. Only $C(5)$ is a graph G with even edges such that $Z(G) = 5$. However, for any candidates of $A^{(2)}$, there does not exists $G_{3,2}$ such that $G_{3,2} \vee A^{(2)} \vee G_{3,2} = C(5)$. □

Next we show three lemmas to determine the shape of $B^{(2)}$.

Lemma 4.7. *Let $A^{(2)} = C(\ddot{5})$ and $G_{4,3} = C(\dot{2})$. The Hosoya index $Z(G_{7,4} \vee B^{(2)} \vee G_{7,4})$ does not equal 56 for connected graphs $B^{(2)}$ and $G_{7,4}$ such that $Z(B^{(2)}) = 12$, $Z(G_{7,4} \vee A^{(2)} \vee G_{7,4}) = 33$, and $Z(G_{4,3} \vee B^{(2)} \vee G_{4,3}) = 24$.*

Proof. First consider the case where $G_{7,4} = C(\dot{15})$. In this case, we have $G_{7,4} \vee A^{(2)} \vee G_{7,4} = C(33)$, which implies $Z(G_{7,4} \vee A^{(2)} \vee G_{7,4}) = 33$. If we choose two different base points of $B^{(2)}$ for the one-point union $G_{7,4} \vee B^{(2)} \vee G_{7,4}$, then the graph $G_{7,4} \vee B^{(2)} \vee G_{7,4}$ contains $C(15, 1, \dots, 1, 15)$ as a subgraph. Since

$$Z(C(15, 1, \dots, 1, 15)) \geq Z(C(15, 15)) = 15 \cdot 15 + 1 > 56,$$

we obtain

$$Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) > 56.$$

If we choose the same base points v of $B^{(2)}$ for left and right one-point unions of $G_{7,4} \vee B^{(2)} \vee G_{7,4}$, then

$$Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) = Z(B^{(2)} \vee C(\dot{29})).$$

Let B_v be the restriction of $B^{(2)}$ to vertices other than the vertex v. Since

$$Z(B^{(2)} \vee C(\dot{29})) = 28Z(B_v) + Z(B^{(2)}) = 28Z(B_v) + 12,$$

we obtain

$$Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) \neq 56.$$

Next we consider the case where $G_{7,4} \neq C(\dot{15})$. In this case, there exits a vertex u of the graph $G_{7,4}$ such that the distance between u and the base point is greater than or equal to 2. In other words, the graph $G_{7,4}$ contains $C(\dot{1}, 2)$ as a subgraph with a base point. Hence

$$Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) \geq Z(C(\dot{1}, 2) \vee B^{(2)} \vee C(\dot{1}, 2)).$$

Let B_u (*resp.* B_v, $B_{u,v}$) be the restriction of $B^{(2)}$ to vertices other than the left (*resp.* right, both) base point of $B^{(2)}$ for the one-point sum $G_{7,4} \vee B^{(2)} \vee G_{7,4}$. If $u \neq v$, then we have

$$Z(C(\dot{1}, 2) \vee B^{(2)} \vee C(\dot{1}, 2)) = 4Z(B^{(2)}) + 2Z(B_u) + 2Z(B_v) + B_{u,v}.$$

Since $Z(B^{(2)}) = 12$, we have

$$\begin{aligned}
&Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) \\
&\geq Z(C(\dot{1}, 2) \vee B^{(2)} \vee C(\dot{1}, 2)) \\
&= 4Z(B^{(2)}) + 2Z(B_u) + 2Z(B_v) + B_{u,v} \\
&\geq 48 + 2Z(B_v) + 2Z(B_u) + 1.
\end{aligned}$$

If $Z(B_v), Z(B_u) \geq 2$, then $Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) > 57$. If $Z(B_v) \leq 1$ and $Z(B^{(2)}) = 12$, then the graph $B^{(2)}$ is $C(\dot{1}, \dot{11})$. However, in this case, $B_u = C(11)$ and $Z(B_u) = 11 \geq 2$.

If $u = v$, then the graph $C(\dot{1}, 2) \vee B^{(2)} \vee C(\dot{1}, 2)$ is $B^{(2)} \vee C(2, \dot{1}, 2)$. Since $Z(B^{(2)} \vee C(2, \dot{1}, 2)) = 4Z(B_u) + 4Z(B^{(2)})$, we have

$$\begin{aligned} Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) &\geq 4Z(B_u) + 4Z(B^{(2)}) \\ &= 4Z(B_u) + 48. \end{aligned}$$

Hence, if $B^{(2)} \notin \left\{ C(\ddot{k}), Q_3(1,1,\ddot{k}), C(\ddot{k}, 2) \right\}$, then

$$Z(C(\dot{1}, 1, 1) \vee B^{(2)} \vee C(\dot{1}, 1, 1)) > 56.$$

If the graph $B^{(2)}$ is $C(\ddot{k})$, $Q_3(1,1,\ddot{k})$ or $C(\ddot{k}, 2)$, then the graph $B^{(2)}$ is either $C(\ddot{12})$ or $Q_3(1,1,5)$ since $Z(B^{(2)}) = 12$. However, since $Z(C(14)) = 14$ and $Z(Q_3(1,1,7)) = 16$, these two graphs do not satisfy the equation $Z(G_{4,3} \vee B^{(2)} \vee G_{4,3}) = 24$. □

Lemma 4.8. *Let $G_{3,2} = C(\dot{3})$, $G_{4,3} = C(\dot{4})$. For a connected graph $B^{(2)}$ satisfying $Z(G_{3,2} \vee B^{(2)} \vee G_{3,2}) = 12$, the Hosoya index $Z(G_{4,3} \vee B^{(2)} \vee G_{4,3})$ does not equal 24.*

Proof. Since $G_{3,2} = C(\dot{3})$ and $Z(G_{3,2} \vee B^{(2)} \vee G_{3,2}) = 12$, the graph $B^{(2)}$ is either $Q_3(1,1,\ddot{1})$ or $C(\ddot{8})$. Hence $Z(G_{4,3} \vee B^{(2)} \vee G_{4,3})$ equals $Z(Q_3(1,1,7)) = 16$ or $Z(C(14)) = 14$. □

Lemma 4.9. *Let $G_{3,2} = C(\dot{2})$, and $G_{4,3} = C(\dot{3})$. Let $B^{(2)}$ be a connected graph such that $Z(G_{3,2} \vee B^{(2)} \vee G_{3,2}) = 12$. If $B^{(2)} \neq C(\dot{1}, 2, \dot{1})$, then $Z(G_{4,3} \vee B^{(2)} \vee G_{4,3})$ does not equal 24.*

Proof. First we consider the case where the graph $G_{3,2} \vee B^{(2)} \vee G_{3,2}$ is either $Q_3(1,1,5)$ or $C(12)$. In this case, similarly to Lemma 4.8, it follows that $Z(G_{4,3} \vee B^{(2)} \vee G_{4,3})$ is $Z(Q_3(1,1,7)) = 16$ or $Z(C(13)) = 14$, which are not equal to 24.

Next we consider the case where the graph $G_{3,2} \vee B^{(2)} \vee G_{3,2}$ is neither $Q_3(1,1,5)$ nor $C(12)$. Since

$$Z(G_{3,2} \vee B^{(2)} \vee G_{3,2}) = Z(C(\dot{2}) \vee B^{(2)} \vee C(\dot{2})) = 12,$$

candidates of the graph $G_{3,2} \vee B^{(2)} \vee G_{3,2}$ are $Q_3(3,1,2)$ and $C(2,2,2)$. Hence candidates of $B^{(2)}$ are the following:

$$Q_3(\ddot{1}, 1, 2), \qquad Q_3(\dot{2}, 1, \dot{1}), \qquad C(\dot{1}, \dot{1}, 2), \qquad C(\dot{1}, 2, \dot{1}).$$

Since $G_{4,3} = C(\dot{3})$, we have

$$Z(G_{4,3} \vee B^{(2)} \vee G_{4,3}) = \begin{cases} Z(Q_3(5,1,2)) = 18 & (B^{(2)} = Q_3(\ddot{1}, 1, 2)) \\ Z(Q_3(4,1,3)) = 20 & (B^{(2)} = Q_3(\dot{2}, 1, \dot{1})) \\ Z(C(3,3,2)) = 23 & (B^{(2)} = C(\dot{1}, \dot{1}, 2)), \end{cases}$$

which implies $Z(G_{4,3} \vee B^{(2)} \vee G_{4,3}) \neq 24$. □

Next we show a lemma to determine $G_{7,4}$.

Lemma 4.10. *Let $G_{7,4}$ and $B^{(2)}$ be connected graphs. Assume that $B^{(2)} = C(\dot{1}, 2, \dot{1})$. If $G_{7,4} \neq C(\dot{1}, 3)$, then $Z(G_{7,4} \vee B^{(2)} \vee G_{7,4})$ does not equal* 56.

Proof. First consider the case where the graph $G_{7,4}$ contains $C(\dot{3})$ as a subgraph with a base point. If the graph $G_{7,4}$ contains $C(\dot{2}, 2)$ as a subgraph with a base points, then

$$\begin{aligned} Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) &\geq Z(C(2,2,2,2,2)) \\ &\geq Z(C(2,2)) \cdot Z(C(2,2,2)) = 5 \cdot 12 > 56. \end{aligned}$$

If the graph $G_{7,4}$ contains $Q_3(1,1,\dot{2})$ as a subgraph with a base points, then

$$\begin{aligned} Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) &\geq Z(Q_3(1,1,2)) \cdot Z(Q_3(1,1,2;1,1)) \\ &= 6 \cdot 14 > 56. \end{aligned}$$

If $G_{7,4} = Q_3(1,1,\dot{1})$, then

$$Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) = 48 < 56.$$

Therefore, if the graph $G_{7,4}$ contains $C(\dot{3})$ as a subgraph with a base point, then $Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) \neq 56$.

Next consider the case where the graph $G_{7,4}$ does not contain $C(\dot{3})$ as a subgraph with a base point. If $G_{7,4} = C(\dot{1}, 1, 2)$, then

$$Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) = Z(C(2,1,1,2,1,1,2)) = 5 \cdot 13 + 3 \cdot 5 > 56.$$

If $G = C(\dot{1}, 3)$, then $Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) = Z(C(3,1,2,1,3)) = 56$. Hence, if the graph $G_{7,4}$ contains $C(\dot{1}, 1, 2)$ as a proper subgraph with a base point, then $Z(G_{7,4} \vee B^{(2)} \vee G_{7,4}) > 56$. □

Finally we show the following lemma to determine $C^{(2)}$.

Lemma 4.11. *Let $G_{3,2} = C(\dot{2})$, $G_{4,3} = C(\dot{3})$, $G_{7,4} = C(\dot{1}, 3)$. Let $C^{(2)}$ be a connected graphs satisfying $Z(G_{3,2} \vee C^{(2)} \vee G_{3,2}) = 13$ and $Z(G_{7,4} \vee C^{(2)} \vee G_{7,4}) = 65$. If $C^{(2)} \neq C(\dot{1}, 1, 1, \dot{1})$, then $Z(G_{4,3} \vee C^{(2)} \vee G_{4,3})$ does not equal* 25*,*

Proof. It follows that

$$\begin{aligned} &Z(G_{7,4} \vee C^{(2)} \vee G_{7,4}) \\ =&Z(C(\dot{1}, 3) \vee C^{(2)} \vee C(\dot{1}, 3)) \\ =&Z(C(\dot{1}, 3) \vee C^{(2)} \vee C(\dot{1}, 1)) + 2Z(C(\dot{1}, 3) \vee C^{(2)}) \\ =&Z(C(\dot{1}, 1) \vee C^{(2)} \vee C(\dot{1}, 1)) + 2Z(C^{(2)} \vee C(\dot{1}, 1)) \\ &+ 2Z(C(\dot{1}, 1) \vee C^{(2)}) + 4Z(C^{(2)}) \\ \geq&Z(C(\dot{1}, 1) \vee C^{(2)} \vee C(\dot{1}, 1)) + 8Z(C^{(2)}). \end{aligned}$$

Since $G_{3,2} = C(\dot{1}, 1)$ and $Z(G_{3,2} \vee C^{(2)} \vee G_{3,2}) = 13$, we have

$$65 = Z(G_{7,4} \vee C^{(2)} \vee G_{7,4}) \geq 13 + 8Z(C^{(2)}).$$

Hence $Z(C^{(2)}) \leq 6$.

Consider the case where $C^{(2)} = C(6)$. Since the graph $G_{3,2}$ is $C(\dot{2})$, we have

$$Z(G_{3,2} \vee C^{(2)} \vee G_{3,2}) = \begin{cases} Z(C(8)) = 8 & (C^{(2)} = C(\ddot{6})) \\ Z(C(6,2)) = 13 & (C^{(2)} = C(\dot{5}, \dot{1})) \\ Z(C(5,3)) = 16 & (C^{(2)} = C(5, \ddot{1})) \\ Z(C(2,4,2)) = 20 & (C^{(2)} = C(\dot{1}, 4, \dot{1})). \end{cases}$$

Hence the graph $C^{(2)}$ is $C(\dot{5}, \dot{1})$. On the other hand, since the graph $G_{4,3}$ is $C(\dot{3})$, we have $Z(G_{4,3} \vee C^{(2)} \vee G_{4,3}) = Z(C(3,7)) = 22$.

Consider the case where $C^{(2)} \neq C(6)$. Since $Z(C^{(2)}) \leq 6$, the number of edges in the graph $C^{(2)}$ is less than or equal to 4. Since $Z(G_{3,2} \vee C^{(2)} \vee G_{3,2}) = 13$, candidates of the graph $G_{3,2} \vee C^{(2)} \vee G_{3,2} = C(\dot{2}) \vee C^{(2)} \vee C(\dot{2})$ are the following:

$$C(2,1,1,2), \qquad C(3,4), \qquad Q_4(1,1,1,3).$$

Since $Z(Q_4(1,1,1,1)) = 7 > 4$, the graph $C^{(2)}$ is not $Q_4(1,1,1,1)$. If the graph $G_{3,2} \vee C^{(2)} \vee G_{3,2}$ is the caterpillar $C(2,1,1,2)$, then the graph $C^{(2)}$ is $C(\dot{1}, 1, 1, \dot{1})$. Hence we consider only the case where $G_{3,2} \vee C^{(2)} \vee G_{3,2} = C(3,4)$. In this case, candidates of the graph $C^{(2)}$ are the following:

$$C(\ddot{1}, 4), \qquad C(1, \dot{1}, \dot{2}, 1), \qquad C(3, \ddot{2}).$$

Hence we have

$$Z(G_{4,3} \vee C^{(2)} \vee G_{4,3}) = \begin{cases} Z(5,3,1) = 21 & (C^{(2)} = C(\ddot{1}, 4)) \\ Z(4,4,1) = 21 & (C^{(2)} = C(\dot{2}, \dot{3})) \\ Z(1,2,6) = 19 & (C^{(2)} = C(3, \ddot{2})). \end{cases}$$

□

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