Graphs, Compositions, Polynomials and Applications

by

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Declaration

I declare that this thesis is my own, unaided work. It is being submitted for the degree of Doctor of Philosophy at the University of the Witwatersrand, Johannesburg. It has not been submitted before for any degree or examination at any other University.

____ (Signature of candidate)

22nd day of January 20 18 in Wits

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— Thokozani Ncambalala

Abstract

In this thesis, we study graph compositions of graphs and two graph polynomials, the k-defect polynomials and the Hosoya polynomials. This study was motivated by the fact that it is known that the number of compositions for certain graphs can be extracted from their k-defect polynomials, for example trees and cycles. We want to investigate if these results can be extended to other classes of graphs, in particular to theta and multibridge graphs. Furthermore we want to investigate if we can mimic these results of k-defect polynomials to Hosoya polynomials of graphs. In particular, investigating if the Hosoya polynomials of graphs can be computed using, similar methods to k-defect polynomials.

We start the investigation by improving the upper bound for the number of graph compositions of any graph. Thereafter, we give the exact number of graph composition of theta and 4-bridge graphs. We then find explicit expressions of the k-defect polynomials of a theta graph via its bad coloring polynomial. Furthermore, we find explicit expressions for the Hosoya polynomials of multibridge graphs and q-vertex joins of graphs with diameter 1 and 2.

Contents

Chapter 1

Introduction

The concept of graph compositions of graphs was introduced in 2001 by Knopfmacher and Mays [25]. Graph compositions of several families of graphs have been discussed in the literature, [5, 23, 25, 28, 29]. In addition, in 2012, Mphako-Banda [28], showed that there is a one to one correspondence between the number of graph compositions of a graph and the number of closed sets of that graph. In 2016, Mphako-Banda and Werner [29] used the principle of inclusion and exclusion for counting graph compositions of suspended Y-trees.

The k-defect polynomial of a graph H was first studied in 1969 by Crapo [13] when studying vertex coloring of graphs. In [8], Brylawski and Oxley showed that the k-defect polynomial of a graph H, counts the number of ways of coloring H with λ colors and having exactly k monochromatic edges. In [27], Mphako, generalized some properties of the chromatic polynomials to k-defect polynomials. In particular, it was shown in this work that the leading coeffient of any k-defect polynomial of certain classes of graphs is equal to the number of closed sets of size k.

The Wiener polynomial was introduced in 1947 by Harold Wiener [34] and later as Hosoya polynomial by Hosoya [22] in 1988. There is no recipe formula for finding the Hosoya polynomial of a graph, see [1, 10, 14, 16, 17, 19, 21, 24, 35, 36]. Hence finding the recipe formula is important.

1.1 Overview of Thesis

In this section we give a brief outline of the results of this thesis in each chapter.

In Chapter 2, we state and prove some of the results of this thesis. We state and prove one of the results of this chapter, a new sharper bound for graph compositions of any graph H. Finally, we give the main result of this chapter, the formula for the number of graph compositions of a theta graph and a four bridge graph.

In Chapter 3, we discuss three graph polynomials, chromatic, k-defect and bad coloring polynomials. The two polynomials, the k-defect and the bad coloring polynomials are the main subjects of discussion in this chapter. In particular, one of the results of this chapter is the formula for the bad coloring polynomial of an m-bridge graph. Finally, we give the main result of this chapter, the explicit expresssion of the k-defect polynomial of a theta graph.

In Chapter 4, we use the concept of distances in graphs and the principle of inclusion-exclusion to get our result. The main result of this chapter, is the explicit expression of the Hosoya polynomial of a uniform multibridge graph. We conclude this chapter, by stating the Wiener index of uniform multibridge from the Hosoya polynomial of uniform multibridge.

In Chapter 5, we introduce a graph operation called the q-vertex join for any graph of diameter 1 and 2. We then state and prove the main result of this chapter, the Hosoya polynomial of the q-vertex join of a diameter 1 and 2 graph. Finally, we give the Wiener index of the q-vertex join of a diameter 1 and 2 graph.

1.2 Basic Definitions

In this section we define some basic concepts in graph theory that are useful to this thesis.

A *graph* is an ordered triple $H = (E(H), V(H), I_H)$ where $V(H)$ is a non-emptyset of elements, $E(H)$ is a finite set of elements disjoint from $V(H)$ and I_H is an incidence relation that associates each element of $E(H)$, an unordered pair of elements of $V(H)$. The elements of the set $V(H)$ are called the *vertices* and elements of the set $E(H)$ are called the *edges* of the graph H. Thus for an edge e of H, we write $I_H(e) = \{v, w\}$ and the vertices v and w are called the *ends* of the edge e or we say , e is incident with v and w. In addition, we say vertices, v and w are *adjacent* or are *neighbours*. The number of edges incident with vertex w is called the *degree* of vertex w. A *hand-shaking* lemma is the sum of all the degrees of vertices in a graph and this sum is equal to twice the number of edges of a graph, that is, $2|E(H)|$. A set of edges of graph H is called a set of *parallel edges* if all the edges in the set have the same ends. A *loop* is an edge whose two ends are the same. A *bridge* is an edge in a connected graph whose removal will separate the graph into two disconnected components. A *sub-graph* H_1 of a graph H is a graph such that $E(H_1) \subseteq E(H)$ and $V(H_1) \subseteq V(H)$. A graph H is *disconnected* if it has two or more components. A *simple graph* is a graph without any parallel edges or loops.

In a graph H, a *walk* is an alternating sequence of vertices and edges, $w_0, e_1, w_1, e_2, w_2, e_3, \cdots, e_n, w_n$ beginning and ending with vertices in which w_{i-1} and w_i are the ends of the edge e_i. A walk in a graph H, is *closed* if $w_0 = w_n$ and is open otherwise. A *trail* is a walk in which all the edges in it are distinct. A trail is a *path* in which all the vertices in it are distinct. A closed trail in which all the vertices in it are distinct is called *cycle*. The *length* of a walk is the number of edges in it.

A *regular graph* is a graph in which all the vertices are of degree k for $k \geq 1$. Let H be a graph on n vertices with c connected components, the *rank* of H, denoted by $r(H)$, is defined to be $r(H) = n - c$. The *nullity* of H, denoted by $n(H)$, is defined to be $n(H) = |E| - r(H)$. A *closed set* X of size k, is the largest rank-r sub-graph of H containing X. In the following example, we illustrate some of the defined concepts which will be heavily used in this work.

Example 1.2.1. Let H be a graph of order 9 corresponding to the diagram in Figure 1.1. Then, rank of H is $9 - 1$. If the two edges e_1 and e_2 are deleted from H, we get the sub-graph X of H of size 8 with two components and 9 vertices, corresponding to the diagram in Figure 1.2. Thus $r(X) = 9 - 2 = 7$, but $r(X \cup \{e_i\}) = 9 - 1 = 8$, for $i = 1$ or 2. Thus X is the largest rank-7 sub-graph of H containing X. Thus, the sub-graph X, is closed in H. If two edges e_1 and e_6 are deleted from H, we get the sub-graph Y of H, of size 8 with one component and 9 vertices, corresponding to the diagram in Figure 1.3. Then, $r(Y) = 9 - 2 = 7 = r(Y \cup \{e_i\})$ for $i = 1$ or 6. Thus, Y is not the largest rank-7 sub-graph of H containing Y. Therefore the sub-graph Y, is not closed in H.

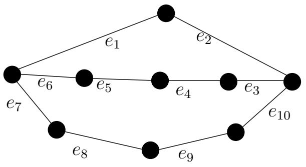

Figure 1.1: The graph H

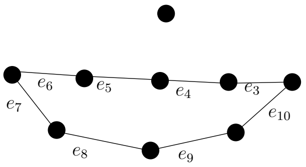

Figure 1.2: The graph X

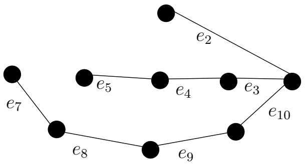

Figure 1.3: The graph Y

1.3 Graph Operations

In this section we define some graph operations in graph theory that are useful to this thesis.

(i) An edge contraction of an edge $e \in H$, denoted by H/e, is the operation of removing an edge e from a graph H, while at the same time merging the two vertices that it previously joined.

(ii) An edge deletion of an edge $e \in H$ denoted by $H\backslash e$, refers to the operation of removing e from a graph H, without merging the two vertices that it previously joined.

(iii) If H is a graph with some parallel edges and loops, we obtain a simple graph of H, by merging each class of parallel edges into one edge and deleting all the loops of H.

(iv) Given vertex disjoint graphs H_1 and H_2, then $H_1 \vee H_2$, is the graph in which each vertex of H_1 is adjacent to every vertex of H_2.

Let H be a graph with vertex set $V(H) = \{h_1, h_2, \cdots, h_n\}$, edge set $E(H)$ and let a vertex $w \notin V(H)$. A vertex join of a graph H, is the graph denoted by $\hat{H}$, with vertex set $V(\hat{H}) = \{h_1, h_2, \cdots, h_n\} \cup \{w\}$ and edge set $E(\hat{H}) = E(H) \cup \{\{h_1, w\}, \{h_2, w\}, \cdots, \{h_n, w\}\}$.
An *Eulerian orientation* of an undirected graph H is an assignment of a direction to each edge of H such that, at each vertex v, the indegree of v equals the outdegree of v.

1.4 Classes of Graphs

In this section, we define some well known classes of graphs in graph theory that are useful to this thesis. A *tree* on n vertices, is a graph, denoted by t_n, in which any two

vertices are connected by only one path or alternatively, a connected graph without any cycle. There are different types of trees in graph theory, one type which will be frequently mentioned in this work is a path. A tree is called a *path*, denoted by P_n, if all the vertices are of degree two at most. An *Eulerian graph* is a graph with every vertex of even degree. A *cycle graph*, denoted by C_n, is a closed trail in which all the vertices in it are distinct. A *complete graph* on n vertices, is a graph, denoted by K_n, in which all the vertices are adjacent to each other, that is it each vertex have $n-1$ neighbours. This means K_n is $n-1$ regular. A *strongly regular* graph on n vertices, is a k-regular graph denoted by $srg(n, k, \lambda, \mu)$, such that if there exists an integer λ such that for every pair of vertices u and v that are adjacent in $srg(n, k, \lambda, \mu)$, then there are λ vertices w that are adjacent to both u and v and if there exists an integer μ such that for every pair of vertices u and v that are not adjacent in $srg(n, k, \lambda, \mu)$, then there are μ vertices w that are adjacent to both u and v. A *wheel graph* on n vertices, denoted by W_n is the join $k_1 \vee C_n$, of k_1 and C_n. A *bipartite graph*, is a graph in which its vertex set can be divided into two disjoint sets U_1 and U_2 such that each edge of the graph has one end in U_1 and the other end in U_2. In particular, it is called a *complete bipartite graph*, denoted by $K_{p,q}$, if every vertex in U_1 is adjacent to each vertex in U_2 and vise versa where $|U_1| = p$ and $|U_2| = q$.
We now define the class of graphs which is the main body of study in this work.

Definition 1.4.1. A *theta graph* is a graph consisting of a pair of end vertices joined by three internally disjoint paths of lengths $b_1, b_2, b_3 \geq 1$. A theta graph is denoted by θ_{b_1,b_2,b_3}. The graph H corresponding to the diagram in Figure 1.1 is an example of a theta graph, $\theta_{2,4,4}$.

The concept of theta graph has been extended to multibridge graphs.

Definition 1.4.2. An *m-bridge graph* is a graph consisting of a pair of end vertices joined by m internally disjoint paths of lengths $a_1, a_2, a_3, \cdots, a_m \geq 1$. An m-bridge graph is denoted by $\theta_{a_1,a_2,a_3,\cdots,a_m}$. If $m = 2$, it is a cycle graph and if $m = 3$, it is called a theta graph.

1.5 Graph Polynomials

There are many polynomials associated with a graph. Polynomials of graphs play a very crucial role in graph theory as they encode information about a graph.
In this section we will define and give some properties of two polynomials of graphs that are well studied in graph theory and are very useful to this work. We start by defining the chromatic polynomial of a graph and state some of its known properties. Finally, we define the Tutte polynomial of a graph and state some of its known properties.
The chromatic polynomial of graph H, denoted by $\chi(H;\lambda)$ is a polynomial in one variable λ.

Definition 1.5.1. The *chromatic polynomial* of a graph H, denoted by $\chi(H;\lambda)$, with c connected components, has the following expansion:

$$\chi(H;\lambda) = \sum_{A \subseteq E(H)} (-1)^{|A|} \lambda^{c}.$$

The following proposition states some of the known properties of the chromatic polynomial.

Proposition 1.5.2. *Let H be a graph. Then*

(i) n is the degree of the polynomial, which is the number of vertices of H.

(ii) each coefficient a_i is an integer.

(iii) the coefficient of λ^n is one i.e $a_n = 1$.

(iv) the coefficient of λ^{n-1} is $a_{n-1} = -m$, where m is the number of edges of H.

(v) the constant term of $\chi(H;\lambda)$ is zero.

(vi) the coefficients a_i alternate in sign such that $\sum_{i=1}^{n} a_i = 0$.

The Tutte polynomials of a graph H denoted by $T(H;x,y)$ is a polynomial in two variables x and y.

Definition 1.5.3. Let $H=(V(H),E(H))$ be a graph. The *tutte polynomial* of H has the following expansion:

$$T(H;x,y)=\sum_{A\subseteq E(H)}(x-1)^{r(E(H))-r(A)}(y-1)^{n(A)}$$

where $r(A)$ is the rank and $n(A)$ is the nullity of A.

The following proposition states some of the known properties of the Tutte polynomial.

Proposition 1.5.4. *Let H be a graph and $T(H;x,y)$ the Tutte polynomial of H. Then*

(i) $\chi(H;\lambda)=(-1)^{r(E(H)}\lambda^{c}T(H;1-\lambda,0)$ *where c is the number of components of H.*

(ii) $T(H;0,0)$ *corresponds to the characteristic function of the empty graph.*

(iii) $T(H;1,2)$ *corresponds to the number of connected spanning sub-graphs.*

(iv) $T(H;2,2)$ *corresponds to the number of spanning sub-graphs.*

(v) $T(H;0,-1)$ *corresponds to the characteristic function of Eulerian graphs.*

(vi) $T(H;-2,0)$ *corresponds to the number of Eulerian orientations.*

Chapter 2

Graph Compositions of Theta Graphs

2.1 Introduction

In this chapter, we start by giving a brief history of graph compositions and a brief history of theta graphs. Then we state and prove one of the results of this chapter, an improved upper bound of graph compositions. Thereafter, we give another result of this chapter, an explicit expression for the number of graph compositions of theta graphs. In addition, we verify our formula for the number of graph compositions of theta graphs which falls in other classes of graphs with already known formulae for the number of graph compositions. Finally, we extend the results for the number of graph compositions of theta graphs to the number of graph compositions of 4-bridge graphs.

2.2 Brief History of Graph Compositions and Theta Graphs

In this section, we give a brief history of graph compositions and theta graphs. We close this section, by stating and illustrating some useful known concepts and definitions from the literature which are relevant to this chapter.

The concept of graph compositions of graphs was introduced in [25], Knopfmacher and Mays. In this original work, generalization of both ordinary compositions of positive integers and partitions of finite sets were given. Furthermore formulas, generating functions and recurrence relations for counting compositions of several families of graphs were discussed. In addition, the upper and the lower bound of graph compositions were set. As a follow up in [31], Ridley and Mays gave a formula for finding compositions of the union of two graphs. After 2004, the literature in graph compositions extended in many directions. In [5], Bajguz introduced a new construction of counting graph compositions of tree-like graphs. In [23], Huq used an alternative approach by using exponential generating functions for counting graph compositions of bipartite graphs. In [28], Mphako-Banda showed that counting the number of graph compositions of a graph is equivalent to counting the number of closed sets of that graph. Recently, in [29], Mphako-Banda and Werner used the principle of inclusion-exclusion for counting graph compositions of suspended Y-trees.

The class of theta graphs is well developed and studied in the literature. Here we give a sample of different directions of studies on theta graphs found in the literature. This class of graphs was first introduced in [26], Loerinc, when studying the chromatic uniqueness of the generalised theta graph. In [20], Eichhorn et al. discussed edge-bandwidth of theta graphs and set the upper and lower bounds for edge-bandwidth for a theta graph. In [7], Jason discussed the chromatic roots of generalized theta graphs and showed that the roots of the chromatic polynomial of a k-array generalized theta graph all lie in the disc $|z-1| \leq [1+o(1)]k/logk$. In [11], Carraher et al. proved that

the sum-paintability of a theta graph with r internally disjoint paths of lengths 2 is $2r + min_{l,m \in N}\{m + l : m(l - m) + \binom{m}{2} \leq r\}$. In [4], Archdeacon, the characterization of planarity was discussed by using a theta graph.
We need the following concepts and theory from the literature.

Definition 2.2.1 ([25])**.** Let H be a labeled graph with vertex set $V(H)$. A composition of H is a partition of $V(H)$ into vertex sets of connected induced sub-graphs of H.

Thus a composition provides a set of connected induced sub-graphs of H,
$\{H_1;H_2; \ . \ . \ . \ ;H_m\}$, with the properties that

$$\bigcup_{m=0}^{\infty} V(H_m) = V(H) \quad \text{and for} \quad i \neq j; \quad V(H_i) \bigcap V(H_j) = \varnothing.$$

Recall from Chapter 1 that if H is a graph on n vertices with c connected components, then the rank of H is denoted by $r(H) = n - c$. In addition, a closed set X of size k, is the largest rank-r sub-graph of H containing X. Recall that the size of a graph H is the number of edges of H.

The following theorem is useful to this chapter. We state, without proof, the theorem in graph compositions [28].

Theorem 2.2.2 ([28])**.** *Let H be a labelled graph with vertex set $V(H)$ and edge set $E(H)$. Let $\mathcal{C}_o(H)$ be the set of all distinct compositions of H such that*
$C(H) = |\mathcal{C}_o(H)|$. Let $\gamma(H)$ be the set of distinct closed sets in H, such that γ_i is a set of distinct closed sets in $\gamma(H)$ of size i. Then $\mathcal{C}(H) = \sum_{i=0}^{|E(H)|} |\gamma_i|$.

We state a basic theorem on the principle of inclusion-exclusion which is widely known in literature, we refer the reader to [9] for the proof. This theorem plays a crucial role in this work.

Theorem 2.2.3. Given a finite set of objects which may or may not have any of the properties $1, 2, 3, \cdots n$, let $P(j_1, \cdots, j_r)$ be the number of objects which have at least the r properties $j_1, \cdots, j_r$. Then the number of objects in the set having at least one of the properties is

$$\begin{array}{cccccccc}
 & P(1) & + & P(2) & + & \cdots & + & P(n) \\
- & P(1,2) & - & P(1,3) & - & \cdots & - & P(n-1,n) \\
+ & P(1,2,3) & + & P(1,2,4) & + & \cdots & + & P(n-2,n-1,n) \\
- & \cdots & & & & & & \\
\vdots & \vdots & & & & & & \\
+ & (-1)^{n-1}P(1,2,\cdots,n). & & & & & &
\end{array}$$

Since this theorem plays a crucial role in this work, to clarify the use of this theorem, we give the following example on application of the principle of inclusion-exclusion in counting the number of graph compositions of a graph H.

Example 2.2.4.

Let H be a graph shown in Figure 1.1. Let γ_{j-1}, where $j \in \{1, 2, \cdots, 11\}$ be the property that a sub-graph of H of size $j-1$ is closed in H. We denote the number of closed sets of size $j-1$ in H by $|\gamma_{j-1}|$. Let $\bar{\gamma}_{j-1}$ be the property that a sub-graph of H of size $j-1$ is non-closed in H. We denote the number of non-closed sets of size $j-1$ in H by $|\bar{\gamma}_{j-1}|$. Therefore from Theorem 2.2.2, the sub-graphs of H with size 0 up to 4 are all closed in H, thus the number of closed sets of size 0 up to 4 is $\sum_{j=1}^{5} |\gamma_{j-1}| = \sum_{j=1}^{5} \binom{10}{j-1}$. For the sub-graphs of H with size 5 up to 8, each size includes both closed and non-close sub-graphs of H. There are $\binom{10}{5}$ sub-graphs of size 5 in H. The number of non-closed sub-graphs with size 5 in H are $|\bar{\gamma}_5| = 2\begin{pmatrix}6\\5\end{pmatrix}$. Therefore the number of closed sets of size 5 is $|\gamma_5| = \begin{pmatrix}10\\5\end{pmatrix} - |\bar{\gamma}_5|$. There are $\binom{10}{6}$ sub-graphs of size 6 in H. The number of non-closed sub-graphs with size 6 in H is $|\bar{\gamma}_6| = 2\begin{pmatrix}6\\5\end{pmatrix}\begin{pmatrix}4\\1\end{pmatrix}$. Thus the number of closed sets of 6 is $|\gamma_6| = \begin{pmatrix}10\\6\end{pmatrix} - |\bar{\gamma}_6|$. Similarly for the closed sets of size

7 we have $|\bar{\gamma}_7| = 2\binom{6}{5}\binom{4}{2} + \binom{8}{7}$, hence $|\gamma_7| = \binom{10}{7} - |\bar{\gamma}_7|$, and for the closed sets of size 8 we have $|\bar{\gamma}_8| = 2\binom{2}{1}\binom{4}{1} + \binom{4}{1}\binom{4}{1}$, hence $|\gamma_8| = \binom{10}{8} - |\bar{\gamma}_8|$. There are no closed sets of size 9 in H, hence $|\gamma_9| = 0$. There is only one closed set of size 10 in H, that is H itself, thus $|\gamma_{10}| = 1$.

Here is the summary of the number of closed sets of H from size 0 to size 10.

$$\begin{aligned}
|\gamma_0| &= \binom{10}{0} = 1 \\
|\gamma_1| &= \binom{10}{1} = 10 \\
|\gamma_2| &= \binom{10}{2} = 45 \\
|\gamma_3| &= \binom{10}{3} = 120 \\
|\gamma_4| &= \binom{10}{4} = 210 \\
|\gamma_5| &= \binom{10}{5} - 2\binom{6}{5} = 240 \\
|\gamma_6| &= \binom{10}{6} - 2\binom{6}{5}\binom{4}{1} = 162 \\
|\gamma_7| &= \binom{10}{7} - 2\binom{6}{5}\binom{4}{2} - \binom{8}{7} = 40 \\
|\gamma_8| &= \binom{10}{8} - 2\binom{2}{1}\binom{4}{1} - \binom{4}{1}\binom{4}{1} = 13 \\
|\gamma_9| &= 0 \\
|\gamma_{10}| &= \binom{10}{10} = 1.
\end{aligned}$$

Hence applying Theorem 2.2.2, the graph compositions of the graph H is

$$C(H) = \sum_{i=0}^{10} |\gamma_i| = 842.$$

2.3 Bounds of Graph Compositions

In this section, we discuss an improved upper bound for the number of graph compositions of a graph H on n vertices. The upper bound and the lower bound were set in [25].

Theorem 2.3.1 ([25]). *Let H be a connected graph with n vertices, then the number of graph compositions of a graph H, is roughly bounded by, $C(t_n) \leq C(H) \leq C(K_n)$.*

Let C be a cycle in a graph H. The path $C - e$ where $e \in E(C)$ is called a broken cycle of H.

Lemma 2.3.2. *Let H be any graph on n vertices. Then any sub-graph X of H containing a broken cycle of H is a non-closed in H.*

Proof. Let $E(H) = \{e_1, e_2, \cdots e_{m-1}, e_m, a_1, a_2 \cdots a_t\}$ be edge set of H such that $|E(H)| = m + t$. Let a cycle C_m be a sub-graph of H such that

$$E(C_m) = \{e_1, e_2, \cdots e_{m-1}, e_m\} \subset E(H)$$

and let X be a sub-graph of H such that

$$E(X) = \{e_1, e_2, \cdots e_{m-1}, a_1, a_2 \cdots a_l\} \subset E(H)$$

where $l \leq t$. Then $E(X)$ contains a broken cycle $\{e_1, e_2, \cdots e_{m-1}\}$ of $E(C_m)$. Moreover, $r(X) = r(X \cup \{e_m\})$ thus X is not the largest rank-r sub-graph containing X. Therefore X is a non-closed sub-graph. □

Theorem 2.3.3. *Let H be a graph with edge set $E(H)$ and vertex set $V(H)$. Then the number of graph compositions of H is,*

$$2^{|V(H)|-1} \leq C(H) \leq 2^{|E(H)|}.$$

Proof. The number of graph compositions is equal to the number of closed sets of H, as established in [28]. The number of closed sets of different sizes can be found by the principle of inclusion-exclusion. The number of closed sets of size k is equal to $\binom{|E(H)|}{k} - Q_k$ where $Q_k \geq 0$, is the number of non-closed sets of size k. Since there are

$|E(H)|$ edges, k ranges from 0 to $|E(H)|$. Thus in total we have the number of closed sets of H to be

$$\begin{aligned} C(H) &= \binom{|E(H)|}{0} - Q_0 + \binom{|E(H)|}{1} - Q_1 + \cdots \\ &\quad + \binom{|E(H)|}{k} - Q_k + \cdots + \binom{|E(H)|}{|E(H)|} - Q_{|E(H)|} \\ &= 2^{|E(H)|} - \sum_{i=0}^{|E(H)|} Q_i. \end{aligned}$$

But $\sum_{i=0}^{|E(H)|} Q_i \geq 0$, thus $C(H) \leq 2^{|E(H)|}$. □

We can get the exact number or some sharper bounds of graph compositions for certain classes of graphs just by studying $\displaystyle\sum_{i=0}^{|E(H)|} Q_i$. The following proposition is known in the literature, see [25].

Proposition 2.3.4. *Let*

(i) t_n *be a tree on* n *vertices, then* $\displaystyle\sum_{i=0}^{|E(t_n)|} Q_i = 0$.

(ii) C_n *be a cycle graph on* n *vertices, then* $\displaystyle\sum_{i=0}^{|E(C_n)|} Q_i = n$.

It is clear that Q_i will be determined by the cycles and the intersection of the cycles in a graph H. Hence the following proposition follows from Lemma 2.3.2.

Proposition 2.3.5. *Let* H *be a graph on* $|E(H)|$ *edges, with 2 cycles,* C_n *and* C_m*. Then*

$$\sum_{i=0}^{|E(H)|} Q_i = (n2^m + m2^n - mn)2^{|E(H)|-m-n}$$

if $E(C_n) \cap E(C_m) = \emptyset$.

Proof. Let H be a graph on $|E(H)|$ edges, with 2 cycles, C_n and C_m. We consider three cases:

Case 1. The broken cycles are in C_n, while in C_m there are no broken cycles, then there are $\binom{n}{1}(2^m - \binom{m}{1})2^{|E(H)|-n-m}$ possibilities.

Case 2. The broken cycles are in C_m, while in C_n there are no broken cycles, then there are $\binom{m}{1}(2^n - \binom{n}{1})2^{|E(H)|-n-m}$ possibilities.

Case 3. The broken cycles are in both C_m and C_n, then there are $\binom{m}{1}\binom{n}{1}2^{|E(H)|-n-m}$ possibilities. Combining the three cases we obtain

$$\sum_{i=0}^{|E(H)|} Q_i = (n2^m + m2^n - mn)2^{|E(H)|-m-n}.$$

□

The following result follows directly from the Proposition 2.3.5.

Corollary 2.3.6. *Let H be a graph on $|E(H)|$ edges, with 2 cycles, C_n and C_m. Then*

$$C(H) = 2^{|E(H)|} - (n2^m + m2^n - mn)2^{|E(H)|-m-n}$$

if $E(C_n) \cap E(C_m) = \emptyset$.

2.4 Graph Compositions of Theta Graphs

In this section, we give an explicit formula of the number of graph compositions of a theta graph. We now calculate $\sum_{i=0}^{|E(H)|} Q_i$ for theta graphs and hence find the number of compositions of a theta graph.

Recall from Definition 1.4.1, that a theta graph denoted by θ_{b_1,b_2,b_3} is a graph consisting of a pair of end vertices joined by three internally disjoint paths of lengths $b_1, b_2, b_3 \geq 1$. The following proposition gives some properties derived from the definition of theta graphs which are useful to this work. For the purpose of logical reasoning in this work, we take $b_1 \leq b_2 \leq b_3$.

Proposition 2.4.1. *Let H be a theta graph θ_{b_1,b_2,b_3}. Then* *(i) the size of H is $b_1 + b_2 + b_3 = \beta$.*

(ii) any edge of a theta graph belongs to two cycles of H.

(iii) there are three cycles in H, namely, $C_{b_1+b_2}$ $C_{b_1+b_3}$ and $C_{b_2+b_3}$.

We find Q_k where $0 \leq k \leq b_1 + b_2 + b_3$ for theta graph.

Lemma 2.4.2. *Let θ_{b_1,b_2,b_3} be a theta graph and $b_1 \leq b_2 \leq b_3$. Then*

$$Q_k = \begin{cases} 0, & 0 \leq k \leq b_1 + b_2 - 2 \text{ and } k = b_1 + b_2 + b_3 \\ b_1 + b_2 + b_3, & k = b_1 + b_2 + b_3 - 1. \end{cases}$$

Proof. Let $0 \leq k \leq b_1 + b_2 - 2$, then it is clear that the smallest cycle in θ_{b_1,b_2,b_3} has $b_1 + b_2$ edges. Hence no broken cycle with fewer than $b_1 + b_2 - 2$ edges. Therefore there are no non-closed sub-graphs of size k by Lemma 2.3.2.
If we let $k = b_1 + b_2 + b_3$, then there is no broken cycle since it is the whole graph. If we let $k = b_1 + b_2 + b_3 - 1$, then there is only one edge of the theta graph missing. By Proposition 2.4.1, each edge is in a cycle, therefore each sub-graph of this form will have a broken cycle. □

We only need to find Q_k for $b_1 + b_2 - 1 \leq k \leq b_1 + b_2 + b_3 - 2$.

Lemma 2.4.3. *Let θ_{b_1,b_2,b_3} be a theta graph and let $b_1 + b_2 - 1 \leq k \leq b_2 + b_3 - 2$. Then*

$$Q_k = \binom{b_1 + b_2}{b_1 + b_2 - 1}\binom{b_3}{k - b_1 - b_2 + 1}.$$

Proof. These are all the sub-graphs containing a broken cycle of $C_{b_1+b_2}$ and some edges in b_3 such that $b_1 + b_2 - 1 \leq k \leq b_1 + b_2 + (b_3 - b_2 - 2)$ since $b_3 \geq b_2$. The broken cycle of $C_{b_1+b_2}$ can be chosen in $\binom{b_1 + b_2}{b_1 + b_2 - 1}$ ways, and the other remaining edges in $\binom{b_3}{k - b_1 - b_2 + 1}$ ways. □

Lemma 2.4.4. *Let* θ_{b_1,b_2,b_3} *be a theta graph and let* $b_1+b_3-1 \le k \le b_2+b_3-2$. *Then*

$$\begin{aligned} Q_k &= \binom{b_1+b_2}{b_1+b_2-1}\binom{b_3}{k-b_1-b_2+1} \\ &\quad +\binom{b_1+b_3}{b_1+b_3-1}\binom{b_2}{k-b_1-b_3+1}. \end{aligned}$$

Proof. For $b_1+b_3-1 \le k \le b_2+b_3-2$, there are two possible broken cycles that is, $C_{b_1+b_2}$ and $C_{b_1+b_3}$. The broken cycles of $C_{b_1+b_2}$ can be chosen in $\binom{b_1+b_2}{b_1+b_2-1}$ ways, and the other remaining edges in $\binom{b_3}{k-b_1-b_2+1}$ ways. The broken cycles of $C_{b_1+b_3}$ can be chosen in $\binom{b_1+b_3}{b_1+b_3-1}$ ways, and the other remaining edges in $\binom{b_2}{k-b_1-b_3+1}$ ways. ☐

Lemma 2.4.5. *Let* θ_{b_1,b_2,b_3} *be a theta graph and let* $b_2+b_3-1 \le k \le b_1+b_2+b_3-3$. *Then*

$$\begin{aligned} Q_k &= \binom{b_1+b_2}{b_1+b_2-1}\binom{b_3}{k-b_1-b_2+1} \\ &\quad +\binom{b_1+b_3}{b_1+b_3-1}\binom{b_2}{k-b_1-b_3+1} \\ &\quad +\binom{b_2+b_3}{b_2+b_3-1}\binom{b_1}{k-b_2-b_3+1}. \end{aligned}$$

Proof. For $b_2+b_3-1 \le k \le b_1+b_2+b_3-3$, there are three possible broken cycles that is, $C_{b_1+b_2}$, $C_{b_1+b_3}$ and $C_{b_2+b_3}$. The broken cycles of $C_{b_1+b_2}$ can be chosen in $\binom{b_1+b_2}{b_1+b_2-1}$ ways, and the other remaining edges in $\binom{b_3}{k-b_1-b_2+1}$ ways. The broken cycles of $C_{b_1+b_3}$ can be chosen in $\binom{b_1+b_3}{b_1+b_3-1}$ ways, and the other remaining edges in $\binom{b_2}{k-b_1-b_3+1}$ ways. Finally the broken cycles of $C_{b_2+b_3}$ can be chosen in $\binom{b_2+b_3}{b_2+b_3-1}$ ways, and the other remaining edges in $\binom{b_1}{k-b_2-b_3+1}$ ways. ☐

Lemma 2.4.6. *Let* θ_{b_1,b_2,b_3} *be a theta graph and let* $k = b_1+b_2+b_3-2$. *Then*

$$Q_k = b_1b_2 + b_1b_3 + b_2b_3.$$

Proof. Firstly, we consider the term b_1b_2. This is the number of sub-graphs containing broken cycles of $C_{b_1+b_3}$ and $C_{b_2+b_3}$, where one edge is missing in b_1 and the other missing edge is in b_2. Secondly, we consider the term b_1b_3. This is the number of sub-graphs containing broken cycles of $C_{b_1+b_2}$ and $C_{b_2+b_3}$, where one edge is missing in b_1 and the other missing edge is in b_3. Finally, we consider the term b_2b_3. This is the number of sub-graphs containing broken cycles of $C_{b_1+b_2}$ and $C_{b_1+b_3}$, where one edge is missing in b_2 and the other missing edge is in b_3. $\square$

The following theorem is a direct result of the Lemma 2.4.2, Lemma 2.4.3, Lemma 2.4.4, Lemma 2.4.5 and Lemma 2.4.6.

Theorem 2.4.7. *Let $H = \theta_{b_1,b_2,b_3}$ be a theta graph and let $\beta = b_1 + b_2 + b_3$. Then the number of graph compositions of H,*

$$\begin{aligned} C(H) &= 2^{\beta} + \beta + b_1b_2 + b_1b_3 + b_2b_3 \\ &\quad -(b_1+b_2)2^{b_3} - (b_2+b_3)2^{b_1} - (b_1+b_3)2^{b_2}. \end{aligned}$$

Proof. Let $\beta = b_1 + b_2 + b_3$. Then in Lemma 2.4.3, Lemma 2.4.4 and Lemma 2.4.5 we have the term $\binom{b_1+b_2}{b_1+b_2-1}\binom{b_3}{k-b_1-b_2+1}$, for $b_1 + b_2 - 1 \leq k \leq \beta - 3$. Now we get

$$\begin{aligned} \sum_{k=b_1+b_2-1}^{\beta-3} \binom{b_1+b_2}{b_1+b_2-1}\binom{b_3}{k-b_1-b_2+1} &= \sum_{k=0}^{b_3-2} \binom{b_1+b_2}{b_1+b_2-1}\binom{b_3}{k} \\ &= (b_1+b_2)(2^{b_3} - b_3 - 1). \end{aligned}$$

Similarly in Lemma 2.4.4 and Lemma 2.4.5 we have the term $\binom{b_1+b_3}{b_1+b_3-1}\binom{b_2}{k-b_1-b_3+1}$, for $b_1 + b_3 - 1 \leq k \leq \beta - 3$ we get

$$\begin{aligned} \sum_{k=b_1+b_3-1}^{\beta-3} \binom{b_1+b_3}{b_1+b_3-1}\binom{b_2}{k-b_1-b_3+1} &= \sum_{k=0}^{b_2-2} \binom{b_1+b_3}{b_1+b_3-1}\binom{b_2}{k} \\ &= (b_1+b_3)(2^{b_2} - b_2 - 1). \end{aligned}$$

Similarly for the term $\binom{b_2+b_3}{b_2+b_3-1}\binom{b_1}{k-b_2-b_3+1}$ in *Lemma* 2.4.5 we get

$$\begin{aligned}\sum_{k=b_2+b_3-1}^{\beta-3}\binom{b_2+b_3}{b_2+b_3-1}\binom{b_1}{k-b_2-b_3+1} &= \sum_{k=0}^{b_1-2}\binom{b_2+b_3}{b_2+b_3-1}\binom{b_1}{k}\\ &= (b_2+b_3)(2^{b_1}-b_1-1).\end{aligned}$$

Now combining $(b_1+b_2)(2^{b_3}-b_3-1)$, $(b_1+b_3)(2^{b_2}-b_2-1)$ and $(b_2+b_3)(2^{b_1}-b_1-1)$ we get the total number of non-closed sets ranging from size b_1+b_2-1 to $\beta-3$

$$\begin{aligned}\sum_{k=b_1+b_2-1}^{\beta-3} Q_k &= (b_2+b_3)2^{b_1}+(b_1+b_3)2^{b_2}+(b_1+b_2)2^{b_3}-2\beta\\ &\quad -2(b_1b_2+b_1b_3+b_2b_3).\end{aligned}$$

From 2.4.2 and Lemma 2.4.6 the combined number of non-closed sets are $\beta+b_1b_2+b_1b_3+b_2b_3$.

Therefore the total number of non-closed sets in H

$$\begin{aligned}\sum_{k=0}^{\beta} Q_k &= (b_2+b_3)2^{b_1}+(b_1+b_3)2^{b_2}+(b_1+b_2)2^{b_3}\\ &\quad -\beta-(b_1b_2+b_1b_3+b_2b_3).\end{aligned}$$

The total number of sub-graphs of H is 2^{β}. Hence the number of graph compositions of H

$$C(H) = 2^{\beta}-\sum_{k=0}^{\beta} Q_k.$$

□

We now use Theorem 2.4.5 to count the number of graph compositions of $\theta_{2,4,4}$ in Example 2.2.4, then for $b_1=2$ and $b_2=b_3=4$

$$Q_k = \begin{cases} 0, & 0\le k\le 4 \text{ and } k=10\\ 10, & k=9.\end{cases}$$

$$
\begin{aligned}
Q_5 &= 2\binom{6}{5} = 12 \\
Q_6 &= 2\binom{6}{5}\binom{4}{1} = 48 \\
Q_7 &= 2\binom{6}{5}\binom{4}{2} + \binom{8}{7} = 80 \\
Q_8 &= 2 \times 4 + 2 \times 4 + 4 \times 4 = 32.
\end{aligned}
$$

Now applying Theorem 2.4.7 we obtain

$$
\begin{aligned}
C(\theta_{2,4,4}) &= 2^{10} - \sum_{k=0}^{10} Q_k \\
&= 2^{10} - 12 - 48 - 80 - 32 - 10 - 0 \\
&= 842.
\end{aligned}
$$

This is the same number of graphs compositions we obtained in Example 2.2.4.

2.5 Verifying Graph Compositions of a Theta Graph with other known formulas

In this section, we verify our formula for graph compositions of a theta graph, with graph compositions of other classes of graphs containing certain theta graphs, that has been given in the literature.

The suspended Y-tree on n vertices, $\widetilde{Y_n}$, discussed in [29] is a theta graph θ_{b_1,b_2,b_3} where $b_1 = b_2 = 2$ and $n = b_3 + 2$. Hence we can verify the number of compositions of a suspended Y-tree on n vertices by using Theorem 2.4.7 with the substitutions $b_1 = b_2 = 2$ and $n = b_3 + 2$.

Theorem 2.5.1 ([29])**.** *Let $\widetilde{Y_n}$ be a suspended Y-tree on n vertices. The number of graph compositions of $\widetilde{Y_n}$,*

$$C(\widetilde{Y_n}) = 3(2^n - n) - 2.$$

Proof.

$$\begin{aligned}
C(\widetilde{Y_n}) &= C(\theta_{2,2,b_3}) \\
&= 2^{4+b_3} + (4 + b_3 + 4 + 2b_3 + 2b_3 - (4)2^{b_3} - (2 + b_3)2^2 - (2 + b_3)2^2. \\
&= 4(2^{(b_3+2)}) - 2^{(b_3+2)} - (3b_3) - (8) \\
&= 3(2^n - n) - 2.
\end{aligned}$$

□

In [31], the formula for counting graph compositions of a ladder graph was given as $C(L_n) = \dfrac{(3+\sqrt{10})^n - (3-\sqrt{10})^n}{\sqrt{10}}$. Therefore $C(L_3) = 74$, which is the number of graph compositions of the graph corresponding to the diagram in Figure 2.1. But by definition of a theta graph, $L_3 = \theta_{1,3,3}$. Hence, applying Theorem 2.4.4, where $b_1 = 1$, and $b_2 = b_3 = 3$, we get $C(\theta_{1,3,3}) = 74$.

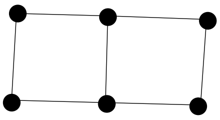

Figure 2.1: The graph L_3

In [25], graph compositions for several classes graphs were discussed including the complete graph with one edge missing K_n^-, wheel graph W_n and a bipartite graph $K_{m,n}$. The formula for counting graph compositions of a complete graph with one edge missing was given as $B(n) - B(n-2)$, where $B(n)$ is the n^{th} bell number. Therefore $C(K_4^-) = 13$, which is the number of graph compositions of the graph corresponding to the diagram in Figure 2.2. But by definition of a theta graph, $K_4^- = \theta_{1,2,2}$. Hence, applying Theorem 2.4.4 where $b_1 = 1$, and $b_2 = b_3 = 2$, we get $C(\theta_{1,2,2}) = 13$.
The formula for counting graph compositions of a wheel graph was given as $C(W_n) = 3C(W_{n-1}) - C(W_{n-2}) + n - 2$, where $C(W_1) = C(W_2) = 2$. Therefore, $C(W_3) = 5$, which is the number of graph compositions of the graph corresponding to the diagram

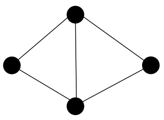

Figure 2.2: The graph K_4^-

in Figure 2.3. But by definition of a theta graph, $W_3 = \theta_{1,1,2}$. Hence, applying Theorem 2.4.4 where $b_1 = b_2 = 1$, and $b_3 = 2$, we get $C(\theta_{1,1,2}) = 5$.

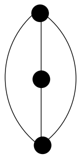

Figure 2.3: The graph W_3

The formula for counting graph compositions of a bipartite graph was given as $C(K_{m,n}) = \sum_{i=1}^{m+1} a_{n,i} i^n$ for $a_{m,n} = \sum_{i=0}^{m-1} \binom{m-1}{i} a_{m-1-i,n-1} - \sum_{i=1}^{m-1} \binom{m-1}{i} a_{m-1-i,n}$ where $a_{m,0} = 0$ for $m > 0$, $a_{0,1} = 1$ and $a_{0,n} = 0$ for $n > 1$. Therefore, $C(K_{2,3}) = 34$, which is the number of graph compositions of the graph corresponding to the diagram in Figure 2.4(a). But by definition of a theta graph, $K_{2,3} = \theta_{2,2,2}$. Hence, applying Theorem 2.4.4, where $b_1 = b_2 = b_3 = 2$ we get $C(\theta_{2,2,2}) = 5$.

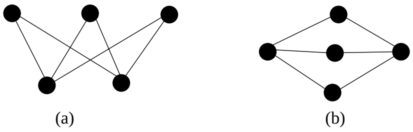

Figure 2.4: The graphs (a)$K_{2,3}$ and (b) $\theta_{2,2,2}$

2.6 Graph Composition of a 4-bridge Graph

In this section, we extend the results on the number of compositions of a theta graph to a 4-bridge graph. We count $\sum_{i=0}^{|E(H)|} Q_i$ where H is a 4-bridge graph. Finally, we give the number of compositions of a 4-bridge graph. Recall from Definition 1.4.2, that 4-bridge graph, denoted by θ_{a_1,a_2,a_3,a_4} is a graph consisting of a pair of end vertices joined by four internally disjoint paths of lengths $a_1, a_2, a_3, a_4 \geq 1$. The graphs corresponding to the diagrams in Figure 2.5, are examples of 4-bridge graphs, $\theta_{2,2,2,2}$ and $\theta_{2,3,4,5}$. For the purpose of logical reasoning in this work, we take $a_1 \leq a_2 \leq a_3 \leq a_4$.

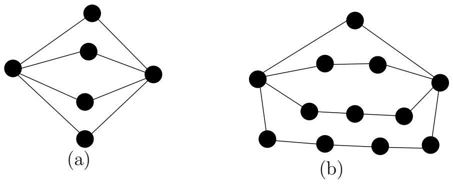

Figure 2.5: The graph $(a) = \theta_{2,2,2,2}$ and graph $(b) = \theta_{2,3,4,5}$

Proposition 2.6.1. *Let H be a 4-bridge graph θ_{a_1,a_2,a_3,a_4}. Then*

(i) the size of H is $a_1 + a_2 + a_3 + a_4 = n$.

(ii) any edge of a 4-bridge graph belongs to three cycles of H.

(iii) there are $\binom{4}{2} = 6$ cycles in H, namely, $C_{a_1+a_2}$, $C_{a_1+a_3}$, $C_{a_1+a_4}$, $C_{a_2+a_3}$, $C_{a_2+a_4}$ and $C_{a_3+a_4}$.

We find Q_k where $0 \leq k \leq a_1 + a_2 + a_3 + a_4$ for a 4-bridge graph.

Lemma 2.6.2. *Let $H = \theta_{a_1,a_2,a_3,a_4}$ be a 4-bridge graph, then the number of non-closed sets of size k is*

$$Q_k = \begin{cases} 0, & 0 \leq k \leq a_1 + a_2 - 2 \textit{ and } k = a_1 + a_2 + a_3 + a_4 \\ a_1 + a_2 + a_3 + a_4, & k = a_1 + a_2 + a_3 + a_4 - 1. \end{cases}$$

Proof. Let $0 \leq k \leq a_1 + a_2 - 2$, then it is clear that the smallest cycle in θ_{a_1,a_2,a_3,a_4} has $a_1 + a_2$ edges. Hence there is no broken cycle with fewer than $a_1 + a_2 - 2$ edges and therefore no non-closed sub-graph of size k by lemma 2.3.2.

If we let $k = a_1 + a_2 + a_3 + a_4$, then there is no broken cycle since it is the whole graph.

If we let $k = a_1 + a_2 + a_3 + a_4 - 1$, then there is only one edge of the theta graph missing. By Proposition 2.4.1, each edge is in a cycle, therefore each sub-graph of this form will have a broken cycle. □

The following four lemmas, lemma 2.6.3, lemma 2.6.4, lemma 2.6.5 and lemma 2.6.6 give the number of non-closed sets for $a_1 + a_2 - 1 \leq k \leq a_1 + a_2 + a_3 + a_4 - 2$.

Lemma 2.6.3. *Let $H = \theta_{a_1,a_2,a_3,a_4}$ be a 4-bridge graph, then the non-closed sets, Q_k of size k of H where $a_1 + a_2 + a_3 + a_4 = n$, $k = n - t$, $a_1 + a_2 - 1 \leq k \leq n - 4$ and $4 \leq t \leq a_3 + a_4 + 1$ is*

$$\begin{aligned} Q_k &= \binom{a_1}{t-1}(a_2 + a_3 + a_4) + \binom{a_2}{t-1}(a_1 + a_3 + a_4) \\ &\quad + \binom{a_3}{t-1}(a_1 + a_2 + a_4) + \binom{a_4}{t-1}(a_1 + a_2 + a_3). \end{aligned}$$

Proof. Let $a_1+a_2+a_3+a_4 = n$, $k = n-t$, $a_1+a_2-1 \leq k \leq n-4$ and $4 \leq t \leq a_3+a_4+1$, where k is the size in the sub-graph of H and t is the number of missing edges of the sub-graph of H. If there are t missing edges in H, such that $t - 1$ edges are missing from a_i for $1 \leq i \leq 4$ and the other missing edge is from a_j for $1 \leq j \leq 4$ where $i \neq j$, then by Lemma 2.3.2 the broken cycles can be formed in four different ways, giving the following four cases.

Case 1. If there are $t - 1$ edges missing in a_1, then the other missing edge will be from a_2, with broken cycles $C_{a_2+a_3}$ and $C_{a_2+a_4}$ or from a_3, with broken cycles $C_{a_2+a_3}$

and $C_{a_3+a_4}$ or from a_4, with broken cycles $C_{a_2+a_4}$ and $C_{a_3+a_4}$. Thus the number of non-closed sub-graphs of H is $\binom{a_1}{t-1}(a_2+a_3+a_4)$.

Case 2. If there are $t-1$ edges missing in a_2, then the other missing edge will be from a_1 or from a_3 or from a_4. Thus the number of non-closed sub-graphs of H is $\binom{a_2}{t-1}(a_1+a_3+a_4)$.

Case 3. If there are $t-1$ edges missing in a_3, then the other missing edge will be from a_1 or from a_2 or from a_4. Thus the number of non-closed sub-graphs of H is $\binom{a_3}{t-1}(a_1+a_2+a_4)$.

Case 4. If there are $t-1$ edges missing in a_4, then the other missing edge will be from a_1 or from a_2 or from a_3. Thus the number of non-closed sub-graphs of H is $\binom{a_4}{t-1}(a_1+a_2+a_3)$. If we combine these four cases we get the required results. $\square$

Lemma 2.6.4. *Let $H=\theta_{a_1,a_2,a_3,a_4}$ be a 4-bridge graph. Then the non-closed sets, Q_k of size k of H where $a_1+a_2+a_3+a_4=n$, $k=n-t$, $a_1+a_2-1\le k\le n-4$ and $4\le t\le a_3+a_4+1$ is*

$$\begin{aligned} Q_k &= \binom{a_1}{t-2}(a_2a_3+a_2a_4+a_3a_4)+\binom{a_2}{t-2}(a_1a_3+a_1a_4+a_3a_4) \\ &\quad +\binom{a_3}{t-2}(a_1a_2+a_2a_4+a_1a_4)+\binom{a_4}{t-2}(a_2a_3+a_1a_3+a_1a_2). \end{aligned}$$

Proof. Let $a_1+a_2+a_3+a_4=n$, $k=n-t$, $a_1+a_2-1\le k\le n-4$ and $4\le t\le a_3+a_4+1$, where k is the size in the sub-graph of H and t is the number of missing edges of the sub-graph of H. If there are t missing edges in H, such that $t-2$ edges are missing from a_i for $1\le i\le 4$ and the other two missing edges are each from a_j for $1\le j\le 4$ and a_l for $1\le l\le 4$ where $i\ne j\ne l$, then by Lemma 2.3.2, the broken cycles can be formed in four different ways, giving the following four cases.

Case 1. If there are $t-2$ edges missing in a_1, then the other two missing edges each will be from a_2 and a_3 or each from a_3 and a_4 or each from a_2 and a_4. Thus the number of non-closed sub-graphs of H is $\binom{a_1}{t-2}(a_2a_3+a_2a_4+a_3a_4)$.

Case 2. If there are $t-2$ edges missing in a_2, then the other two missing edges each will be from a_1 and a_3 or each from a_1 and a_4 or each from a_3 and a_4. Thus the number of non-closed sub-graphs of H is $\binom{a_2}{t-2}(a_1a_3 + a_1a_4 + a_3a_4)$.

Case 3. If there are $t-2$ edges missing in a_3, then the other two missing edges each will be from a_1 and a_2 or each from a_1 and a_4 or each from a_2 and a_4. Thus the number of non-closed sub-graphs of H is $\binom{a_3}{t-2}(a_1a_2 + a_2a_4 + a_1a_4)$.

Case 4. If there are $t-2$ edges missing in a_4, then the other two missing edges each will be from a_1 and a_2 or each from a_1 and a_3 or each from a_2 and a_3. Thus the number of non-closed sub-graphs of H is $\binom{a_4}{t-2}(a_2a_3 + a_1a_3 + a_1a_2)$. If we combine these four cases we get the required results. □

Lemma 2.6.5. *Let $H = \theta_{a_1,a_2,a_3,a_4}$ be a 4-bridge graph, then the non-closed sets, Q_k of size k of H where $a_1 + a_2 + a_3 + a_4 = n$, $k = n - t$, $a_1 + a_2 - 1 \leq k \leq n - 5$ and $5 \leq t \leq a_3 + a_4 + 1$ is*

$$\begin{aligned}
Q_k &= (a_3 + a_4)\left[\binom{a_1 + a_2}{t-1} - \binom{a_1}{t-1} - a_1\binom{a_2}{t-2} - a_2\binom{a_1}{t-2} - \binom{a_2}{t-1}\right] \\
&\quad +(a_2 + a_3)\left[\binom{a_1 + a_4}{t-1} - \binom{a_1}{t-1} - a_1\binom{a_4}{t-2} - a_4\binom{a_1}{t-2} - \binom{a_4}{t-1}\right] \\
&\quad +(a_2 + a_4)\left[\binom{a_1 + a_3}{t-1} - \binom{a_1}{t-1} - a_1\binom{a_3}{t-2} - a_3\binom{a_1}{t-2} - \binom{a_3}{t-1}\right] \\
&\quad +(a_1 + a_3)\left[\binom{a_2 + a_4}{t-1} - \binom{a_2}{t-1} - a_2\binom{a_4}{t-2} - a_4\binom{a_2}{t-2} - \binom{a_4}{t-1}\right] \\
&\quad +(a_1 + a_4)\left[\binom{a_2 + a_3}{t-1} - \binom{a_2}{t-1} - a_2\binom{a_3}{t-2} - a_3\binom{a_2}{t-2} - \binom{a_3}{t-1}\right] \\
&\quad +(a_1 + a_2)\left[\binom{a_3 + a_4}{t-1} - \binom{a_3}{t-1} - a_3\binom{a_4}{t-2} - a_4\binom{a_3}{t-2} - \binom{a_4}{t-1}\right].
\end{aligned}$$

Proof. Let $a_1+a_2+a_3+a_4 = n$, $k = n-t$, $a_1+a_2-1 \leq k \leq n-5$ and $5 \leq t \leq a_3+a_4+1$, where k is the size in the sub-graph of H and t is the number of missing edges of the sub-graph of H. If there are t missing edges in a sub-graph of H, such that one edge is missing from a_i for $1 \leq i \leq 4$ and from the other $t-1$ missing edges, then there are at least two edges missing from a_j for $1 \leq j \leq 4$ and also at least two edges missing from a_l for $1 \leq l \leq 4$ where $i \neq j \neq l$. Then by Lemma 2.3.2, the broken cycles can be formed in six different ways, giving six cases. We prove only one case, as the proofs for the other five cases are similar. Consider the case for the term

$$(a_3 + a_4)\left[\binom{a_1 + a_2}{t-1} - \binom{a_1}{t-1} - a_1\binom{a_2}{t-2} - a_2\binom{a_1}{t-2} - \binom{a_2}{t-1}\right].$$

Here considering the above notation we have $i = 3$ or $i = 4$ for a_i then $j = 1$ from a_j and $l = 2$ from a_l. Therefore if there are t missing edges in a sub-graph of H, then one edge is missing from a_3 or a_4 and there are at least two edges missing from a_1 and also at least two edges missing from a_2. We have the broken cycle $C_{a_3+a_4}$. Then we have the following expression for $5 \leq t \leq a_3 + a_4 + 1$.

$$\binom{a_3}{1}\sum_{r=2}^{t-3}\binom{a_1}{r}\binom{a_2}{t-1-r} + \binom{a_4}{1}\sum_{r=2}^{t-3}\binom{a_1}{r}\binom{a_2}{t-1-r}.$$

This expression this results from the case where one edge is missing in a_3, and hence there are r edges missing in a_1 and $t - 1 - r$ edges missing in a_2, or if there is one edge missing in a_4, then there are r edges missing in a_1 and $t - 1 - r$ edges missing in a_2. The conditions $2 \leq r \leq t - 3$ and $5 \leq t \leq a_3 + a_4 + 1$, ensure that there are at least two edges missing in each of a_1 and a_2. From Chapter 3 Proposition 3.6.2 [Vandermonde convolution]

$$\sum_{i=0}^{r}\binom{b_1}{r-i}\binom{b_2}{i} = \binom{b_1 + b_2}{r}.$$

We have that

$$\begin{aligned}
\sum_{r=2}^{t-3}\binom{a_1}{r}\binom{a_2}{t-1-r} &= \sum_{r=0}^{t-1}\binom{a_1}{r}\binom{a_2}{t-1-r} - \binom{a_1}{0}\binom{a_2}{t-1} - \binom{a_1}{1}\binom{a_2}{t-2} \\
&\quad - \binom{a_1}{t-2}\binom{a_2}{1} - \binom{a_1}{t-1}\binom{a_2}{0} \\
&= \binom{a_1 + a_2}{t-1} - \binom{a_2}{t-1} - a_1\binom{a_2}{t-2} - a_2\binom{a_1}{t-2} - \binom{a_1}{t-1}.
\end{aligned}$$

Hence, we obtain the required result,

$$
\begin{aligned}
& a_3\sum_{r=2}^{t-3}\binom{a_1}{r}\binom{a_2}{t-1-r}+a_4\sum_{r=2}^{t-3}\binom{a_1}{r}\binom{a_2}{t-1-r}\\
= & \ (a_3+a_4)\left[\binom{a_1+a_2}{t-1}-\binom{a_2}{t-1}-a_1\binom{a_2}{t-2}-a_2\binom{a_1}{t-2}-\binom{a_1}{t-1}\right].
\end{aligned}
$$

□

Lemma 2.6.6. *If $H=\theta_{a_1,a_2,a_3,a_4}$ is a 4-bridge graph, then the number of non-closed sets of size k, Q_k of H, for $n-3\le k\le n-2$ are*

$$
Q_k = \begin{cases} a_1a_2a_3+a_1a_3a_4+a_1a_2a_4+a_2a_3a_4+\binom{a_1}{2}(a_2+a_3+a_4) & \\ +\binom{a_2}{2}(a_1+a_3+a_4)+\binom{a_3}{2}(a_1+a_2+a_4)+\binom{a_4}{2}(a_1+a_2+a_3), & k=n-3\\ a_1a_2+a_1a_3+a_2a_3+a_1a_4+a_2a_4+a_3a_4, & k=n-2. \end{cases}
$$

Proof. Let $k=n-3$, we compute Q_k. Firstly, we consider the term $a_1a_2a_3$. The number of sub-graphs containing broken cycles of $C_{a_1+a_4}$, $C_{a_2+a_4}$ and $C_{a_3+a_4}$, where one edge is missing in each a_1, a_2, and a_3. Secondly, we consider the term $a_1a_3a_4$. The number of sub-graphs containing broken cycles of $C_{a_1+a_2}$, $C_{a_2+a_3}$ and $C_{a_2+a_4}$, where one edge is missing in each a_1, a_3, and a_4. The two terms $a_1a_2a_4$ and $a_2a_3a_4$ are obtained in a similar manner. Thirdly, we consider the term $\binom{a_1}{2}(a_2+a_3+a_4)$. The number of sub-graphs such that two edges are missing from a_1 and one edge is missing from a_2 or a_3 or a_4. The other three terms are obtained in a similar manner that is $\binom{a_2}{2}(a_1+a_3+a_4)$, $\binom{a_3}{2}(a_1+a_2+a_4)$ and $\binom{a_4}{2}(a_1+a_2+a_3)$ are obtained in a similar manner. Thus

$$
\begin{aligned}
Q_{n-3} = & \ a_1a_2a_3+a_1a_3a_4+a_1a_2a_4+a_2a_3a_4+\binom{a_1}{2}(a_2+a_3+a_4)\\
& +\binom{a_3}{2}(a_1+a_2+a_4)+\binom{a_4}{2}(a_1+a_2+a_3)+\binom{a_2}{2}(a_1+a_3+a_4).
\end{aligned}
$$

Let $k = n - 2$. We now compute Q_k. Firstly, we consider the term a_1a_2, the number of sub-graphs containing broken cycles of $C_{a_1+a_3}$, $C_{a_1+a_4}$, $C_{a_2+a_3}$ and $C_{a_2+a_4}$, where one edge is missing in a_1 and the other missing edge is in a_2. Secondly we consider the term a_1a_3, the number of sub-graphs containing broken cycles of $C_{a_1+a_2}$, $C_{a_1+a_4}$, $C_{a_3+a_4}$ and $C_{a_2+a_3}$, where one edge is missing in a_1 and the other missing edge is in a_3. The other four terms are obtained in a similar manner that is a_2a_3, a_1a_4, a_2a_4 and a_3a_4. Thus

$$Q_{n-2} = a_1a_2 + a_1a_3 + a_2a_3 + a_1a_4 + a_2a_4 + a_3a_4.$$

□

In Theorem 2.6.7 as in Theorem 2.4.7, we use the results of lemma 2.6.2, lemma 2.6.3, lemma 2.6.4, lemma 2.6.5, lemma 2.6.6 and Theorem 2.2.2 to obtain the formula for the graph compositions of θ_{a_1,a_2,a_3,a_4}.

Theorem 2.6.7. *Let $H = \theta_{a_1,a_2,a_3,a_4}$ be a 4-bridge graph such that $a_1+a_2+a_3+a_4 = n$, $p = a_1a_2 + a_1a_3 + a_2a_3 + a_1a_4 + a_2a_4 + a_3a_4$, $q = a_1a_2a_3 + a_1a_3a_4 + a_1a_2a_4 + a_2a_3a_4$, $w_1 = a_2a_3 + a_2a_4 + a_3a_4$, $w_2 = a_1a_3 + a_1a_4 + a_3a_4$, $w_3 = a_1a_2 + a_2a_4 + a_1a_4$, $w_4 = a_2a_3 + a_1a_3 + a_1a_2$. Then the graph composition of H is*

$$\begin{aligned} \mathcal{C}(H) &= 2^n - n - p - q + \sum_{j=1}^{4} w_j 2^{a_j} + \sum_{j=1}^{4} (n - a_j) 2^{a_j} \\ &\quad -(a_2 + a_3)2^{a_1+a_4} - (a_1 + a_4)2^{a_2+a_3} - (a_2 + a_4)2^{a_1+a_3} \\ &\quad -(a_1 + a_2)2^{a_3+a_4} - (a_3 + a_4)2^{a_1+a_2} - (a_1 + a_3)2^{a_2+a_4}. \end{aligned}$$

2.7 Conclusion

In this chapter, we obtained a new upper bound for the number of graph compositions of any graph. We have given a procedure for obtaining graph compositions via non-closed sets. We summed up all total numbers of non-closed sets of different sizes of a graph and then subtracted this number from the total number of sub-graphs of a graph. We presented this procedure, using the cases of a theta graph and a 4-bridge graph.

Chapter 3

k-defect Polynomials of Theta Graphs

3.1 Introduction

In this chapter, we start by discussing some of the known theory which is useful to this work, on the chromatic polynomials, the k-defect polynomials, and the bad coloring polynomials. Finally, we state and prove the main result of this chapter, the explicit expression of the k-defect polynomial of a theta graph.

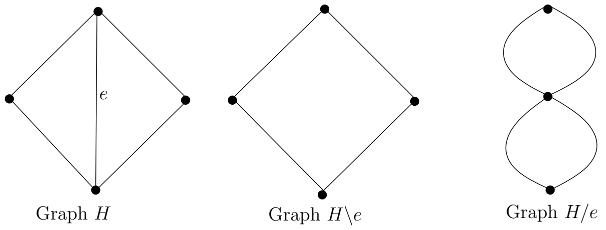

Figure 3.1:

In this chapter, and all the examples in each section, the referred graph H and its minors will be as shown in the diagrams of Figure 3.1, unless otherwise stated. A graph obtained after deletion, contraction or a combination of these operations is known as a minor. Let H be a graph and X a sub-graph of H. We denote a minor obtained by contracting X from H by H/X. The graphs will be denoted as follows: $H = \theta_{1,2,2}$ is a theta graph, $H\backslash e$, is the minor, H delete edge e, and H/e is the minor, H contract edge e.

3.2 Chromatic Polynomials of Graphs

In this section, we give a brief introduction to chromatic polynomials. The chromatic polynomial of a graph was first defined in 1912 by Birkhoff [6] in an attempt to solve the four color problem. In 1968, Read [30], wrote an introductory paper on chromatic polynomials which generated a lot of interest and activated the study of chromatic polynomials. Since then, there is a lot of literature on chromatic polynomials, most of which has been summarized in a book [18].

Let $H = (V, E)$ be a graph. A coloring of a graph H is an assignment of colors to each vertex of H. A coloring of H in which adjacent vertices are not allowed to have the same color is called a proper coloring. The chromatic polynomial, $\chi(H; \lambda)$, is a function which is associated with a graph H and expresses the number of different proper colorings of H with λ colors. The following four propositions summarize some of the well known properties of the chromatic polynomial of a graph, which are useful to this work. We refer the reader to [30] for further details.

There are several known methods for computing the chromatic polynomial of a graph H. We state without proof the following proposition which gives one of the methods for computing the chromatic polynomial of a graph H.

Proposition 3.2.1. *Let H be a graph with the set of edges $E(H)$ and an edge $f \in E(H)$. Then*

(a) if f is neither a loop nor a bridge, $\chi(H, \lambda) = \chi(H\backslash f; \lambda) - \chi(H/f; \lambda)$.

(b) if $f \in E(H)$ and f is a bridge, $\chi(H, \lambda) = (\lambda - 1)\chi(H\backslash f; \lambda)$.

(c) if f is a loop, $\chi(H,\lambda)=0$.

Proposition 3.2.2. *Let H be a graph of order n. Then*

(a) the degree of $\chi(H;\lambda)$ is n.

(b) the leading coefficient of $\chi(H;\lambda)$ is 1.

Proposition 3.2.3. *The chromatic polynomial*

(a) of a tree t_n on n vertices is given by $\chi(t_n;\lambda)=\lambda(\lambda-1)^{n-1}$.

(b) of a cycle graph C_n on n vertices is given by $\chi(C_n;\lambda)=(\lambda-1)^n+(-1)^n(\lambda-1)$.

Proposition 3.2.4. *Let H be a graph with some parallel edges and H' be the simple graph of H. Then $\chi(H;\lambda)=\chi(H';\lambda)$.*

The following example demonstrates, how to apply the stated propositions and method in computing the chromatic polynomial of a graph H.

Example 3.2.5.

Recall, in the diagrams shown in Figure 3.1, H is a theta graph $\theta_{1,2,2}$, $H\backslash e$, is the minor of H obtained after deleting e and H/e is the minor of H obtained after contracting e. We start the computation of the chromatic polynomial of H using the deletion and contraction method stated in Proposition 3.2.1.

$$\begin{aligned}
\chi(H;\lambda) &= \chi(H\backslash e;\lambda)-\chi(H/e;\lambda) \text{ by Propositions 3.2.1 and 3.3.5}\\
&= \chi(C_4;\lambda)-\chi(P_3;\lambda) \text{ by Propositions 3.2.4}\\
&= (\lambda-1)^4+(-1)^4(\lambda-1)-\lambda(\lambda-1)^2 \text{ by Propositions 3.2.3}\\
&= \lambda^4-5\lambda^3+8\lambda^2-4\lambda.
\end{aligned}$$

3.3 k-defect Polynomials of Graphs

In this section we introduce the k-defect polynomial and some of its known properties which are useful in this thesis. We close this section by giving an example of computing the 1-defect polynomial of a theta graph.

The k-defect polynomial of a graph H was first studied in 1969 by Crapo [13] when studying vertex coloring of graphs. In [8], Brylawski and Oxley showed that the k-defect polynomial of a graph H, denoted by $\phi_k(H;\lambda)$, counts the number of ways of coloring H with λ colors and having exactly k monochromatic edges. In [27], Mphako, generalized some properties of the chromatic polynomials to k-defect polynomials and in addition, found explicit expressions of k-defect polynomials of certain matroids. Unlike the chromatic polynomial, there is very limited literature on the k-defect polynomials. For a detailed introduction on the k-defect polynomials, we refer the reader to [27].

Let H be a vertex colored graph with the set of edges $E(H)$. A coloring of a graph H in which adjacent vertices have the same color is called a bad coloring. An edge f of the graph H is called bad or monochromatic if it joins two vertices of the same color. The following trivial proposition is a direct result of the definition of the k-defect polynomial of any graph.

Proposition 3.3.1. *Let H be a graph with edge set $E(H)$.*

(a) if $k > |E(H)|$, then $\phi_k(H;\lambda) = 0$.

(b) if $k = |E(H)|$, then $\phi_k(H;\lambda) = \lambda$.

(c) if $k = 0$, then $\chi(H;\lambda) = \phi_0(H;\lambda)$ where $\chi(H;\lambda)$ is the chromatic polynomial of H.

Recall from Chapter 1, the two well known graph operations, deletion and contraction of a graph.

Proposition 3.3.2 and Proposition 3.3.3 outlines some known properties of the k-defect polynomials useful to this work.

Proposition 3.3.2 ([27])**.** *Let H be a graph with edge set $E(H)$. Then*

(a) the leading coefficient of $\phi_k(H;\lambda)$ is the number of closed sets of size k with smallest rank possible for a closed set of size k.

(b)

$$\phi_k(H;\lambda) = \sum_{X\in L(H),|X|=k} \chi(H/X;\lambda)$$

where $L(H)$ is the set of all closed sets of H and the graph H has at least one closed set of size k. Otherwise $\phi_k(H;\lambda) = 0$.

The k-defect polynomial of a graph can also be computed recursively using Proposition 3.3.3.

Proposition 3.3.3 ([27])**.** *Let H be a graph with edge set $E(H)$. Then*

$$\phi_k(H;\lambda) = \phi_k(H\backslash e;\lambda) - \phi_k(H/e;\lambda) + \phi_{k-1}(H/e;\lambda).$$

The following proposition states some known explicit expressions of the k-defect polynomials which are useful in this thesis.

Proposition 3.3.4. *The k-defect polynomial*

(a) of a tree t_n on n vertices is given by

$$\phi_k(t_n;\lambda) = \binom{n-1}{k}\lambda(\lambda-1)^{n-1-k}.$$

(b) of a cycle graph C_n on n vertices is given by

$$\phi_k(C_n;\lambda) = \binom{n}{k}\left[(\lambda-1)^{n-k} + (-1)^{n-k}(\lambda-1)\right].$$

The following proposition is a direct result from the definition of a k-defect polynomial. This proposition can be useful in reducing the number of steps in the computation of the k-defect polynomial.

Proposition 3.3.5. *Let H be a graph such that every edge has a parallel class of at least $m > 1$ edges. Then the k-defect polynomial, $\phi_{m-1}(H;\lambda) = 0$.*

Proof. It is clear that if we color any adjacent pair of vertices in the graph H with one color, we already have at least m bad edges. □

We close this section by demonstrating the recursive method of computing the k-defect polynomial. We compute the 1-defect polynomial of a theta graph, $\theta_{1,2,2}$, in Example 3.3.6.

Example 3.3.6.

Recall, in the diagrams shown in Figure 3.1, H is a theta graph $\theta_{1,2,2}$, $H\backslash e$, and H/e is the minor of H obtained after deleting e and H/e is the minor of H obtained after contracting e. We start the computation of the k-defect polynomial of H using the deletion and contraction method stated in Proposition 3.3.3.

$$\begin{aligned}
\phi_1(H;\lambda) &= \phi_1(H\backslash e;\lambda) - \phi_1(H/e;\lambda) + \phi_0(H/e;\lambda) \\
&= \phi_1(C_4;\lambda) + 0 + \chi(H/e;\lambda) \text{ by Propositions 3.2.3 and 3.3.5} \\
&= 4(\lambda^3 - 3\lambda^2 + 2\lambda) + \lambda(\lambda-1)^2 \text{ by Propositions 3.3.1 and 3.3.4} \\
&= 5\lambda^3 - 14\lambda^2 + 9\lambda.
\end{aligned}$$

3.4 Bad Coloring Polynomials of Graphs

In this section we introduce the bad coloring polynomial of a graph H denoted by $\widetilde{B}(H;\lambda,S)$, also known as the coboundary polynomial $B(H;\lambda,S)$ in the literature for matroids. We state some of the known properties of the bad coloring polynomial which are useful in this thesis. Note that finding the coboundary polynomial is equivalent to finding the bad coloring polynomial since $\lambda^{-c(H)}\widetilde{B}(H;\lambda,S) = B(H;\lambda,S)$ where $c(H)$ is the number of components of the graph H. It should also be noted that most of the work known in the literature is on the coboundary polynomial of a graph. We close this section by giving an example of computing the bad coloring polynomial of a theta graph and verifying the relationship between the bad coloring polynomial , the k-defect polynomial and the chromatic polynomial.

Let H be a graph with edge set $E(H)$. The bad coloring polynomial of H is a polynomial with two independent variables λ and S, denoted by $\widetilde{B}(H;\lambda;S)$. We define $\widetilde{B}(H;\lambda;S)$ as

$$\widetilde{B}(H;\lambda,S)=\lambda^{c(H)}B(H;\lambda;S)=\lambda^{c(H)}\sum_{A\subseteq E(H)}(S-1)^{|A|}\lambda^{r(E(H))-r(A)}.$$

The bad coloring polynomial was first studied as a generating function in S by Crapo [9].

Proposition 3.4.1 ([9]). *Let H be a graph with edge set $E(H)$. The bad coloring polynomial of H,*

$$\widetilde{B}(H;\lambda;S)=\sum_{k=0}^{|E(H)|}\phi_k(H;\lambda)S^k$$

where $\phi_k(H;\lambda)$ is the k-defect polynomial of the graph H.

For further details on the theory of the bad coloring polynomial, we refer the reader to [8, 13, 27].

We now state without proof some propositions on the coboundary polynomial (bad coloring polynomial) of a graph H which are useful to this work.

Proposition 3.4.2. *Let H be a graph with the set of edges $E(H)$ and $f\in E(H)$. Then*

(a) $B(H;\lambda,S)=B(H\backslash f;\lambda,S)+(S-1)B(H/f;\lambda,S)$, *where f is neither a loop nor a bridge.*

(b) $B(H;\lambda,S)=(S+\lambda-1)B(H/f;\lambda,S)$, *where f is a bridge.*

(c) $B(H;\lambda,S)=SB(H\backslash f;\lambda,S)$, *where f is a loop.*

Proposition 3.4.3. *Let H_1 and H_2 be two graphs and let $H_1 \bullet H_2$ be the vertex gluing of H_1 and H_2. The*

$$B(H_1 \bullet H_2; \lambda, S) = B(H_1; \lambda, S)B(H_2\lambda, S).$$

By applying Proposition 3.3.4 and Proposition 3.4.1, we get

Proposition 3.4.4. *The bad coloring polynomial*

(a) of a tree t_n on n vertices is given by

$$\widetilde{B}(t_n; \lambda, S) = \sum_{k=0}^{|E(t_n)|} \phi_k(t_n; \lambda)S^k = \sum_{k=0}^{n-1} \binom{n-1}{k} \lambda(\lambda - 1)^{n-1-k} S^k.$$

(b) of a cycle graph C_n on n vertices is given by

$$\widetilde{B}(C_n; \lambda, S) = \sum_{k=0}^{|E(C_n)|} \phi_k(C_n; \lambda)S^k = \sum_{k=0}^{n} \binom{n}{k} \left[(\lambda - 1)^{n-k} + (-1)^{n-k}(\lambda - 1)\right] S^k.$$

In the following example we illustrate how to compute the bad coloring polynomial of a theta graph.

Example 3.4.5.

Now we apply Proposition 3.4.2 repeatedly to compute the bad coloring polynomial of the theta graph $\theta_{1,2,2}$. The diagrams shown in Figure 3.2 is a theta graph $\theta_{1,2,2} = H$, the minor $H\backslash e$, the minor H/e, the minor $H/e\backslash f$, and the minor $H/e/f$.

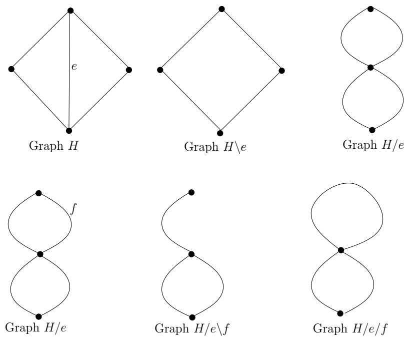

Figure 3.2:

$$\begin{aligned}
\lambda^{-1}\widetilde{B}(H;\lambda,S) &= B(H;\lambda,S)\\
&= B(H\backslash e;\lambda,S)+(S-1)B(H/e;\lambda,S)\\
&= B(C_4;\lambda,S)+(S-1)B(H/e;\lambda,S)\\
&= B(C_4;\lambda,S)+(S-1)\left[B(H/e\backslash f;\lambda,S)+(S-1)B(H/e/f;\lambda,S)\right]\\
&= B(C_4;\lambda,S)+(S-1)\left[(S+\lambda-1)B(C_2;\lambda,S)+S(S-1)B(C_2;\lambda,S)\right]\\
&= B(C_4;\lambda,S)+(S-1)(S+\lambda-1)B(C_2;\lambda,S)+S(S-1)^2B(C_2;\lambda,S)\\
&= (S+\lambda-1)^3+(S+\lambda-1)(S-1)[(S+\lambda-1)+(S-1)S]\\
&\quad +(S-1)[(S+\lambda-1)^2+(S-1)(S+\lambda-1)+(S-1)^2S]\\
&\quad +(S-1)^2S[(S+\lambda-1)+(S-1)S]\\
&= (S+\lambda-1)^3+2(S-1)(S+\lambda-1)^2+(S-1)^2(S+\lambda-1)\\
&\quad +2(S-1)^2(S+\lambda-1)S+(S-1)^3S+(S-1)^3S^2.
\end{aligned}$$

Therefore the bad coloring polynomial of H,

$$\begin{aligned}
&\widetilde{B}(H;\lambda,S)\\
= {}&\lambda^1\left[(S+\lambda-1)^3+2(S-1)(S+\lambda-1)^2+(S-1)^2(S+\lambda-1)\right.\\
&\left.+\,2(S-1)^2(S+\lambda-1)S+(S-1)^3S+(S-1)^3S^2\right].
\end{aligned}$$

Now we write the bad coloring polynomial in Example 3.4.5 as a generating function in S.

$$\begin{aligned}\widetilde{B}(\theta_{1,2,2};\lambda,S) &= \lambda S^5\\ &\quad +0\\ &\quad +(2\lambda^2-2\lambda)S^3\\ &\quad +(4\lambda^2-4\lambda)S^2\\ &\quad +(5\lambda^3-14\lambda^2+9\lambda)S\\ &\quad +(\lambda^4-5\lambda^3+8\lambda^2-4\lambda)S^0.\end{aligned}$$

By Proposition 3.4.1, we know that the coefficient of S^k in the generating function is the k-defect polynomial. The case $k=0$, is verified since the chromatic polynomial found in Example 3.2.5 is equal to the coefficient of S^0 in the generating function. Similarly, the case of $k=1$, is verified since the 1-defect polynomial found in Example 3.3.6 is equal to the coefficient of S^1.

3.5 Bad Coloring Polynomial of an m-bridge Graph

In this section, we start by computing the bad coloring polynomial of a theta graph. Finally, we find an explicit expression of the bad coloring polynomial for an m-bridge graph. We close the section, by verifying the results of bad coloring polynomial of theta graph found in Section 3.4.

Recall from Definition 1.4.2 that an m-bridge graph is a graph consisting of a pair of end vertices joined by m internally disjoint paths of lengths $a_1, a_2, a_3, \cdots, a_m \geq 1$. And is denoted by $\theta_{a_1,a_2,a_3,\cdots,a_m}$.

Let H be any theta graph, θ_{a_1,a_2,a_3}. Note that a theta graph is an m-bridge graph with $m=3$. Since the bad coloring polynomial of any cycle graph is known, see, Proposition 3.4.4, we therefore express our formulae in terms of bad coloring polynomials of cycle graphs.

We need the following two lemmas to state and prove the main results of this section.

Lemma 3.5.1. *Let C_n be a cycle graph of order n. Then*

$$\widetilde{B}(C_n;\lambda,S)=\lambda\left[\sum_{i=1}^{n}(S+\lambda-1)^{n-i}(S-1)^{i-1}+(S-1)^n\right].$$

Proof.

$$\begin{aligned}
&\lambda^{-1}\widetilde{B}(C_n;\lambda,S)\\
=\;& B(C_n;\lambda,S)\\
=\;& B(C_n\backslash e;\lambda,S)+(S-1)B(C_n/e;\lambda,S)\\
=\;& (S+\lambda-1)^{n-1}+(S-1)B(C_{n-1};\lambda,S)\\
=\;& (S+\lambda-1)^{n-1}+(S-1)(S+\lambda-1)^{n-2}+(S-1)^2B(C_{n-2};\lambda,S)\\
=\;& (S+\lambda-1)^{n-1}+(S-1)(S+\lambda-1)^{n-2}+(S-1)^2(S+\lambda-1)^{n-3}\\
&+(S-1)^3B(C_{n-3};\lambda,S)\\
=\;& (S+\lambda-1)^{n-1}+(S-1)(S+\lambda-1)^{n-2}+(S-1)^2(S+\lambda-1)^{n-3}\\
&+(S-1)^3(S+\lambda-1)^{n-4}+\cdots+(S-1)^{n-2}(S+\lambda-1)+(S-1)^{n-1}B(C_1;\lambda,S)\\
=\;& (S+\lambda-1)^{n-1}+(S-1)(S+\lambda-1)^{n-2}+(S-1)^2(S+\lambda-1)^{n-3}\\
&+(S-1)^3(S+\lambda-1)^{n-4}+\cdots+(S-1)^{n-2}(S+\lambda-1)+(S-1)^{n-1}S\\
=\;& (S+\lambda-1)^{n-1}+(S-1)(S+\lambda-1)^{n-2}+(S-1)^2(S+\lambda-1)^{n-3}\\
&+(S-1)^3(S+\lambda-1)^{n-4}+\cdots+(S-1)^{n-2}(S+\lambda-1)\\
&+(S-1)^{n-1}S-(S-1)^{n-1}+(S-1)^{n-1}\\
=\;& (S+\lambda-1)^{n-1}+(S-1)(S+\lambda-1)^{n-2}+(S-1)^2(S+\lambda-1)^{n-3}\\
&+(S-1)^3(S+\lambda-1)^{n-4}+\cdots+(S-1)^{n-2}(S+\lambda-1)+(S-1)^n+(S-1)^{n-1}\\
=\;& \sum_{i=1}^{n}(S+\lambda-1)^{n-i}(S-1)^{i-1}+(S-1)^n.
\end{aligned}$$

Therefore,

$$\widetilde{B}(C_n;\lambda,S)\;=\;\lambda\left[\sum_{i=1}^{n}(S+\lambda-1)^{n-i}(S-1)^{i-1}+(S-1)^n\right].$$

$\square$

Lemma 3.5.2. *The recursive formula of the bad coloring polynomial of an m-bridge graph, $\theta_{a_1,a_2,\cdots,a_m}$, is given by*

$$\begin{aligned}
\lambda^{-1}\widetilde{B}(\theta_{a_1,a_2,\cdots,a_m};\lambda,S) &= B(\theta_{a_1,a_2,\cdots,a_m};\lambda,S)\\
&= \left[B(C_{a_1},\lambda,S)-(S-1)^{a_1}\right]B(\theta_{a_2,a_3,\cdots,a_m};\lambda,S)\\
&\quad +(S-1)^{a_1}\prod_{i=1}^{m-1}B(C_{a_{i+1}};\lambda,S).
\end{aligned}$$

Proof. Without loss of generality, we show the result for $m=4$. Let $H=\theta_{a_1,a_2,a_3,a_4}$, then

$$\begin{aligned}
&B(H;\lambda,S)\\
= {}&(S+\lambda-1)^{a_1-1}B(\theta_{a_2,a_3,a_4};\lambda,S)+(S-1)B(\theta_{a_1-1,a_2,a_3,a_4};\lambda,S)\\
= {}&(S+\lambda-1)^{a_1-1}B(\theta_{a_2,a_3,a_4};\lambda,S)+(S-1)(S+\lambda-1)^{a_1-2}B(\theta_{a_2,a_3,a_4};\lambda,S)\\
&+(S-1)^2B(\theta_{a_1-2,a_2,a_3,a_3};\lambda,S)\\
= {}&(S+\lambda-1)^{a_1-1}B(\theta_{a_2,a_3,a_4};\lambda,S)+(S-1)(S+\lambda-1)^{a_1-2}B(\theta_{a_2,a_3,a_4};\lambda,S)\\
&+(S-1)^2(S+\lambda-1)^{a_1-3}B(\theta_{a_2,a_3,a_4};\lambda,S)+(S-1)^3B(\theta_{a_1-3,a_2,a_3,a_3},\lambda,S)\\
= {}&\left[(S+\lambda-1)^{a_1-1}+(S-1)(S+\lambda-1)^{a_1-2}\right]B(\theta_{a_2,a_3,a_4};\lambda,S)\\
&+\left[(S-1)^2(S+\lambda-1)^{a_1-3}+(S-1)^3(S+\lambda-1)^{a_1-4}\right]B(\theta_{a_2,a_3,a_4};\lambda,S)\\
&+\cdots+(S-1)^{a_1-2}(S+\lambda-1)B(\theta_{a_2,a_3,a_4};\lambda,S)+(S-1)^{a_1-1}B(\theta_{1,a_2,a_3,a_4};\lambda,S)\\
= {}&\left[(S+\lambda-1)^{a_1-1}+(S-1)(S+\lambda-1)^{a_1-2}\right]B(\theta_{a_2,a_3,a_4};\lambda,S)\\
&+\left[(S-1)^2(S+\lambda-1)^{a_1-3}+(S-1)^3(S+\lambda-1)^{a_1-4}\right]B(\theta_{a_2,a_3,a_4};\lambda,S)\\
&+\left[\cdots+(S-1)^{a_1-2}(S+\lambda-1)+(S-1)^{a_1-1}\right]B(\theta_{a_2,a_3,a_4};\lambda,S)\\
&+(S-1)^{a_1}B(C_{a_2}\bullet C_{a_3}\bullet C_{a_4};\lambda,S).
\end{aligned}$$

We apply Proposition 3.4.3 to the vertex gluing of C_{a_2}, C_{a_3} and C_{a_4} to a single vertex, thereafter simplify as follows:

$$\begin{aligned}
& B(H;\lambda,S) \\
= \; & \left[(S+\lambda-1)^{a_1-1}+(S-1)(S+\lambda-1)^{a_1-2}\right]B(\theta_{a_2,a_3,a_4};\lambda,S) \\
& +\left[(S-1)^2(S+\lambda-1)^{a_1-3}+(S-1)^3(S+\lambda-1)^{a_1-4}\right]B(\theta_{a_2,a_3,a_4};\lambda,S) \\
& +\left[\cdots+(S-1)^{a_1-2}(S+\lambda-1)+(S-1)^{a_1-1}\right]B(\theta_{a_2,a_3,a_4};\lambda,S) \\
& +(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S)B(C_{a_4};\lambda,S) \\
= \; & \left[(S+\lambda-1)^{a_1-1}+(S-1)(S+\lambda-1)^{a_1-2}\right]B(\theta_{a_2,a_3,a_4};\lambda,S) \\
& +\left[(S-1)^2(S+\lambda-1)^{a_1-3}+(S-1)^3(S+\lambda-1)^{a_1-4}\right]B(\theta_{a_2,a_3,a_4};\lambda,S) \\
& +\left[\cdots+(S-1)^{a_1-2}(S+\lambda-1)+(S-1)^{a_1-1}\right]B(\theta_{a_2,a_3,a_4};\lambda,S) \\
& +\left[(S-1)^{a_1}-(S-1)^{a_1}\right]B(\theta_{a_2,a_3,a_4};\lambda,S) \\
& +(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S)B(C_{a_4};\lambda,S).
\end{aligned}$$

Now we gather all the coefficients of $B(\theta_{a_2,a_3,a_4};\lambda,S)$ and apply Lemma 3.5.1 to get the bad coloring polynomial

$$\begin{aligned}
\widetilde{B}(H;\lambda,S) &= \lambda B(H;\lambda,S) \\
&= \lambda\left[B(C_{a_1};\lambda,S)-(S-1)^{a_1}\right]B(\theta_{a_2,a_3,a_4};\lambda,S) \\
&\quad +\lambda(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S)B(C_{a_4};\lambda,S).
\end{aligned}$$

□

We are in a position to state and prove one of results of this chapter.

Theorem 3.5.3. *Let H be a theta graph, θ_{a_1,a_2,a_3}, with $1 \le a_1 \le a_2 \le a_3$. The bad coloring polynomial,*

$$\begin{aligned}
\widetilde{B}(H;\lambda,S) &= \lambda B(H;\lambda,S) \\
&= \lambda B(C_{a_2+a_3};\lambda,S)\left[B(C_{a_1};\lambda,S)-(S-1)^{a_1}\right] \\
&\quad +\lambda(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S).
\end{aligned}$$

Proof.

$$\begin{aligned}
& B(H;\lambda,S) \\
= \;& (S+\lambda-1)^{a_1-1}B(C_{a_2+a_3};\lambda,S)+(S-1)B(\theta_{a_1-1,a_2,a_3};\lambda,S) \\
= \;& (S+\lambda-1)^{a_1-1}B(C_{a_2+a_3};\lambda,S)+(S-1)(S+\lambda-1)^{a_1-2}B(C_{a_2+a_3};\lambda,S) \\
& +(S-1)^2B(\theta_{a_1-2,a_2,a_3};\lambda,S) \\
= \;& (S+\lambda-1)^{a_1-1}B(C_{a_2+a_3};\lambda,S)+(S-1)(S+\lambda-1)^{a_1-2}B(C_{a_2+a_3};\lambda,S) \\
& +(S-1)^2(S+\lambda-1)^{a_1-3}B(C_{a_2+a_3};\lambda,S)+(S-1)^3B(\theta_{a_1-3;a_2,a_3},\lambda,S) \\
= \;& \left[(S+\lambda-1)^{a_1-1}+(S-1)(S+\lambda-1)^{a_1-2}\right]B(C_{a_2+a_3};\lambda,S) \\
& +\left[(S-1)^2(S+\lambda-1)^{a_1-3}+(S-1)^3(S+\lambda-1)^{a_1-4}\right]B(C_{a_2+a_3};\lambda,S) \\
& +\cdots+(S-1)^{a_1-2}(S+\lambda-1)B(C_{a_2+a_3};\lambda,S)+(S-1)^{a_1-1}B(\theta_{1,a_2,a_3};\lambda,S) \\
= \;& \left[(S+\lambda-1)^{a_1-1}+(S-1)(S+\lambda-1)^{a_1-2}\right]B(C_{a_2+a_3};\lambda,S) \\
& +\left[(S-1)^2(S+\lambda-1)^{a_1-3}+(S-1)^3(S+\lambda-1)^{a_1-4}\right]B(C_{a_2+a_3};\lambda,S) \\
& +\left[\cdots+(S-1)^{a_1-2}(S+\lambda-1)+(S-1)^{a_1-1}\right]B(C_{a_2+a_3};\lambda,S) \\
& +(S-1)^{a_1}B(C_{a_2}\bullet C_{a_3};\lambda,S).
\end{aligned}$$

We apply Proposition 3.4.3 to the vertex gluing $C_{a_2}\bullet C_{a_3}$ and simplify the equation further.

$$\begin{aligned}
& B(H;\lambda,S) \\
= \;& \left[(S+\lambda-1)^{a_1-1}+(S-1)(S+\lambda-1)^{a_1-2}\right]B(C_{a_2+a_3};\lambda,S) \\
& +\left[(S-1)^2(S+\lambda-1)^{a_1-3}+(S-1)^3(S+\lambda-1)^{a_1-4}\right]B(C_{a_2+a_3};\lambda,S) \\
& +\left[\cdots+(S-1)^{a_1-2}(S+\lambda-1)+(S-1)^{a_1-1}\right]B(C_{a_2+a_3};\lambda,S) \\
& +(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S)
\end{aligned}$$

$$\begin{aligned}
&= \left[(S+\lambda-1)^{a_1-1}+(S-1)(S+\lambda-1)^{a_1-2}\right]B(C_{a_2+a_3};\lambda,S)\\
&\quad+\left[(S-1)^2(S+\lambda-1)^{a_1-3}+(S-1)^3(S+\lambda-1)^{a_1-4}\right]B(C_{a_2+a_3};\lambda,S)\\
&\quad+\left[\cdots+(S-1)^{a_1-2}(S+\lambda-1)+(S-1)^{a_1-1}\right]B(C_{a_2+a_3};\lambda,S)\\
&\quad+\left[(S-1)^{a_1}-(S-1)^{a_1}\right]B(C_{a_2+a_3};\lambda,S)\\
&\quad+(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S)\\
&= \left[B(C_{a_1};\lambda,S)-(S-1)^{a_1}\right]B(C_{a_2+a_3};\lambda,S)\\
&\quad+(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S).
\end{aligned}$$

We multiply by λ to get the bad coloring polynomial. □

We now extend the results stated in Theorem 3.5.3 to an m-bridge graph for $m \geq 3$.

Theorem 3.5.4. *Let H be an m-bridge graph, $\theta_{a_1,a_2,\cdots,a_m}$, with $1 \leq a_1 \leq a_2 \cdots \leq a_m$. The bad coloring polynomial,*

$$\begin{aligned}
\lambda^{-1}\widetilde{B}(H;\lambda,S) &= B(H;\lambda,S)\\
&= B(C_{a_{m-1}+a_m};\lambda,S)\prod_{i=1}^{m-2}\left[B(C_{a_i};\lambda,S)-(S-1)^{a_i}\right]\\
&\quad+\sum_{j=1}^{m-3}(S-1)^{a_{j+1}}\prod_{i=1}^{m-j-1}B(C_{a_{i+j+1}};\lambda,S)\prod_{r=1}^{j}\left[B(C_{a_r};\lambda,S)-(S-1)^{a_r}\right]\\
&\quad+(S-1)^{a_1}\prod_{i=1}^{m-1}B(C_{a_{i+1}};\lambda,S).
\end{aligned}$$

Proof. The proof is by induction. The base case is a 3-bridge graph. Thus, case $m = 3$, is true by Theorem 3.5.3. We assume that the result is true for an $(m-1)$-

bridge graph where $m \geq 4$. Thus,

$$\begin{aligned}
& B(\theta_{a_1,a_2,\cdots,a_{m-1}};\lambda,S) \\
= \; & B(C_{a_{m-2}+a_m-1};\lambda,S)\prod_{i=1}^{m-3}\left[B(C_{a_i};\lambda,S)-(S-1)^{a_i}\right] \\
& +\sum_{j=1}^{m-4}(S-1)^{a_{j+1}}\prod_{i=1}^{m-j-2}B(C_{a_{i+j+1}};\lambda,S)\prod_{r=1}^{j}\left[B(C_{a_r};\lambda,S)-(S-1)^{a_r}\right] \\
& +(S-1)^{a_1}\prod_{i=1}^{m-2}B(C_{a_{i+1}};\lambda,S).
\end{aligned}$$

Now we consider an m-bridge graph. By Lemma 3.5.2 we know that

$$\begin{aligned}
B(\theta_{a_1,a_2,\cdots,a_m};\lambda,S) \;=\; & \left[B(C_{a_1};\lambda,S)-(S-1)^{a_1}\right]B(\theta_{a_2,a_3,\cdots,a_m};\lambda,S) \\
& +(S-1)^{a_1}\prod_{i=1}^{m-1}B(C_{a_{i+1}};\lambda,S).
\end{aligned}$$

In addition we know that $\theta_{a_2,a_3,\cdots,a_m}$ is the $(m-1)$-bridge graph.

$$\begin{aligned}
& B(\theta_{a_2,a_3,\cdots,a_m},\lambda,S) \\
= \; & B(C_{a_{m-1}+a_m},\lambda,S)\prod_{i=2}^{m-2}\left[B(C_{a_i},\lambda,S)-(S-1)^{a_i}\right] \\
& +\sum_{j=2}^{m-3}(S-1)^{a_{j+1}}\prod_{i=1}^{m-j-1}B(C_{a_{i+j+1}},\lambda,S)\prod_{r=2}^{j}\left[B(C_{a_r},\lambda,S)-(S-1)^{a_r}\right] \\
& +(S-1)^{a_2}\prod_{i=2}^{m-1}B(C_{a_{i+1}},\lambda,S).
\end{aligned}$$

Hence the result. □

We now verify Theorem 3.5.4 by substituting $m = 3$, $a_1 = 1$ and $a_2 = a_3 = 2$, and compare the results with the answer found in Example 3.4.5.

Example 3.5.5.

The diagrams shown in Figure 3.2 is a theta graph $\theta_{1,2,2} = H$, and its the minors. We now compute the bad coloring polynomial of H using Theorem 3.5.4 where $a_1 = 1$

and $a_2 = a_3 = 2$.

$$\begin{aligned}
\lambda^{-1}\widetilde{B}(H;\lambda,S) &= B(\theta_{1,2,2};\lambda,S) \\
&= B(C_4;\lambda,S)\left[B(C_1;\lambda,S)-(S-1)\right]+(S-1)B(C_2;\lambda,S)B(C_2;\lambda,S) \\
&= (S+\lambda-1)^3+(S-1)(S+\lambda-1)^2+(S-1)^2B(C_2;\lambda,S) \\
&\quad +(S-1)\left[(S+\lambda-1)+(S-1)S\right]\left[(S+\lambda-1)+(S-1)S\right] \\
&= (S+\lambda-1)^3+(S-1)(S+\lambda-1)^2 \\
&\quad +(S-1)^2(S+\lambda-1)+(S-1)^3S \\
&\quad +(S-1)\left[(S+\lambda-1)^2+2(S-1)(S+\lambda-1)S+(S-1)^2S^2\right] \\
&= (S+\lambda-1)^3+2(S-1)(S+\lambda-1)^2+(S-1)^2(S+\lambda-1) \\
&\quad +2(S-1)^2(S+\lambda-1)S+(S-1)^3S+(S-1)^3S^2.
\end{aligned}$$

Hence the bad coloring polynomial of $\theta_{1,2,2} = H$ is given by

$$\begin{aligned}
\widetilde{B}(H;\lambda,S) &= \lambda\left[(S+\lambda-1)^3+2(S-1)(S+\lambda-1)^2+(S-1)^2(S+\lambda-1)\right. \\
&\quad \left.+\,2(S-1)^2(S+\lambda-1)S+(S-1)^3S+(S-1)^3S^2\right].
\end{aligned}$$

Thus we get the same answer as in Example 3.4.5, verifying our result.

3.6 The k-defect Polynomials of a Theta Graph

In this section, we apply Proposition 3.4.1 and Theorem 3.5.3 to find the explicit expressions of the k-defect polynomials of a theta graph. We conclude this section by verifying the results with Example 3.3.6.

Recall from Section 3.4,

Proposition 3.4.1 Let H be a graph with edge set $E(H)$. The bad coloring polynomial of H,

$$\widetilde{B}(H;\lambda,S) = \sum_{k=0}^{|E(H)|} \phi_k(H;\lambda)S^k$$

where $\phi_k(H;\lambda)$ is the k-defect polynomial of the graph H.

Recall from Section 3.5

Theorem 3.5.3 Let H be a theta graph, θ_{a_1,a_2,a_3}, with $1 \leq a_1 \leq a_2 \leq a_3$. The bad coloring polynomial,

$$\begin{aligned}\lambda^{-1}\widetilde{B}(H;\lambda,S) &= B(C_{a_2+a_3};\lambda,S)\left[B(C_{a_1};\lambda,S)-(S-1)^{a_1}\right] \\ &\quad +(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S).\end{aligned}$$

Recall from Definition 3.3.4 that the bad coloring polynomial of a cycle graph C_n on n vertices,

$$\widetilde{B}(C_n;\lambda,S)=\sum_{k=0}^{|E(C_n)|}\phi_k(C_n;\lambda)S^k=\sum_{k=0}^{n}\binom{n}{k}\left[(\lambda-1)^{n-k}+(-1)^{n-k}(\lambda-1)\right]S^k.$$

We are going to use the equation

$$\phi_k(C_n;\lambda)=\binom{n}{k}\left[(\lambda-1)^{n-k}+(-1)^{n-k}(\lambda-1)\right]$$

to find the k-defect polynomial of the theta graph. Since we know the bad coloring polynomial of a theta graph, we can rewrite it as a generating function in S, then applying Proposition 3.4.1, the k-defect polynomial of the theta graph is the coefficient of S^k. But in this case, we do not need to rewrite it as a generating function in order to find the coefficient of S^k, we manipulate the bad coloring polynomial of a theta graph from Theorem 3.5.3, and write it as a sum of three products,

$$B(C_{a_2+a_3};\lambda,S)B(C_{a_1};\lambda,S)+(-1)(S-1)^{a_1}B(C_{a_2+a_3};\lambda,S)+(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S).$$

We then find the coefficient of S^k in each of the three products. Summing these coefficients will give the k-defect polynomial of the theta graph. To ease notation, in this section, $[S^k]\,[P(\lambda,S)]$ will denote the coefficient of S^k in the polynomial $P(\lambda,S)$. We state, without proof, the following two well known propositions, which will be useful in this section. We refer the reader to [33] for further details.

Proposition 3.6.1. *Let* $H(S) = \sum_{i=0}^{\infty} h_i S^i$, $G(S) = \sum_{i=0}^{\infty} g_i S^i$ *and* $F(S) = \sum_{i=0}^{\infty} f_i S^i$ *be three generating functions such that* $H(S) = G(S)F(S)$. *Then*

$$h_k = \sum_{i=0}^{k} g_i f_{k-i}.$$

Proposition 3.6.2. *[Vandermonde convolution] Let* b_1, b_2 *and* r *be natural numbers, then*

$$\sum_{i=0}^{r} \binom{b_1}{r-i}\binom{b_2}{i} = \binom{b_1+b_2}{r}.$$

use the following lemma, Lemma 3.6.3, Lemma 3.6.4 and Lemma 3.6.6, to find and simplify the coefficient of S^k for each of the three products of the bad coloring polynomial of a theta graph,

$$B(C_{a_2+a_3};\lambda,S)B(C_{a_1};\lambda,S)+(-1)(S-1)^{a_1}B(C_{a_2+a_3};\lambda,S)+(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S).$$

Recall that $[S^k]\,[P(\lambda,S)]$ will denote the coefficient of S^k in the polynomial $P(\lambda,S)$. We start by simplifying the product $B(C_{a_2+a_3};\lambda,S)B(C_{a_1};\lambda,S)$.

Lemma 3.6.3. *The coefficient of* S^k *in the product* $B(C_{a_2+a_3};\lambda,S)B(C_{a_1};\lambda,S)$,

$$\begin{aligned}
& [S^k]\,[B(C_{a_2+a_3},\lambda,S)B(C_{a_1},\lambda,S)] \\
= \; & \frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}\left((\lambda-1)^{n-k}+(-1)^{n-k}(\lambda-1)^2\right) \\
& +\frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}\left((-1)^{a_1-k+i}(\lambda-1)^{a_2+a_3+1-i}\right) \\
& +\frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}\left((-1)^{a_2+a_3-i}(\lambda-1)^{a_1-k+i+1}\right).
\end{aligned}$$

Proof.

$$\begin{aligned}
& [S^k]\left[B(C_{a_2+a_3};\lambda,S)B(C_{a_1},\lambda,S)\right] \\
= & \sum_{i=0}^{k}\phi_i(C_{a_2+a_3},\lambda)\phi_{k-i}(C_{a_1},\lambda) \text{ by Proposition 3.6.1} \\
= & \sum_{i=0}^{k}\left(\frac{1}{\lambda}\binom{a_2+a_3}{i}(\lambda-1)^{a_2+a_3-i}+(-1)^{a_2+a_3-i}(\lambda-1)\right) \\
\times & \left(\frac{1}{\lambda}\binom{a_1}{k-i}(\lambda-1)^{a_1-k+i}+(-1)^{a_1-k+i}(\lambda-1)\right) \text{ by Proposition 3.3.4} \\
= & \frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}\left((\lambda-1)^{n-k}+(-1)^{a_2+a_3-i}(\lambda-1)^{a_1-k+i+1}\right) \\
& +\frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}\left((-1)^{a_1-k+i}(\lambda-1)^{a_2+a_3+1-i}+(-1)^{n-k}(\lambda-1)^2\right) \\
= & \frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}\left((\lambda-1)^{n-k}+(-1)^{n-k}(\lambda-1)^2\right) \\
& +\frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}\left((-1)^{a_1-k+i}(\lambda-1)^{a_2+a_3+1-i}+(-1)^{a_2+a_3-i}(\lambda-1)^{a_1-k+i+1}\right).
\end{aligned}$$

Simplifying and applying Proposition 3.6.2, we get

$$\begin{aligned}
& [S^k]\left[B(C_{a_2+a_3};\lambda,S)B(C_{a_1},\lambda,S)\right] \\
= & \frac{1}{\lambda^2}\binom{n}{k}\left((\lambda-1)^{n-k}+(-1)^{n-k}(\lambda-1)^2\right) \\
& +\frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}\left((-1)^{a_1-k+i}(\lambda-1)^{a_2+a_3+1-i}+(-1)^{a_2+a_3-i}(\lambda-1)^{a_1-k+i+1}\right).
\end{aligned}$$

□

We now simplify the second product $(-1)(S-1)^{a_1}B(C_{a_2+a_3};\lambda,S)$.

Lemma 3.6.4. *The coefficient of S^k in the product $(-1)(S-1)^{a_1}B(C_{a_2+a_3};\lambda,S)$,*

$$\begin{aligned}
& [S^k]\left[(-1)(S-1)^{a_1}B(C_{a_2+a_3};\lambda,S)\right] \\
= & \frac{1}{\lambda^2}\binom{n}{k}(-1)^{n-k+1}\lambda(\lambda-1) \\
& +\frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}(-1)^{a_1-k+i+1}\lambda(\lambda-1)^{a_2+a_3-i}.
\end{aligned}$$

Proof. We make use of the k-defect polynomial of a cycle graph given in Proposition 3.3.4 and the binomial theorem for the coefficients in $(S-1)^{a_1}$.

$$\begin{aligned}
& [S^k]\left[(-1)(S-1)^{a_1}B(C_{a_2+a_3};\lambda,S)\right] \\
= & -\sum_{i=0}^{k}\phi_i(C_{a_2+a_3},\lambda)\binom{a_1}{k-i}(-1)^{a_1-k+i} \\
= & \sum_{i=0}^{k}\frac{1}{\lambda}\binom{a_2+a_3}{i}\left[(\lambda-1)^{a_2+a_3-i}+(-1)^{a_2+a_3-i}(\lambda-1)\right]\frac{\lambda}{\lambda}\binom{a_1}{k-i}(-1)^{a_1-k+i+1} \\
= & \frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}\left[(-1)^{a_1-k+i+1}\lambda(\lambda-1)^{a_2+a_3-i}+(-1)^{n-k+1}\lambda(\lambda-1)\right] \\
= & \frac{1}{\lambda^2}\binom{n}{k}(-1)^{n-k+1}\lambda(\lambda-1) \\
& +\frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}(-1)^{a_1-k+i+1}\lambda(\lambda-1)^{a_2+a_3-i}.
\end{aligned}$$

□

Now adding and simplifying the results of Lemma 3.6.3 and Lemma 3.6.4 we get Corollary 3.6.5, the coefficient of S^k in $B(C_{a_2+a_3};\lambda,S)\left[B(C_{a_1};\lambda,S)-(S-1)^{a_1}\right]$.

Corollary 3.6.5.

$$\begin{aligned}
& [S^k]\left[B(C_{a_2+a_3};\lambda,S)\left[B(C_{a_1};\lambda,S)-(S-1)^{a_1}\right]\right] \\
= & \frac{1}{\lambda^2}\binom{n}{k}\left[(\lambda-1)^{n-k}+(-1)^{n-k+1}(\lambda-1)\right] \\
& +\frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}\left[(-1)^{a_1-k+i+1}(\lambda-1)^{a_2+a_3-i}+(-1)^{a_2+a_3-i}(\lambda-1)^{a_1-k+i+1}\right].
\end{aligned}$$

Finally, we simplify the third product $(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S)$.

Lemma 3.6.6. *The coefficient of S^k in the product $(S-1)^{a_1}B(C_{a_2},\lambda,S)B(C_{a_3},\lambda,S)$,*

$$\begin{aligned}
&[S^k]\left[(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S)\right]\\
= \;& \frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}(-1)^{a_1-k+i}(\lambda-1)^{a_2+a_3-i}\\
&+\frac{1}{\lambda^2}\sum_{j=0}^{k}\binom{a_1+a_2}{j}\binom{a_3}{k-j}(-1)^{a_1+a_2-j}(\lambda-1)^{a_3-k+j+1}\\
&+\frac{1}{\lambda^2}\sum_{r=0}^{k}\binom{a_2}{k-r}\binom{a_1+a_3}{r}(-1)^{a_1+a_3-r}(\lambda-1)^{a_2-k+r+1}\\
&+\frac{1}{\lambda^2}\binom{n}{k}(-1)^{n-k}(\lambda-1)^2.
\end{aligned}$$

Proof.

$$\begin{aligned}
&[S^k]\left[(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S)\right]\\
= \;& \sum_{r=0}^{k}\binom{a_1}{r}(-1)^{a_1-r}\sum_{i=0}^{k-r}\phi_i(C_{a_2},\lambda)\phi_{k-r-i}(C_{a_3},\lambda)\\
= \;& \sum_{r=0}^{k}\binom{a_1}{r}(-1)^{a_1-r}\sum_{i=0}^{k-r}\frac{1}{\lambda}\binom{a_2}{i}\left[(\lambda-1)^{a_2-i}+(-1)^{a_2-i}(\lambda-1)\right]\\
&\times\frac{1}{\lambda}\binom{a_3}{k-r-i}\left[(\lambda-1)^{a_3-k+r+i}+(-1)^{a_3-k+r+i}(\lambda-1)\right]\\
= \;& \frac{1}{\lambda^2}\sum_{r=0}^{k}\sum_{i=0}^{k-r}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}(-1)^{a_1-r}(\lambda-1)^{a_2+a_3-k+r}\\
&+\frac{1}{\lambda^2}\sum_{r=0}^{k}\sum_{i=0}^{k-r}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}(-1)^{a_1+a_2-i-r}(\lambda-1)^{a_3-k+r+i+1}\\
&+\frac{1}{\lambda^2}\sum_{r=0}^{k}\sum_{i=0}^{k-r}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}(-1)^{a_1+a_3-k+i}(\lambda-1)^{a_2-i+1}\\
&+\frac{1}{\lambda^2}\sum_{r=0}^{k}\sum_{i=0}^{k-r}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}(-1)^{a_1+a_2+a_3-k}(\lambda-1)^{2}.
\end{aligned}$$

There are four terms in $[S^k]\left[(S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S)\right]$ which we can simplify separately.

(i) We simplify the first term,

$$\frac{1}{\lambda^2}\sum_{r=0}^{k}\sum_{i=0}^{k-r}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}\left[(-1)^{a_1-r}(\lambda-1)^{a_2+a_3-k+r}\right].$$

$$\begin{aligned}&\frac{1}{\lambda^2}\sum_{r=0}^{k}\sum_{i=0}^{k-r}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}(-1)^{a_1-r}(\lambda-1)^{a_2+a_3-k+r}\\ =\ &\frac{1}{\lambda^2}\sum_{r=0}^{k}\binom{a_1}{r}\binom{a_2+a_3}{k-r}(-1)^{a_1-r}(\lambda-1)^{a_2+a_3-k+r}.\end{aligned}$$

Let $i=k-r$, then we get

$$\begin{aligned}&\frac{1}{\lambda^2}\sum_{r=0}^{k}\binom{a_1}{r}\binom{a_2+a_3}{k-r}(-1)^{a_1-r}(\lambda-1)^{a_2+a_3-k+r}\\ =\ &\frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}(-1)^{a_1-k+i}(\lambda-1)^{a_2+a_3-i}.\end{aligned}$$

(ii) We simplify the second term

$$\frac{1}{\lambda^2}\sum_{r=0}^{k}\sum_{i=0}^{k-r}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}(-1)^{a_1+a_2-i-r}(\lambda-1)^{a_3-k+r+i+1}$$

by interchanging the order of summation as follows; We see that $0\le i\le k-r$, then $0\le r\le i+r\le k$. Let $j=i+r$, thus $0\le r\le j\le k$. Therefore

$$\begin{aligned}&\frac{1}{\lambda^2}\sum_{r=0}^{k}\sum_{i=0}^{k-r}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}(-1)^{a_1+a_2-i-r}(\lambda-1)^{a_3-k+r+i+1}\\ =\ &\frac{1}{\lambda^2}\sum_{j=0}^{k}\sum_{r=0}^{j}\binom{a_1}{r}\binom{a_2}{j-r}\binom{a_3}{k-j}(-1)^{a_1+a_2-j}(\lambda-1)^{a_3-k+j+1}\\ =\ &\frac{1}{\lambda^2}\sum_{j=0}^{k}\binom{a_1+a_2}{j}\binom{a_3}{k-j}(-1)^{a_1+a_2-j}(\lambda-1)^{a_3-k+j+1}.\end{aligned}$$

(iii) We simplify the third term

$$\frac{1}{\lambda^2}\sum_{r=0}^{k}\sum_{i=0}^{k-r}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}(-1)^{a_1+a_3+i}(\lambda-1)^{a_2-i+1}$$

by interchanging the order of summation as follows, we see that $i \leq k-r$, then $i+r \leq k$, thus $r \leq k-i$. Therefore

$$\begin{aligned} & \frac{1}{\lambda^2}\sum_{r=0}^{k}\sum_{i=0}^{k-r}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}(-1)^{a_1+a_3-k+i}(\lambda-1)^{a_2-i+1} \\ = & \frac{1}{\lambda^2}\sum_{i=0}^{k}\sum_{r=0}^{k-i}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}(-1)^{a_1+a_3-k+i}(\lambda-1)^{a_2-i+1} \\ = & \frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2}{i}\binom{a_1+a_3}{k-i}(-1)^{a_1+a_3-k+i}(\lambda-1)^{a_2-i+1} \end{aligned}$$

Now let $i = k-r$, then we get

$$\frac{1}{\lambda^2}\sum_{r=0}^{k}\binom{a_2}{k-r}\binom{a_1+a_3}{r}(-1)^{a_1+a_3-r}(\lambda-1)^{a_2-k+r+1}.$$

(iv) We simplify the last term $\frac{1}{\lambda^2}\sum_{r=0}^{k}\sum_{i=0}^{k-r}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}(-1)^{a_1+a_2+a_3-k}(\lambda-1)^2$, the we get

$$\begin{aligned} & \frac{1}{\lambda^2}\sum_{r=0}^{k}\sum_{i=0}^{k-r}\binom{a_1}{r}\binom{a_2}{i}\binom{a_3}{k-r-i}(-1)^{a_1+a_2+a_3-k}(\lambda-1)^2 \\ = & \frac{1}{\lambda^2}\sum_{r=0}^{k}\binom{a_1}{r}\binom{a_2+a_3}{k-r}(-1)^{a_1+a_2+a_3-k}(\lambda-1)^2 \\ = & \frac{1}{\lambda^2}\binom{a_1+a_2+a_3}{k}(-1)^{a_1+a_2+a_3-k}(\lambda-1)^2 \\ = & \frac{1}{\lambda^2}\binom{n}{k}(-1)^{n-k}(\lambda-1)^2. \end{aligned}$$

□

We are in a position to state the main result of this section. To get Theorem 3.6.7 we use the results of Lemma 3.6.6 and Corollary 3.6.5.

Theorem 3.6.7. *Let θ_{a_1,a_2,a_3} be a theta graph with $1 \leq a_1 \leq a_2 \leq a_3$ and $a_1+a_2+a_3 = n$. Then the k-defect polynomial for θ_{a_1,a_2,a_3} is*

$$\begin{aligned}\phi_k(\theta_{a_1,a_2,a_3};\lambda) &= \frac{1}{\lambda}\binom{n}{k}\left[(\lambda-1)^{n-k}+(-1)^{n-k}(\lambda-1)(\lambda-2)\right]\\ &\quad +\frac{1}{\lambda}\sum_{j=1}^{3}\sum_{i=0}^{k}\binom{a_j}{k-i}\binom{n-a_j}{i}(-1)^{n-a_j+i}(\lambda-1)^{a_j+i-k+1}.\end{aligned}$$

where $0 \leq k \leq n$.

Proof.

$$\begin{aligned}[S^k]\left[\lambda^{-1}\widetilde{B}(\theta_{a_1,a_2,a_3};\lambda,S)\right] &= [S^k]\left[B(\theta_{a_1,a_2,a_3};\lambda,S)\right]\\ &= [S^k]\left[B(C_{a_2+a_3};\lambda,S)\left[B(C_{a_1};\lambda,S)-(S-1)^{a_1}\right]\right.\\ &\quad \left.+\left[S^k\right](S-1)^{a_1}B(C_{a_2};\lambda,S)B(C_{a_3};\lambda,S)\right]\\ &= \lambda^{-1}\phi_k(\theta_{a_1,a_2,a_3};\lambda).\end{aligned}$$

To get $\phi_k(\theta_{a_1,a_2,a_3};\lambda)$ we apply Lemma 3.6.6 and Corollary 3.6.5, and gather like terms.

$$\begin{aligned}\lambda^{-1}\phi_k(\theta_{a_1,a_2,a_3};\lambda) &= \frac{1}{\lambda^2}\binom{n}{k}\left[(\lambda-1)^{n-k}+(-1)^{n-k+1}(\lambda-1)\right]+\frac{1}{\lambda^2}\binom{n}{k}(-1)^{n-k}(\lambda-1)^2\\ &\quad -\frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}(-1)^{a_1-k+i}(\lambda-1)^{a_2+a_3-i}\\ &\quad +\frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}(-1)^{a_1-k+i}(\lambda-1)^{a_2+a_3-i}\\ &\quad +\frac{1}{\lambda^2}\sum_{i=0}^{k}\binom{a_2+a_3}{i}\binom{a_1}{k-i}(-1)^{a_2+a_3-i}(\lambda-1)^{a_1-k+i+1}\\ &\quad +\frac{1}{\lambda^2}\sum_{r=0}^{k}\binom{a_2}{k-r}\binom{a_1+a_3}{r}(-1)^{a_1+a_3-r}(\lambda-1)^{a_2-k+r+1}\\ &\quad +\frac{1}{\lambda^2}\sum_{j=0}^{k}\binom{a_1+a_2}{j}\binom{a_3}{k-j}(-1)^{a_1+a_2-j}(\lambda-1)^{a_3-k+j+1}.\end{aligned}$$

Finally, we simply the terms to get the required result as

$$\begin{aligned}
\phi_k(\theta_{a_1,a_2,a_3};\lambda) &= \frac{1}{\lambda}\binom{n}{k}\left[(\lambda-1)^{n-k}+(-1)^{n-k}(\lambda-1)(\lambda-2)\right] \\
&\quad +\frac{1}{\lambda}\sum_{i=0}^{k}\binom{a_1}{k-i}\binom{n-a_1}{i}(-1)^{n-a_1+i}(\lambda-1)^{a_1+i-k+1} \\
&\quad +\frac{1}{\lambda}\sum_{i=0}^{k}\binom{a_2}{k-i}\binom{n-a_2}{i}(-1)^{n-a_2+i}(\lambda-1)^{a_2+i-k+1} \\
&\quad +\frac{1}{\lambda}\sum_{i=0}^{k}\binom{a_3}{k-i}\binom{n-a_3}{i}(-1)^{n-a_3+i}(\lambda-1)^{a_3+i-k+1} \\
&= \frac{1}{\lambda}\binom{n}{k}\left[(\lambda-1)^{n-k}+(-1)^{n-k}(\lambda-1)(\lambda-2)\right] \\
&\quad +\frac{1}{\lambda}\sum_{j=1}^{3}\sum_{i=0}^{k}\binom{a_j}{k-i}\binom{n-a_j}{i}(-1)^{n-a_j+i}(\lambda-1)^{a_j+i-k+1}.
\end{aligned}$$

□

We now verify that Example 3.3.6 give us the same answer when we apply it to Theorem 3.6.7,

Example 3.6.8.

Recall, in the diagrams shown in Figure 3.1, H is a theta graph $\theta_{1,2,2}$. Thus if $H = \theta_{a_1,a_2,a_3}$ then $a_1 = 1$ and $a_2 = a_3 = 2$. Now we apply Theorem 3.6.7 to compute the 1-defect polynomial of H.

$$\begin{aligned}
\phi_1(\theta_{1,2,2};\lambda) &= \frac{1}{\lambda}\binom{5}{1}\left[(\lambda-1)^{5-1}+(-1)^{5-1}(\lambda-1)(\lambda-2)\right] \\
&\quad +\frac{1}{\lambda}\sum_{i=0}^{1}\binom{1}{1-i}\binom{5-1}{i}(-1)^{5-1+i}(\lambda-1)^{1+i-1+1} \\
&\quad +\frac{2}{\lambda}\sum_{i=0}^{1}\binom{2}{1-i}\binom{5-2}{i}(-1)^{5-2+i}(\lambda-1)^{2+i-1+1}
\end{aligned}$$

$$
\begin{aligned}
&= \frac{5}{\lambda}\left[(\lambda-1)^4+(-1)^4(\lambda-1)(\lambda-2)\right] \\
&\quad +\frac{1}{\lambda}\left[\lambda-1-4(\lambda-1)^2\right] \\
&\quad +\frac{2}{\lambda}\left[-2(\lambda-1)^2+3(\lambda-1)^3\right] \\
&= \frac{1}{\lambda}\left[5\lambda^4-20\lambda^3+30\lambda^2-20\lambda+5+5\lambda^2-15\lambda+10\right] \\
&\quad +\frac{1}{\lambda}\left[\lambda-1-4\lambda^2+8\lambda-4\right] \\
&\quad +\frac{1}{\lambda}\left[-4\lambda^2+8\lambda-4+6\lambda^3-18\lambda^2+18\lambda-6\right] \\
&= \frac{1}{\lambda}\left[5\lambda^4-14\lambda^3+9\lambda^2\right] \\
&= 5\lambda^3-14\lambda^2+9\lambda.
\end{aligned}
$$

Thus we get the same answer as in Example 3.3.6, verifying our result.

3.7 Conclusion

In this chapter we used the known theory on the coboundary polynomials to find the bad coloring polynomial of a theta graph and multibridge graphs. The bad coloring polynomial can be expressed as a generating function in S where the coefficient of S^k is the k-defect polynomial of a graph. In this chapter, we did not exactly express the bad coloring polynomial as a generating function, we split the bad coloring polynomial of a theta graph into three products whose sum gives the bad coloring polynomial and then extracted the coefficients of S^k in each product. Finally, we added the three extracted coefficients of S^k to get the k-defect polynomial of the theta graph. We verified our theorem with an example.

Chapter 4

Hosoya Polynomial of Uniform Multibridge Graphs

4.1 Introduction

In this chapter, we start by giving a brief history on Hosoya polynomials. Then we state without proof, some explicit expressions of Hosoya polynomials of certain classes of graphs. We illustrate with an example how to compute the Hosoya polynomial of a graph. We give the main result of this chapter, the Hosoya polynomial of uniform multibridge graphs. Finally we apply some results of this chapter to chemical graphs.

4.2 Brief History and Properties of Hosoya Polynomial of a Graph

In this section, we give a brief history of the Hosoya polynomial of a graph and some of its known properties. In particular, we start with the brief history of the Wiener index and hyper-Wiener index.

The Wiener index was introduced in 1947 by Harold Wiener [34]. Wiener used this index as a tool for obtaining the boiling points of alkanes. This study of the Wiener index attracted the attention of chemists and mathematicians. There is a well developed relationship between chemistry and graph theory, such that in chemical graphs, the vertices of the graph correspond to the atoms of the molecule and the edges represent the chemical bonds. We need the concept of diameter in graph theory to be able to define the Wiener index of a graph.

Definition 4.2.1. The distance, $d(u, v)$ between any two vertices u and v in a graph H is the length of a shortest path between them. The diameter D of H is given by $D := max_{u,v \in V(H)}\{d(u, v)\}$.

Definition 4.2.2. Let H be a connected graph and $V(H) = \{u_1, u_2, \cdots, u_n\}$ be the vertex set of H, the Wiener index of the graph H, is given by

$$W(H) = \frac{1}{2} \sum_{i=1,j=1}^{n} d(u_i, u_j).$$

In addition, the hyper-Wiener index of a graph H is

$$WW(H) = W(H) + \frac{1}{2} \sum_{i=1,j=1}^{n} d^2(u_i, u_j).$$

Sagan, et al. in 1996, see [32], studied the Wiener polynomial of a graph as a generating function in q. In their study, it was shown that the derivative of the Wiener polynomial was the q-analog of the Wiener index of a graph. Some properties of the Wiener polynomial were given and explicit expressions of the Wiener polynomials of certain classes of graphs were given.

The Hosoya polynomial of a graph was studied independently as a generating function about distance distributing, by Hosoya in 1988, see [22]. The Hosoya polynomial is defined for a connected graph H as

$$\mathcal{H}(H, z) = \sum_{w=1}^{D} d(H, w) z^w$$

where $d(H, w) \geq 1$ is the number of vertex pairs at distance w. It was shown in this study that the Hosoya polynomial has applications to two important topological indices, the Wiener index and hyper-Wiener index. Thus, the Wiener index is given by the first derivative of the Hosoya polynomial, $\mathcal{H}(H, z)$, at $z = 1$, and it is shown in [12] that the hyper-Wiener index is given by half of the second derivative of the Hosoya polynomial $z\mathcal{H}(H, z)$ at $z = 1$. Hence it is clear that the Hosoya Polynomial is just another name of the Wiener polynomial. Hence in the literature, we have two names for the same polynomial, the Wiener polynomial and the Hosoya polynomial. In this work we have chosen to use the Hosoya polynomial.

Since then, the study of Hosoya polynomials has been taken in many directions by both chemists and mathematicians. One direction of study is finding explicit expressions of the Hosoya polynomial of certain classes of graphs, for example, see [1, 10, 14, 16, 17, 19, 21, 24, 35, 36]. Another new direction is solving for the roots of Hosoya polynomials, for example see [2, 3].

In this chapter, our goal is to find an explicit expression of Hosoya polynomial of uniform multibridge graphs.

4.3 Some Known Results on Hosoya Polynomial of a Graph

In this section, we give some properties of the Hosoya polynomials known in the literature. We then give without proof, some known Hosoya polynomials of some classes of graphs.

The following theorem summarizes some of the known properties of the Hosoya polynomial and we refer the reader to [22, 32] for further details.

Theorem 4.3.1. *Let H be a graph, $E(H)$ be the edge set and $V(H)$ be the vertex set of H. Let $\mathcal{H}(H, z)$ be the Hosoya polynomial of H. Then*

(i) the degree of $\mathcal{H}(H, z)$ is the diameter of H.

(ii) the coefficient of z in $\mathcal{H}(H, z)$ is $|E(H)|$.

(iii) *the coefficient of* z^0 *in* $\mathcal{H}(H, z)$ *is zero.*

(iv) $\mathcal{H}(H, 1) = \binom{|V(H)|}{2}$.

(v) $\frac{d}{dz}\mathcal{H}(H, z)|_{z=1} = W(H) = \sum_{w=1}^{D} wd(H, w)$.

(vi) $\frac{1}{2}\frac{d^2}{dz^2}z\mathcal{H}(H, z)|_{z=1} = WW(H) = W(H) + \frac{1}{2}\sum_{w=1}^{D} w^2 d(H, w)$.

The following two theorems give the Hosoya polynomials of commonly used graphs in mathematics, complete, cycle, path, bipartite and wheel graphs, see [32].

Theorem 4.3.2 ([32])**.** *The Hosoya polynomial of*

(i) *a complete graph* K_n *is*

$$\mathcal{H}(K_n, z) = \binom{n}{2} z.$$

(ii) *a complete bipartite graph* $K_{n,m}$ *is*

$$\mathcal{H}(K_{n,m}, z) = nmz + \left[\binom{n}{2} + \binom{m}{2}\right] z^2.$$

(iii) *a wheel graph* W_n *is*

$$\mathcal{H}(W_n, z) = (2n-2)z + \frac{[(n-1)(n-4)]}{2} z^2.$$

It is of special interest to note that unlike many graph polynomials, the Hosoya polynomials of even and odd cycles have different formulae. Similarly, non isomorphic trees of the same size have different formulae of the Hosoya polynomial.

Theorem 4.3.3 ([32])**.** *The Hosoya polynomial of*

(i) *an even cycle* C_{2n} *is*

$$\mathcal{H}(C_{2n}, z) = 2n \sum_{i=1}^{n-1} z^i + nz^n.$$

(ii) an odd cycle C_{2n+1} is

$$\mathcal{H}(C_{2n+1}, z) = (2n+1)\sum_{i=1}^{n} z^i.$$

(iii) a path P_n is

$$\mathcal{H}(P_n, z) = \sum_{i=1}^{n-1}(n-i)z^i.$$

As a consequence of Theorem 4.3.3, we get the following corollary.

Corollary 4.3.4 ([32])**.** *The Wiener index of*

(i) an even cycle C_{2n} is

$$W(C_{2n}) = \frac{(2n)^3}{8}.$$

(ii) an odd cycle C_{2n+1} is

$$W(C_{2n+1}) = \frac{(2n+2)(2n+1)(2n)}{8}.$$

(iii) a path P_n is

$$W(P_n) = \binom{n+1}{3}.$$

Theorem 4.3.5 ([16])**.** *Let H be a distance-regular graph having the intersection array $\{b_0, b_1, \cdots, b_{D-1}; c_1 = 1, c_2, \cdots, c_D\}$ Then the Hosoya polynomial of H is*

$$\mathcal{H}(H, z) = \frac{nb_0}{2}\left(z + \sum_{i=2}^{D} \frac{\prod_{j=1}^{i-1} b_j}{\prod_{j=2}^{i} c_j} z^i\right).$$

Corollary 4.3.6 ([16])**.** *Let $H = srg(n, k, \lambda, \mu)$, be a strongly regular graph. Then the Hosoya polynomial of H is*

$$\mathcal{H}(H, z) = \frac{n}{2}(kz + (n-k-1)z^2).$$

The following two theorems state some known Hosoya polynomials of chemical graphs.

Theorem 4.3.7 ([1]). *The Hosoya polynomial of an m-pentagonal-chain $G(m,S)$ for $m \geq 5$,*

$$\begin{aligned}\mathcal{H}(G(m,S),z) &= (3m+2)+(4m+1)z+(7m-2)z^2+(7m-8)z^3+(7m-14)z^4 \\ &+ (8m-22)z^5+\sum_{k=6}^{m+1}[9(m-k)+21]z^k+4z^{m+2}.\end{aligned}$$

Theorem 4.3.8 ([35]). *The Hosoya polynomial of TUC4C8(S), $T(p,q)$, for $p \geq 1$ and $q \geq 2$, where*

(i) $q \leq p$

$$\begin{aligned}\mathcal{H}(T(p,q);z) &= 2pq+\frac{4pz^{2p+1}(z+1)(z^q-1)}{(z-1)^3} \\ &- \frac{2pq(z+1)^2((z^2+1)(z^{2p}-1)+z^{2p}+1)}{(z-1)(z^3-1)} \\ &+ \frac{2pz(z+1)(z(z^2+1)(z^{3q}-1)-(z^2+z+1)^2(z^{2q}-1))}{(z-1)(z^3-1)^2}.\end{aligned}$$

(ii) $q > p$

$$\begin{aligned}\mathcal{H}(T(p,q);z) &= 2pq+\frac{2pz(z+1)(z^p-1)(z^{2q}+z^{2p}-z^p-1)}{(z-1)^3} \\ &+ \frac{2pz^2(z+1)(z^2+1)(z^{3p}-1)}{(z-1)(z^3-1)^2} \\ &- \frac{2p(z+1)^2(q(z^p-1)((z^2+1)(z^p+1)-z^{2p+1})+pz^{3p+1})}{(z-1)(z^3-1)}.\end{aligned}$$

The following theorem gives the Hosoya polynomial of a graph that is obtained from a graph operation, vertex-attaching, of some other graphs. This graph operation has application in chemical graphs.

Theorem 4.3.9 ([15])**.** *Let H be a connected graph obtained by point-attaching from $H_1, \ . \ . \ . \ ,H_k$, and let $x_{i\rightarrow j}$ and δ_{ij} be as as defined in [15].*

$$\mathcal{H}(H,z) = \sum_{i=1}^{k} \mathcal{H}(H_i,z) + \sum_{i,j\in\binom{|k|}{2}} \left(\mathcal{H}_{x_{i\rightarrow j}}(H_i,z).\mathcal{H}_{x_{j\rightarrow i}}(H_j,z)z^{\delta_{ij}}\right).$$

4.4 Computing Hosoya Polynomial of a Theta Graph

In this section, we start by giving an example of computing the Hosoya polynomial of a theta graph, $\theta_{3,3,3}$ using the definition of Hosoya polynomial. We then close the section by demonstrating how to compute the Hosoya polynomial of the same theta graph, $\theta_{3,3,3}$, using the principle of inclusion-exclusion.

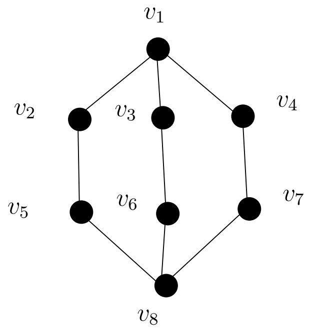

Figure 4.1: The graph $\theta_{3,3,3}$

Example 4.4.1.

Recall from Section 4.2, the definition of the Hosoya polynomial of a connected graph H,

$$\mathcal{H}(H,z) = \sum_{w=1}^{D} d(H,w)z^w$$

where $d(H, w) \geq 1$ is the number of vertex pairs at distance $w \geq 1$. we start by finding D, the diameter of $\theta_{3,3,3}$.

Recall that the diameter D of a graph H is given by $D := max_{u,v \in V(H)}\{d(u, v)\}$. Therefore, the diameter of $\theta_{3,3,3}$ is the distance of a pair of vertices with the largest distance from each other. In Table 4.1, we summarize the distances of all pairs of vertices of the graph , $\theta_{3,3,3}$, corresponding to the diagram in Figure 4.1.

Distance	**no. of pairs**	**The pairs of vertices**
3	7	$\{v_1, v_8\}$, $\{v_2, v_6\}$, $\{v_2, v_7\}$, $\{v_3, v_7\}$, $\{v_3, v_5\}$, $\{v_4, v_5\}$, $\{v_4, v_6\}$.
2	12	$\{v_1, v_5\}$, $\{v_1, v_6\}$, $\{v_1, v_7\}$, $\{v_2, v_3\}$, $\{v_2, v_4\}$, $\{v_2, v_8\}$, $\{v_3, v_4\}$, $\{v_3, v_8\}$, $\{v_4, v_8\}$, $\{v_5, v_6\}$, $\{v_5, v_7\}$, $\{v_5, v_7\}$.
1	9	pairs of vertices for each edge.

Table 4.1:

It is clear from Table 4.1 that the diameter of $\theta_{3,3,3}$ is 3, hence the Hosoya polynomial of $\theta_{3,3,3}$, $\mathcal{H}(\theta_{3,3,3}; z) = 9z + 12z^2 + 7z^3$.

Hence the Wiener index of $W(\theta_{3,3,3})$,

$$\begin{aligned} W(\theta_{3,3,3}) &= \frac{d}{dz}(9z + 12z^2 + 7z^3)|_{z=1} \\ &= 9 + 24z + 21z^2|_{z=1} \\ &= 54 \end{aligned}$$

In preparation for the main result of this chapter, we explore the use of the principle of inclusion-exclusion, described in Section 2.2, in computing the Hosoya polynomial of a theta graph, $\theta_{3,3,3}$. From Chapter 1, Definition 1.4.1 and Chapter 2, Proposition 2.4.1, we know that $\theta_{3,3,3}$ has three cycles, each of these cycle has order 6, and has three internally disjoint paths of order 4 each. The graph $\theta_{3,3,3}$, corresponding to the diagram in Figure 4.1, has three cycles, denoted $\widehat{C}_i$, and three internally disjoint paths, denoted $\widehat{P}_i$, namely,

$$\begin{aligned}
\widehat{C}_1 &= \{v_1v_2, v_2v_5, v_5v_8, v_8v_6, v_6v_3, v_3v_1\} \\
\widehat{C}_2 &= \{v_1v_4, v_4v_7, v_7v_8, v_8v_6, v_6v_3, v_3v_1\} \\
\widehat{C}_3 &= \{v_1v_2, v_2v_5, v_5v_8, v_8v_7, v_7v_4, v_4v_1\} \\
\widehat{P}_1 &= \{v_1v_2, v_2v_5, v_5v_8\} \\
\widehat{P}_2 &= \{v_8v_6, v_6v_3, v_3v_1\} \\
\widehat{P}_3 &= \{v_1v_4, v_4v_7, v_7v_8\}
\end{aligned}$$

We note that path $\widehat{P}_1 \subseteq \widehat{C}_1$ and $\widehat{P}_1 \subseteq \widehat{C}_3$, path $\widehat{P}_2 \subseteq \widehat{C}_2$ and $\widehat{P}_2 \subseteq \widehat{C}_1$ and path $\widehat{P}_3 \subseteq \widehat{C}_2$ and $\widehat{P}_3 \subseteq \widehat{C}_3$.

We now compute the Hosoya polynomial of $\theta_{3,3,3}$ in terms of the Hosoya polynomials of $\widehat{C}_1$, $\widehat{C}_2$, $\widehat{C}_3$, $\widehat{P}_1$, $\widehat{P}_2$ and $\widehat{P}_3$ using the principle of inclusion-exclusion.

In the Table 4.2, we summarize the distances of all pairs of vertices of the sub-graph $\widehat{C}_1$ of $\theta_{3,3,3}$.

Distance	**no. of pairs**	**The pairs of vertices**
1	6	$\{v_1, v_2\}, \{v_2, v_5\}, \{v_5, v_8\}, \{v_8, v_6\}, \{v_6, v_3\}, \{v_3, v_1\}$.
2	6	$\{v_1, v_5\}, \{v_2, v_8\}, \{v_5, v_6\}, \{v_8, v_3\}, \{v_6, v_1\}, \{v_3, v_2\}$.
3	3	$\{v_1, v_8\}, \{v_2, v_6\}, \{v_5, v_3\}$.

Table 4.2:

Hence from Table 4.2, the Hosoya polynomial of $\widehat{C}_1$ is $\mathcal{H}(\widehat{C}_1, z) = 6z + 6z^2 + 3z^3$. Similarly, $\mathcal{H}(\widehat{C}_2, z) = \mathcal{H}(\widehat{C}_3, z) = 6z + 6z^2 + 3z^3$.

In Table 4.3, we summarize the distances of all pairs of vertices of the sub-graph $\widehat{P}_1 \subseteq \widehat{C}_1$ of $\theta_{3,3,3}$.

Hence from Table 4.3, the Hosoya polynomial of $\widehat{P}_1$ is $\mathcal{H}(\widehat{P}_1, z) = 3z + 2z^2 + z^3$. Similarly, $\mathcal{H}(\widehat{P}_2, z) = \mathcal{H}(\widehat{P}_3, z) = 3z + 2z^2 + z^3$.

Distance	**no. of pairs**	**The pairs of vertices**
1	3	$\{v_1, v_2\}, \{v_2, v_5\}, \{v_5, v_8\}.$
2	2	$\{v_1, v_5\}, \{v_2, v_8\}.$
3	1	$\{v_1, v_8\}.$

Table 4.3:

It is clear from Table 4.2 and Table 4.3, since $\widehat{P}_1 \subseteq \widehat{C}_1$, that all the vertex pairs at distance $w \in \{1, 2, 3\}$ in the path $\widehat{P}_1$ appear also as vertex pairs at distance $w \in \{1, 2, 3\}$ respectively, in $\widehat{C}_1$. Similarly, these vertex pairs will also appear as vertex pairs at distance $w \in \{1, 2, 3\}$ respectively, in $\widehat{C}_3$.

A similar argument indicates that, all the vertex pairs at distance $w \in \{1, 2, 3\}$ in the path $\widehat{P}_2$ also appear as vertex pairs at distance $w \in \{1, 2, 3\}$ respectively, in $\widehat{C}_1$ and $\widehat{C}_2$ and all the vertex pairs at distance $w \in \{1, 2, 3\}$ in the path $\widehat{P}_3$ also appear as vertex pair at distance $w \in \{1, 2, 3\}$ respectively, in $\widehat{C}_2$ and $\widehat{C}_3$.

It is clear that we have covered all vertex pairs of $\theta_{3,3,3}$, in some cycle of the graph. Hence by the principle of inclusion-exclusion, we include all the vertex pairs by adding the Hosoya polynomials of the three cycles of the graph, then we exclude the repeated vertex pairs, by subtracting the Hosoya polynomial of the three paths. Finally, we add the term z^3 to cover the vertex pair $\{v_1, v_8\}$ which has been added three times and subtracted three times, in the Hosoya polynomials of cycles and paths, respectively.

$$\begin{aligned}
\mathcal{H}(\theta_{3,3,3}; z) &= \mathcal{H}(\widehat{C}_1, z) + \mathcal{H}(\widehat{C}_2, z) + \mathcal{H}(\widehat{C}_3, z) - \mathcal{H}(\widehat{P}_1, z) - \mathcal{H}(\widehat{P}_2, z) - \mathcal{H}(\widehat{P}_3, z) + z^3 \\
&= 3(6z + 6z^2 + 3z^3) - 3(3z + 2z^2 + z^3) + z^3 \\
&= 9z + 12z^2 + 7z^3.
\end{aligned}$$

4.5 The Hosoya Polynomial of Uniform Multibridge Graphs

In this section, we state some properties of an m-bridge graph. Then we state and prove the main result of this chapter, the formulas for the Hosoya polynomial of a uniform multibridge graph.

Recall from Chapter 1, Definition 1.4.2, that an m-bridge graph is a graph consisting of a pair of end vertices joined by $m \geq 2$ internally disjoint paths of lengths $b_1, b_2, \cdots, b_m \geq 1$ and is denoted by $\theta_{b_1,b_2,b_3,\cdots,b_m}$. There are many paths in an m-bridge graph, but of much interest in this work are the internally disjoint paths of lengths $b_1, b_2, \cdots, b_m \geq 1$ which define the graph. To ease notation in this chapter, we denoted these internally disjoint paths of lengths $b_1, b_2, \cdots, b_m$ of an m-bridge graph, by $\widehat{P}_{b_1}, \widehat{P}_{b_2}, \widehat{P}_{b_3}, \cdots, \widehat{P}_{b_m}$ respectively. Note that $\widehat{P}_{b_i}$ has order $b_i + 1$ for all $i \in \{1, 2, \cdots, m\}$. An m-bridge graph is simply a cycle graph if $m = 2$ and is a theta graph if $m = 3$. A cycle of an m-bridge graph, will be denoted by $C_{b_i+b_j}$ if it connects two internally disjoint paths, of lengths b_i and b_j. If $b_i = b$, for all $i \in \{1, 2, \cdots, m\}$ in $\theta_{b_1,b_2,b_3,\cdots,b_m}$, then the m-bridge graph is said to be uniform. We denote a uniform m-bridge graph by $\theta_m(b)$.

The following proposition stating some properties of an m-bridge graph, is a direct result from the definition of an m-bridge graph, and is useful to this work.

Proposition 4.5.1. *Let H be an m-bridge graph $\theta_{b_1,b_2,b_3,\cdots,b_m}$. Then*

(i) the size of H is $\displaystyle\sum_{i=1}^{m} b_i$.

(ii) the order of H is $\displaystyle\sum_{i=1}^{m} b_i - m + 2$.

(iii) any path $\widehat{P}_{b_i}$ of an m-bridge graph belongs to $m - 1$ cycles of H.

(iv) there are $\binom{m}{2}$ cycles in H given by $C_{b_i+b_j}$, and $i \neq j$.

Corollary 4.5.2. *Let H be a uniform m-bridge graph, $\theta_m(b)$. Then*

- *(i) the size of H is mb.*
- *(ii) the order of H is $m(b-1)+2$.*
- *(iii) there are m isomorphic internally disjoint paths, $\widehat{P}_b$ in H.*
- *(iv) every cycle of H is even.*

In order to apply the principle of inclusion-exclusion in the main results of Theorem 4.5.4, we need the following Lemma.

Lemma 4.5.3. *Let H be an m-bridge graph $\theta_{b_1,b_2,b_3,\cdots,b_m}$. Then every pair of vertices in H belong to some cycle of the graph H.*

Proof. Let H be an m-bridge graph $\theta_{b_1,b_2,b_3,\cdots,b_m}$. Let the two vertices that connect the m internally disjoint paths of H be u and v. We consider four cases as follows.
Case 1. Assume that the pair of vertices is the one that connects the m internally disjoint paths of H, that is, u and v. This pair appears once in each of the m internally disjoint paths and $\binom{m}{2}$ cycles in H respectively, as it connects all the m internally disjoint paths in H. Therefore the pair $\{u, v\}$ is in all the $\binom{m}{2}$ cycles in H.
Case 2. Assume that the pair of vertices include exactly one of u and v, and another vertex in any of the m internally disjoint paths. Then the two vertices are in the same path $\widehat{P}_{b_l}$, where $1 \le l \le m$. Then by Proposition 4.5.1 part (iii) the pair of vertices belong to $m-1$ cycles, as $\widehat{P}_{b_l}$, belong to $m-1$ cycles.
Case 3. Consider a pair of vertices that does not include u and v. Assume that these two vertices are in the same path $\widehat{P}_{b_l}$, where $1 \le l \le m$. Then by Proposition 4.5.1 part (iii) the pair of vertices belong to $m-1$ cycles, as $\widehat{P}_{b_l}$, belong to $m-1$ cycles.
Case 4. Consider a pair of vertices that does not include u and v. Assume that these two vertices are in different internally disjoint paths $\widehat{P}_{b_i}$ and $\widehat{P}_{b_j}$ respectively, where $i \neq j$ for $i, j \in \{1, 2, \cdots, m\}$. Then by Proposition 4.5.1 part (iv) the pair of vertices are in exactly one cycle $C_{b_i+b_j}$.

Thus every pair of vertices in H belong to some cycle. $\square$

From Lemma 4.5.3 **Case 1, 2, 3,** we conclude that only those pairs of vertices that appear in the same path $\widehat{P}_{b_l}$, where $1 \leq l \leq m$, will always appear in more than one cycle, that is in $m-1$ or $\binom{m}{2}$ cycles.
But from Lemma 4.5.3 **Case 4,** we conclude that, if two vertices appear in different internally disjoint paths $\widehat{P}_{b_i}$ and $\widehat{P}_{b_j}$ respectively, where $i \neq j$ for $i, j \in \{1, 2, \cdots, m\}$, then the pair of vertices will always appear in exactly one cycle $C_{b_i+b_j}$.
We are now ready to prove the main results of this chapter.

Theorem 4.5.4. *Let $H = \theta_m(b)$ be a uniform m-bridge graph. The Hosoya polynomial of H is*

$$\mathcal{H}(H, z) = \binom{m}{2}\mathcal{H}(C_{2b}, z) - m(m-2)\mathcal{H}(\widehat{P}_b, z) + \binom{m-1}{2}z^b.$$

Proof. Let $H = \theta_m(b)$ be a uniform m-bridge graph and the two vertices that connect the m internally disjoint paths be u and v. From Proposition 4.5.1 and Corollary 4.5.2, we know that H has $\binom{m}{2}$ even cycles. Thus the sum of Hosoya polynomials for all the cycles in H is $\binom{m}{2}\mathcal{H}(C_{2b}, z)$. By Lemma 4.5.3, each pair of vertices of H belongs to some cycle, hence each pair of vertex contributes to the counted sum of Hosoya polynomials for all the cycles in H. By Lemma 4.5.3, some vertex pairs appear in more than one cycle of H. Hence we need to remove the repetitions in the sum of Hosoya polynomials for all the cycles in H.
By Definition 1.4.2, there are m internally disjoint paths in H, denoted $\widehat{P}_b$. By Proposition 4.5.1, part (iii), any of these paths, $\widehat{P}_b$, of an m-bridge graph belongs to $m-1$ cycles of H. Hence $\mathcal{H}(\widehat{P}_b, z)$ contributes to the Hosoya polynomial of $m-1$ cycles. So we let, each path contribute to the Hosoya polynomial of one cycle, thus we remove it $m-2$ times. Hence for all the m paths, from $\binom{m}{2}\mathcal{H}(C_{2b}, z)$, we remove $\mathcal{H}(\widehat{P}_b, z)$, $m(m-2)$ times, that is

$$\binom{m}{2}\mathcal{H}(C_{2b}, z) - m(m-2)\mathcal{H}(\widehat{P}_b, z).$$

To complete the proof, we note that the vertex pair, u and v appears in each cycle and in each path. Moreover, the distance between u and v is equal to b. By definition of the Hosoya polynomial, contributes the term z^b. Since there are $\binom{m}{2}$ cycles in H, the vertex pair u and v have contributed $\binom{m}{2}z^b$ in the sum $\binom{m}{2}\mathcal{H}(C_{2b}, z)$ and $m(m-2)z^b$ in $m(m-2)\mathcal{H}(\widehat{P}_b, z)$. But we need the vertex pair to contribute only once in the Hosoya polynomial of H. Thus, since $m(m-2) \geq \binom{m}{2}$ for $m \geq 3$, we need to find k such that $\binom{m}{2}z^b - m(m-2)z^b + kz^b = z^b$. Thus, solving for k in the following equation, $\binom{m}{2} - m(m-2) + k = 1$

$$\begin{aligned} 1 &= \binom{m}{2} - m(m-2) + k \\ &= \frac{m(m-1)}{2} - m(m-2) + k \\ &= m\left[\frac{(m-1)}{2} - m + 2\right] + k. \end{aligned}$$

Therefore

$$\begin{aligned} k &= 1 - m\left[\frac{(m-1)}{2} - m + 2\right] \\ &= 1 + m\left[m - 2 + \frac{(1-m)}{2}\right] \\ &= 1 + m\left[\frac{2m - 4 + 1 - m}{2}\right] \\ &= 1 + m\left[\frac{m-3}{2}\right] \\ &= \frac{2}{2} + \frac{m^2 - 3m}{2} \\ &= \frac{m^2 - 3m + 2}{2} \\ &= \frac{(m-1)(m-2)}{2} \\ &= \binom{m-1}{2}. \end{aligned}$$

Therefore, the Hosoya polynomial of H, is

$$\binom{m}{2}\mathcal{H}(C_{2b}, z) - m(m-2)\mathcal{H}(\widehat{P}_b, z) + \binom{m-1}{2}z^b.$$

$\square$

We now give the explicit expression of the Hosoya polynomial of uniform m-bridge graph.

Theorem 4.5.5. *Let $H = \theta_m(b)$ be a uniform m-bridge graph. The Hosoya polynomial of H is*

$$\mathcal{H}(H, z) = \sum_{i=1}^{b-1} \left(m(m-2)(i-1) + mb\right) z^i + \left(\frac{(b-1)m(m-1)}{2} + 1\right) z^b.$$

Proof. Substituting the Hosoya polynomials of an even cycle and the Hosoya polynomial of a path graph given by Theorem 4.3.3 in the expression of the Hosoya polynomial of a uniform m-bridge graph given in Theorem 4.5.4, we get the required result. $\square$

As a consequence of Theorem 4.5.4 and Corollary 4.3.4, we get the Wiener index of a uniform m-bridge graph, stated in the following corollary.

Corollary 4.5.6. *Let $H = \theta_m(b)$ be a uniform m-bridge graph. The Wiener index of H is,*

$$W(H) = b + \frac{b(b-1)m\left((2b-1)m - (b-5)\right)}{6}.$$

In Example 4.4.1, the Hosoya polynomial of $\theta_{3,3,3}$, is given as

$$\mathcal{H}(\theta_{3,3,3}; z) = 9z + 12z^2 + 7z^3.$$

Now substituting $m = 3$ and $b = 3$, in Theorem 4.5.5, we verify our result.

$$\begin{aligned}
\mathcal{H}(\theta_{3,3,3}; z), z) &= \sum_{i=1}^{3-1} \left(3(3-2)(i-1) + 3 * 3\right) z^i + \left(\frac{(3-1)3(3-1)}{2} + 1\right) z^3. \\
&= (0+9)z + (3+9)z^2 + (6+1)z^3 \\
&= 9z + 12z^2 + 7z^3.
\end{aligned}$$

In Example 4.4.1 we found the Wiener index of $\theta_{3,3,3}$ to be $W(\theta_{3,3,3}) = 54$. Now substituting $m = 3$ and $b = 3$, in Corollary 4.5.6, we get

$$W(\theta_{3,3,3}) = 3 + \frac{3(3-1)3\left((2 \times 3 - 1)3 - (3-5)\right)}{6} = 54$$

verifying our result.

4.6 Some Application to Chemical Graphs

We note that if m is equal to 3 in $\theta_m(b)$, then we have a theta graph with all three internally disjoint paths equal to b. This class of graphs is called *bridged bi-cyclic* alkanes in mathematical chemistry. There are two bridged bi-cyclic alkanes that correspond to the class of graphs $\theta_3(b)$, with the Hosoya polynomial

$$\mathcal{H}(\theta_3(b), z) = 3\mathcal{H}(C_{2b}, z) - 3\mathcal{H}(\widehat{P}_b, z) + z^b.$$

We have the *bicyclo[2.2.2]octane* which is $\theta_3(3) = \theta_{3,3,3}$ and the *bicyclo[3.3.3]undecane* which is $\theta_3(4) = \theta_{4,4,4}$. Therefore, from Example 4.4.1 the Hosoya polynomial of bicyclo[2.2.2]octane is $\mathcal{H}(\theta_{3,3,3}; z) = 9z + 12z^2 + 7z^3$. While the Hosoya polynomial of bicyclo[3.3.3]undecane is

$$\mathcal{H}(\theta_3(4), z) = 3\mathcal{H}(C_8, z) - 3\mathcal{H}(\widehat{P}_4, z) + z^4 = 12z + 15z^2 + 18z^3 + 10z^4.$$

The Wiener indices are $W(\theta_{3,3,3}) = 54$ and $W(\theta_{4,4,4}) = 136$.

4.7 Conclusion

We illustrated with an example how to compute the Hosoya polynomial of a graph. We explored and used the principle of inclusion and exclusion to get the formula of the Hosoya polynomial for a uniform multibridge graph. Finally, we showed how these results can be applied to mathematical chemistry.

Chapter 5

The Hosoya Polynomial of q-vertex Joins

5.1 Introduction

In this chapter, we extend the concept of vertex join of a graph to a q-vertex join. We discuss some properties of q-vertex joins of a graph. Finally, we give a formula for the Hosoya polynomial of a q-vertex join of a graph with diameter at most 2.
Recall that $d(u, v)$ denote a minimum distance between any two vertices u and v in a graph H and the diameter D of H is given by $D := max_{u,v \in V(H)}\{d(u, v)\}$. A graph with maximum distance equal to 1 or 2 between pairs of vertices is said to be a graph with diameter 1 or 2 respectively.
The Hosoya polynomial of any graph with diameter 2 is known, see [3].

Proposition 5.1.1 ([3])**.** *Let H be a graph on edge set $E(H)$ and let $V(H)$ be vertex set of H, with $|V(H)|$ vertices and $|E(H)|$ edges and with diameter two. Then the Hosoya polynomial of H*

$$\mathcal{H}(H, z) \;=\; |E(H)|z + \left[\binom{|V(H)|}{2} - |E(H)|\right] z^2.$$

Let H be a graph with vertex set $V(H) = \{h_1, h_2, \cdots, h_n\}$, edge set $E(H)$ and let a vertex $w \notin V(H)$. A vertex join of a graph H, is the graph denoted by $\hat{H}$, with vertex set $V(\hat{H}) = \{h_1, h_2, \cdots, h_n\} \cup \{w\}$ and edge set $E(\hat{H}) = E(H) \cup \{\{h_1, w\}, \{h_2, w\}, \cdots, \{h_n, w\}\}$. To ease notation, We shall call an edge $e \in \{\{h_1, w\}, \{h_2, w\}, \cdots, \{h_n, w\}\}$ a join edge and a vertex w a join vertex.

If each join edge of a vertex join, $\hat{H}$, is replaced by a path P_{q+1}, the resulting graph is called a q-vertex join of a graph H, denoted by $\hat{H}_q$. A path P_{q+1} in a q-vertex join which replaced a join edge of $\hat{H}$ is called a join path. We denote a join path by $\hat{P}_{q+1}$ and to ease notation, we label the n join paths as $\hat{P}_{q+1_1}, \hat{P}_{q+1_2}, \cdots, \hat{P}_{q+1_n}$, if $\hat{P}_{q+1_j}$ is the join path from vertex h_j to vertex w. In addition, $\hat{P}_{q+1} \cong P_{q+1}$. Furthermore, a cycle of a q-vertex join, which contain two join paths and one or two edges of H, is called a join cycle. We denote a join cycle with one edge of H by $\hat{C}_{2q+1}$ and a join cycle with two edges of H by $\hat{C}_{2q+2}$. Moreover, $\hat{C}_{2q+1} \cong C_{2q+1}$ and $\hat{C}_{2q+2} \cong C_{2q+2}$. The following Proposition 5.1.2 states some properties of a q-vertex join, which can be extracted from the definition.

Proposition 5.1.2. *Let H be a diameter 2 graph of order n and size m. Let $\hat{H}_q$ be a q-vertex join of H. Then*

(i) the order of $\hat{H}_q$ is equal to $qn + 1$.

(ii) the number of join paths in $\hat{H}_q$ is equal to n.

(iii) the size of $\hat{H}_q$ is equal to $m + qn$.

Lemma 5.1.3 and Lemma 5.1.5 state some properties of a q-vertex join which are needed in the proofs of the main results of this chapter.

Lemma 5.1.3. *Let H be a diameter 2 graph of order n and size m. Let $\hat{H}_q$ be a q-vertex join of H. Then*

(i) the total number of join cycles, $\hat{C}_{2q+1}$ in $\hat{H}_q$ is m.

(ii) the total number of join cycles, $\hat{C}_{2q+2}$ in $\hat{H}_q$ is $\binom{n}{2} - m$.

(iii) the total number of join cycles in $\hat{H}_q$ is equal to $\binom{n}{2}$.

Proof. (i) Consider an edge $e = \{v_i, v_j\}$ of H, such that $v_i, v_j \in V(H)$ such that the join paths $\hat{P}_{q+1_i}, \hat{P}_{q+1_j}$ joins the join vertex w and vertices v_i, v_j respectively. It is clear that a walk starting at v_i to w through $\hat{P}_{q+1_i}$ to v_j through $\hat{P}_{q+1_j}$ back to v_i is a join cycle, since $\{v_i, v_j\}$ is an edge of $\hat{H}_q$ and $\hat{P}_{q+1_i} \neq \hat{P}_{q+1_j}$. There are m edges, in H, hence m join cycles of the form $\hat{C}_{2q+1}$.

(ii) We just need to count the number of pairs of vertices in H, that are at distance 2 from each other. The rest of the argument is similar to proof of part (i). From Proposition 5.1.1 we know that the number of pairs of vertices at distance 2 from each other in H are $\binom{n}{2} - m$. Hence $\binom{n}{2} - m$ join cycles of the form $\hat{C}_{2q+2}$.

(iii) Combining part (i) and part (ii) we get $\binom{n}{2}$.

□

Corollary 5.1.4. *Let H be a diameter 2 graph of order n and size m. Let $\hat{H}_q$ be a q-vertex join of H. Then*

(i) $\hat{C}_{2q+1} = \hat{P}_{q+1_i} \cup \hat{P}_{q+1_j} \cup (v_i, v_j)$ and

(ii) $\hat{C}_{2q+2} = \hat{P}_{q+1_i} \cup \hat{P}_{q+1_j} \cup (v_i, v_t) \cup (v_t, v_j)$ where $(v_i, v_t) \cup (v_t, v_j) \cong P_3$.

Lemma 5.1.5. *Let H be a diameter 2 graph of order n and size m. Let $\hat{H}_q$ be a q-vertex join of H. Then every vertex pair in $\hat{H}_q$ belong to some joint cycle in $\hat{H}_q$.*

Proof. There are four cases to be considered:

Case 1. A pair of vertices $v_i, v_j \in V(H)$ are either at distance 1 or 2 from each other since H is a diameter 2 graph. By proof of Lemma 5.1.3, each of these pairs of vertices belong to a join cycle.

Case 2. A pair of vertices $v_t, v_j \in V(\hat{P}_{q+1_j})$ such that both vertices are in the same join path $\hat{P}_{q+1_j}$ and $v_t \notin V(H)$. By definition of a join cycle each of these pairs of vertices belong to a join cycle.

Case 3. A pair of vertices v_i, v_t such that $v_i \in V(H)$ and $v_t \in V(\hat{P}_{q+1_j})$ and $w \neq v_t \neq v_j$. By definition the join path $\hat{P}_{q+1_j}$, joins vertex w and vertex $v_j \in V(H)$ in the q-vertex join. Thus $v_j \in V(\hat{P}_{q+1_j})$. But by part (i) v_i, v_j is on the join cycle, in particular the join cycle $\hat{P}_{q+1_i} \cup \hat{P}_{q+1_j} \cup (v_i, v_j)$ by proof of Lemma 5.1.3 part (i). Since $v_t \in V(\hat{P}_{q+1_j})$ then, a pair v_i, v_t is on this join cycle.

Case 4. A pair of vertices v_r, v_t such that $v_r, v_t \notin V(H)$, $v_r \neq w \neq v_t$, $v_r \in V(\hat{P}_{q+1_i})$ and $v_t \in V(\hat{P}_{q+1_j})$. Let $v_i, v_j \in V(H)$, such that $v_i \in V(\hat{P}_{q+1_i})$ and $v_j \in V(\hat{P}_{q+1_j})$. If $d(v_i, v_j) = 1$, then $v_r, v_t \in \hat{C}_{2q+1}$, while if $d(v_i, v_j) = 2$, then $v_r, v_t \in \hat{C}_{2q+2}$.

Thus every vertex pair in $\hat{H}_q$ belong to some join cycle in $\hat{H}_q$.

□

5.2 The Hosoya Polynomial of q-vertex Joins

In this section, we start by proving the Hosoya polynomials of the q-vertex join for graphs with diameter 1 and 2, that is $\hat{H}_q$, then we obtain the Wiener index of $\hat{H}_q$. Finally we state the Hosoya polynomial of some well known graphs with diameter 2 in the form $\hat{H}_q$. These graphs are complete bipartite, wheel and strongly regular graphs. We also include the Hosoya polynomial of uniform m-bridge graph $\theta_m(2)$ as it has diameter two. We start with the Hosoya polynomials of q-vertex join for graphs with diameter 1. Since all graphs of diameter 1 are complete graphs, it is interesting to find the Hosoya polynomials of the q-vertex join for complete graphs. Lemma 5.2.1 and Lemma 5.2.2 are useful to prove Theorem 5.2.3.

Lemma 5.2.1. *Let K_n be a complete graph of order n and let $\hat{K}_{nq}$ be the q-vertex join of K_n. Then there are $\binom{n}{2}$ join cycles of the form $\hat{C}_{2q+1}$ in $\hat{K}_{n_q}$.*

Proof. All vertex pairs are joined by an edge hence the result by Lemma 5.1.3 part (i). □

Lemma 5.2.2. *Let K_n be a complete graph of order n and let $\hat{K_{n_q}}$ be the q-vertex join of K_n. Then every vertex pair in $\hat{K_{n_q}}$ belong to some cycle in $\hat{K_{n_q}}$.*

Proof. The proof is similar to proof of Lemma 5.1.5. □

Theorem 5.2.3 gives us the Hosoya polynomial of q-vertex join for graphs with diameter 1, which is one of the main results of this chapter.

Theorem 5.2.3. *Let $H = K_n$ a complete graph of order n and let $\hat{H}_q$ be the q-vertex join of K_n. Then the Hosoya polynomial of $\hat{H}_q$,*

$$\mathcal{H}(\hat{H}_q, z) \;=\; \binom{n}{2}\mathcal{H}(\hat{C}_{2q+1}, z) - n(n-2)\mathcal{H}(\hat{P}_{q+1}, z).$$

Proof. We use the principle of inclusion-exclusion in this proof and the fact that $\hat{P}_{q+1} \cong P_{q+1}$ and $\hat{C}_{2q+1} \cong C_{2q+1}$. From Lemma 5.2.1 and Lemma 5.2.2, we know that every vertex pair in $\hat{H}_q$ belong to some cycle $\hat{C}_{2q+1}$. Hence the Hosoya polynomial of $\hat{H}_q$ can be found in terms of join cycles and join paths.

By Lemma 5.2.1 the number of join cycles of size $2q+1$ in $\hat{H}_q$ is $\binom{n}{2}$. Therefore the sum of the Hosoya polynomials of all the join cycles of $\hat{H}_q$ is $\binom{n}{2}\mathcal{H}(\hat{C}_{2q+1}, z)$.

By Corollary 5.1.4, $\hat{C}_{2q+1} = \hat{P}_{q+1_i} \cup \hat{P}_{q+1_j} \cup (v_i, v_j)$. Since v_i is paired with all the other $(n-1)$ vertices, this implies that the path $\hat{P}_{q+1_i}$ will appear in $(n-1)$ join cycles. Thus the Hosoya polynomial of each join path $\hat{P}_{q+1_i}$ is in the Hosoya polynomials of $(n-1)$ join cycles. But we need the Hosoya polynomial of $\hat{P}_{q+1_i}$ to contribute once in the total sum, thus we remove the $(n-2)$ repetitions. We do this to all the n join paths, to get the Hosoya polynomial of $\hat{H}_q$,

$$\mathcal{H}(\hat{H}_q, z) = \binom{n}{2}\mathcal{H}(\hat{C}_{2q+1}, z) - n(n-2)\mathcal{H}(\hat{P}_{q+1}, z).$$

□

We now compute the Hosoya polynomials of q-vertex join for graphs with diameter 2. Lemma 5.2.4 gives us the Hosoya polynomial of q-vertex join for the path P_3, which we are going to use to prove Theorem 5.2.3.

Lemma 5.2.4. *Let $H = P_3$ be a path on three vertices and let $\hat{H}_q$ be the q-vertex join of P_3. Then the Hosoya polynomial of $\hat{H}_q$,*

$$\mathcal{H}(\hat{H}_q, z) \quad = \quad 2\mathcal{H}(\hat{C}_{2q+1}, z) + \frac{q}{q+1}\mathcal{H}(\hat{C}_{2q+2}, z) - 3\mathcal{H}(\hat{P}_{q+1}, z).$$

Proof. We are going to use the fact that $\hat{P}_{q+1} \cong P_{q+1}$, $\hat{C}_{2q+1} \cong C_{2q+1}$ and $\hat{C}_{2q+2} \cong C_{2q+2}$. Let $H = P_3$ and $V(H) = \{v_1, v_2, v_3\}$ such that $d(v_1, v_2) = d(v_2, v_3) = 1$ and $d(v_1, v_3) = 2$. It is clear by Corollary 5.1.4 that in $\hat{H}_q$, there are three join cycles,

$$\hat{P}_{q+1_1} \cup \hat{P}_{q+1_2} \cup (v_1, v_2) \cong \hat{P}_{q+1_2} \cup \hat{P}_{q+1_3} \cup (v_2, v_3) \cong \hat{C}_{2q+1}$$

and

$$\hat{P}_{q+1_1} \cup \hat{P}_{q+1_3} \cup (v_1, v_2) \cup (v_2, v_3) \cong \hat{C}_{2q+2}.$$

Thus the contribution of the three join cycles to the Hosoya polynomial of $\hat{H}_q$ is less than or equal to $2\mathcal{H}(\hat{C}_{2q+1}, z) + \mathcal{H}(\hat{C}_{2q+2}, z)$. We now remove all the repeated pairs of vertices in the three join cycles.

(i) Each join path is appearing twice in the three join cycles, so we remove $\mathcal{H}(\hat{P}_{q+1}, z)$ from $2\mathcal{H}(\hat{C}_{2q+1}, z)$ and we remove $2\mathcal{H}(\hat{P}_{q+1}, z)$ from $\mathcal{H}(\hat{C}_{2q+2}, z)$.

(ii) The edge of H namely, (v_1, v_2) is appearing in 2 join cycles and so is the edge (v_2, v_3), hence we remove the term $2z$ from $\mathcal{H}(\hat{C}_{2q+2}, z)$.

(iii) Consider all the distances from v_2 to any vertex but w in the two join paths $\hat{P}_{q+1_1}$, $\hat{P}_{q+1_3}$ and in the join cycle $\hat{C}_{2q+2}$. These distances have been included already in the 2 join cycles, hence we remove the term $2z^2 + 2z^3 + \cdots + 2z^q$ from $\mathcal{H}(\hat{C}_{2q+2}, z)$.

(iv) We note that the shortest distance between v_2 and w is q, that is via the join path $\hat{P}_{{q+1}_2}$, but in the cycle $\hat{C}_{2q+2}$ the shortest distance between v_2 and w is $q+1$, which is more than q, thus we must also remove z^{q+1} from $\mathcal{H}(\hat{C}_{2q+2}, z)$.

Therefore, in total, we have $2z + 2z^2 + 2z^3 + \cdots + 2z^q + z^{q+1}$ additional terms to be excluded from $\mathcal{H}(\hat{C}_{2q+2}, z)$. Recall that the Hosoya polynomial of an even cycle C_{2n} is $\mathcal{H}(C_{2n}, z) = 2n \sum_{i=1}^{n-1} z^i + nz^n$. Now we note that

$$\begin{aligned}
\sum_{i=1}^{q} 2z^i + z^{q+1} &= \frac{q+1}{q+1}\left[\sum_{i=1}^{q} 2z^i + z^{q+1}\right] \\
&= \frac{1}{q+1}\left[2(q+1)\sum_{i=1}^{q} z^i + (q+1)z^{q+1}\right] \\
&= \frac{1}{q+1}\mathcal{H}(\hat{C}_{2q+2}, z).
\end{aligned}$$

Then we obtain

$$\mathcal{H}(\hat{C}_{2q+2}, z) - 2\mathcal{H}(\hat{P}_{q+1}, z) - \frac{1}{q+1}\mathcal{H}(\hat{C}_{2q+2}, z)$$

which simplifies to $\frac{q}{q+1}\mathcal{H}(\hat{C}_{2q+2}, z) - 2\mathcal{H}(\hat{P}_{q+1}, z)$.

We combine all the results as follows

$$\begin{aligned}
\mathcal{H}(\hat{H}_q, z) &= 2\mathcal{H}(\hat{C}_{2q+1}, z) - \mathcal{H}(\hat{P}_{q+1}, z) + \frac{q}{q+1}\mathcal{H}(\hat{C}_{2q+2}, z) \\
&\quad -2\mathcal{H}(\hat{P}_{q+1}, z) \\
&= 2\mathcal{H}(\hat{C}_{2q+1}, z) + \frac{q}{q+1}\mathcal{H}(\hat{C}_{2q+2}, z) - 3\mathcal{H}(\hat{P}_{q+1}, z).
\end{aligned}$$

Thus we get the required results. $\square$

There are many classes of diameter 2 graphs, for example complete bipartite, wheel, strongly regular and uniform multibridge $\theta_m(2)$ graphs. Now we prove the main results of this chapter in Theorem 5.2.5, the Hosoya polynomial of q-vertex join of diameter 2 graphs. We are going to use the fact that $\hat{P}_{q+1} \cong P_{q+1}$, $\hat{C}_{2q+1} \cong C_{2q+1}$ and $\hat{C}_{2q+2} \cong C_{2q+2}$.

Theorem 5.2.5. *Let H be a diameter 2 graph of size m and order n and let $\mathcal{H}(H,z)$ be the Hosoya polynomial of H. Then the Hosoya polynomial of the q-vertex join, $\hat{H}_q$,*

$$\begin{aligned}\mathcal{H}(\hat{H}_q,z) &= m\mathcal{H}(\hat{C}_{2q+1},z)+\frac{q}{q+1}\left(\binom{n}{2}-m\right)\mathcal{H}(\hat{C}_{2q+2},z)\\ &\quad -n(n-2)\mathcal{H}(\hat{P}_{q+1},z).\end{aligned}$$

Proof. From Lemma 5.1.3 there are m join cycles $\hat{C}_{2q+1}$ and $\binom{n}{2}-m$ join cycles $\hat{C}_{2q+2}$ in $\hat{H}_q$. From Lemma 5.1.5 we know that every vertex pair in $\hat{H}_q$ belong to some join cycle $\hat{C}_{2q+1}$ or $\hat{C}_{2q+2}$ and by Corollary 5.1.4 each join cycle has 2 join paths, thus the Hosoya polynomial of $\hat{H}_q$ can be expressed in terms of the Hosoya polynomials of join cycles and Hosoya polynomials of join paths.

By Lemma 5.1.3, we have m join cycles of the form $\hat{C}_{2q+1}$ in $\hat{H}_q$. Hence these join cycles contribute the term $m\mathcal{H}(\hat{C}_{2q+1},z)$ to the Hosoya polynomial of $\hat{H}_q$. As in the proof of Lemma 5.2.4 we need to remove the Hosoya polynomials of some of the join paths $\hat{P}_{q+1}$ that are found in more than 1 join cycle.

Let $V(H)=\{v_1,v_2,v_3,\cdots,v_n\}$ be the vertex set of H and let the degree of vertex v_i be $a_i \geq 1$ for $1 \leq i \leq n$. Recall that the hand-shake lemma states that the sum of all the degrees of vertices of a graph is equal to twice the number of edges of a graph. Therefore graph H of size m implies $\sum_{i=1}^{n} a_i = 2m$.

Now we consider the degree of vertices of H in order to count the number of repetitions of $\mathcal{H}(\hat{P}_{q+1_i},z)$ in $m\mathcal{H}(\hat{C}_{2q+1},z)$.

It is clear by definition that each join path $\hat{P}_{q+1_i}$ with $v_i \in V(\hat{P}_{q+1_i})$ is paired with a_i join paths to form a_i join cycles of the form $\hat{C}_{2q+1}$.

Thus the Hosoya polynomials of each join path $\hat{P}_{q+1_i}$ is repeated a_i-1 times in the a_i join cycles of the form $\hat{C}_{2q+1}$.

We compute all the repetitions of $\mathcal{H}(\hat{P}_{q+1_i},z)$ from $m\mathcal{H}(\hat{C}_{2q+1},z)$, as follows

$$\begin{aligned}\sum_{i=1}^{n}(a_i-1) &= \sum_{i=1}^{n}a_i - n\\ &= 2m-n.\end{aligned}$$

Therefore the repeated number of $\mathcal{H}(\hat{P}_{q+1_i},z)$ is $[2m-n]\,\mathcal{H}(\hat{P}_{q+1},z)$. Thus we exclude $[2m-n]\,\mathcal{H}(\hat{P}_{q+1},z)$ from $m\mathcal{H}(\hat{C}_{2q+1},z)$ to get

$$m\mathcal{H}(\hat{C}_{2q+1},z)-[2m-n]\,\mathcal{H}(\hat{P}_{q+1},z).$$

In $\hat{H}_q$ we consider the sum of the Hosoya polynomials of the $\binom{n}{2}-m$ join cycles of the form $\hat{C}_{2q+2}$ which is $\left(\binom{n}{2}-m\right)\mathcal{H}(\hat{C}_{2q+2},z)$. From Lemma 5.2.4 we know that there are $2\mathcal{H}(\hat{P}_{q+1},z)+\frac{1}{q+1}\mathcal{H}(\hat{C}_{2q+2},z)$ repetitions from $\mathcal{H}(\hat{C}_{2q+2},z)$.

Thus from $\left(\binom{n}{2}-m\right)\mathcal{H}(\hat{C}_{2q+2},z)$, there term

$\left[\binom{n}{2}-m\right]\left(2\mathcal{H}(\hat{P}_{q+1},z)+\frac{1}{q+1}\mathcal{H}(\hat{C}_{2q+2},z)\right)$ is a repetition.

Therefore we exclude all repetitions from $\left(\binom{n}{2}-m\right)\mathcal{H}(\hat{C}_{2q+2},z)$ to get

$$\begin{aligned}&\left[\binom{n}{2}-m\right]\left(\mathcal{H}(\hat{C}_{2q+2},z)-2\mathcal{H}(\hat{P}_{q+1},z)-\frac{1}{q+1}\mathcal{H}(\hat{C}_{2q+2},z)\right)\\ =\ &\left[\binom{n}{2}-m\right]\left(\frac{q}{q+1}\mathcal{H}(\hat{C}_{2q+2},z)-2\mathcal{H}(\hat{P}_{q+1},z)\right).\end{aligned}$$

We combine all the results and obtain $\mathcal{H}(\hat{H}_q,z)$ as follows

$$\begin{aligned}\mathcal{H}(\hat{H}_q,z) &= m\mathcal{H}(\hat{C}_{2q+1},z)-[2m-n]\,\mathcal{H}(\hat{P}_{q+1},z)\\ &\quad+\left[\binom{n}{2}-m\right]\left(\frac{q}{q+1}\mathcal{H}(\hat{C}_{2q+2},z)-2\mathcal{H}(\hat{P}_{q+1},z)\right)\\ &= m\mathcal{H}(\hat{C}_{2q+1},z)+\left[\binom{n}{2}-m\right]\frac{q}{q+1}\mathcal{H}(\hat{C}_{2q+2},z)\\ &\quad-[2m-n]\,\mathcal{H}(\hat{P}_{q+1},z)-\left[\binom{n}{2}-m\right]2\mathcal{H}(\hat{P}_{q+1},z)\end{aligned}$$

$$\begin{aligned}
&= m\mathcal{H}(\hat{C}_{2q+1},z) + \left[\binom{n}{2} - m\right]\frac{q}{q+1}\mathcal{H}(\hat{C}_{2q+2},z) \\
&\quad - [2m-n]\,\mathcal{H}(\hat{P}_{q+1},z) - [n(n-1)-2m]\,\mathcal{H}(\hat{P}_{q+1},z) \\
&= m\mathcal{H}(\hat{C}_{2q+1},z) + \left[\binom{n}{2} - m\right]\frac{q}{q+1}\mathcal{H}(\hat{C}_{2q+2},z) \\
&\quad - [n(n-1)-n]\,\mathcal{H}(\hat{P}_{q+1},z) \\
&= m\mathcal{H}(\hat{C}_{2q+1},z) + \left[\binom{n}{2} - m\right]\frac{q}{q+1}\mathcal{H}(\hat{C}_{2q+2},z) \\
&\quad -n(n-2)\mathcal{H}(\hat{P}_{q+1},z).
\end{aligned}$$

$\square$

We now verify the results of Theorem~join8, from Chapter 4 in Theorem 4.3.1 part (iv), we know that for any graph H of order n have $\mathcal{H}(H,1) = \binom{n}{2}$, the number of pair of vertices for H. Now $\hat{H}_q$ has $qn+1$ vertices, thus

$$\begin{aligned}
\mathcal{H}(\hat{H}_q,1) &= m\mathcal{H}(\hat{C}_{2q+1},1) + \frac{q}{q+1}\left(\binom{n}{2} - m\right)\mathcal{H}(\hat{C}_{2q+2},1) \\
&\quad -n\,[n-2]\,\mathcal{H}(\hat{P}_{q+1},1) \\
&= m\binom{2q+1}{2} + \frac{q}{q+1}\left(\binom{n}{2} - m\right)\binom{2q+2}{2} \\
&\quad -n\,[n-2]\binom{q+1}{2} \\
&= m\frac{(2q+1)2q}{2} + \frac{q}{q+1}\left(\binom{n}{2} - m\right)\frac{(2q+2)(2q+1)}{2} \\
&\quad -n\,[n-2]\,\frac{(q+1)q}{2} \\
&= \frac{m(2q+1)2q}{2} + \frac{q(2q+1)n(n-1)}{2} - \frac{m(2q+1)2q}{2} \\
&\quad -\frac{n(n-2)(q+1)q}{2} \\
&= \frac{nq}{2}\left[(2q+1)(n-1) - (n-2)(q+1)\right] \\
&= \frac{nq}{2}\left[2qn + n - 2q - 1 - qn + 2q - n + 2\right].
\end{aligned}$$

Hence we conclude that

$$\begin{aligned}\mathcal{H}(\hat{H}_q, 1) &= \frac{nq}{2}\,[qn+1] \\ &= \binom{qn+1}{2}.\end{aligned}$$

Recall from Chapter 4 in Corollary 4.3.4, that the Wiener indices of even cycles, odd cycles and paths are $W(C_{2q+2}) = (2q+2)^3/8$, $W(C_{2q+1}) = (2q+2)(2q+1)(2q)/8$ and $W(P_{q+1}) = \binom{q+2}{3}$ respectively. From Theorem 5.2.3, the Wiener index of $\hat{K_{n_q}} = \hat{H}_q$ should be in terms of odd cycles and paths as follows,

$$W(\hat{H}_q) = \binom{n}{2} W(\hat{C}_{2q+1}) - n\,(n-2)\,W(\hat{P}_{q+1}).$$

Thus if we simplify $W(\hat{H}_q)$ we get Corollary 5.2.6 for the Wiener index of $\hat{H}_q$.

Corollary 5.2.6. *Let $H = K_n$ a complete graph of order n and let $\hat{H}_q$ be the q-vertex join of K_n. Then the Wiener index of $\hat{H}_q$,*

$$W(\hat{H}_q) = n\binom{q+1}{2}\left[\frac{4nq-n-2q+5}{6}\right].$$

From Theorem 5.2.5, the Wiener index of $\hat{H}_q$ should be in terms of even cycles, odd cycles and paths as follows,

$$\begin{aligned}W(\hat{H}_q) &= mW(\hat{C}_{2q+1}) + \frac{q}{q+1}\left(\binom{n}{2} - m\right) W(\hat{C}_{2q+2}) \\ &\quad - n\,[n-2]\,W(\hat{P}_{q+1}).\end{aligned}$$

Thus if we simplify $W(\hat{H}_q)$ we get Corollary 5.2.7 for the Wiener index of $\hat{H}_q$.

Corollary 5.2.7. *Let H be a diameter 2 graph of size m and order n and let $\mathcal{H}(H, z)$ be the Hosoya polynomial of H. Then the Wiener index of $\hat{H}_q$,*

$$W(\hat{H}_q) = \binom{q+1}{2}\left[n\frac{(1-q+n+2qn)}{3} - m\right].$$

We apply Theorem 5.2.5, Theorem 4.3.3, Theorem 4.5.4 and Corollary 4.3.6 to get the results of Corollary 5.2.8.

Corollary 5.2.8. *Let H be a graph with diameter 2 and let $\mathcal{H}(H, z)$ be the Hosoya polynomial of H. Then if H is*

(i) a complete bipartite graph $K_{n,m}$, then for the q-vertex join of $K_{n,m}$, $\hat{H}_q$ we get

$$\begin{aligned}\mathcal{H}(\hat{H}_q, z) &= mn\mathcal{H}(\hat{C}_{2q+1}, z) + \frac{q}{q+1}\left(\binom{m}{2} + \binom{n}{2}\right)\mathcal{H}(\hat{C}_{2q+2}, z)\\ &\quad -(m+n)(m+n-2)\mathcal{H}(\hat{P}_{q+1}, z).\end{aligned}$$

(ii) a wheel graph W_n, then for the q-vertex join of W_n, $\hat{H}_q$ we get

$$\begin{aligned}\mathcal{H}(\hat{H}_q, z) &= (2n-2)\mathcal{H}(\hat{C}_{2q+1}, z) + \frac{q}{q+1}\left(\frac{(n-1)(n-4)}{2}\right)\mathcal{H}(\hat{C}_{2q+2}, z)\\ &\quad -n(n-2)\mathcal{H}(\hat{P}_{q+1}, z).\end{aligned}$$

(iii) a strongly regular graph $srg(n, k, \lambda, \mu)$, then for the q-vertex join of $srg(n, k, \lambda, \mu)$, $\hat{H}_q$ we get

$$\begin{aligned}\mathcal{H}(\hat{H}_q, z) &= \frac{nk}{2}\mathcal{H}(\hat{C}_{2q+1}, z) + \frac{q}{q+1}\left(\frac{n(n-k-1)}{2}\right)\mathcal{H}(\hat{C}_{2q+2}, z)\\ &\quad -n(n-2)\mathcal{H}(\hat{P}_{q+1}, z).\end{aligned}$$

(iv) a uniform m-bridge graph $\theta_m(2)$*, then for the q-vertex join of* $\theta_m(2)$*,* $\hat{H}_q$ *we get*

$$\begin{aligned}\mathcal{H}(\hat{H}_q, z) &= 2m\mathcal{H}(\hat{C}_{2q+1}, z) + \frac{q}{q+1}\left(\binom{m+2}{2} - 2m\right)\mathcal{H}(\hat{C}_{2q+2}, z) \\ &\quad -m(m+2)\mathcal{H}(\hat{P}_{q+1}, z).\end{aligned}$$

5.3 Conclusion

We introduced a graph operation called a q-vertex join of any graph. Using the known results on the Hosoya polynomials of diameter 2 graphs, we explored and used the principle of inclusion and exclusion to find the Hosoya polynomial and Wiener index of a q-vertex join of graph H with diameter at most 2.

Chapter 6

Conclusion

Firstly, in Chapter 2, we obtained a new upper bound for the number of graph compositions of any graph. We then gave a method, for obtaining graph compositions via non-closed sets. In particular we demonstrated this method, using the cases of a class of theta graphs and 4-bridge graphs.

Secondly, in Chapter 3, we discussed the known theory on bad coloring polynomials. Then we found bad coloring polynomial of a theta graph and multibridge graph. We then extracted coefficients of S^k from the bad coloring polynomial of a theta graph to get the k-defect polynomials of the theta graph. We finally verified our theorem with an example.

Thirdly, in Chapter 4, we used the principle of inclusion-exclusion and got an explicit express of the Hosoya polynomial of uniform multibridge graphs. Finally we explained the results to mathematical chemistry.

Finally, in Chapter 5, we used the principle of inclusion-exclusion and found the formula for the Hosoya polynomials and Wiener indices of a q-vertex join of graphs with diameter at most 2.

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