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HOSOYA POLYNOMIAL OF A MULTI-BRIDGE GRAPH

T. NCAMBALALA[1], E. G. MPHAKO-BANDA[1], §

ABSTRACT. Explicit expressions of the Hosoya polynomials of some classes of graphs are known. In this paper we find an explicit expression for the Hosoya polynomial of the multibridge graph. Finally we give some examples of multi-bridge graphs which are chemical graphs.

Keywords: Hosoya polynomial, Wiener index, uniform multi-bridge graph, graph distance, inclusion-exclusion principle.

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1. Introduction

The Wiener index which was introduced in 1947 by H. Wiener [9] as a tool for obtaining the boiling points of alkanes, has 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.

If we let $d(u, v)$ denote the minimum distance between any two vertices u and v and $D = max_{u,v\in V(G)}\{d(u, v)\}$ the diameter of a connected graph G with vertex set $V(G) = \{u_1, u_2, \cdots, u_n\}$ the Wiener index of the graph G,

$$W(G) = \frac{1}{2}\sum_{u_i\in V(G)}^{n} d(u_i, G).$$

Sagan, et al.[8], studied the Wiener polynomial as a generating function in q and showed that the derivative of the Wiener polynomial is the q-analog of the Wiener index of a graph. In addition, some properties and explicit expressions of the Wiener polynomials of certain classes of graphs were given.

In 1988, Hosoya[2] independently studied a polynomial about distance distributing for a connected graph G. This polynomial is called the Hosoya polynomial and is given as a

[1] School of Mathematics, University of the Witwatersrand, P/Bag 3, WITS, 2050, RSA.
e-mail: Thokozani.ncambalala@wits.ac.za; ORCID: https://orcid.org/0000-0003-0241-4971.
e-mail: eunice.mphako-banda@wits.ac.za; ORCID: https://orcid.org/0000-0002-8149-7850.
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generating function,

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

where $d(G,w)\geq 1$ is the number of vertex pairs at distance w. The Hosoya polynomial has application to an important topological index, the Wiener index. In particular, the Wiener index is given by the first derivative of the Hosoya polynomial, $H(G,z)$, at $z=1$ which implies that the Hosoya Polynomial is the same as the Wiener polynomial.

Just like many graph polynomials, there are many research directions for the Hosoya polynomial for both chemists and mathematicians. One direction of study is finding explicit expressions of the Hosoya polynomial of certain classes of graphs, for example [1, 3, 4, 5, 6, 7, 10, 11]. In this paper, we follow this research direction.

For many graph polynomials, even and odd cycles have the same formula, but for the Hosoya polynomial, even and odd cycles have different formulae. Similarly, non isomorphic trees of the same size have different formulae of the Hosoya polynomial.

Theorem 1.1 ([8]). *The Hosoya polynomial of*

(i) an even cycle C_{2n} *is* $H(C_{2n},z)=2n\sum_{i=1}^{n-1} z^i+nz^n$.

(ii) an odd cycle C_{2n+1} *is* $H(C_{2n+1},z)=(2n+1)\sum_{i=1}^{n} z^i$.

(iii) a path P_n *is* $H(P_n,z)=\sum_{i=1}^{n-1}(n-i)z^i$.

2. The Hosoya Polynomial of Uniform m-bridge Graphs

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 paper are the internally disjoint paths of lengths $b_1,b_2,\cdots,b_m\geq 1$ which define the graph. To ease notation, we denote 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 $i\in\{1,2,\cdots,m\}$. A 2-bridge graph is simply a cycle graph and 3-bridge graph is a theta graph. 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 $i\in\{1,2,\cdots,m\}$, then $\theta_{b_1,b_2,b_3,\cdots,b_m}$, is said to be a uniform m-bridge graph denoted by $\theta_m(b)$.

Let G be an m-bridge graph $\theta_{b_1,b_2,b_3,\cdots,b_m}$, then the size of G is $\sum_{i=1}^{m} b_i$ and the order of G is $\sum_{i=1}^{m} b_i-m+2$. Furthermore, any path $\widehat{P}_{b_i}$ of an m-bridge graph belongs to $m-1$ cycles of G and there are $\binom{m}{2}$ cycles in G given by $C_{b_i+b_j}$ for $i\neq j$. Of special interest to this work, if G is a uniform m-bridge graph, $\theta_m(b)$, then the size of G is mb and the order of G is $m(b-1)+2$. In addition there are m isomorphic internally disjoint paths, $\widehat{P}_b$ in G and every cycle of G is even.

A vertex cycle cover of a graph G is a set of cycles which are subgraphs of G and contain all vertices of G. Since in this work we are discussing vertex pairs, we extend the vertex cycle cover concept to vertex pair cycle cover which correspond to a set of cycles that are subgraphs of G and contain all vertex pairs of G.

Lemma 2.1. *Let G be an m-bridge graph $\theta_{b_1,b_2,b_3,\cdots,b_m}$. Then every pair of vertices in G belong to some cycle of the graph G, that is G has a vertex pair cycle cover.*

Proof. Let G be an m-bridge graph $\theta_{b_1,b_2,b_3,\cdots,b_m}$. Let the two vertices that connects the m internally disjoint paths of G be u and v. We consider four cases as follows.

Case 1. Consider the pair of vertices u and v, the pair that connects the m internally disjoint paths of G. This pair appear once in each of the m internally disjoint paths and $\binom{m}{2}$ cycles in G respectively, as it connects all the m internally disjoint paths in G. Therefore the pair $\{u, v\}$ is in all the $\binom{m}{2}$ cycles in G.

Case 2. Consider a pair of vertices having exactly one vertex in $\{u, v\}$ and another vertex in any of the m internally disjoint paths not in $\{u, v\}$. Then the two vertices are on the same path $\widehat{P}_{b_l}$, where $1 \leq l \leq m$. Then, 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 and these two vertices are on the same path $\widehat{P}_{b_l}$, where $1 \leq l \leq m$. Then, 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 and 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, the pair of vertices are in exactly one cycle $C_{b_i+b_j}$.

Thus every pair of vertices in G belong to some cycle. Hence G has a vertex pair cycle cover. □

From Lemma 2.1, **Cases 1, 2** and **3**, we conclude that only those pairs of vertices that appear in the same path, namely $\widehat{P}_{b_l}$, where $1 \leq l \leq m$, will appear in more than one cycle. From **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 appear in exactly one cycle $C_{b_i+b_j}$.

Lemma 2.2. *Let G be a uniform m-bridge graph $\theta_m(b)$, Then the shortest path between any pair of vertices in G lie on at least one cycle C_{2b} of G.*

Proof. Let G be a uniform m-bridge graph $\theta_m(b)$. Let the two vertices that connect the m internally disjoint paths of G be u and v. We consider four cases as follows.

Case 1. Consider the pair of vertices u and v, the pair that connects the m internally disjoint paths of G. Then the shortest path between the pair u and v is through any of the m internally disjoint paths. Hence the shortest paths are in all the $\binom{m}{2}$ cycles in G.

Case 2. Consider a pair of vertices having exactly one vertex in $\{u, v\}$ and another vertex in any of the m internally disjoint paths not in $\{u, v\}$. Then the two vertices are on the same path $\widehat{P}_{b_l}$, where $1 \leq l \leq m$. Thus the shortest path between the pair is within $\widehat{P}_{b_l}$ and the shortest path 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 and these two vertices are on the same path $\widehat{P}_{b_l}$, where $1 \leq l \leq m$. Then the shortest path between the pair is within $\widehat{P}_{b_l}$ and shortest path between the pair 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 and 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 the shortest path between the pair is of vertices is in exactly one cycle C_{2b}. Thus the shortest path between any pair of vertices in G lie on at least one cycle C_{2b} of G. □

We note that the diameter of any cycle C_{2b} in G is b. Hence the maximum possible distance between any pair of vertices in G is equal to b. On the other hand we can find the shortest path between any pair of vertices in G using the following method. If a pair is on the same path $\widehat{P}_{b_j}$, it is clear. If a pair is on the same cycle but not on the the same path, say vertex $w \in V(\widehat{P}_{b_i})$ and vertex $x \in V(\widehat{P}_{b_j})$, where $w, x \notin \{u, v\}$, from vertex w to vertex x there are exactly two paths connecting theses two vertices on the cycle. Then the shortest path is the one with length less than b.

Theorem 2.1. *Let $G = \theta_m(b)$ be a uniform m-bridge graph. Then the Hosoya polynomial of G,*

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

Proof. Let $G = \theta_m(b)$ be a uniform m-bridge graph and let u and v be the two vertices that connect the m internally disjoint paths. We know that G has $\binom{m}{2}$ even cycles. Thus the sum of the Hosoya polynomials of all the cycles in G is $\binom{m}{2}H(C_{2b}, z)$. By Lemma 2.1, each pair of vertices of G belongs to some cycle and by Lemma 2.2 the shortest path between any pair of vertices in G lie on at least one cycle C_{2b} of G. Hence each pair of vertex contributes to the counted sum of Hosoya polynomials for all the cycles in G. By Lemma 2.1, some vertex pairs appear in more than one cycle of G. Hence we need to remove the repetitions in the sum of the Hosoya polynomials of all the cycles in G.

There are m internally disjoint paths in G, denoted by $\widehat{P}_b$. Each of these paths, $\widehat{P}_b$, of an m-bridge graph belongs to $m-1$ cycles of G. Hence, $H(\widehat{P}_b, z)$ contributes to the Hosoya polynomial of $m-1$ cycles. But each path should contribute to the Hosoya polynomial of one cycle only, thus we remove it $m-2$ times. Hence for all the m paths, from $\binom{m}{2}H(C_{2b}, z)$, we remove $H(\widehat{P}_b, z)$, $m(m-2)$ times, that is

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

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, this vertex pair contributes the term z^b. Since there are $\binom{m}{2}$ cycles in G, the vertex pair u and v have contributed $\binom{m}{2}z^b$ in the sum $\binom{m}{2}H(C_{2b}, z)$ and $m(m-2)z^b$ in $m(m-2)H(\widehat{P}_b, z)$. But we need the vertex pair to contribute only once in the Hosoya polynomial of G. 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, $\binom{m}{2} - m(m-2) + k = 1$

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

Therefore

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

Therefore, the Hosoya polynomial of G, is

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

□

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

Corollary 2.1. *Let $G = \theta_m(b)$ be a uniform m-bridge graph. Then the Hosoya polynomial of G,*

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

As a consequence of Corollary 2.1 and definition of the Wiener index, we state the Wiener index of a uniform m-bridge graph.

Corollary 2.2. *Let $G = \theta_m(b)$ be a uniform m-bridge graph. Then the Wiener index of G is,*

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

3. Conclusions

We note that some m-bridge graphs are chemical graphs. In particular, $\theta_3(b)$ contains a class of chemical graphs called *bridged bicyclic* alkanes in mathematical chemistry. For example, the two bridged bicyclic alkanes, the bicyclo[2.2.2]octane and the bicyclo[3.3.3]undecane correspond to $\theta_3(3)$ and $\theta_3(4)$ respectively. Hence, the Hosoya polynomial of bicyclo[2.2.2]octane,

$$H(\theta_3(3), z) = 3H(C_6, z) - 3H(\widehat{P}_3, z) + z^3 = 9z + 12z^2 + 7z^3$$

and the Hosoya polynomial of bicyclo[3.3.3]undecane,

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

Finally, the Wiener index of the bicyclo[2.2.2]octane, $W(\theta_3(3)) = 54$ and the Wiener index of the bicyclo[3.3.3]undecane $W(\theta_3(4)) = 136$.

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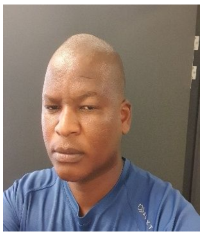

Thokozani Ncambalala is a lecturer of mathematics at the University of the Witwatersrand, Johannesburg where he received his PhD in pure mathematics specializing in graph polynomials in January 2018. Further, he holds an Honors degree and a Masters degree in mathematics from the same University. He started teaching mathematics at the University of the Witwatersrand in 2015 as a junior lecturer. He has supervised three honor research projects and he is currently supervising a master student in graph theory. His research interest is in graph theory, mainly in graph polynomials and enumerative combinatorics.

Eunice Gogo Mphako-Banda has numerous postgraduate qualifications - Postgraduate Diploma in Mathematics from the University of Sheffield and MSc in Mathematics from the University of Manchester, United Kingdom. Further, she has a PhD in Discrete Mathematics from Victoria University of Wellington, New Zealand. She is currently working at the University of the Witwatersrand, School of Mathematics. Her research interests currently include - matroid theory, knot theory and graph theory.