Iranian Journal of Mathematical Chemistry, Vol. 4, No.2, December 2013, pp. 213 – 220

IJMC

The Hyper–Zagreb Index of Graph Operations

G. H. SHIRDEL[a,•]**, H. REZAPOUR**[a] **AND A. M. SAYADI**[b]

[a] *Department of Mathematic, Faculty of Basic Sciences, University of Qom, Qom, Iran*
[b] *School of Mathematic, Statistics and Computer Science, University of Tehran, Tehran, Iran*

(*Received July 1, 2013; Accepted November 11, 2013*)

ABSTRACT

Let *G* be a simple connected graph. The first and second Zagreb indices have been introduced as $M_1(G) = \sum_{v\in V(G)} \deg_G(v)^2$ and $M_2(G) = \sum_{uv\in E(G)} \deg_G(u)\deg_G(v)$, respectively, where $\deg_G v(\deg_G u)$ is the degree of vertex $v(u)$. In this paper, we define a new distance-based named Hyper–Zagreb as $HM(G) = \sum_{e=uv\in E(G)} (\deg_G(u) + \deg_G(v))^2$. In this paper, the Hyper–Zagreb index of the Cartesian product, composition, join and disjunction of graphs are computed.

Keywords: Hyper–Zagreb index, Zagreb index, graph operation.

1. INTRODUCTION

In this paper, it is assumed that G is a connected graph with vertex and edge sets V(G) and E(G), respectively. We consider only simple connected graphs, i.e. connected graphs without loops and multiple edges. For a graph G, the degree of a vertex v is the number of edges incident to v, denoted by $\deg_G v$. A topological index Top(G) of a graph G, is a number with this property that for every graph H isomorphic to G, Top(H) = Top(G). Usage of topological indices in chemistry began in 1947 when chemist Harold Wiener developed the most widely known topological descriptor, the Wiener index, and used it to determine physical properties of types of alkanes known as paraffin. In a graph theoretical language the Wiener index is equal to the sum of distances between all pairs of vertices of the respective graph. For a nice survey in this topic we encourage the reader to consult [14].

• Corresponding author (Email: shirdel81math@gmail.com).

Numerous other indices have been defined. The Zagreb indices have been introduced more than thirty years ago by Gutman and Trinajestić [6]. They are defined as:

$$M_1(G) = \sum_{v \in V(G)} \deg(v)^2$$

$$M_2(G) = \sum_{uv \in V(G)} \deg(u)\deg(v).$$

We encourage the reader to consult [1, 5, 16, 17, 18] for historical background, computational techniques and mathematical properties of Zagreb indices. We define the Hyper−Zagreb index as:

$$HM(G) = \sum_{e=uv \in E(G)} (\deg_G(u) + \deg_G(v))^2 .$$

The Cartesian product $G \times H$ of graphs G and H has the vertex set $V(G \times H) = V(G) \times V(H)$ and $(a,x)(b,y)$ is an edge of $G \times H$ if $a = b$ and $xy \in E(H)$, or $ab \in E(H)$ and $x = y$.

The join $G + H$ of graphs G and H is a graph with vertex set $V(G) \bigcup V(H)$ and edge set $E(G) \bigcup E(H) \bigcup \{uv : u \in V(G) \text{ and } v \in V(H)\}$.

The composition $G[H]$ or ($G o H$) of graphs G and H with disjoint vertex sets V(G) and V(H) and edge sets E(G) and E(H) is the graph with vertex set $V(G) \times V(H)$ and $u = (u_1, v_1)$ is adjacent to $v = (u_2, v_2)$ whenever u_1 is adjacent to u_2 or $u_1 = u_2$ and v_1 is adjacent to v_2 .

The symmetric difference $G \oplus H$ of two graphs G and H is the graph with vertex set $V(G) \times V(H)$ and

$$E(G \oplus H) = \{(u_1, u_2)(v_1, v_2) \mid u_1 v_1 \in E(G) \text{ or } u_2 v_2 \in E(H) \text{ but not both}\}.$$

The tensor product $G \otimes H$ of two graphs G and H is the graph with vertex set $V(G) \times V(H)$ and $E(G \otimes H) = \{u_1, u_2)(v_1, v_2) \mid u_1 v_1 \in E(G) \text{ and } u_2 v_2 \in E(H)\}$.

The corona product $G * H$ is defined as the graph obtained from G and H by taking one copy of G and $|V(G)|$ copies of H and then joining by an edge each vertex of the i th copy of H is named (H, i) with the i th vertex of G.

2. NEW GRAPH INVARIANT

In this section, we define the Hyper−Zagreb index of a graph and some exact formulae for the Hyper−Zagreb index of some well−known graphs are presented. We begin with the definition and crucial lemma related to distance properties of some graph operations.

Let us begin with a few examples, then we will give a crucial lemma related to distance properties of some graph operations. Our main results are applications of this lemma in computing exact formulae for some graph operations under Hyper–Zagreb index.

Example 1. In this example the Hyper–Zagreb index of some well-known graphs are calculated. We first consider the complete graph K_n. Then the degree of any vertex in this graph is $n-1$, thus

$$HM(K_n) = \sum_{e=uv\in E(kn)} (\deg_{k_n}(u) + \deg_{k_n}(v))^2 = 2n(n-1)^3 .$$

Let $K_{m,n}$ denote a complete bipartite graph. Then we have:

$$\mathrm{HM}(\mathrm{K}_{\mathrm{m,n}}) = \sum_{\mathrm{e=uv}\in \mathrm{E}(\mathrm{K}_{\mathrm{m,n}})} (\deg_{\mathrm{K}_{\mathrm{m,n}}}(\mathrm{u}) + \deg_{\mathrm{k}_{\mathrm{m,n}}}(\mathrm{v}))^2 = \mathrm{mn}(\mathrm{m}+\mathrm{n})^2.$$

For a cycle graph with n vertices, we have:

$$HM(C_n) = \sum_{e=uv\in E(C_n)} (\deg_{C_n}(u) + \deg_{C_n}(v))^2 = 16n .$$

For a path with n vertices, we have:

$$HM(P_n) = \sum_{e=uv\in E(P_n)} (\deg_{p_n}(u) + \deg_{p_n}(v))^2 = 16n - 30 .$$

For wheel on $n+1$ vertices, we have:

$$HM(W_n) = \sum_{e=uv\in E(W_n)} (\deg_{W_n}(u) + \deg_{W_n}(v))^2 = n(n^2 + 6n + 45) .$$

Finally, for a ladder graph with $2n$ vertices, $n \geq 3$, the Hyper–Zagreb index can be computed by the following formula:

$$HM(L_{2n}) = \sum_{e=uv\in E(L_{2n})} (\deg_{L_{2n}}(u) + \deg_{L_{2n}}(v))^2 = 108n - 156 .$$

Lemma 1. Let G and H be two connected graphs, then we have:

(a) $|V(G\times H)| = |V(G\vee H)| = |V(G[H])| = |V(G\oplus H)| = |V(G)||V(H)|$,

$|E(G\times H)| = |E(G)||V(H)| + |V(G)||E(H)|$,

$|E(G+H)| = |E(G)| + |E(H)| + |V(G)||V(H)|$,

$|E(G[H])| = |E(G)||V(H)|^2 + |E(G)||V(G)|$,

$|E(G\vee H)| = |V(G)||V(H)|^2 + |E(G)||V(G)|^2 - 2|E(G)||E(H)|$,

$|E(G\oplus H)| = |E(G)||V(H)|^2 + |E(H)||V(G)|^2 - 4|E(G)||E(H)|$.

(b) $G\times H$ is connected if and only if G and H are connected.

(c) If (a,b) is a vertex of $G\times H$ then $\deg_{G\times H}((a,b))=\deg_G(a)+\deg_H(b)$.

(d) If (a,b) is a vertex of $G[H]$ then $\deg_{G[H]}((a,b))=|V(G)|\deg_G(a)+\deg_H(b)$.

(e) If (a,b) is a vertex of $G\oplus H$ or $G\vee H$, we have:

$$\deg_{G\oplus H}((a,b))=|V(H)|\deg_G(a)+|V(G)|\deg_H(b)-2\deg_G(a)\deg_H(b).$$

$$\deg_{G\vee H}((a,b))=|V(H)|\deg_G(a)+|V(G)|\deg_H(b)-\deg_G(a)\deg_H(b).$$

(f) If a is a vertex of $G+H$ then, we have:

$$\deg_{G+H}(a)=\begin{cases}\deg_G(a)+|V(H)| & a\in V(G)\\ \deg_H(a)+|V(G)| & a\in V(H)\end{cases}$$

Proof: The parts (a) and (b) are consequence of definitions and some famous results of the book of Imrich and Klavzar [7]. For the proof of (c-f) we refer to [8].

Theorem 1. Let G and H be graphs. Then we have:

$$\begin{aligned}\mathrm{HM}(G+H)=&\ \mathrm{HM}(G)+\mathrm{HM}(H)+5(|V(G)|M_1(H)+|V(H)|M_1(G))\\ &+8\left(|V(G)|^2|E(H)|+|V(H)|^2|E(G)|+|E(G)||E(H)|\right)\\ &+|V(G)||V(H)|\left((|V(H)|+|V(G)|)^2+4(|E(G)|+|E(H)|\right).\end{aligned}$$

Proof: From the definition we know:

$$E(G+H)=E(G)\cup E(H)\cup\{uv:u\in V(G),v\in V(H)\}$$

So, we have:

$$\begin{aligned}\mathrm{HM}(G+H)=&\sum_{uv\in E(G+H)}(\deg_{G+H}u+\deg_{G+H}v)^2\\ =&\sum_{uv\in E(H)}(\deg_{G+H}u+\deg_{G+H}v)^2\\ &+\sum_{uv\in E(G)}(\deg_{G+H}u+\deg_{G+H}v)^2\\ &+\sum_{uv\in\{uv:u\in v(G),v\in V(H)\}}(\deg_{G+H}u+\deg_{G+H}v)^2.\end{aligned}$$

It is easy to see that:

$$\sum_{uv\in A}(\deg_{G+H}u+\deg_{G+H}v)^2=HM(H)+4|V(G)|\left(M_1(H)+|V(G)||E(H)|\right) \quad (1)$$

and similarly we have:

$$\sum_{uv\in B}(\deg_{G+H}u+\deg_{G+H}v)^2 = HM(H)+4|V(H)|\left(M_1(G)+|V(H)||E(G)|\right). \quad (2)$$

Finally, we can write:

$$\sum_{uv\in C}(\deg_{G+H}u+\deg_{G+H}v)^2 = \sum_{\substack{u\in V(G)\\ v\in V(H)}}\left(\deg_G u+|V(H)|+\deg_G v+|V(G)|\right)^2$$

$$= |V(G)|M_1(H)+|V(H)|M_1(G)+8|E(G)||E(H)|$$

$$+|V(G)||V(H)|\left((|V(H)|+|V(G)|)^2+4(|E(G)|+|E(H)|\right)$$

$$+4\left(|V(G)|^2|E(H)|+|V(H)|^2|E(G)|\right). \quad (3)$$

Combining these three equations ((1), (2), (3)) will complete the proof.

Theorem 2. Let G and H be graphs. Then we have:

$$HM(G\times H)=|V(G)|HM(H)+|V(H)|HM(G)+8|E(G)|M_1(H)+8|E(H)|M_1(G)+16|E(G)||E(H)|$$

Proof: From the definition of the Cartesian product of graphs, we have:

$$E(G\times H)=\{(a,x)(b,y): ab\in E(G),\ x=y\ or\ xy\in E(H),\ a=b\}$$

therefore we can write:

$$HM(G\times H)=\sum_{(a,x)(b,y)\in E(G\times H)}\left(\deg_{G\times H}(a,x)+\deg_{G\times H}(b,y)\right)^2$$

$$+\sum_{\substack{(a,x)(a,y)\\ xy\in E(H)}}\left(\deg_{G\times H}(a,x)+\deg_{G\times H}(a,y)\right)^2$$

$$=\sum_{\substack{(a,x)(b,x)\\ xy\in E(G)}}\left(\deg_{G\times H}(a,x)+\deg_{G\times H}(b,x)\right)^2$$

$$+\sum_{a\in V(G)}\sum_{xy\in E(H)}\left(2\deg_G a+\deg_H x+\deg_H y\right)^2$$

$$=\sum_{x\in V(H)}\sum_{ab\in E(G)}\left(2\deg_H x+\deg_G a+\deg_G b\right)^2$$

This implies that,

$$|V(G)|HM(H)+|V(H)|HM(G)+8|E(G)|M_1(H)+8|E(H)|M_1(G)+16|E(G)||E(H)|.$$

Theorem 3. Let G and H be graphs. Then we have:

$$HM(G[H]) = |V(H)|^4 HM(G) + |V(G)|HM(H) + 2|E(G)||V(H)|M_1(H) + 8|V(H)||E(H)|(|E(G)|M_1(H) + 2M_1(G)|V(H)|).$$

Proof: From the definition of the composition $G[H]$ we have:

$$HM(G[H]) = \sum_{\substack{(a,x)(b,y)\in E(G[H])\\ ab\in E(G)}} (\deg_{G[H]}(a,x) + \deg_{G[H]}(b,y))^2 + \sum_{\substack{(a,x)(a,y)\in E(G[H])\\ xy\in E(H)}} (\deg_{G[H]}(a,x) + \deg_{G[H]}(a,y))^2.$$

So we have:

$$\sum_{\substack{(a,x)(b,y)\in E(G[H])\\ ab\in E(G)}} (\deg_{G[H]}(a,x) + \deg_{G[H]}(b,y))^2$$
$$= \sum_{x\in V(H)} \sum_{y\in V(H)} \sum_{ab\in E(G)} (|V(H)|\deg_G(a) + \deg_H(x) + |V(H)|\deg_G(b) + \deg_H(y))^2$$
$$= \sum_{x\in V(H)} \sum_{y\in V(H)} \left(|V(H)|^2 HM(G) + |E(G)|(\deg_H(x) + \deg_H(y))^2 + 2|V(H)|M_1(G)(\deg_H(x) + \deg_H(y))\right)$$
$$= |V(H)|^4 HM(G) + 2|E(G)||V(H)|M_1(H) + 8|E(G)||V(H)||E(H)| + 8M_1(G)|V(H)|^2|E(H)|. \qquad (4)$$

Moreover,

$$\sum_{\substack{(a,x)(a,y)\in E(G[H])\\ xy\in E(H)}} (\deg_{G[H]}(a,x) + \deg_{G[H]}(a,y))^2$$
$$= \sum_{a\in V(G)} \sum_{xy\in E(H)} (2|V(H)|\deg_G(a) + \deg_H(x) + \deg_H(y))^2$$
$$= \sum_{a\in V(G)} \left(4|E(H)||V(H)|^2 \deg_G{}^2(a) + HM(H) + 4|V(H)|\deg_G(a)M_1(H)\right)$$
$$= 4M_1(G)|E(H)||V(H)|^2 + |V(G)|HM(H) + 8M_1(H)|V(H)||E(H)|. \qquad (5)$$

It is easy to see that the summation of (4) and (5) complete the proof.

Theorem 4. Let G and H be graphs. Then we have:

$$HM(G*H) = HM(G) + |V(G)|HM(H) + 5|V(H)|M_1(G) + 5|V(G)|M_1(H) + 4|V(H)||E(G)|(2|V(H)| + 1) + 8|E(H)|(|V(G)| + |E(G)|) + |V(G)||V(H)|(|V(H)|^3 + 2|V(H)| + 4|E(H)|).$$

Proof: Let $A = E(G)$, $B = E(H,i)$ and $C = edges\ between\ G\ and\ (H,i)$ then:

$$\sum_{uv\in A} (\deg_{G*H} u + \deg_{G*H} v)^2 = \sum_{uv\in A} \left((\deg_G u + |V(H)|) + (\deg_G v + |V(H)|)\right)^2$$

$$= HM(G) + 4|V(H)|(|E(G)| + M_1(G)). \quad (6)$$

$$\sum_{uv\in B} (\deg_{G*H} u + \deg_{G*H} v)^2 = \sum_{i=1}^{|V(G)|} \sum_{uv\in E(H)} (\deg_H u + 1 + \deg_H v + 1)^2$$
$$= |V(G)|(4|E(H)| + HM(H) + 4M_1(H)). \quad (7)$$

$$\sum_{uv\in c} (\deg_{G*H} u + \deg_{G*H} v)^2 = \sum_{\substack{uv\in C \\ \{u\in V(G), v\in V(H,i)\}}} ((\deg_G u + |V(H)|) + (\deg_H v + 1))^2$$
$$= |V(G)||V(H)|(|V(H)|^2 + 1 + 4|E(H)| + 2|V(H)|) + 4|V(H)|^2|E(G)|$$
$$+ |V(H)|M_1(G) + |V(G)|M_1(H) + 4|E(H)|(|V(G)| + 2|E(G)|). \quad (8)$$

Combining these three equations ((6), (7), (8)) complete the proof.

3. FUTURE WORK

In addition, further research we seek to generalize the above theorems for n graph. Then you can see the similarities between generalization of the first and second Zagreb and their generalization to Hayper−Zagreb index of graphs.

REFERENCES

1. J. Braun, A. Kerber, M. Meringer, C. Rucker, Similarity of molecular descriptors: the equivalence of Zagreb indices and walk counts, MATCH Commun. Math. Comput. Chem. **54** (2005) 163–176.
2. M.V. Diudea, I. Gutman, L. Jantschi, Molecular Topology, Huntington, NY, 2001.
3. A. A. Dobrynin, R. Entringer, I. Gutman, Wiener index of trees: Theory and applications, Acta Appl. Math. **66** (2001) 211–249.
4. A. A. Dobrynin, I. Gutman, S. Klavžar, P. Zigert, Wiener index of hexagonal systems, Acta Appl. Math. **72** (2002) 247–294.
5. I. Gutman, K.C. Das, The first Zagreb index 30 years after, MATCH Commun. Math. Comput. Chem. **50** (2004) 83–92.
6. I. Gutman, N. Trinajstić, Graph theory and molecular orbitals, Total −electron energy of alternant hydrocarbons, Chem. Phys. Lett. **17** (1972) 535–538.
7. W. Imrich, S. Klavžar, Product Graphs: Structure and Recognition, John Wiley & Sons, New York, USA, 2000.
8. M. H. Khalifeh, H. Yousefi−Azari, A. R. Ashrafi, The Hyper−Wiener index of graph operations, Comput. Math. Appl. **56** (2008) 1402–1407.

9. M. H. Khalifeh, H. Yousefi−Azari, A. R. Ashrafi, Vertex and edge PI indices of Cartesian product graphs, Discrete Appl. Math. **156** (2008) 1780−1789.
10. S. Klavžar, A. Rajapakse, I. Gutman, The Szeged and the Wiener index of graphs, Appl. Math. Lett. **9** (1996) 45−49.
11. S. Nikolić, G. Kovačević, A. Milićević, N. Trinajstić, The Zagreb indices 30 years after, Croat. Chem. Acta **76** (2003) 113−124.
12. B. E. Sagan, Y.−N. Yeh, P. Zhang, The Wiener polynomial of a graph, Int. J. Quantum. Chem. **60** (5) (1996) 959−969.
13. N. Trinajstić, Chemical Graph Theory, CRC Press, Boca Raton, FL, 1992.
14. H. Wiener, Structural determination of the paraffin boiling points, J. Am. Chem. Soc. **69** (1947) 17−20.
15. H. Yousefi−Azari, B. Manoochehrian, A. R. Ashrafi, The PI index of product graphs, Appl. Math. Lett. **21** (6) (2008) 624−627.
16. B. Zhou, I. Gutman, Relations between Wiener, hyper-Wiener and Zagreb indices, Chem. Phys. Lett. **394** (2004) 93−95.
17. B. Zhou, Zagreb indices, MATCH Commun. Math. Comput. Chem. **52** (2004) 113−118.
18. B. Zhou, I. Gutman, Further properties of Zagreb indices, MATCH Commun. Math. Comput. Chem. **54** (2005) 233−239.