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ON HYPER–ZAGREB INDEX AND COINDEX

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A b s t r a c t. Let G be a graph with vertex set $\mathbf{V}$ and edges set $\mathbf{E}$. By $d(v)$ is denoted the degree of its vertex v. Two much studied degree–based graph invariants are the first and second Zagreb indices, defined as $M_1 = \sum_{u \in \mathbf{V}} d(u)^2$ and $M_2 = \sum_{uv \in \mathbf{E}} d(u)\, d(v)$. A recently proposed new invariant of this kind is the hyper–Zagreb index, defined as $HZ = \sum_{uv \in \mathbf{E}} [d(u) + d(v)]^2$. The basic relations between this index and its coindex for a graph G and its complement $\overline{G}$ are determined.

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1. *Introduction*

Let G be a graph of order n with vertex set $\mathbf{V}(G) = \{v_1, v_2, \ldots, v_n\}$ and edge set $\mathbf{E}(G)$. The degree of the vertex $v \in \mathbf{V}(G)$, denoted by $d_G(v) = d(v)$, is the number of first neighbors of v in the graph G.

The complement $\overline{G}$ of the graph G is the graph with vertex set $\mathbf{V}(G)$, in which two vertices are adjacent if and only if they are not adjacent in G.

In the contemporary mathematico–chemical literature, there exist several dozens of vertex–degree–based molecular structure descriptors [8, 10, 15]. Of these, the two Zagreb indices belong among the oldest molecular structure descriptors [17, 12, 3, 13, 11]. The *first Zagreb index* is defined as

$$M_1 = M_1(G) = \sum_{v \in \mathbf{V}(G)} d(v)^2 \tag{1.1}$$

and satisfies the identity [4, 5]

$$M_1(G) = \sum_{uv \in \mathbf{E}(G)} \big[d(u) + d(v)\big], \tag{1.2}$$

whereas the *second Zagreb index* is defined as

$$M_2 = M_2(G) = \sum_{uv \in \mathbf{E}(G)} d(u)\, d(v)\,.$$

The index M_1 was conceived in 1972 [16], whereas M_2 was first time considered a few years later [14]. For historical details see [11]. For details of the mathematical theory of the Zagreb indices see the booklet [20] and the more than hundred pages long survey [2].

Recently [7], a modification $F(G)$ of the first Zagreb index was re-introduced. This vertex–degree-based graph invariant was first time encountered in 1972, in the paper [16], but was eventually disregarded. The "forgotten" index F is defined as [7]

$$F = F(G) = \sum_{v \in \mathbf{V}(G)} d(v)^3\,.$$

Its main properties have been established in [7, 9].

In 2008, bearing in mind Eq. (1.2), Došlić put forward the first Zagreb coindex, defined as [4]

$$\overline{M}_1 = \overline{M}_1(G) = \sum_{uv \notin \mathbf{E}(G)} \big[d(u) + d(v)\big], \tag{1.3}$$

whereas the second Zagreb coindex was defined analogously as

$$\overline{M}_2 = \overline{M}_2(G) = \sum_{uv \notin \mathbf{E}(G)} d(u)\, d(v)\,. \tag{1.4}$$

In Eqs. (1.3) and (1.4) is it assumed that $u \neq v$.

Eq. (1.2) happens to be just a special case of a much more general relation. Let v be a vertex of the graph G, and let $\Phi(v)$ be any quantity associated to (or determined by) v.

Theorem 1.1 ([6]). *Let $X(G)$ be a graph invariant of the form*

$$X(G) = \sum_{v \in \mathbf{V}(G)} \Phi(v)\,.$$

Then the following edge–decomposition of X holds:

$$X(G) = \sum_{uv \in \mathbf{E}(G)} \left[\frac{\Phi(u)}{d(u)} + \frac{\Phi(v)}{d(v)} \right].$$

As another special case of Theorem 1.1, we have

$$F(G) = \sum_{uv \in \mathbf{E}(G)} \left[d(u)^2 + d(v)^2 \right]$$

which implies that the respective F-coindex is

$$\overline{F}(G) = \sum_{uv \notin \mathbf{E}(G)} \left[d(u)^2 + d(v)^2 \right].$$

The first Zagreb and F indices and coindices are mutually related as follows:

Theorem 1.2. *Let G be a graph with n vertices and m edges. Then*

$$\overline{M}_1(G) = 2m(n-1) - M_1(G), \tag{1.5}$$

$$M_1(\overline{G}) = n(n-1)^2 - 4m(n-1) + M_1(G), \tag{1.6}$$

$$\overline{M}_1(\overline{G}) = 2m(n-1) - M_1(G),$$

$$\overline{F}(G) = (n-1)M_1(G) - F(G),$$

$$F(\overline{G}) = n(n-1)^3 - 4m(n-1)^2 + 3(n-1)M_1(G) - F(G),$$

$$\overline{F}(\overline{G}) = 2m(n-1)^2 - 2(n-1)M_1(G) + F(G).$$

Especially intriguing is a special case of the above theorem, namely:

Corollary 1.1 ([13]). *Let G be any graph and $\overline{G}$ its complement. Then*

$$\overline{M}_1(G) = \overline{M}_1(\overline{G})\,.$$

There is no analogous relation for the F-index.

In this paper we are concerned with a recent extension of the Zagreb–index concept, namely with the so-called *hyper–Zagreb index*.

2. *Hyper–Zagreb index*

The hyper–Zagreb index, defined as

$$HZ = HZ(G) = \sum_{uv \in \mathbf{E}(G)} \big[d(u) + d(v)\big]^2 \tag{2.1}$$

was put forward in 2013 by the Iranian mathematicians Shirdel, Rezapour, and Sayad [19]. This definition was evidently motivated by Eq. (1.2). From Eq. (2.1), it can be immediately recognized that the hyper–Zagreb index is closely related with its much older congeners, namely that

$$HZ(G) = F(G) + 2M_2(G)\,.$$

In parallel with the other, previously conceived coindices, the hyper–Zagreb coindex is defined as

$$\overline{HZ} = \overline{HZ}(G) = \sum_{uv \notin \mathbf{E}(G)} \big[d(u) + d(v)\big]^2\,. \tag{2.2}$$

These new vertex–degree–based graph invariants were then studied in several subsequent papers [1, 21, 18]. In all four papers [19, 1, 21, 18], the authors were concerned with the hyper–Zagreb index and coindex of various graph transformations (such as join, disjunction, composition, Cartesian product, corona and edge–corona products, and similar). However, the fundamental relations, analogous to Theorem 1.2, were not reported in [19, 1, 21, 18]. In order to fill this gap, we now establish the following:

Theorem 2.1. *Let G be a graph with n vertices and m edges. Let the hyper–Zagreb index and coindex be defined via Eqs. (2.1) and (2.2). Then*

$$\overline{HZ}(G) = 4m^2 + (n-2)M_1(G) - HZ(G), \tag{2.3}$$

$$\begin{aligned} HZ(\overline{G}) &= 2n(n-1)^3 - 12m(n-1)^2 + 4m^2, \\ &\quad +(5n-6)M_1(G) - HZ(G), \end{aligned} \tag{2.4}$$

$$\overline{HZ}(\overline{G}) = 4m(n-1)^2 + 4(n-1)M_1(G) + HZ(G)\,. \tag{2.5}$$

3. *Proof of identity (2.3)*

In view of Eqs. (2.1) and (2.2),

$$HZ(G)+\overline{HZ}(G)=\left(\sum_{uv\in\mathbf{E}(G)}+\sum_{uv\notin\mathbf{E}(G)}\right)\big[d(u)+d(v)\big]^2$$

$$=\frac{1}{2}\left[\sum_{u\in\mathbf{V}(G)}\sum_{v\in\mathbf{V}(G)}\big[d(u)+d(v)\big]^2-\sum_{v\in\mathbf{V}(G)}\big[d(v)+d(v)\big]^2\right]$$

$$=\frac{1}{2}\left[\sum_{u\in\mathbf{V}(G)}\sum_{v\in\mathbf{V}(G)}\big[d(u)^2+d(v)^2+2d(u)\,d(v)\big]-4\sum_{v\in\mathbf{V}(G)}d(v)^2\right]$$

$$=\frac{1}{2}\left[n\sum_{u\in\mathbf{V}(G)}d(u)^2+n\sum_{v\in\mathbf{V}(G)}d(v)^2+2\left(\sum_{u\in\mathbf{V}(G)}d(u)\right)\left(\sum_{v\in\mathbf{V}(G)}d(v)\right)\right.$$

$$\left.-4\sum_{v\in\mathbf{V}(G)}d(v)^2\right]$$

$$=\frac{1}{2}\Big[nM_1(G)+nM_1(G)+2(2m)(2m)-4M_1(G)\Big],$$

where we have taken into account Eq. (1.1) and the fact that the sum of vertex degrees is equal to twice the number of edges. Thus,

$$HZ+\overline{HZ}=(n-2)M_1+4m^2,$$

which directly implies identity (2.3).

4. *Proof of identity (2.4)*

By Eq. (2.1),

$$HZ(\overline{G})=\sum_{uv\in\mathbf{E}(\overline{G})}\big[d_{\overline{G}}(u)+d_{\overline{G}}(v)\big]^2.$$

Recalling that $d_{\overline{G}}(v)=n-1-d_G(v)$, and that

$$\sum_{uv\in\mathbf{E}(\overline{G})}=\sum_{uv\notin\mathbf{E}(G)},$$

we get

$$\begin{aligned} HZ(\overline{G}) &= \sum_{uv \notin \mathbf{E}(G)} \big[n-1-d_G(u)+n-1-d_G(v)\big]^2 \\ &= \sum_{uv \notin \mathbf{E}(G)} \Big[4(n-1)^2 + \big[d(u)+d(v)\big]^2 - 4(n-1)\big[d(u)+d(v)\big]\Big] \\ &= 4(n-1)^2\left[\binom{n}{2} - m\right] + \overline{HZ}(G) - 4(n-1)\overline{M}_1(G)\,. \end{aligned} \tag{4.1}$$

Now, by substituting into (4.1) the expressions for $\overline{HZ}(G)$, Eq. (2.3), and for $\overline{M}_1(G)$, Eq. (1.5), we arrive at

$$\begin{aligned} HZ(\overline{G}) &= 4(n-1)^2\left[\binom{n}{2} - m\right] + \Big[4m^2 + (n-2)M_1(G) - HZ(G)\Big] \\ &\quad -4(n-1)\Big[2m(n-1) - M_1(G)\Big] \end{aligned}$$

which directly leads to formula (2.4).

5. *Proof of identity (2.5)*

Eq. (2.3) can be rewritten as

$$\overline{HZ}(\overline{G}) = 4\overline{m}^2 + (n-2)M_1(\overline{G}) - HZ(\overline{G}),$$

where $\overline{m}$ is the number of edges of the complement $\overline{G}$, i.e., $\overline{m} = \binom{n}{2} - m$. Then by using Eqs. (1.6) and (2.4),

$$\begin{aligned} \overline{HZ}(\overline{G}) &= 4\left[\binom{n}{2} - m\right]^2 + (n-2)\Big[n(n-1)^2 - 4m(n-1) + M_1(G)\Big] \\ &\quad -\Big[2n(n-1)^3 - 12m(n-1)^2 + 4m^2 + (5n-6)M_1(G) - HZ(G)\Big], \end{aligned}$$

which after appropriate calculation renders the identity (2.5).

REFERENCES

[1] B. Basavanagoud, S. Patil, *A note on hyper–Zagreb index of graph operations*, Iran. J. Math. Chem. **7** (2016), 89–92.

[2] B. Borovićanin, K. C. Das, B. Furtula, I. Gutman, *Zagreb indices: Bounds and extremal graphs*, MATCH Commun. Math. Comput Chem., forthcoming.

[3] K. C. Das, I. Gutman, *Some properties of the second Zagreb index*, MATCH Commun. Math. Comput. Chem. **52** (2004), 103–112.

[4] T. Došlić, *Vertex–weighted Wiener polynomials for composite graphs*, Ars Math. Contemp. **1** (2008), 66–80.

[5] T. Došlić, B. Furtula, A. Graovac, I. Gutman, S. Moradi, Z. Yarahmadi, *On vertex–degree–based molecular structure descriptors*, MATCH Commun. Math. Comput Chem. **66** (2011), 613–626.

[6] T. Došlić, T. Réti, D. Vukičević, *On the vertex degree indices of connected graphs*, Chem. Phys. Lett. **512** (2011), 283–286.

[7] B. Furtula, I. Gutman, *A forgotten topological index*, J. Math. Chem. **53** (2015), 1184–1190.

[8] B. Furtula, I. Gutman, M. Dehmer, *On structure–sensitivity of degree–based topological indices*, Appl. Math. Comput. **219**, (2013) 8973–8978.

[9] B. Furtula, I. Gutman, Ž. Kovijanić Vukićević, G. Lekishvili, G. Popivoda, *On an old/new degree–based topological index*, Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.) **148** (2015), 19–31.

[10] I. Gutman, *Degree–based topological indices*, Croat. Chem. Acta **86** (2013) 351–361.

[11] I. Gutman, *On the origin of two degree–based topological indices*, Bull. Acad. Serbe Sci. Arts (Cl. Sci. Math. Natur.) **146** (2014), 39–52.

[12] I. Gutman, K. C. Das, *The first Zagreb index 30 years after*, MATCH Commun. Math. Comput. Chem. **50** (2004), 83–92.

[13] I. Gutman, B. Furtula, Ž. Kovijanić Vukićević, G. Popivoda, *On Zagreb indices and coindices*, MATCH Commun. Math. Comput. Chem. **74** (2015), 5–16.

[14] I. Gutman, B. Ruščić, N. Trinajstić, C. F. Wilcox, *Graph theory and molecular orbitals. XII. Acyclic polyenes*, J. Chem. Phys. **62** (1975), 3399–3405.

[15] I. Gutman, J. Tošović, *Testing the quality of molecular structure descriptors. Vertex–degree–based topological indices*, J. Serb. Chem. Soc. **78** (2013), 805–810.

[16] I. Gutman, N. Trinajstić, *Graph theory and molecular orbitals. Total π-electron energy of alternant hydrocarbons*, Chem. Phys. Lett. **17** (1972), 535–538.

[17] S. Nikolić, G. Kovačević, A. Miličević, N. Trinajstić, *The Zagreb indices 30 years after*, Croat. Chem. Acta **76** (2003), 113–124.

[18] K. Pattabiraman, M. Vijayaragavan, *Hyper Zagreb indices and its coindices of graphs*, Bull. Int. Math. Virt. Inst. **7** (2017), 31–41.

[19] G. H. Shirdel, H. Rezapour, A. M. Sayadi, *The hyper–Zagreb index of graph operations*, Iran. J. Math. Chem. **4** (2013), 213–220.

[20] D. Stevanović, *Mathematical Properties of Zagreb Indices*, Akademska misao, Beograd, 2014 (in Serbian).

[21] M. Veylaki, M. J. Nikmehr, *The third and hyper–Zagreb coindices of some graph operations*, J. Appl. Math. Comput. **50** (2016), 315–325.

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