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RELATIONS BETWEEN WIENER, HYPER−WIENER AND SOME ZAGREB TYPE INDICES

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ABSTRACT. In this paper, some inequalities between the Wiener, hyper-Wiener, first Zagreb, second Zagreb, first reformulated Zagreb, second reformulated Zagreb and the general Zagreb indices of a simple graph are given. Our results improve some earlier bonds between these graph invariants.

Keywords: Topological index, Wiener index, Hyper-Wiener index, Zagreb indices, Reformulated Zagreb index.

INTRODUCTION

A **graph** is a pair $G = (V, E)$ in which V is a non-empty set and $E \subseteq P_2(V) = \{\{x, y\} | x \neq x \in V\}$. If each element of V has at most four mates in V, then the graph G is called a **molecular graph**. Topological indices are maps from molecular graphs into real numbers, such that this mapping is invariant under graph isomorphisms. These indices are widely used in chemistry for relationship between molecular structures and molecular properties of a given complex (DEVILLERS and BALABAN, 2000). The **Wiener index** (WIENER, 1947) and **Zagreb group indices** (GUTMAN and TRINAJSTIĆ, 1972; GUTMAN and FURTULA, 2003) are some of the most studied topological indices both by chemists and mathematicians. In a similar way as Zagreb group indices, the first and second **reformulated Zagreb indices** were defined (ILIĆ and ZHOU, 2012). In addition if α is an arbitrary real number except from 0 and 1, then (LI and ZHENG, 2005) introduced the **general Zagreb index** of a graph. The most important generalization of Wiener index is the **hyper-Wiener index** (KLEIN *et al.*, 1995). We will define these graph invariant later.

Let $G = (V, E)$ be a simple connected graph and $u, v \in V$. The distance between u and v, $d_G(u, v)$, is defined as the minimum length of a shortest path connecting them. A graph invariant is said to be **distance-based** if it can be defined by distance function $d_G(-,-)$. The Wiener and hyper-Wiener indices of G are defined as follows:

$W(G) = \sum_{\{u,v\}\subset V(G)} d_G(u,v)$,

$WW(G) = \frac{1}{2}[W(G) + \sum_{\{u,v\}\subset V(G)} d_G(u,v)^2]$.

These are the most important distance-based topological indices of a graph.

Suppose G is a simple graph and $v \in V(G)$. The notation $deg(v)$ used for the degree of v in G. A topological index is said to be **degree-based** if it can be defined as the function $deg(-)$. The Zagreb and reformulated Zagreb group indices are most important degree-based topological indices of G. These topological indices, as well as, the general Zagreb index of G are defined as follows:

$M_1(G) = \sum_{v\in V(G)} deg_G(v)^2 \& M_2(G) = \sum_{uv\in E(G)} deg_G(u)deg_G(v)$,

$EM_1(G) = \sum_{e\in E(G)} deg_G(e)^2 \& EM_2(G) = \sum_{e\sim f} deg_G(e)deg_G(f)$,

$M_1^\alpha(G) = \sum_{u\in V(G)} deg_G(u)^\alpha$.

Here, $e{\sim}f$ means that the edges e and f have a common vertex, the notation $deg_G(u)$ is used for the degree of vertex v in G and for an edge $e = uv$, $deg_G(e) = deg_G(u) + deg_G(v) - 2$ denotes the degree of the edge e. It is easy to prove that $M_1(G) = \sum_{uv\in E(G)} [deg_G(u) + deg_G(v)]$.

It is clear that $M_1^2(G) = M_1(G)$. The graph invariant $M_1^3(G)$ is called the **forgotten topological index** and denoted by $F(G)$; $F(G) = \sum_{u\in V(G)} deg_G(u)^3$ (FURTULA and GUTMAN, 2015). We encourage the interested readers to consult papers (GUTMAN *et al.*, 1997; KLAVŽAR *et al.*, 2000; NIKOLIĆ *et al.*, 2003; XING *et al.*, 2011) for more information on this topic.

It is natural to try to establish relations between the degree-based and distance-based topological indices. (ZHOU and GUTMAN, 2004) obtained some bounds on Wiener and hyper-Wiener indices, in terms of the first Zagreb index for molecular graphs with girth greater than four. BEHTOI *et al.* (2011) deduced inequalities for Wiener and hyper-Wiener indices, in terms of M_1, M_2 and the number of hexagons. DAS *et al.* (2015) continued the previous works by considering Szeged, PI, and Wiener polarity indices, as distance-based indices, and the first and second Zagreb indices.

The aim of this paper is to bring new inequalities, relating W, WW, M_1, M_2, EM_1, EM_2, F and M_1^4. In addition our results correct some minor errors in previous works.

PRELIMINARIES

Let $G = (V(G), E(G))$ be a simple connected graph with n vertices and m edges, respectively. The diameter of G, denoted by $diam(G)$, is defined as the largest distance between vertices of G. The length of a shortest cycle in G is called the girth of G, denoted by $g(G)$. If G does not contain a cycles, then we set $g(G) = \infty$. Let k be a nonnegative integer. Then $d(G,k)$ denotes the number of pairs of vertices in G with distance k. Note that $d(G,k) = 0$, for every $k > diam(G)$, and $d(G,1) = m$. It is easy to check that

$\sum_{k\geq 1} d(G,k) = \binom{n}{2} \& W(G) = \sum_{k\geq 1} kd(G,k)$,

$WW(G) = \frac{1}{2}\sum_{k\geq 1} k(k+1)d(G,k)$.

ZHO and GUTMAN (2004) showed that the equality $d(G,2) = \frac{1}{2}M_1(G) - m$ holds for graphs that do not contain triangles and/or quadrangles; in fact $g(G) > 4$. We may extend this result as:

Lemma 2.1 *Let G be a graph with s squares, m edges and $g(G) \geq 4$. Then $d(G,2) = \frac{1}{2}M_1(G) - m - 2s$.*

Proof. Since $g(G) \geq 4$, for each square in G there are exactly two pairs of vertices of distance two and hence two distinct paths of length two in G. It follows that

$$d(G,2) = \sum_{u\sim v\sim x} 1 - 2s = \sum_{v\in V(G)} deg_G(v)\left[\frac{deg_G(v)-1}{2}\right] - 2s = \frac{1}{2}M_1(G) - m - 2s,$$

as desired.

BEHTOI *et al.* (2011) explained that if $g(G) > 4$ and G has h hexagons, then $d(G,3) = M_2(G) - M_1(G) + m - 3h$. Suppose G is a cycle with 5 vertices, then $g(G) = 5$ and $d(G,3) = 0$, but $M_2(G) - M_1(G) + m - 3h = 10 - 10 + 5 - 3\times 0 = 5$. In fact, $d(G,3) = M_2(G) - M_1(G) + m - 3h$ holds when $g(G) \geq 6$, since we conclude from $g(G) \geq 6$ that each hexagon in G has exactly three pairs of vertices of distance three and so two distinct paths of size three in G. Hence,

$$\begin{aligned} d(G,3) &= \sum_{w\sim u\sim v\sim x} 1 - 3h \\ &= \sum_{u\sim v} (deg_G(u) - 1)(deg_G(v) - 1) - 3h \\ &= \sum_{u\sim v} [deg_G(u)deg_G(v) - (deg_G(u) + deg_G(v)) + 1] - 3h \\ &= M_2(G) - M_1(G) + m - 3h. \end{aligned}$$

This observation yields the following lemma;

Lemma 2.2 *If G is a graph with h hexagons, m edges and $g(G) \geq 6$, then $d(G,3) = M_2(G) - M_1(G) + m - 3h$.*

We are now ready to extend this result to the case that G has exactly c octagons and $g(G) \geq 8$.

Lemma 2.3 *Let G be a graph with c octagons, n vertices and m edges. If $A(G) = \sum_{e\sim f,e=uv,f=vx} (deg_G(v) - 1)(deg_G(e) + deg_G(f))$ and $g(G) \geq 8$, then $d(G,4) = EM_2(G) - A(G) + \frac{1}{2}M_1^4(G) - \frac{3}{2}F(G) + \frac{3}{2}M_1(G) - m - 4c$.*

Proof. Since $g(G) \geq 8$, for each octagon in G there are exactly four pairs of vertices of distance four and hence two distinct paths of length four in G. Therefore,

$$\begin{aligned} d(G,4) &= \sum_{w\sim u\sim v\sim x\sim z} 1 - 4c \\ &= \sum_{u\sim v\sim x} (deg_G(u) - 1)(deg_G(x) - 1) - 4c \\ &= \sum_{e\sim f,e=uv,f=vx} \big(deg_G(e) - (deg_G(v) - 1)\big)\big(deg_G(f) - (deg_G(v) - 1)\big) - 4c \\ &= \sum_{e\sim f,e=uv,f=vx} [deg_G(e)deg_G(f) - deg_G(e)(deg_G(v) - 1) \\ &\quad -(deg_G(v) - 1)deg_G(f) + (deg_G(v) - 1)^2] - 4c \\ &= \sum_{e\sim f,e=uv,f=vx} deg_G(e)deg_G(f) + \sum_{e\sim f,e=uv,f=vx} (deg_G(v) - 1)^2 - 4c \\ &\quad - \sum_{e\sim f,e=uv,f=vx} (deg_G(v) - 1)(deg_G(e) + deg_G(f)). \end{aligned}$$

So, by definition,

$$d(G,4) = EM_2(G) - \sum_{e\sim f, e=uv, f=vx} (deg_G(v)-1)(deg_G(e)+deg_G(f))$$
$$+\sum_{v\in V(G)} \binom{deg_G(v)}{2}(deg_G(v)-1)^2 - 4c$$
$$= EM_2(G) - \sum_{e\sim f, e=uv, f=vx} (deg_G(v)-1)(deg_G(e)+deg_G(f))$$
$$+\frac{1}{2}\sum_{v\in V(G)} [deg_G^4(v) - 3deg_G^3(v) + 3deg_G^2(v) - deg_G(v)] - 4c$$
$$= EM_2(G) - \sum_{e\sim f, e=uv, f=vx} (deg_G(v)-1)(deg_G(e)+deg_G(f))$$
$$+\frac{1}{2}M_1^4(G) - \frac{3}{2}F(G) + \frac{3}{2}M_1(G) - m - 4c$$
$$= EM_2(G) - A(G) + \frac{1}{2}M_1^4(G) - \frac{3}{2}F(G) + \frac{3}{2}M_1(G) - m - 4c.$$

This completes the proof.

From the previous lemma, we conclude that:

Corollary 2.4 *Let G be a graph with c octagons, n vertices, m edges and $g(G) \geq 8$. Then* $\sum_{k\geq 5} d(G,k) = \frac{n(n-1)}{2} - [M_1(G) + M_2(G) + EM_2(G) - A(G) + \frac{1}{2}M_1^4(G) - \frac{3}{2}F(G) - 4c]$.

MAIN RESULTS

Suppose G is a connected simple graph with n vertices and m edges. Then the Wiener, hyper-Wiener, Zagreb indices and general Zagreb indices satisfy the following relations:

Theorem 3.1 *Suppose that G is a graph with c octagons, n vertices, m edges and $g(G) \geq 8$. If $\delta'(G) = \delta' = min\{deg_G(v) | v \in V(G) and deg_G(v) \neq 1\}$, then*

1. $W(G) \geq \frac{5n(n-1)}{2} + \frac{3}{2}F(G) + (\delta'-1)EM_1(G) + 4c - (2m + EM_2(G) + M_1(G) + 2M_2(G) + \frac{1}{2}M_1^4(G))$,
2. $WW(G) \geq \frac{1}{2}W(G) + \frac{1}{2}[\frac{25n(n-1)}{2} + \frac{27}{2}F(G) + 9(\delta'-1)EM_1(G) + 36c - (10m + 9EM_2(G) + 8M_1(G) + 16M_2(G) + \frac{9}{2}M_1^4(G))]$,
3. $WW(G) \geq \frac{1}{2}[15n(n-1) + 15F(G) + 10(\delta'-1)EM_1(G) + 40c - (12m + 10EM_2(G) + 9M_1(G) + 18M_2(G) + 5M_1^4(G))]$,
4. $WW(G) \geq 3W(G) + 3F(G) + 2(\delta'-1)EM_1(G) + 8c - (2EM_2(G) + \frac{3}{2}M_1(G) + 3M_2(G) + M_1^4(G))$.

The equality in all four cases will hold if and only if the distance between any two vertices in G is not greater than 5 and $\{deg_G(v) | v \in V(G)$ and $deg_G(v) \neq 1\} = \{\delta'\}$.

Proof. From what has already been proved in section 2, we have:

$$(1) W(G) = \sum_{k\geq 1} kd(G,k) = d(G,1) + 2d(G,2) + 3d(G,3) + 4d(G,4) + \sum_{k\geq 5} kd(G,k)$$
$$\geq m + M_1(G) - 2m + 3M_2(G) - 3M_1(G) + 3m + 4EM_2(G) - 4A(G)$$
$$+2M_1^4(G) - 6F(G) + 6M_1(G) - 4m - 16c + 5\sum_{k\geq 5} d(G,k)$$
$$= m + M_1(G) - 2m + 3M_2(G) - 3M_1(G) + 3m + 4EM_2(G) - 4A(G)$$
$$+2M_1^4(G) - 6F(G) + 6M_1(G) - 4m - 16c + \frac{5n(n-1)}{2} - 5M_1(G)$$
$$-5M_2(G) - 5EM_2(G) + 5A(G) - \frac{5}{2}M_1^4(G) + \frac{15}{2}F(G) + 20c$$
$$\geq \frac{5n(n-1)}{2} + \frac{3}{2}F(G) + (\delta'-1)EM_1(G) + 4c$$

$$-(2m+EM_2(G)+M_1(G)+2M_2(G)+\frac{1}{2}M_1^4(G)).$$

The last inequality follows from $A(G)\geq(\delta'-1)EM_1(G)$.

$$(2)WW(G)=\frac{1}{2}\sum_{k\geq1}k(k+1)d(G,k)=\frac{1}{2}W(G)+\frac{1}{2}\sum_{k\geq1}k^2d(G,k)$$
$$=\frac{1}{2}W(G)+\frac{1}{2}[d(G,1)+4d(G,2)+9d(G,3)+16d(G,4)+\sum_{k\geq5}k^2d(G,k)]$$
$$\geq\frac{1}{2}W(G)+[\frac{m}{2}+M_1(G)-2m+\frac{9}{2}M_2(G)-\frac{9}{2}M_1(G)+\frac{9}{2}m+8EM_2(G)$$
$$-8A(G)+4M_1^4(G)-12F(G)+13M_1(G)-8m-32c+\frac{25}{2}\sum_{k\geq5}d(G,k)$$
$$=\frac{1}{2}W(G)-5m+\frac{9}{2}M_2(G)-\frac{9}{2}M_1(G)+8EM_2(G)-8A(G)$$
$$+4M_1^4(G)-12F(G)+12M_1(G)+18c+\frac{25n(n-1)}{4}+\frac{75}{4}F(G)$$
$$-\frac{25}{2}M_1(G)-\frac{25}{2}M_2(G)-\frac{25}{2}EM_2(G)+\frac{25}{2}A(G)-\frac{25}{4}M_1^4(G)$$
$$\geq\frac{1}{2}W(G)+\frac{25n(n-1)}{4}+\frac{27}{4}F(G)+\frac{9}{2}(\delta'-1)EM_1(G)+18c$$
$$-(5m+\frac{9}{2}EM_2(G)+4M_1(G)+8M_2(G)+\frac{9}{4}M_1^4(G))$$

in which the last inequality follows from $A(G)\geq(\delta'-1)EM_1(G)$. The inequality (3) is a direct consequence of (1) and (2).

$$(4)WW(G)=\frac{1}{2}\sum_{k\geq1}k(k+1)d(G,k)=\frac{1}{2}W(G)+\frac{1}{2}\sum_{k\geq1}k^2d(G,k)$$
$$=\frac{1}{2}W(G)+\frac{1}{2}[d(G,1)+4d(G,2)+9d(G,3)+16d(G,4)+\sum_{k\geq5}k^2d(G,k)]$$
$$\geq\frac{1}{2}W(G)+M_1(G)-5m+\frac{9}{2}M_2(G)+\frac{15}{2}M_1(G)+8EM_2(G)-8A(G)$$
$$+4M_1^4(G)-12F(G)-32c+\frac{5}{2}\sum_{k\geq5}kd(G,k)$$
$$=\frac{1}{2}W(G)-5m+\frac{17}{2}M_1(G)+\frac{9}{2}M_2(G)+8EM_2(G)$$
$$-8A(G)+4M_1^4(G)-12F(G)-32c$$
$$+\frac{5}{2}[W(G)-(d(G,1)+2d(G,2)+3d(G,3)+4d(G,4))]$$
$$=3W(G)-5m+\frac{17}{2}M_1(G)+\frac{9}{2}M_2(G)+8EM_2(G)$$
$$-8A(G)+4M_1^4(G)-12F(G)-32c$$
$$+5m-10M_1(G)-\frac{15}{2}M_2(G)-10EM_2(G)$$
$$+10A(G)-5M_1^4(G)+15F(G)+40c$$
$$=3W(G)+3F(G)+2A(G)+8c$$
$$-(2EM_2(G)+\frac{3}{2}M_1(G)+3M_2(G)+M_1^4(G))$$
$$\geq3W(G)+3F(G)+2(\delta'-1)EM_1(G)+8c$$
$$-(2EM_2(G)+\frac{3}{2}M_1(G)+3M_2(G)+M_1^4(G))$$

in which the last inequality is a consequence of $A(G)\geq(\delta'-1)EM_1(G)$. Equality in $(1-4)$ hold if and only if $\sum_{k\geq5}kd(G,k)=5\sum_{k\geq5}d(G,k)(or\sum_{k\geq5}k^2d(G,k)=25\sum_{k\geq5}d(G,k))$ and $A(G)=(\delta'-1)EM_1(G)$. Therefore, these equalities can be occurred if and only if the distance between any two vertices of the graph G is not greater than 5 and $\{deg_G(v)|v\in V(G)\text{and }deg_G(v)\neq1\}=\{\delta'\}$.

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