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Some New Relations between Wiener, Hyper–Wiener and Zagreb Indices

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Abstract

Gutman and Zhou (Relations between Wiener, hyper-Wiener and Zagreb indices, Chemical Physics Letters 394 (2004) 93-95) obtained some bounds on Wiener and hyper-Wiener indices, in term of the first Zagreb index in molecular graphs with girth greater than four. We obtain new inequalities for Wiener and hyper–Wiener indices, in terms of the first and the second Zagreb indices and the number of hexagons in these graphs. These inequalities improve the bounds obtained by Gutman and Zhou and are the best possible bounds. Using these relations we obtain a bound on the second Zagreb index in terms of the first Zagreb index, for hexagon–free graphs.

1 Introduction

Throughout this paper we consider connected simple graphs, i. e., graphs without loops and multiple edges. Our notations are standard and mainly taken from [1]. Let $G = (V(G), E(G))$ be a graph with vertex set $V(G)$ and edge set $E(G)$. We denote by $d(x, y)$, $N(x)$ and $\deg(x)$, the distance between vertices x and y, vertices in distance one with vertex x and the degree of x, respectively. The diameter of G, denoted by diam(G), is defined as the largest distance between vertices of G. We also denote by $g(G)$ the girth of the graph G which is defined as the length of the smallest (induced) cycle in G, if G has at least one cycle, and is defined to be infinite if G has no cycle. Thus the girth of trees and more generally the girth of the forests is defined to be infinite.

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A topological index is a number related to a graph which is structural invariant, that is to say it is fixed under graph automorphisms. The Wiener index, denoted by W, is perhaps the most studied topological indices from application and theoretical view points. This index is defined as the sum of all distances between vertices of the graph. Randić introduced an extension of the Wiener index for trees, and this has come to be known as the hyper-Wiener index, denoted by WW. Klein et al. [2] generalized this extension to cyclic structures as

$$WW(G) = \frac{1}{2} \sum_{\{u,v\} \subseteq V(G)} \left(d(u,v) + d(u,v)^2 \right) \ .$$

The graph invariant hyper-Wiener is also a distance based graph invariant. For every k, $1 \leq k \leq \mathrm{diam}(G)$, let $d(G,k)$ denotes the number of pairs of vertices in $V(G)$ with distance k, i. e.,

$$d(G,k) := |\{\{x,y\} \mid x,y \in V(G),\ d(x,y) = k\}| \ .$$

Note that we have $d(G,k) = 0$ for every $k > \mathrm{diam}(G)$. Clearly $\sum_{k \geq 1} d(G,k) = \frac{n(n-1)}{2}$ and it is evidently obtained that

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

The graph invariants M_1 and M_2, the first and the second Zagreb indices respectively, were firstly considered in 1972, see [3], are not distance based graph invariants. They are defined as

$$M_1(G) := \sum_{xy \in E(G)} (\deg(x) + \deg(y)) = \sum_{x \in V(G)} \deg(x)^2$$

and

$$M_2(G) := \sum_{xy \in E(G)} \deg(x) \deg(y) \ .$$

This expressions which now are called the Zagreb indices were deduced within the study of the dependence of total π-electron energy on molecular structures [3] and are measures of branching of the molecular carbon-atom skeleton [4]. For recent research on Zagreb indices see [5, 6], the articles published in this issue, and the references cited therein.

Recently Gutman and Zhou, using the expression of $d(G,2)$ in terms of the first Zagreb index and the number of edges, obtained some bounds on Wiener and hyper-Wiener indices, in term of the first Zagreb index, the number of vertices and edges in the graph G with girth greater than four [7]. In fact, for a simple triangle and square free graph G they proved that

$$W(G) \geq \frac{3}{2}n(n-1) - m - \frac{1}{2}M_1$$

and

$$WW(G) \geq 3n(n-1) - 2m - \frac{3}{2}M_1 \quad , \quad WW(G) \geq 2W(G) - \frac{1}{2}M_1 \ .$$

In this note we obtain some new inequities for Wiener and hyper-Wiener indices of a graph, in term of the first and the second Zagreb indices and the number of hexagons (induced cycles of size six). We show that these inequalities improve the bounds obtained by Gutman and Zhou and are the best possible bounds. In what follows we use M_1 and M_2 instated of $M_1(G)$ and $M_2(G)$ when there is no confusing.

2 Main Results

Let $G = (V(G), E(G))$ be an arbitrary graph. For every adjacent vertices $x, y \in V(G)$ we have $d(x, y) = 1$ and vice versa. So $d(G, 1)$ is equal to the number of edges of the graph G, that is $d(G, 1) = |E(G)|$.

Lemma 1. Let G be a graph with h hexagons, m edges and $g(G) > 4$. Then
(i) $d(G, 2) = \frac{1}{2}M_1 - m$
(ii) $d(G, 3) = M_2 - M_1 + m - 3h$.

Proof. Let $x, y \in V(G)$ be two vertices of distance two in G and xzy be a path of size two between them. Then we have $z \in N(x) \cap N(y)$ and so $N(x) \cap N(y) \neq \emptyset$. Conversely, if x_1, y_1 are two distinct (non-adjacent) vertices with $N(x_1) \cap N(y_1) \neq \emptyset$, then we must have $d(x_1, y_1) = 2$, since G has no triangle. Note also that G has no square and so $|N(x_1) \cap N(y_1)| = 1$. Thus there is a bijection between the sets $\{\{x, y\} \mid d(x, y) = 2\}$ and $\{\{x, y\} \mid x \neq y, \exists z \in V(G) : x, y \in N(z)\}$, and so we have

$$d(G,2) = \sum_{z \in V(G)} \binom{\deg(z)}{2} = \frac{1}{2}\left(\sum_{z \in V(G)} \deg(z)^2 - \sum_{z \in V(G)} \deg(z)\right) = \frac{1}{2}M_1 - m \ .$$

Similarly if x, y are two vertices of distance three in G and xz_1z_2y be a path of size three between them, then $z_1z_2 \in E(G)$, $x \in N(z_1) - z_2$ and $y \in N(z_2) - z_1$. Conversely, if x, y are two (distinct) vertices such that there exist $z_1z_2 \in E(G)$ with $x \in N(z_1) - z_2$

and $y \in N(z_2) - z_1$, then $d(x,y) = 3$. Note that in this case, since $g(G) > 4$, we have $x \notin N(z_2)$, $y \notin N(z_1)$ and $xy \notin E(G)$. Since G has no square, there is a unique (shortest) path of size two between each pair of vertices of distance two in G. But in each hexagon in G there are exactly three pairs of vertices of distance three with two distinct (shortest) paths of size three in G. Thus according to the above arguments we have

$$\begin{aligned} d(G,3) &= \sum_{z_1 z_2 \in E(G)} (\deg(z_1) - 1)(\deg(z_2) - 1) - 3h \\ &= \sum_{z_1 z_2 \in E(G)} (\deg(z_1)\deg(z_2) - (\deg(z_1) + \deg(z_2)) + 1) - 3h \\ &= M_2 - M_1 + m - 3h \end{aligned}$$

which completes the proof of lemma. ■

Theorem 2. If G is a graph with h hexagons, m edges and $g(G) > 4$, then $W(G) \geq 2(n(n-1) - m) - M_2 + 3h$ and equality holds if and only if $\operatorname{diam}(G) \leq 4$.

Proof. By the definitions and using the above lemma we obtain that

$$\begin{aligned} W(G) = \sum_{k \geq 1} kd(G,k) &= d(G,1) + 2d(G,2) + 3d(G,3) + \sum_{k \geq 4} kd(G,k) \\ &= m + 2\left(\frac{1}{2}M_1 - m\right) + 3(M_2 - M_1 + m - 3h) + \sum_{k \geq 4} kd(G,k) \\ &= 3M_2 - 2(M_1 - m) - 9h + \sum_{k \geq 4} kd(G,k) \\ &\geq 3M_2 - 2(M_1 - m) - 9h \\ &+ 4\left(\binom{n}{2} - m - (\frac{1}{2}M_1 - m) - (M_2 - M_1 + m - 3h)\right) \\ &= 2(n(n-1) - m) - M_2 + 3h\ . \end{aligned}$$

This bound is the best possible since for the path with five vertices P_5, we have $W(P_5) = 20$ and $M_2(P_5) = 12$. In fact this bound is attained for all graphs with diameter at most four. ■

Obviously we have

$$3\sum_{k \geq 3} d(G,k) \leq 3d(G,3) + 4\sum_{k \geq 4} d(G,k)\ .$$

Since the left hand side of the above inequality is used by Gutamn and Zhou as a lower bound for $\sum_{k \geq 3} kd(G,k)$ and our lower bound takes in to the account the right hand side of above inequality, so our lower bound for $W(G)$ is greater and so

$$3\binom{n}{2} - \frac{1}{2}\,M_1 - m \leq 2(n(n-1) - m) - M_2 + 3h\ .$$

This observation yields the following corollary.

Corollary 3. With the notations and conditions of Theorem 2, we have $M_2 \leq \frac{1}{2}(M_1 + n(n-1) - 2m)$.

The following theorem gives us two lower bounds for the hyper-Wiener index.

Theorem 4. If G is a graph with h hexagons, m edges and $g(G) > 4$, then
(i) $WW(G) \geq 5n(n-1) - 6m - 4M_2 + \frac{1}{2}M_1 + 12h$
(ii) $WW(G) \geq \frac{5}{2}W(G) - m + \frac{1}{2}M_1 - \frac{3}{2}M_2 + \frac{9}{2}h$
and in above inequalities, equality holds if and only if $\mathrm{diam}(G) \leq 4$.

Proof. By the definition of hyper-Wiener in terms of $d(G,K)$'s and by using Lemma 1 we obtain that

$$\begin{aligned}
WW(G) &= \frac{1}{2}\sum_{k\geq 1} k(k+1)d(G,k) \\
&= d(G,1) + 3d(G,2) + 6d(G,3) + \frac{1}{2}\sum_{k\geq 4}(k^2+k)d(G,k) \\
&= m + 3(\frac{1}{2}M_1 - m) + 6(M_2 - M_1 + m - 3h) + \frac{1}{2}\sum_{k\geq 4}(k^2+k)d(G,k) \\
&= 6M_2 + 4m - \frac{9}{2}M_1 - 18h + \frac{1}{2}\sum_{k\geq 4}(k^2+k)d(G,k) \\
&\geq 6M_2 + 4m - \frac{9}{2}M_1 - 18h + 10\sum_{k\geq 4} d(G,k) \\
&= 6M_2 + 4m - \frac{9}{2}M_1 - 18h \\
&+ 10\left(\binom{n}{2} - m - (\frac{1}{2}M_1 - m) - (M_2 - M_1 + m - 3h)\right) \\
&= 5n(n-1) - 6m - 4M_2 + \frac{1}{2}\,M_1 + 12h\ .
\end{aligned}$$

This proves the first case. For the second one we compute

$$
\begin{aligned}
WW(G) &= \frac{1}{2}\left(W(G)+\sum_{k\geq 1} k^2 d(G,k)\right)\\
&= \frac{1}{2}W(G)+\frac{1}{2}d(G,1)+2d(G,2)+\frac{9}{2}d(G,3)+\frac{1}{2}\sum_{k\geq 4} k^2 d(G,k)\\
&\geq \frac{1}{2}W(G)+\frac{1}{2}d(G,1)+2d(G,2)+\frac{9}{2}d(G,3)+\frac{4}{2}\sum_{k\geq 4} k d(G,k)\\
&= \frac{1}{2}W(G)+3m-\frac{7}{2}M_1+\frac{9}{2}(M_2-3h)\\
&+ 2\left(W(G)-m-2\left(\frac{1}{2}M_1-m\right)-3(M_2-M_1+m-3h)\right)\\
&= \frac{5}{2}W(G)-m+\frac{1}{2}M_1-\frac{3}{2}M_2+\frac{9}{2}h\ .
\end{aligned}
$$

Note that all of the above inequalities turn to equalities if and only if $d(G,k)=0$, for $k\geq 5$, that is if and only if $\mathrm{diam}(G)\leq 4$, which completes the proof of theorem. ■

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