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The Relationships between Wiener Index, Stability Number and Clique Number of Composite Graphs

[1]T. DOŠLIĆ, [2]M. GHORBANI AND [3]M. A. HOSSEINZADEH
[1]Faculty of Civil Engineering, University of Zagreb, Kačićeva 26, 10000 Zagreb, Croatia
[2]Department of Mathematics, Faculty of Science, Shahid Rajaei, Teacher Training University, Tehran, 16785-136, I. R. Iran
[3]Department of Mathematical Science, Sharif University of Technology, Tehran, 11365-9415, I. R. Iran
[1]doslic@grad.hr, [2]mghorbani@srttu.edu, [3]ma.hoseinzade@gmail.com

Abstract. Some new relations have been established between Wiener indices, stability numbers and clique numbers for several classes of composite graphs that arise via graph products. For three of considered operations we show that they make a multiplicative pair with the clique number.

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1. Introduction

The Wiener index is a distance-based topological invariant much used in the study of the structure-property and the structure-activity relationships of various classes of biochemically interesting compounds [12]. It has been also much researched from the purely mathematical viewpoint, giving rise to a vast corpus of literature over the last decades. A number of derivative invariants have been investigated and many formulas for particular classes of graphs were obtained. We refer the reader to a comprehensive survey of results for trees by Dobrynin, Entringer and Gutman as an illustration of that effort [1]. Typical results of such work are usually formulas expressing the Wiener index of graphs from the considered class *via* some other graph invariants [4,7,8]. Another line of research, started by a paper by Yeh and Gutman [14], has been concerned with establishing the relationship between the Wiener index of a composite graph and Wiener indices of its components. (By a composite graph we mean a graph that arises from two or more graphs *via* binary operations known as graph products [3].) The main goal of the present paper is to investigate how the Wiener index of a composite graph can be expressed in terms of the Wiener indices and the clique numbers of its components.

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In the next section we give the necessary definitions and some preliminary results. Section 3 is concerned with six types of graph products and the behavior of the clique and the stability number under those operations. The fourth section contains the main results, i.e., the explicit formulas for the relationship between Wiener index and the clique and stability numbers of the considered composite graphs. The paper is concluded by a short section containing a couple of results not fitting in the other sections and outlining some possible directions for future research.

2. Definitions and preliminaries

Our notation is standard and mainly taken from standard books of graph theory such as, e.g., [11]. All graphs considered in this paper are simple and connected. The vertex and edge sets of a graph G are denoted by $V(G)$ and $E(G)$, respectively.

A **stable set** in a graph is a set of vertices no two of which are adjacent. (Stable sets are also commonly known as **independent sets**.) A stable set in a graph is **maximum** if the graph contains no larger stable set and **maximal** if the set cannot be extended to a larger stable set; a maximum stable set is necessarily maximal, but not conversely. The cardinality of any maximum stable set in a graph G is called the **stability number** of G and is denoted by $\alpha(G)$.

A **clique** in a graph is a set of mutually adjacent vertices. The maximum size of a clique in a graph G is called the **clique number** of G and denoted by $\omega(G)$. Clearly, a set of vertices S is a clique of a simple graph G if and only if it is a stable set of its complement $\overline{G}$. In particular, $\alpha(G) = \omega(\overline{G})$.

The **distance** $d_G(x,y)$ between two vertices x and y of $V(G)$ is defined as the length of any shortest path in G connecting x and y. The **Wiener index** $W(G)$ of a graph G is defined as

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

where $d_G(u,v)$ denotes the distance between vertices u and v in G.

3. Composite graphs

In this section we introduce six classes of composite graphs that arise via graph products and study the way their stability number and clique number depend on the stability and clique number(s) of their components. For the case of stability number we rely heavily on the classical paper by Nowakowski and Rall [6], while for the clique numbers we provide proofs. The mentioned reference is mostly concerned with the question when a given pair of a graph product $G \otimes H$ and a graph invariant $i(G)$ is multiplicative, i.e., under what conditions we have that either $i(G \otimes H) \leq i(G)i(H)$ or $i(G \otimes H) \geq i(G)i(H)$. For the stability number the question is answered in positive for five out of the six graph products considered here. For three of those five products we will show that they also make a multiplicative pair with the clique number, while the remaining two products treat the clique number in a markedly different manner. Finally, the sixth product does not make a multiplicative pair with neither stability number nor the clique number.

We introduce the products roughly in the order of decreased multiplicativity with respect to the considered invariants. We start from the strong product and disjunction, that form multiplicative pairs with both stability and clique number. The lexicographic product behaves even better, achieving equalities in both cases. We proceed with Cartesian product and the symmetric difference and conclude our list with operation of join.

3.1. Strong product

For given graphs G_1 and G_2 their **strong product** $G_1 \boxtimes G_2$ is defined as the graph on the vertex set $V(G_1) \times V(G_2)$ with vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ connected by an edge if and only if either ($u_1 = v_1$ and $u_2v_2 \in E(G_2)$) or ($u_2 = v_2$ and $u_1v_1 \in E(G_1)$) or ($u_1v_1 \in E(G_1)$ and $u_2v_2 \in E(G_2)$).

Lemma 3.1. $\alpha(G \boxtimes H) \geq \alpha(G)\alpha(H)$ *and* $\omega(G \boxtimes H) = \omega(G)\omega(H)$.

Proof. The first claim follows from reference [6, Lemma 2.7 and Table 1].

In order to prove the second result, suppose that $C = \{u_1, u_2, \cdots, u_{\omega(G)}\}$ and $C' = \{v_1, v_2, \cdots, v_{\omega(H)}\}$ are maximum cliques of G and H, respectively. We claim that $C \times C'$ is a clique of $G \boxtimes H$. For this consider the vertices $a = (u_i, v_j),\ b = (u_k, v_l) \in C \times C'$, where $1 \leq i, k \leq \omega(G)$ and $1 \leq j, l \leq \omega(H)$. We distinguish three cases. In the first case, $u_i = u_k$. Then, since $v_jv_l \in E(H)$, we have $ab \in E(G \boxtimes H)$. Similarly, when $v_j = v_l$, we have $ab \in E(G \boxtimes H)$ since $u_iu_k \in E(G)$. Finally, in the third case, when $u_i \neq u_k, v_j \neq v_l$, we must have $ab \in E(G \boxtimes H)$, since $u_iu_k \in E(G)$ and $v_jv_l \in E(H)$. Hence, $\omega(G \boxtimes H) \geq \omega(G)\omega(H)$.

Let $C \subseteq \{(u_1, v_1), (u_1, v_2), \cdots, (u_1, v_s), \cdots, (u_r, v_1), \cdots, (u_r, v_s)\}$ be a maximum clique of $G \boxtimes H$, where $r \leq |V(G)|$ and $s \leq |V(H)|$. For every $1 \leq i < j \leq r$, we have $u_iu_j \in E(G)$. Thus, $r \leq \omega(G)$. On the other hand, for every $1 \leq i < j \leq s$, we have $v_iv_j \in E(H)$ and so, $s \leq \omega(H)$. Hence, $\omega(G \boxtimes H) \leq \omega(G)\omega(H)$. ∎

3.2. Disjunction

The **disjunction** $G_1 \vee G_2$ of two graphs G_1 and G_2 is the graph with vertex set $V(G_1) \times V(G_2)$ in which (u_1, v_1) is adjacent with (u_2, v_2) whenever u_1 is adjacent with u_2 in G_1 or v_1 is adjacent with v_2 in G_2.

Lemma 3.2. $\alpha(G \vee H) \geq \alpha(G)\alpha(H)$ *and* $\omega(G \vee H) \geq \omega(G)\omega(H)$.

Again, the claim about the stability number follows from reference [6]. The proof of second claim is similar to the proof for the strong product and we omit the details.

3.3. Composition

The composition $G = G_1[G_2]$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph with vertex set $V_1 \times V_2$ and $u = (u_1, v_1)$ is adjacent with $v = (u_2, v_2)$ whenever (u_1 is adjacent with u_2) or ($u_1 = u_2$ and v_1 is adjacent with v_2). The composition of two graphs is also known as their lexicographic product.

Theorem 3.1. $\alpha(G[H]) = \alpha(G)\alpha(H)$ *and* $\omega(G[H]) = \omega(G)\omega(H)$.

Proof. Again, the first claim is established in reference [6, Lemma 2.8].

To prove the second inequality suppose that $C = \{u_1, \cdots, u_{\omega(G)}\}$ and $C' = \{v_1, \cdots, v_{\omega(H)}\}$ are maximum cliques of G and H, respectively. Furthermore consider the vertices $a = (u_i, v_j),\ b = (u_k, v_l) \in C \times C'$, where $1 \leq i, k \leq \omega(G)$ and $1 \leq j, l \leq \omega(H)$. We distinguish two cases. In the first case, $u_i = u_k$. Since $v_jv_l \in E(H)$, we have $ab \in E(G[H])$. In the second case, $u_i \neq u_k$. Since $u_iu_k \in E(G)$ and $v_jv_l \in E(H)$, we must have $ab \in E(G[H])$. So $C \times C^{'}$ is a clique of $G[H]$ and thus $\omega(G[H]) \geq \omega(G)\omega(H)$. The proof of the converse inequality follows as in the case of strong product. ∎

3.4. Cartesian product

For given graphs G_1 and G_2 their **Cartesian product** $G_1 \Box G_2$ is defined as the graph on the vertex set $V(G_1) \times V(G_2)$ with vertices $u = (u_1, u_2)$ and $v = (v_1, v_2)$ connected by an edge if and only if either ($u_1 = v_1$ and $u_2v_2 \in E(G_2)$) or ($u_2 = v_2$ and $u_1v_1 \in E(G_1)$).

The Cartesian product of more than two graphs is defined inductively, $G_1 \Box \ldots \Box G_s = (G_1 \Box \ldots \Box G_{s-1}) \Box G_s$. We denote $G_1 \Box G_2 \Box \cdots \Box G_s$ by $\Box_{i=1}^{s} G_i$. If $G_1 = G_2 = \cdots = G_s = G$, we have the s-th Cartesian power of G and denote it by G^s.

The following bounds on $\alpha(G \Box H)$ were derived by Vizing [10] in 1963.

Theorem 3.2. *For any graphs G and H,*

(i) $\alpha(G \Box H) \leq \min\{\alpha(G)|V(H)|, \alpha(H)|V(G)|\}$
(ii) $\alpha(G \Box H) \geq \alpha(G)\alpha(H) + \min\{|V(G)| - \alpha(G), |V(H)| - \alpha(H)\}$.

The first inequality in the following lemma, although weaker than the Vising's one, is better suited for generalization to Cartesian products with more than two factors.

Lemma 3.3. $\alpha(G \Box H) \geq \alpha(G)\alpha(H)$ *and* $\omega(G \Box H) \geq \max\{\omega(G), \omega(H)\}$.

Proof. Besides following from Theorem 3.2, the first inequality was also established in [6] where it was shown that the Cartesian product and the independence number form a multiplicative pair (see Lemma 2.7 and Table 1 of the reference).

Regarding the second inequality, we can suppose that $\max\{\omega(G), \omega(H)\} = \omega(G)$, because the Cartesian product is commutative. Let $C = \{u_1, u_2, \cdots, u_{\omega(G)}\}$ be a maximum clique of G, $v \in V(H)$ and $K \subset V(G \Box H)$, such that $K = \{(u_1, v), (u_2, v), \ldots, (u_{\omega(G)}, v)\}$. It is easy to see that for $1 \leq i, j \leq \omega(G)$ and $i \neq j$ we have $u_iu_j \in E(G)$ and so K is a clique in $G \Box H$. That completes the proof. ∎

Corollary 3.1. $\alpha(\Box_{i=1}^{s} G_i) \geq \prod_{i=1}^{s} \alpha(G_i)$ *and* $\omega(\Box_{i=1}^{s} G_i) \geq \max\{\omega(G_1), \omega(G_2), \cdots, \omega(G_s)\}$.

Example 3.1. The C_4 nanotubes and nanotori arise as Cartesian products of paths and cycles and of two cycles, respectively. By using the above results combining them with known values for the stability numbers of paths and cycles, we obtain the following explicit formulas for C_4 nanotubes and nanotori. We denote $R = P_n \Box C_m$ and $S = C_k \Box C_m$ and assume $k, m \geq 3$.

$$\alpha(R) \geq \lceil n/2 \rceil \lfloor m/2 \rfloor + \min\{\lfloor n/2 \rfloor, \lceil m/2 \rceil\}, \quad \omega(R) = 2 + \delta_{m,3},$$
$$\alpha(S) \geq \lfloor m/2 \rfloor \lfloor k/2 \rfloor + \min\{\lceil m/2 \rceil, \lceil k/2 \rceil\}, \quad \omega(S) = 2 + \max\{\delta_{m,3}, \delta_{k,3}\}.$$

Here $\delta_{p,3} = 1$ if $p = 3$ and 0 otherwise.

3.5. Symmetric difference

The **symmetric difference** $G_1 \oplus G_2$ of two graphs G_1 and G_2 is the graph with vertex set $V(G_1) \times V(G_2)$ in which (u_1, v_1) is adjacent with (u_2, v_2) whenever u_1 is adjacent with u_2 in G_1 or v_1 is adjacent with v_2 in G_2, but not both together.

Lemma 3.4. $\alpha(G \oplus H) \geq \alpha(G)\alpha(H)$ *and* $\omega(G \oplus H) \geq \max\{\omega(G), \omega(H)\}$.

The proof is similar to the proof for the case of Cartesian product and we omit the details.

3.6. Join

The join $G = G_1 + G_2$ of graphs G_1 and G_2 with disjoint vertex sets V_1 and V_2 and edge sets E_1 and E_2 is the graph union $G_1 \cup G_2$ together with all the edges joining V_1 and V_2. The definition generalizes to the case of $s \geq 3$ graphs in a straightforward manner. The following formula for the number of edges is easily verified by induction on s.

Lemma 3.5. *Let G_i, $i = 1,\ldots,s$, be some graphs. Then*

$$|E(G_1 + \cdots + G_s)| = \sum_{i=1}^{s} |E(G_i)| + \frac{1}{2}\sum_{i=1}^{s} |V(G_i)| \sum_{j=1, j\neq i}^{s} |V(G_j)|.$$

Theorem 3.3. $\alpha(G+H) = \max\{\alpha(G), \alpha(H)\}$ *and* $\omega(G+H) = \omega(G) + \omega(H)$.

Proof. Without loss of generality we can suppose $\max\{\alpha(G), \alpha(H)\} = \alpha(G)$. Let $S = \{u_1, u_2, \cdots, u_{\alpha(G)}\}$ be the maximum stable set of G. For every pair (u_i, u_j), $1 \leq i, j \leq \alpha(G)$. $i \neq j$, of S, the edge u_iu_j is not in $E(G)$ and so $u_iu_j \notin E(G+H)$. This implies the S is a stable set of $G+H$. In other words, $\alpha(G+H) \geq \max\{\alpha(G), \alpha(H)\}$.

Conversely, suppose that $S^{'}$ is a maximum stable set of $G+H$. The elements of $S^{'}$ do not belong to $V(G)$ and $V(H)$ simultaneously. If $S^{'} \subset V(G)$, then $\alpha(G+H) \leq \alpha(G)$, else $\alpha(G+H) \leq \alpha(H)$. Therefore $\alpha(G+H) \leq \max\{\alpha(G), \alpha(H)\}$. For an arbitrary clique C of $G+H$ we can suppose $C = C_1 \cup C_2$ in which $C_1 \subseteq V(G)$ and $C_2 \subseteq V(H)$. It is easy to see that $|C_1| \leq \omega(G)$ and $|C_2| \leq \omega(H)$. So, $\omega(G+H) \leq \omega(G) + \omega(H)$. Clearly $\omega(G+H) \geq \omega(G) + \omega(H)$ and this completes the proof. ∎

As a consequence, we have the following formulas for a join of more than two graphs. $\alpha(G_1 + \cdots + G_s) = \max\{\alpha(G_1), \cdots, \alpha(G_s)\}$ and $\omega(G_1 + \cdots + G_s) = \sum_{i=1}^{s} \omega(G_i)$.

4. Main results

Let us denote by E_n the empty (or trivial) graph on n vertices and let $G(n_1, n_2)$ $(n_1, n_2 \in \mathbb{N})$ be the join of complete graph K_{n_1} and E_{n_2}. It is easy to see that $G(1,n) \cong S_n$ and $G(n-1,1) \cong K_n$, where S_n is the star graph on $n+1$ vertices. By Theorem 3.3, $\alpha(G(n_1,n_2)) = n_2$ and $\omega(G(n_1,n_2)) = n_1 + 1$. In the following let $\omega = \omega(G)$ and $\alpha = \alpha(G)$. Obviously, for a graph on n vertices, $\alpha = 1$ if and only if $G \cong K_n$.

Theorem 4.1. *Let G be a nontrivial graph. Then we have: $W(G) = \omega(\omega-1)/2 + \alpha(\alpha-1)$ if and only if $G \cong K_n$.*

Proof. If $G \cong K_n$ then it is obvious that $W(G) = \omega(\omega-1)/2 + \alpha(\alpha-1)$. Conversely, suppose $W(G) = \omega(\omega-1)/2 + \alpha(\alpha-1)$. Furthermore, let S and C be the maximum stable set and the maximum set of cliques of G respectively. It is easy to see that $W(G) \geq \sum_{u,v\in C} d(u,v) + \sum_{u,v\in S} d(u,v) + \sum_{u\in C, v\in S} d(u,v) \geq \omega(\omega-1)/2 + \alpha(\alpha-1)$. This implies $\sum_{u\in C, v\in S} d(u,v) = 0$. So, $|S| = 1$ and then $\alpha = 1$. Hence G must be equal to K_n and the proof is completed. ∎

Lemma 4.1. $W(G(n_1,n_2)) = \binom{n_1}{2} + 2\binom{n_2}{2} + n_1n_2$.

Proof.

$$W(G(n_1,n_2)) = \sum_{u,v\in K_{n_1}} d(u,v) + \sum_{u,v\in E_{n_2}} d(u,v) + \sum_{u\in K_{n_1}, v\in E_{n_2}} d(u,v)$$

$$= n_1(n_1-1)/2 + n_2(n_2-1) + n_1 n_2 = \binom{n_1}{2} + 2\binom{n_2}{2} + n_1 n_2. \qquad \blacksquare$$

The quantities n_1 and n_2 appear symmetrically in the above relations. By a direct computation one can readily verify that the symmetry remains preserved if the first parameter is decreased by one.

Corollary 4.1. $W(G(n_1-1,n_2)) = \binom{n_1}{2} + 2\binom{n_2}{2} + (n_1-1)(n_2-1)$. $\blacksquare$

Theorem 4.2. $W(G) \geq \omega(\omega-1)/2 + \alpha(\alpha-1) + (\omega-1)(\alpha-1)$ *with equality if and only if* $G \cong G(\omega-1,\alpha)$.

Proof. Let S and C be a maximum stable set and a maximum clique of G, respectively. We have $\forall\, u,v \in C : d(u,v) = 1, \quad \forall\, u,v \in S : d(u,v) \geq 2$. On the other hand, $|S \cap C| \leq 1$. So

$$\begin{aligned} W(G) &\geq \sum_{u,v\in C} d(u,v) + \sum_{u,v\in S} d(u,v) + \sum_{u\in C, v\in S} d(u,v) \\ &\geq \omega(\omega-1)/2 + \alpha(\alpha-1) + (\omega-1)(\alpha-1). \end{aligned}$$

If $G \cong G(\omega-1,\alpha)$, then by Corollary 4.1 the equality holds. Conversely, if $W(G) = \omega(\omega-1)/2 + \alpha(\alpha-1) + (\omega-1)(\alpha-1)$ then $S \cup C = V(G)$. Since $\sum_{u,v\in C} d(u,v) = \omega(\omega-1)/2$, thus $\sum_{u,v\in S} d(u,v) = \alpha(\alpha-1)$ and $\sum_{u\in C,v\in S} d(u,v) = (\omega-1)(\alpha-1)$. This implies $|C \cap S| = 1$. Let $C \cap S = \{u\}$. Since $u \in C$, then for every $v \in C$ we have $uv \in E(G)$. Similarly, $u \in S$ and $\sum_{u\in C,v\in S} d(u,v) = (\omega-1)(\alpha-1)$ results for every $x \in S$ and $y \in C - \{u\}$, $xy \in E(G)$. Therefore $G \cong G(\omega-1,\alpha)$. $\blacksquare$

Theorem 4.3. *Let G be a graph and $n = |V(G)|$. Then* $W(G) \geq (n-\alpha)(n-\alpha-1)/2 + \alpha(n-1)$ *with equality if and only if* $G \cong G(n-\alpha,\alpha)$.

Proof. Let S be a maximum stable set of G. Then

$$\begin{aligned} W(G) &= \sum_{u,v\in G-S} d(u,v) + \sum_{u,v\in S} d(u,v) + \sum_{u\in G-S,\ v\in S} d(u,v) \\ &\geq \binom{n-\alpha}{2} + 2\binom{\alpha}{2} + \alpha(n-\alpha) = (n-\alpha)(n-\alpha-1)/2 + \alpha(n-1). \end{aligned}$$

If the equality holds, then for every $u,v \in V(G) - S$ the edge uv is in $E(G)$ and every vertex of S is adjacent to all vertices of $V(G) - S$. This implies $G \cong G(n-\alpha,\alpha)$. The converse follows from Lemma 4.1. $\blacksquare$

Corollary 4.2. *Let G be an arbitrary graph and $\overline{G}$ be a connected graph. Then*

$$W(\overline{G}) \geq \binom{\alpha}{2} + (\omega-1)(\alpha+\omega-1)$$

with equality if and only if $G \cong E_{\alpha-1} \cup K_\omega$, *and*

$$W(\overline{G}) \geq \binom{n-\omega}{2} + \omega(n-1)$$

with equality if and only if $G \cong E_{n-\omega-1} \cup K_\omega$.

Proof. Follows from Theorem 4.2 and equality $\alpha(\overline{G}) = \omega(G)$. $\blacksquare$

Corollary 4.3. *Let* $\alpha_m = \max\{\alpha_i = \alpha(G_i), 1 \leq i \leq n\}$, $\omega_m = \max\{\omega_i = \omega(G_i), 1 \leq i \leq n\}$, $\omega_m^{'} = \max\{\omega_i = \omega(G_i), 1 \leq i \leq 2\}$, $\omega_\Sigma = \sum_{i=1}^{n} \omega_i$, *and* $n_i = |V(G_i)|$. *We have the following formulas for the Wiener index:*

- $W(G_1 \boxtimes G_2) \geq \binom{\omega_1\omega_2}{2} + (\alpha_1\alpha_2 - 1)(\alpha_1\alpha_2 + \omega_1\omega_2 - 1)$,
- $W(\square_{i=1}^{n} G_i) \geq \binom{\omega_m}{2} + (\Pi_{i=1}^{n}\alpha_i - 1)(\Pi_{i=1}^{n}\alpha_i + \omega_m - 1)$,
- $W(G_1 + G_2 + \cdots + G_n) \geq \binom{\omega_\Sigma}{2} + (\alpha_m - 1)(\alpha_m + \omega_\Sigma - 1)$,
- $W(G_1[G_2]) \geq \binom{\omega_1\omega_2}{2} + (\alpha_1\alpha_2 - 1)(\alpha_1\alpha_2 + \omega_1\omega_2 - 1)$,
- $W(G_1 \vee G_2) \geq \binom{\omega_1\omega_2}{2} + (\alpha_1\alpha_2 - 1)(\alpha_1\alpha_2 + \omega_1\omega_2 - 1)$,
- $W(G_1 \oplus G_2) \geq \binom{\omega_m'}{2} + (\alpha_1\alpha_2 - 1)(\alpha_1\alpha_2 + \omega_m' - 1)$.

5. Digressions and concluding remarks

Here we present a couple of results concerned with uniquely colorable and Hamiltonian graphs that do not fit into other sections.

An s-chromatic graph G is uniquely colorable if it has only one possible proper s-coloring up to permutation of the colors. We refer the reader to [9, 13] for some basic facts about uniquely colorable graphs.

Theorem 5.1. *Let G be a uniquely colorable graph with color classes $V_1, \cdots, V_s$, such that $n_i = |V_i|, 1 \leq i \leq s$. Then*

$$W(G) \geq \frac{1}{2}\left[\sum_{i=1}^{s} n_i^2 + n^2 - 2n\right],$$

with equality if and only if $G \cong K_{n_1,\cdots,n_s}$.

Proof.

$$\begin{aligned} W(G) &= \sum_{x,y\in V(G)} d(x,y) = \frac{1}{2}\sum_{i=1}^{s}\sum_{j=1}^{s}\sum_{x\in V_i}\sum_{y\in V_j} d(x,y) \\ &= \sum_{i=1}^{s}\sum_{x,y\in V_i} d(x,y) + \frac{1}{2}\sum_{i=1}^{s}\sum_{j=1,j\neq i}^{s}\sum_{x\in V_i}\sum_{y\in V_j} d(x,y) \\ &\geq \sum_{i=1}^{s} 2\binom{n_i}{2} + \frac{1}{2}\sum_{i=1}^{s}\sum_{j=1,j\neq i}^{s}\sum_{x\in V_i}\sum_{y\in V_j} 1 = \sum_{i=1}^{s} 2\binom{n_i}{2} + \frac{1}{2}\sum_{i=1}^{s} n_i(n-n_i). \end{aligned}$$

The first claim now follows by simplifying the above result.

Let $W(G) = 1/2\left[\sum_{i=1}^{s} n_i^2 + n^2 - 2n\right]$. Since the vertices of V_i are independent, then for every pair $x,y \in V_i$, we have $d(x,y) \geq 2$. This implies

$$\sum_{i=1}^{s}\sum_{x,y\in V_i} d(x,y) \geq \sum_{i=1}^{s} 2\binom{n_i}{2}. \tag{5.1}$$

Suppose now that $x \in V_i$ and $y \in V_j (1 \leq i < j \leq s)$. Then $d(x,y) \geq 1$ and so,

$$\sum_{i=1}^{s}\sum_{j=1,j\neq i}^{s}\sum_{x\in V_i}\sum_{y\in V_j} d(x,y) \geq \sum_{i=1}^{s} n_i(n-n_i). \tag{5.2}$$

In order to satisfy our assumption, both inequalities must be equalities. The first equality means that the vertices from the same color class are at distance 2; the second equality means that all pairs of vertices belonging to different color classes are adjacent. Hence $G \cong K_{n_1,\cdots,n_s}$. The converse implication is obvious. ∎

Corollary 5.1. *Let G be a graph with chromatic number $\chi(G) = s$ and $n_i = |V_i|$. Then*

$$W(G) \geq \frac{n(n-2)}{2} + \frac{1}{2}\min\left\{\sum_{i=1}^{s} {n_i}^2; \sum_{i=1}^{s} n_i = n\right\},$$

with equality if and only if $G \cong K_{n_1,\cdots,n_s}$.

It is well known that the sum in the right hand side of the above inequality is minimized when all terms are equal to $\lfloor n/s \rfloor$ or $\lceil n/s \rceil$.

Our last result is an observation on Hamiltonian graphs.

Theorem 5.2. *Let G be an n-vertex graph with a Hamiltonian cycle. Then $W(G) \leq W(C_n)$ with equality if and only if $G \cong C_n$.*

Proof. Clearly $W(G) \leq W(C_n)$. Let now $W(G) = W(C_n)$. Since C_n is a sub graph of G, then for every pair of vertices belong to $V(G)$ such as x, y, $d_G(x,y) \leq d_{C_n}(x,y)$. This implies $d_G(x,y) = d_{C_n}(x,y)$ and so $G \cong C_n$. Conversely, if $G \cong C_n$, then $W(G) = W(C_n)$. ∎

Coming back to the main topic of this paper, it would be interesting to further investigate the relationship between the Wiener index and the stability and clique numbers of various classes of graphs. Among classes that could allow for nice and compact formulas are many that have chemical relevance, such as, e.g., benzenoid graphs [2], linear polymers, thorny graphs [5], fullerenes, and others.

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