Another aspect of graph invariants depending on the path metric and an application in nanoscience

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ABSTRACT

The aim of this paper is to find a new expression for distance-based graph invariants of connected graphs having a decomposition into convex subgraphs. We apply this method to Schultz and Gutman indices of graphs. It can be generalized to other distance-based graph invariants. As an application, the Wiener index of the one-pentagonal nanocone is computed.

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1. Introduction and notations

Throughout this paper all graphs are assumed to be simple, finite and connected. A function Top from the class of connected graphs into real numbers with the property that Top(G) = Top(H) whenever G and H are isomorphic is known as a topological index in the chemical literature; see [1]. There are many examples of such functions, especially those based on distances, which are applicable in chemistry. The Wiener index [2], defined as the sum of all distances between pairs of vertices in a graph, is probably the first and most studied such graph invariant, both from a theoretical and a practical point of view; see for instance [3–11].

Suppose G is a graph, x, y ∈ V(G) and λ is a non-zero real number. The distance d(x, y) is the length of a shortest path connecting x and y. We also define d_C(u, v) = d_G(u, v)^λ and W(G) = ∑_{u,v} d_G(u, v)^λ. The Schultz and Gutman indices of a graph G are defined as:

W_s(G) = ∑_{[u,v]⊆V(G)} (deg_C(u) + deg_C(v))d_C(u, v),

W_g(G) = ∑_{[u,v]⊆V(G)} (deg_C(u)deg_C(v))d_C(u, v).

If G and H are graphs such that V(H) ⊆ V(G) and E(H) ⊆ E(G) then H is said to be a subgraph of G, denoted by H ≤ G. If F ⊆ V(G) then the subgraph ⟨F⟩_C of G induced by F is defined by V⟨F⟩_C = F and E⟨F⟩_C = {e ∈ E(G) | [u, v] ⊆ F} is called the induced subgraph of G induced by F. An isometric subgraph L of G is a subgraph in which d_L(u, v) = d_G(u, v), for all

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vertices $u, v \in V(L)$. We write $L \ll G$ to show that $L$ is an isometric subgraph of $G$. Clearly, $F \ll H$ and $H \ll G$ implies that $F \ll G$. Define $N^G_G(v) = \{x \in V(G) | d_G(x, v) < r \}$. By this notation, $|N^G_G(v)| = \deg_v(G) + 1$.

Throughout this paper our notation is standard and taken mainly from [12–14].

**Definition 1.** Suppose $H$ is a subgraph of $G$ and $v \in V(H)$. The vertex $v$ is called boundary vertex of $H$ in $G$, if $|N^G_G(v)| - |N^H_H(v)| > 0$. The set of all boundary vertices of $H$ in $G$ is denoted by $\partial_G(H)$.

The following simple lemma is an immediate consequence of our definition.

**Lemma 1.** Let $G$ and $H$ be graphs, $H \subset G$, $u \in V(H)$ and $v \in V(G) \setminus V(H)$. Then every path connecting $u$ and $v$ contains a vertex of $\partial_G(H)$.

Suppose $P = u_1u_2 \cdots u_nv$ is an arbitrary path connecting $u$ and $v$. Define $P_G(u, v)$ to be the following subgraph:

$$V(P_G(u, v)) = \{u_1, u_2, \ldots, u_n, v\},$$

$$E(P_G(u, v)) = \{u_1u_2, \ldots, u_nv\}.$$

If $w$ is another vertex and $v_1b_1b_2 \cdots b_nw$ is path connecting $v$ and $w$ then $P_G(u, v) + P_G(v, w)$ denotes the following sequence:

$$ua_1a_2 \cdots a_nb_1b_2 \cdots b_nw.$$

Suppose $[a_i]_{i=1}^q \cup [b_j]_{j=1}^r = \emptyset$. Then, $P_G(u, v) + P_G(v, w)$ is a path connecting $u$ and $w$, when $u \neq w$ and a cycle, otherwise. Also, the length of $P_G(u, v)$ is denoted by $|P_G(u, v)|$.

Suppose $G$ is a graph, $H, K$ are subgraphs of $G$. The union and intersection of $H$ and $K$ are denoted by $H \cup K$ and $H \cap K$, respectively. These are defined as:

$$E(H \cup K) = E(H) \cup E(K),$$
$$V(H \cup K) = V(H) \cup V(K),$$
$$E(H \cap K) = E(H) \cap E(K),$$
$$V(H \cap K) = V(H) \cap V(K).$$

The union and intersection of a collection $\{H_i\}_{i=1}^n$ of subgraphs are denoted by $\bigcup_{i=1}^n H_i$ and $\bigcap_{i=1}^n H_i$, respectively.

A subgraph $H$ of $G$ is called convex if any shortest path of $G$ between vertices of $H$ is already in $H$. In other words, $u, v \in V(H)$ with $|P_G(u, v)| = d_G(u, v)$ implies that $P_G(u, v) \subseteq H$. It is clear that convexity is a transitive relation and every convex subgraph is isometric, but its converse is not generally correct.

It is easy to see that for each non-trivial simple graph $G$ and its convex subgraph $H$ containing an edge $e = uw$, $H - e$ is not isometric, since $d_{G\setminus e}(u, v) \neq d_G(u, v) - 1$. So, $H$ is not convex. On the other hand, it is not so difficult to construct a graph $G$ having isometric subgraphs $G_1$ and $G_2$ such that $G_1 \cup G_2$ is not isometric. The same is true for the intersection of $G_1$ and $G_2$. On the other hand, one can construct a graph $G$ having convex subgraphs $G_1$ and $G_2$ such that $G_1 \cup G_2$ is not convex, but the intersection of convex subgraphs have convex component(s). In general, we have the following lemma:

**Lemma 2.** Suppose $\{H_i\}_{i=1}^k$ is a sequence of convex subgraphs of a connected graph $G$. Then each component of $\bigcap_{i=1}^k H_i$ is a convex subgraph of $G$.

The previous lemma is not correct if we interchange the “convex subgraph” into “isometric subgraph”. In the following two lemmas, two criteria for convexity and isometry of subgraphs are proved.

**Lemma 3.** Suppose $H \subset G$. If $\langle V(H)\rangle_C = H$ and there exists an isometric subgraph $I$ of $G$ such that $\partial_G(H) \subseteq \langle V(I)\rangle_C \subseteq \langle V(H)\rangle_C$ then $H \ll G$.

**Proof.** If it is not, take $u, v \in V(H)$ such that $d_G(u, v) < d_H(u, v)$. Suppose $P_G(u, v) = ua_1a_2 \cdots a_nv$ is a shortest path in $G$. Since $\langle V(H)\rangle_C = H$, there exists $i, 1 \leq i \leq n$, such that $a_i \not\in V(H)$. Consider $P_G(u, a_i) + P_G(a_i, v) = P_G(u, v)$ and apply Lemma 1, to obtain vertices $a_i, a_j$ such that $\{a_i, a_j\} \subseteq \partial_G(H)$. Since there is $I \ll G$ such that $\{a_i, a_j\} \subseteq \langle V(I)\rangle_C$, then $d_G(a_i, a_j) = d_H(a_i, a_j)$. Therefore, $d_H(a_i, a_j) \leq d_G(a_i, a_j) + d_G(a_j, a_i)$, which is impossible. $\Box$

**Lemma 4.** Suppose $G$ is a graph and $H \subset G$. If $\langle V(H)\rangle_C = H$ and there exists a convex subgraph $I$ of $G$ such that $\partial_G(H) \subseteq \langle V(I)\rangle_C \subseteq \langle V(H)\rangle_C$ then $H$ is convex.

**Proof.** It is enough to prove that if $u, v \in V(H)$ and $P_G(u, v)$ is a path of length $d_G(u, v)$ then $P_G(u, v) \subseteq H$. If not, since $\langle V(H)\rangle_C = H$ there exists $w \in V(G) \setminus V(H)$ such that $P_G(u, w) + P_G(w, v)$ is a shortest path between $u$ and $v$. By Lemma 1, there are vertices $a_m, a_n \in \partial_G(H)$ such that $a_m \in V(P_G(u, w))$ and $a_n \in V(P_G(v, w))$. Now there are paths $P_G(a_m, w)$ and $P_G(a_n, w)$ such that $P_G(a_m, w) \subseteq P_G(u, w)$, $P_G(a_n, w) \subseteq P_G(w, v)$ and $P_G(a_m, w) + P_G(a_n, w)$ is a shortest path connecting $a_m$ and $a_n$. Moreover, there is a convex subgraph $\langle V(I)\rangle_C \subseteq \langle V(H)\rangle_C$ such that $\partial_G(H) \subseteq \langle V(I)\rangle_C$ and by definition $P_G(a_m, w) + P_G(a_n, w) \subseteq I$ and so $w \in V(H)$ which is a contradiction. $\Box$
2. Main results

The aim of this section is to present a new approach for computing some distance-based invariants of a class of graphs, many classes of chemical graphs are contained. Using our method, it is possible to recalculate easily the main results of papers [15–17]. We encourage the reader to consult papers [18–22] for background materials, as well as basic computational techniques.

**Theorem 1.** Suppose \( F \subseteq E(G) \) such that \( G - F \) is a graph with exactly two components \( G_1 \) and \( G_2 \). If \( G_1 \) and \( G_2 \) are isometric subgraphs of \( G \) then for every \( u \in V(G_1) \) and \( v \in V(G_2) \) there exists a shortest path \( P_F(u, v) \) such that \( |P_F(u, v) \cap F| = 1 \).

**Proof.** Suppose \( e = ab \in F \). Since \( G_1 \) and \( G_2 \) are isometric, \( \{a, b\} \subseteq V(G_1) \) and \( \{a, b\} \subseteq V(G_2) \). We now assume that there exists a shortest path \( P_F(u, v) \) such that \( u \in V(G_1) \), \( v \in V(G_2) \) and \( |P_F(u, v) \cap F| = 1 \), \( \{a, b\} \subseteq V(G_1) \). Since \( G_1 \ll G \), \( G_2 \ll G \) and \( G - F \) is not connected, there are paths \( P_{G_1}(u, a) \) and \( P_{G_2}(a, b) \) such that \( P_{G_1}(u, a) = P_{G_1}(u, a) + P_{G_1}(a, b) + P_{G_2}(b, v) \), and \( P_{G_2}(a, b) = P_{G_2}(a, b) + P_{G_2}(b, v) \), is a path in \( G \) with the property that \( |P_F(u, v) \cap F| = 1 \). This completes the proof. \( \Box \)

**Corollary 1.** Suppose \( G \) is a graph, \( F \subseteq E(G) \) and \( G - F \) is a graph with exactly two components \( G_1 \) and \( G_2 \) such that \( G_1 \ll G \). Choose \( u \in V(G_1) \) and \( v \in V(G_2) \) and define:

\[
S = F \cap \{E(P_F(u, v)) \mid P_F(u, v) = d_G(u, v) \}.
\]

Then for each \( \alpha \in S \) there exists a path \( P_F(u, v) \) such that \( |P_F(u, v) \cap F| = \alpha \).

In **Theorem 1**, replace the term “isometric” by “convex”. Since \( G - F \) is not connected, for arbitrary vertices \( u \in V(G_1) \) and \( v \in V(G_2) \) there are an edge \( ab \in F \) and a shortest path \( P_F(u, v) = P_F(u, a) + P_F(a, b) + P_F(b, v) \) such that \( a \in V(G_1) \) and \( b \in V(G_2) \). Since \( P_F(u, a) \) and \( P_F(b, v) \) are shortest paths of \( G \) and \( G_2 \) are convex, \( P_F(u, v) \subseteq G_1 \) and \( P_F(b, v) \subseteq G_2 \). Thus we have the following corollary:

**Corollary 2.** Suppose \( G \) is a connected graph and \( F \subseteq E(G) \). If \( G - F = G_1 \cup G_2 \), \( u \in V(G_1) \), \( v \in V(G_2) \) and \( G_1, G_2 \) are convex then for every shortest path \( P_F(u, v) \), \( |P_F(u, v) \cap F| = 1 \).

**Lemma 5.** Suppose \( G \) is a graph and \( \{F_i\}_{i=1}^r \) is a partition of the edge set of \( G \) such that for each \( i \), \( G - F_i \), has exactly two components \( G_{i}^1 \) and \( G_{i}^2 \) which are convex. Then there exists a set \( R \) of shortest paths with the property that for each pair of vertices of \( G \) there exists a unique path in \( R \) connecting them and for each \( i \) the following statements hold:

1. If \( P_G(u, v) \in R \), where \( \{u, v\} \subseteq V(G_{i}^1) \) or \( \{u, v\} \subseteq V(G_{i}^2) \) then \( |E(P_G(u, v)) \cap F_i| = 0 \).
2. If \( u \in V(G_{i}^1) \), \( v \in V(G_{i}^2) \) and \( P_G(u, v) \in R \) then \( |E(P_G(u, v)) \cap F_i| = 1 \).

**Proof.** Since the graph \( G - F_i \) has convex components, by definition of convexity the proof of the first part is trivial. To prove 2 we can use either **Corollary 2** or **Theorem 1**, **Corollary 1** and **Lemma 2**, repeatedly. \( \Box \)

Similar to that we said before **Lemma 2**, for every subgraph \( H \) of graph \( G \) and \( e = uv \in E(H) \) the graph \( H - e \) is not isometric and so convex, since \( d_H(u, v) > d_G(u, v) = 1 \). In general, every non-induced subgraph is not isometric and so convex.

**Condition (⋆):** \( G \) is a connected graph with a partition \( \{F_i\}_{i=1}^r \) of \( E(G) \) such that \( G - F_i \) has exactly two components \( G_{i}^1 \) and \( G_{i}^2 \) which are convex, \( 1 \leq i \leq r \).

**Theorem 2.** If \( G \) satisfies the condition (⋆) then \( G \) is bipartite.

**Proof.** Suppose \( C \) is an arbitrary isometric cycle of \( G \). We claim that \( |C \cap F_i| = 0 \) or \( 2 \), \( 1 \leq i \leq r \). If not, \( |C \cap F_i| = 1 \) or \( 2 \), for some \( i \). If \( C \cap F_i = |e| \) then either \( C - e \) is contained in one of the components of \( G - F_i \) or \( G - F_i \) is connected. The latter contradicts condition (⋆). In other case, the component containing \( C - e \) is not an induced subgraph of \( G \) and by the paragraph before condition (⋆) cannot be isometric, contradicting convexity of the components of \( G - F_i \), so \( |C \cap F_i| = 1 \). Now suppose \( t = |C \cap F_i| > 2 \). Consider \( G - F_i \) to find a partition for the edges or vertices of \( C \) into \( t \) paths that are not connected by edges of \( C - F_i \), which may have length 0. By the Pigeonhole principle, at least two members of this partition are contained in one component of \( G - F_i \). Obviously, the component containing more than one part of the partition of \( C - F_i \) is not an induced subgraph of \( G \) and by the paragraph before condition (⋆) it is not isometric leads to a contradiction. Thus \( |C \cap F_i| = 0 \) or 2, and \( \sum_{i=1}^{r} |C \cap F_i| = 2 \). Moreover, \( \{F_i\}_{i=1}^{r} \) is a partition of \( E(G) \) and so \( C \) is an even cycle. On the other hand, if \( G \) has an odd cycle then one can find an isometric odd cycle. This shows that the length of every cycle of \( G \) is even which completes our argument. \( \Box \)

Suppose \( G \) is a graph, \( \lambda \) is a non-zero real number and \( F, L \) are subsets of \( V(G) \). Define:

\[
\lambda D(F, G) = \sum_{u \in V(G)} \sum_{v \in F} d_G^2(u, v),
\]

\[
\lambda D_F(L, F) = \sum_{v \in L} \sum_{u \in F} d_G^2(u, v).
\]
It is easy to see that \( \frac{1}{2} D_C(V(G), V(G)) = \frac{1}{2} D(V(G), G) = W(G) \). If \( \{ F_i \}_{i=1}^n \) is a partition of \( V(G) \) then \( W(G) = \frac{1}{2} \sum_{i=1}^n D_C(F_i, F_j) \). Obviously, if \( F \subseteq V(G) \) and \( (F)_C \ll G \) then \( D_C(F, F) = 2W((F)_C) \). Similar to the Wiener index, one can see that if \( \{ F_i \}_{i=1}^n \) is a partition of \( V(G) \) then \( W(G) = \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n \lambda D_C(F_i, F_j) \). Therefore,

\[
\lambda W(G) = \frac{1}{2} \left[ \sum_{i=1}^n \lambda D_C(V(G), V(G)) \right] = \frac{1}{2} \left[ \lambda D(V(G), G) \right].
\]

On the other hand, if \( F \subseteq V(G) \) and \( (F)_C \ll G \) then \( \lambda D_C(F, F) = 2 \times \lambda W((F)_C) \).

**Theorem 3.** Suppose that the condition \((\ast)\) holds. Then

\[
W(G) = \sum_{i=1}^r \left| V(GF_i(1)) \right| \left| V(GF_i(2)) \right|.
\]

**Proof.** Suppose \( e \in E(G) \) and \( R \) is a set of shortest path connecting vertices of \( G \) such that for each \( u \neq v \in V(G) \), there is a unique shortest path in \( R \) connecting \( u \) and \( v \). Define

\[
n(e) = \sum_{e \in E(G(U, V))} \left| \{ P_G(u, v) \} \cap \{ [u, v] \} \right|.
\]

Then one can see that \( W(G) = \sum_{e \in E(G)} n(e) \). Assume that \( R \) has the properties given in Lemma 5. Apply Lemma 5 to deduce that \( \sum_{e \in E(G)} n(e) = \sum_{e \in E(G)} \sum_{P_G(u, v) \in R} n(e) = \sum_{e \in E(G)} \sum_{P_G(u, v) \in R} |V(GF_i(1))| \left| V(GF_i(2)) \right| \), as desired. \( \square \)

**Theorem 4.** Suppose that condition \((\ast)\) holds, then \( \lambda W(G) = \sum_{i=1}^r \left[ \lambda \sum_{e \in E(G)} \lambda n(e) \right] \), for non-zero real \( \lambda \).

**Proof.** Suppose \( R \) is a set of shortest paths in \( G \), such that for each pair \( (x, y) \) of vertices of \( G \), there exists a unique shortest path in \( R \) connecting \( x \) and \( y \). Set \( B(e) = \{ (u, v) \} \) \( P_G(u, v) \in R \) \( E(P_G(u, v)) \neq \emptyset \) and \( \lambda n(e) = \sum_{[u, v] \in B(e)} d^2(u, v) \). Then, we can see that

\[
\lambda W(G) = \sum_{e \in E(G)} \lambda n(e).
\]

Assume that \( R' \) is a set of shortest paths of \( G \) that satisfies the conditions of the set \( R \) and Lemma 5. Therefore,

\[
\sum_{e \in E(G)} \lambda n(e) = \sum_{u \in V(GF_i(1)) \cap V(GF_i(2))} d^2(u, v) = \lambda D_C(V(GF_i(1)), V(GF_i(2))).
\]

On the other hand, \( V(GF_i(1)) \) and \( V(GF_i(2)) \) constitute a partition of \( V(G) \) and also \( GF_i(1) \) and \( GF_i(2) \) are isometric subgraphs of \( G \). Thus,

\[
\lambda W(G) = \lambda D_C(V(GF_i(1)), V(GF_i(2))) + \lambda W(GF_i(1)) + \lambda W(GF_i(2)).
\]

We now apply (1), (2) and (3) to conclude that

\[
\lambda W(G) = \sum_{e \in E(G)} \lambda n(e) = \sum_{i=1}^r \sum_{e \in E(G)} \lambda n(e)
\]

\[
= \sum_{i=1}^r \left[ \lambda W(G) - \lambda W(GF_i(1)) - \lambda W(GF_i(2)) \right].
\]

This completes our proof. \( \square \)

**Theorem 5.** Suppose that condition \((\ast)\) holds, then

\[
W_+ (G) = \sum_{i=1}^r \left( |E(G)| + 2 |E(GF_i(1))| \left| E(GF_i(2)) \right| + |E(GF_i(1))| \left| E(GF_i(2)) \right| \right),
\]

\[
W_\times (G) = 2 |E(G)|^2 + \sum_{i=1}^r \left( |E(GF_i(1))| \left| E(GF_i(2)) \right| - |F_i|^2 \right),
\]

where \( E = E(G) \) and \( V = V(G) \).
Consider a set $R$ of shortest paths between vertices of $G$ such that for each vertex $a, b \in V(G)$ there is exactly one shortest path connecting $a$ and $b$ in $R$. Suppose there are $k$ paths $P_G(u_1, v_1), P_G(u_2, v_2), \ldots, P_G(u_k, v_k)$ in $R$ containing the edge $e$. Define $\eta_G(e) = \sum_{i=1}^{k} \deg(u_i) + \deg(v_i))$. So $W_+(G) = \sum_{e \in E(G)} \eta_G(e)$. By Lemma 5, there exists a set of shortest path $R$ such that if $u \in GF_1(1), v \in GF_1(2)$ then the shortest path $S(u, v)$ of $R$ connecting $u$ and $v$ has exactly one edge in $F_1$ and if $u, v \in GF_1(1)$ or $u, v \in GF_1(2)$ then $S(u, v)$ does not have an edge in $F_1$. On the other hand, by convexity of components of each $G - F_i$, for every $e \in F_i$, the endpoints of $e$ cannot belong to a unique component of $F_i$. Therefore, we have:

$$
W_+(G) = \sum_{e \in E(G)} \eta_G(e) = \sum_{i=1}^{r} \sum_{e \in F_i} \eta_G(e)
$$

which completes the proof. □

Remark. Suppose $T$ is a tree. By removing an edge of $T$, a forest containing two components, each of them having a boundary vertex, is obtained. Since two components have exactly one boundary vertex then by Lemma 4 they are convex. So, the properties of Theorems 3 and 5 are satisfied. Therefore, we have:

$$
W_+(T) = 4W(T) - 2|E(T)|^2 - |E(T)|,
$$

(4)

$$
W_+(T) = 4W(T) - |E(T)|^2 |V(T)| = W_+(T) + |E(T)|^2.
$$

These results are obtained in [23,24] in a different method.

For graphs satisfying the condition (*), it is possible to apply Lemma 5 to obtain a new method for computing other distance-based graph invariants; see [25] for details.

3. An application in nanoscience

Carbon nanocone originally is discovered by Ge and Sattler in 1994, [26]. These are constructed from a graphene sheet by removing a 60° wedge and joining the edges a cone with a single pentagonal defect at the apex. Removing additional wedges introduces more such defects and reduces the opening angle. A cone with six pentagons has an opening angle of zero and is just a nanotube with one open end.
The aim of this section is to compute the Wiener index of a carbon nanocone $G[n] = \text{CNC}_2[n]$ containing a central pentagon surrounded by $n$ layers of hexagons; see [27,28] and Fig. 1. To do this, we consider the partition of the molecular graph of $G[n]$ into five regions $F_1, F_2, F_3, F_4$ and $F_5$, Fig. 1. Consider the graphs $G_1[n] = (F_1 \cup F_2 \cup F_3)_{G[n]}, G_2[n] = (F_1 \cup F_2)_{G[n]}$ and $G_3[n] = (F_1)_{G[n]}$ depicted in Figs. 2–4, respectively. The subgraphs $\partial G_1[n](G_1[n]), \partial G_1[n](G_2[n])$ and $\partial G_1[n](G_3[n])$ and an isometric subgraph containing them are depicted in Figs. 2–4. By Lemma 2, $G_2[n] \ll G[n]$ and $G_3[n] \ll G[n]$. We are now ready to prove the following theorem:

**Theorem 6.** The Wiener index of the graph $G[n]$ can be expressed as follows:

$$W(G[n]) = 5(W(G_1[n]) - W(G_2[n])).$$

**Proof.** By definition and the symmetry of $G[n]$, the following equalities are satisfied:

$$D(F_1, G[n]) = \sum_{i=1}^{5} D_{G[n]}(F_1, F_i) = D_{G[n]}(F_1, F_1) + 2D_{G[n]}(F_1, F_2) + 2D_{G[n]}(F_1, F_3).$$

$$D_{G[n]}(F_1 \cup F_2, F_1 \cup F_2) = 2D_{G[n]}(F_1, F_1) + 2D_{G[n]}(F_1, F_2),$$

$$D_{G[n]}(F_1 \cup F_2 \cup F_3, F_1 \cup F_2 \cup F_3) = 4D_{G[n]}(F_1, F_2) + 3D_{G[n]}(F_1, F_1) + 2D_{G[n]}(F_1, F_3).$$
To explain, we partition one can find a partition of edges of $M$ are denoted by $M$. We now apply Eqs. (6) and (7).

By the paragraph before this theorem, $G_1[n] \cong (F_1 \cup F_2 \cup F_3)_{G[n]} \ll G[n]$. By Eq. (6),

$$D(F_1, G[n]) = D_{G[n]}(F_1 \cup F_2 \cup F_3, F_1 \cup F_2 \cup F_3) = D_{G[n]}(F_1 \cup F_2, F_1 \cup F_2).$$

Therefore,

$$D(F_1, G[n]) = D_{G[n]}(F_1 \cup F_2 \cup F_3, F_1 \cup F_2 \cup F_3) - D_{G[n]}(F_1 \cup F_2, F_1 \cup F_2).$$

By the paragraph before this theorem,

$$G_1[n] \cong (F_1 \cup F_2 \cup F_3)_{G[n]} \ll G[n].$$

So by Eq. (6),

$$D(F_1, G[n]) = 2W(G_1[n]) - 2W(G_2[n]),$$

and,

$$W(G[n]) = 1/2 \sum_{i=1}^{5} D(F_i, G[n]) = 5/2D(F_j, G[n]). \quad 1 \leq j \leq 5.$$

We now apply Eqs. (7) and (8) to obtain the result.

In Figs. 5 and 6, two hexagonal systems $M(11, 6)$ and $N(9, 5)$ are depicted. The general case of these hexagonal systems are denoted by $M(n, k)$ and $N(n, k)$. Obviously, $M(2n, n) \cong G_1[n]$ and $N(n, n) \cong G_2[n]$. By Lemma 3 and Figs. 5 and 6, one can find a partition of edges of $M(2n, n)$ and a partition of edges of $N(n, n)$ satisfying the conditions of Theorem 4.

To explain, we partition $M(2n, n)$ (and similarly for $N(n, n)$) by cuts drawn in Figs. 5 and 6. By a simple calculations, $g_1 = |V(G_1[n])| = 3(n + 1)^2$ and $g_2 = |V(G_2[n])| = 2(n + 1)^2$. So by Theorem 3 we have:

$$W(G_1[n]) = \frac{g_2^2}{4} + 2 \sum_{i=1}^{n} (g_2 - i^2)^2 + 2 \sum_{i=1}^{n} (g_2 - 2i(n + 1))(2i(n + 1)).$$

$$W(G_2[n]) = \frac{g_2^2}{4} + 2 \sum_{i=1}^{n} (g_2 - i^2)^2 + 2 \sum_{i=1}^{n} (g_2 - 2i(n + 1))(2i(n + 1)).$$
Corollary 3.

\[ W(G[n]) = 15 + 86n + \frac{1135}{6} n^2 + \frac{1205}{6} n^3 + \frac{310}{3} n^4 + \frac{62}{3} n^5. \]

Proof. Apply Theorem 6 and calculations given after this theorem. □

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References


