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WIENER INDEX UNDER GATED AMALGAMATIONS

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Abstract. A subgraph H of a graph G is gated if for every $x \in V(G)$ there exists a vertex u in H such that $d_G(x, v) = d_G(x, u) + d_G(u, v)$ for any $v \in V(H)$. The gated amalgam of graphs G_1 and G_2 is obtained from G_1 and G_2 by identifying their isomorphic gated subgraphs H_1 and H_2 . Two theorems on the Wiener index of gated amalgams are proved. Several known results on the Wiener index of (chemical) graphs are corollaries of these theorems which we demonstrate by gated amalgams of trees and benzenoid systems.

1. INTRODUCTION

The Wiener index is one of the most studied graph invariants in mathematical chemistry. It was introduced in 1947 by Harold Wiener [32] and extensively studied since the middle of the 1970s. The nowadays usual definition of the index was first given by Hosoya in 1971 [23]. In mathematical literature the Wiener index was first considered in [15], and its study is in fact equivalent to the studies of the average distance, cf. [5]. For (starting) information on results on the Wiener index, the chemical meaning of the index and its history we refer to [6, 7, 8, 21, 22, 26, 31] and special issues of MATCH Commun. Math.

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Comput. Chem. [18] and Discrete Appl. Math. [19]. We wish to point out that the theory is especially well elaborated for the Wiener index of trees [12] and hexagonal systems [13].

While studying different classes of chemical graphs, like trees or hexagonal systems, one of the most natural approaches is to build larges graphs from smaller constituents from the same family. For instance, a tree can be recursively build by attaching pendant vertices and similarly, catacondensed hexagonal systems can be build by successively attaching hexagons. Here an edge and a hexagon can be considered as a prime constituents of these classes of graphs, respectively. Moreover, such graphs can also be decomposed into smaller—but not prime—components. For instance, we can glue together two trees along a vertex to obtain a bigger tree and two hexagonal systems along an edge to get a bigger hexagonal system.

Such constructions have been frequently used in the literature to obtain different types of results on the Wiener index. As an example let us just mention investigations of nonisomorphic graphs with the same Wiener index. The main goal of this paper is to unify several such results into a general framework. It turns out that the concept of the gated amalgamation is a natural concept for such a unification, applicable to any graphs, chemical or nonchemical. Roughly speaking, the gated amalgamation is an operation that identifies isomorphic subgraphs of two graphs to obtain a bigger graph, where the distance function is controlled by the distance functions of the constituents.

The paper is organized as follows. In the next section we recall concepts and notions needed, in particular gated sets and amalgamations. In Section 3 our main results are presented and proved. In the last section we deduce three results from the literature as corollaries to our theorems. These results consider the Wiener index under tree transformations, under attaching a hexagon to a catacondensed hexagonal system, and under attaching two hexagonal systems.

2. PRELIMINARIES

All graphs considered are finite, undirected, connected, and without loops and multiple edges. The vertex and edge sets of a graph G are denoted V(G) and E(G). We will shortly write |G| for |V(G)|.

Under distance $d_G(u, v)$ between vertices $u, v \in V(G)$ we mean the usual shortest path distance of G. The distance of a vertex $v \in V(G)$, $d_G(v)$, is the sum of distances between v and all other vertices of G, that is,

$$d_G(v) = \sum_{u \in V(G)} d(v, u).$$

The Wiener index is denoted by W(G) and defined as the sum of distances between all pairs of vertices in G:

$$W(G) = \sum_{\{u,v\} \subseteq V(G)} d_G(u,v) = \frac{1}{2} \sum_{v \in V(G)} d_G(v). \tag{1}$$

A subgraph H of a graph G is called isometric if $d_H(u,v) = d_G(u,v)$ for all $u,v \in V(H)$. The interval I(u,v) between vertices u,v of a connected graph G is the set of vertices of all shortest paths between u and v in G. A subgraph H of a graph G is convex if with any vertices $u,v \in H$ we have $I(u,v) \subseteq V(H)$. A subgraph H of a graph G is called gated in G if for every $x \in V(G)$ there exists a vertex u in H such that $u \in I(x,v)$ for all $v \in V(H)$ [14]. Note that if for some x such a vertex u in V(H) exists, it must be unique. It is then called the gate of x in H and denoted $g_H(x)$, see Fig. 1. It is well-known that the intersection of gated subgraphs is again gated and that a gated subgraph is always convex, cf. [1]. For several additional results on gated subgraphs we refer to [2, 3, 4, 24].

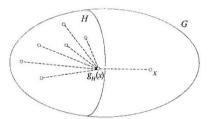


Figure 1: The gate $g_H(x)$ of x in the subgraph H

Let G_1 and G_2 be gated subgraphs of a graph G such that $G_1 \cup G_2 = G$ and $G_1 \cap G_2 \neq \emptyset$. If in addition there are no edges between $G_1 \setminus G_2$ and $G_2 \setminus G_1$ then G is a gated amalgam of G_1 and G_2 , cf. [1]. Equivalent description of the gated amalgamation is the following. Let H_1 be a gated subgraph of a graph G_1 and H_2 a gated subgraph of G_2 , where H_1 and H_2 are isomorphic graphs. Then the gated amalgam of G_1 and G_2 is obtained from G_1 and G_2 by identifying their subgraphs H_1 and H_2 . It is easy to see that these two description are indeed equivalent, see [1, Lemma 1]. We will call G_1 and G_2 covers of the gated amalgam G.

A hexagonal system is 2-connected plane graph in which all inner faces are hexagons (and all hexagons are faces), such that two hexagons are either disjoint or have exactly one common edge, and no three hexagons share a common edge. A hexagonal system is catacondensed if any triple of its hexagons has empty intersection.

Finally, the n-cube Q_n $(n \ge 1)$ is the graph whose vertices are all binary words of length n, two words being adjacent whenever they differ in precisely one place. For instance, Q_1 is the complete graph on two vertices, Q_2 is the 4-cycle, and Q_3 is the usual 3-cube.

3. MAIN RESULTS

In this section we prove our main results—Theorems 1 and 3. In the first theorem we present a formula for W of a gated amalgam G in which the covers G_1 and G_2 of G play symmetric roles. The second result gives a shorter formula for W of a gated amalgam, but in that case the role of the covers is no longer symmetric.

Theorem 1 Let G be the gated amalgam of G_1 and G_2 . Let $G_0 = G_1 \cap G_2$ and let $g_1: G_1 \setminus G_0 \to G_0$ and $g_2: G_2 \setminus G_0 \to G_0$ be the gate maps. Then

$$W(G) = W(G_1) + W(G_2) - W(G_0) + |G_2 \setminus G_1| \sum_{x \in G_1 \setminus G_2} d(x, g_1(x)) + |G_1 \setminus G_2| \sum_{y \in G_2 \setminus G_1} d(y, g_2(y)) + |G_1 \setminus G_2| \sum_{x \in G_1 \setminus G_2} |g_1^{-1}(u)| \cdot |g_2^{-1}(v)| \cdot d_G(u, v).$$

Proof. We first decompose the Wiener index in the following way:

$$W(G) = \sum_{\substack{\{x,y\} \subseteq G_1\\ x \in G_1 \setminus G_2\\ y \in G_1 \setminus G_2}} d_G(x,y) + \sum_{\substack{\{x,y\} \subseteq G_2\\ \{x,y\} \subseteq G$$

As G_0 , G_1 , and G_2 are gated sets, and hence convex, we have:

$$\sum_{\{x,y\}\subseteq G_1} d_G(x,y) + \sum_{\{x,y\}\subseteq G_2} d_G(x,y) - \sum_{\{x,y\}\subseteq G_0} d_G(x,y) = W(G_1) + W(G_2) - W(G_0). \quad (3)$$

To compute the last term of the right-hand side of (2), consider a shortest x, y-path P in G, where $x \in G_1 \setminus G_2$ and $y \in G_2 \setminus G_1$. Note first that P intersects G_0 since there are no edges between $G_1 \setminus G_2$ and $G_2 \setminus G_1$. Let w be the first vertex of P in G_0 while passing P from x to y. Then $d_{G_1}(x,w) = d_{G_1}(x,g_1(x)) + d_{G_1}(g_1(x),w)$. We may thus replace the x, w-subpath of P with a path of equal length but whose first vertex in G_0 is $g_1(x)$. Analogously we may assume that the first vertex of P in G_0 while passing P from y to x is $g_2(y)$. Therefore, since G_0 is convex, we get

$$d_G(x,y) = d_{G_1}(x, g_1(x)) + d_{G_2}(g_1(x), g_2(y)) + d_{G_2}(g_2(y), y),$$

cf. Fig.2. Since all the corresponding subgraph are convex we can further write

$$d_G(x,y) = d_G(x,g_1(x)) + d_G(g_1(x),g_2(y)) + d_G(g_2(y),y).$$

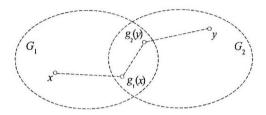


Figure 2: A shortest path between $x \in G_1 \setminus G_2$ and $y \in G_2 \setminus G_1$

Hence the last term of the right-hand side of (2) can be computed as follows:

$$\sum_{\substack{x \in G_1 \backslash G_2 \\ y \in G_2 \backslash G_1}} d_G(x, y) = \sum_{x \in G_1 \backslash G_2} \sum_{y \in G_2 \backslash G_1} \left(d_G(x, g_1(x)) + d_G(g_1(x), g_2(y)) + (d_G(g_2(y), y)) \right)$$

$$= |G_2 \backslash G_1| \sum_{x \in G_1 \backslash G_2} d_G(x, g_1(x)) + |G_1 \backslash G_2| \sum_{y \in G_2 \backslash G_1} d_G(y, g_2(y))$$

$$+ \sum_{(u, v) \in G_0 \times G_0} |g_1^{-1}(u)| \cdot |g_2^{-1}(v)| \cdot d_G(u, v) . \tag{4}$$

Inserting (4) and (3) into (2) the result follows.

We point out that is the last sum of Theorem 1 we sum over all ordered pairs of vertices from G_0 .

Corollary 2 Let G be the graph obtained by an identification of a vertex of a graph G_1 and a vertex of a graph G_2 . Let the identified vertex be w. Then

$$W(G) = W(G_1) + W(G_2) + (|G_2| - 1) \cdot d_{G_1}(w) + (|G_1| - 1) \cdot d_{G_2}(w).$$

Proof. Clearly, G is the gated amalgam of G_1 and G_2 with the intersection w. Now the result follows immediately from Theorem 1.

We continue with the second version of the Wiener index of a graph G that is the gated amalgam of G_1 and G_2 . Now the covers are treated differently which enables us to obtain a shorter expression for W(G). Clearly, in this case W(G) cannot be symmetric with respect to G_1 and G_2 .

Theorem 3 Let G be the gated amalgam of G_1 and G_2 . Let $G_0 = G_1 \cap G_2$ and let $g_1 : G_1 \setminus G_0 \to G_0$ be the gate map from $G_1 \setminus G_0$ to G_0 . Suppose in addition that $G_1 \setminus G_0$ is isometric in G_1 . Then

$$W(G) = W(G_1 \setminus G_0) + W(G_2) + |G_2| \sum_{x \in G_1 \setminus G_2} d(x, g_1(x)) + \sum_{x \in G_0} |g_1^{-1}(x)| \cdot d_{G_2}(x).$$

Proof. We now decompose the Wiener index in the following way:

$$W(G) = \sum_{\{x,y\}\subseteq G_1\backslash G_2} d_G(x,y) + \sum_{\{x,y\}\subseteq G_2} d_G(x,y) + \sum_{\substack{x\in G_1\backslash G_2\\y\in G_2}} d_G(u,v).$$
 (5)

Since $G_1 \setminus G_0$ is isometric by the theorem's assumption, and since G_2 is gated (and hence convex), we have

$$\sum_{\{x,y\}\subseteq G_1\setminus G_2} d_G(x,y) + \sum_{\{x,y\}\subseteq G_2} d_G(x,y) = W(G_1\setminus G_0) + W(G_2). \quad (6)$$

As to the third term of the right-hand side of (5), consider a shortest x, y-path P in G, where $x \in G_1 \setminus G_2$ and $y \in G_2$. Then P intersects G_0 , and let w be the first vertex of P in G_0 while passing P from x to y. Then, by similar arguments as in the proof of Theorem 1 we have

$$d_G(x,y) = d_G(x,w) + d_G(w,y)$$

$$= d_G(x,g_1(x)) + d_G(g_1(x),w) + d_G(w,y)$$

$$= d_G(x,g_1(x)) + d_G(g_1(x),y).$$

Therefore,

$$\sum_{\substack{x \in G_1 \setminus G_2 \\ y \in G_2}} d_G(u, v) = |G_2| \sum_{x \in G_1 \setminus G_2} d(x, g_1(x)) + \sum_{x \in G_1 \setminus G_2} d_{G_2}(g_1(x))$$

$$= |G_2| \sum_{x \in G_1 \setminus G_2} d(x, g_1(x)) + \sum_{x \in G_2} |g_1^{-1}(x)| \cdot d_{G_2}(x). \tag{7}$$

Inserting (6) and (7) into (5) the result follows.

Note that in Theorem 3 we have in addition assumed that $G_1 \setminus G_0$ is isometric in G_1 . This condition is used of aesthetic reasons only. Namely, if $G_1 \setminus G_0$ would not be an isometric subgraph, then $\sum_{\{x,y\}\subseteq G_1\setminus G_2} d_G(x,y)$ cannot be replaced with $W(G_1 \setminus G_0)$. In this case, however, the result can be reformulated as

$$W(G) = \sum_{\{x,y\} \subseteq G_1 \setminus G_2} d_G(x,y) + W(G_2) + |G_2| \sum_{x \in G_1 \setminus G_2} d(x,g_1(x)) + \sum_{x \in G_0} |g_1^{-1}(x)| \cdot d_{G_2}(x).$$

To illustrate Theorems 1 and 3 we consider two examples, a chemical one and a nonchemical one.

Example 1. Consider the hexagonal system from Fig. 3. Theorem 1 will be applied on the left amalgamation, while Theorem 3 on the right one. Note that in both cases $G_0 = K_2$.

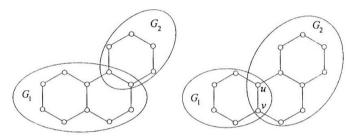


Figure 3: Two gated amalgamations of the phenanthrene

First consider the left amalgamation. Then we have $W(G_1)=109$, $W(G_2)=27$, $|G_2\setminus G_1|=4$, and $|G_1\setminus G_2|=8$. In addition, for the sum of distances of vertices from $G_1\setminus G_2$ to their gates we have $\sum_{x\in G_1\setminus G_2}d(x,g_1(x))=18$, while $\sum_{y\in G_2\setminus G_1}d(y,g_2(y))=6$. Hence,

$$W(G) = 109 + 27 - 1 + 4 \cdot 18 + 8 \cdot 6 + 6 \cdot 2 + 2 \cdot 2 = 271.$$

Next to the right amalgamation and Theorem 3. Then $W(G_1 \setminus G_0) = 10$, $W(G_2) = 109$, $|G_2| = 10$, $\sum_{x \in G_1 \setminus G_2} d(x, g_1(x)) = 1 + 2 + 2 + 1$, while for both vertices x of G_0 we have $|g_1^{-1}(x)| = 2$ and $d_{G_2}(u) = 21$, $d_{G_2}(v) = 25$. Hence we have:

$$W(G) = 10 + 109 + 10 \cdot 6 + 2 \cdot 21 + 2 \cdot 25 = 271$$
.

Example 2. Let G_n , $n \ge 1$, be the graph obtained from two copies Q' and Q'' of the n-cube Q_n by identifying an (n-1)-subcube of Q' with an (n-1)-subcube of Q'', cf. Fig. 4, where G_1 , G_2 , and G_3 are drawn.

Clearly, G_n is a gated amalgam of two *n*-cubes with two (n-1)-cubes as covers. It is well-known, cf. [16, 25], that $W(Q_n) = n \, 2^{2(n-1)}$. Therefore, applying Theorem 1 we easily obtain:

$$W(G_n) = 2 n 2^{2(n-1)} - (n-1)2^{2(n-2)} + 2 \cdot 2^{n-1} 2^{n-1} + 2 (n-1)2^{2(n-2)}$$

= $(9n+7)2^{2(n-2)}$.

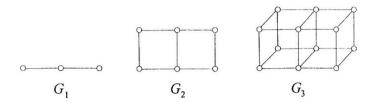


Figure 4: First three graphs G_n , $n \ge 1$

4. THREE SPECIAL CASES

In this section we present three typical examples how Theorems 1 and 3 can be applied. All these examples appeared before in the literature and the list of such examples could well have been extended.

4.1. Wiener index under tree transformations

Rada [30] considered certain tree transformations in order to construct nonisomorphic trees with the same Wiener index. The main idea is to attach a given tree to different vertices of another tree and to consider the corresponding Wiener indices. More precisely, let u and v be vertices of a tree T and let w be a vertex of a tree S. Let T_u be the tree obtained from T and S by identifying u with w, and let T_v be the tree obtained from T and S by identifying v with w, see Fig. 5.

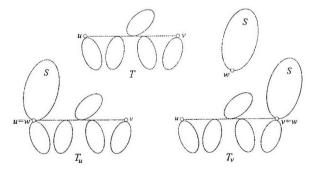


Figure 5: Trees T_u and T_v constructed from trees T and S

We now present the central result of [30] and its short proof.

Theorem 4 Let u, v, T, Tu, Tv, and S be as above. Then

$$W(T_u) - W(T_v) = (|S| - 1) \cdot (d_T(u) - d_T(v)).$$

Proof. Clearly, T_u and T_v are gated amalgams of T and S. Then Corollary 2, applied on T_u and T_v with $G_1 = T$ and $G_2 = S$, gives:

$$W(T_u) = W(T) + W(S) + (|S| - 1) \cdot d_T(u) + (|T| - 1) \cdot d_S(w),$$

$$W(T_v) = W(T) + W(S) + (|S| - 1) \cdot d_T(v) + (|T| - 1) \cdot d_S(w),$$

and the result follows.

It is of interest to closely examine the expression $d_T(u) - d_T(v)$ from the previous theorem. It can be, more generally, computed as follows.

Proposition 5 Let H be a gated subgraph of a connected graph G with the gate map $g_H: G \setminus H \to H$. Let $u, v \in H$, then

$$d_G(u) - d_G(v) = \sum_{y \in H} \left(|g_H^{-1}(y)| \cdot (d(y, u) - d(y, v)) \right) + (d_H(u) - d_H(v)).$$

Proof. Consider a vertex $x \in G \setminus H$. Then $d(x, u) = d(x, g_H(x)) + d(g_H(x), u)$ and $d(x, v) = d(x, g_H(x)) + d(g_H(x), v)$, hence

$$d(x, y) - d(x, y) = d(q_y(x), y) - d(q_y(x), y)$$

We can therefore compute as follows:

$$\begin{split} d_G(u) - d_G(v) &= \sum_{x \in G} (d(u, x) - d(v, x)) \\ &= \sum_{x \in G \setminus H} (d(u, x) - d(v, x)) + \sum_{x \in H} (d(u, x) - d(v, x)) \\ &= \sum_{x \in G \setminus H} (d(g_H(x), u) - d(g_H(x), v)) + (d_H(u) - d_H(v)) \\ &= \sum_{y \in H} \left(|g_H^{-1}(y)| \cdot (d(y, u) - d(y, v)) \right) + (d_H(u) - d_H(v)) \,. \end{split}$$

In the particular case of Theorem 4 we can select the unique u, v-path in T as a gated subgraph. Then Proposition 5 easily implies the expression for $d_T(u) - d_T(v)$ given in [30].

4.2. Attaching a hexagon to a catacondensed hexagonal system

In our second application we consider catacondensed hexagonal systems. Clearly, any such graph can be obtained by a recursive procedure of joining a hexagon to the previously constructed system. Therefore, the following theorem is relevant.

Theorem 6 Let G be a catacondensed hexagonal system and let e = uv be a join edge of G. Let H be the catacondensed hexagonal system obtained from G by removing the pendant hexagon containing e. Then

$$W(G) = W(H) + 2(d_H(u) + d_H(u)) + 6|H| + 10.$$

Proof. Let G_1 be the pendant hexagon of G containing the edge e and set $G_2 = H$. Then G is the gated amalgam of G_1 and G_2 . Moreover, $W(G_1 \setminus G_0) = 10$, $W(G_2) = W(H)$, $\sum_{x \in G_1 \setminus G_2} d(x, g_1(x)) = 6$, and $|g_1^{-1}(u)| = |g_1^{-1}(u)| = 2$. Now the result follows immediately from Theorem 3.

Theorem 6 goes back to Gutman and Polansky [20] and has been applied many times, for instance in [17, 29]. For more related references see [13].

This example is a special case of the following observation. Let G_1 and G_2 be bipartite graphs and let G be a graph obtained from G_1 and G_2 by identifying en edge of G_1 with and edge of G_2 . (Note that G is bipartite as well.) Then G is a gated amalgam of G_1 and G_2 . Indeed, let uv be the edge of G where G_1 and G_2 have been identified. Then for any vertex w of G we have either d(w, u) < d(w, v) or d(w, u) > d(w, v), for otherwise G would not be bipartite. But then the vertex closer to w is its gate.

4.3. Attaching two hexagonal systems

In the previous example we have attached a hexagon to a catacondensed hexagonal system. A more general situation is when two hexagonal systems are glued together along an edge. For this case Polansky and Bonchev [27, 28] obtained the following result, which we prove here using Theorem 1.

Theorem 7 Let G_1, G_2 be arbitrary hexagonal systems and $e_1 = (v_1, u_1) \in E(G_1)$, $e_2 = (v_2, u_2) \in E(G_2)$. If the system G is constructed from G_1 and G_2 by identifying the edges e_1 and e_2 so that the vertex v_1 is identified with the vertex v_2 , then

$$W(G) = W(G_1) + W(G_2)$$

$$+ \frac{1}{2} \Big((|G_2| - 2) (d_{G_1}(v_1) + d_{G_1}(u_1) \Big) + \frac{1}{2} \Big((|G_1| - 2) (d_{G_2}(v_2) + d_{G_2}(u_2) \Big)$$

$$- \frac{1}{2} \Big((d_{G_1}(v_1) - d_{G_1}(u_1)) (d_{G_2}(v_2) - d_{G_2}(u_2)) \Big) - \frac{1}{2} |G_1| |G_2| + 1.$$

Proof. First, G is the gated amalgam of G_1 and G_2 . We next observe that

$$\sum_{x \in G_1 \setminus G_2} d(x, g_1(x)) = \sum_{x \in g_1^{-1}(v_1)} d(x, g_1(x)) + \sum_{x \notin g_1^{-1}(v_1)} d(x, g_1(x))$$

$$= \sum_{x \in g_1^{-1}(v_1)} d(x, v_1) + \sum_{x \notin g_1^{-1}(v_1)} d(x, v_1) - 1.$$
(8)

Analogously we infer that

$$\sum_{x \in G_1 \setminus G_2} d(x, g_1(x)) = \sum_{x \in g_1^{-1}(u_1)} d(x, u_1) + \sum_{x \notin g_1^{-1}(u_1)} d(x, u_1) - 1.$$
 (9)

Combining (8) and (9) we obtain

$$2\sum_{x\in G_1\backslash G_2}d(x,g_1(x)) = d_{G_1}(v_1) + d_{G_1}(u_1) - |G_1|,$$
(10)

and by the symmetry also

$$2\sum_{x \in G_2 \backslash G_1} d(x, g_2(x)) = d_{G_2}(v_2) + d_{G_2}(u_2) - |G_2|, \qquad (11)$$

Set now $|g_1^{-1}(v_1)| = a$, $|g_1^{-1}(u_1)| = b$, $|g_2^{-1}(v_1)| = c$, and $|g_2^{-1}(u_2)| = d$, so that

$$\sum_{(u,v)\in G_0\times G_0} |g_1^{-1}(u)| \cdot |g_2^{-1}(v)| \cdot d_G(u,v) = ad + bc.$$
 (12)

Hence, inserting (10), (11), and (12) into Theorem 1, we get:

$$W(G) = W(G_1) + W(G_2)$$
+ $\frac{1}{2} \left(|G_2| - 2 \right) (d_{G_1}(v_1) + d_{G_1}(u_1) + \frac{1}{2} \left(|G_1| - 2 \right) (d_{G_2}(v_2) + d_{G_2}(u_2) + d_{G_2}(u_2) + d_{G_2}(u_2) \right)$
+ $ad + bc + |G_1| + |G_2| - |G_1| |G_2| - 1$.

Clearly, $|G_1| = a + b + 2$ and $|G_2| = c + d + 2$. Moreover,

$$d_{G_1}(v_1) - d_{G_2}(u_1) = b - a$$

and

$$d_{G_2}(v_2) - d_{G_2}(u_2) = d - c,$$

from which the result easily follows.

The formula of Theorem 7 has been further elaborated by Dobrynin in [9, 10, 11].

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