Wiener number of vertex-weighted graphs and a chemical application

Sandi Klavžar
Department of Mathematics, PEF
University of Maribor
Koroška cesta 160
2000 Maribor, Slovenia

Ivan Gutman *
Institute of Physical Chemistry
Attila József University
P.O.Box 105
H-6701 Szeged, Hungary

Abstract

The Wiener number $W(G)$ of a graph G is the sum of distances between all pairs of vertices of G. If (G, w) is a vertex-weighted graph, then the Wiener number $W(G, w)$ of (G, w) is the sum, over all pairs of vertices, of products of weights of the vertices and their distance. For G being a partial binary Hamming graph, a formula is given for computing $W(G, w)$ in terms of a binary Hamming labeling of G. This result is applied to prove that $W(PH) = W(\widetilde{HS}) + 36W(ID)$, where PH is a phenylene, $\widetilde{HS}$ a pertinently vertex-weighted hexagonal squeeze of PH, and ID the inner dual of the hexagonal squeeze.

1 Introduction

In this paper we are concerned with a graph invariant $W = W(G)$, defined for an arbitrary connected graph G as

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

where $d_G(u, v)$ denotes the length of a shortest path in G between vertices u and v. We call W the *Wiener number*.

The investigation of the quantity W seems to be first undertaken by Harold Wiener [33] almost exactly fifty years ago. Since then there is a continuous record of research activity in this field with no sign of attenuation. Wiener's original article [33] appeared in a chemical journal and was long overlooked by mathematicians. In the meantime the sum of all distances of graphs was studied in quite a few mathematical works. A variety of names for W was proposed: "*gross status*" [19], "*total status*" [4], "*graph distance*"

*Present address: Faculty of Science, P.O.Box 60, YU-34000 Kragujevac, Yugoslavia

[9], "*transmission*" [29] and simply "*sum of all distances*" [11, 37]. In some works the closely related "*mean distance*" [8, 36] or "*average distance*" [1, 6] were considered. The name "*Wiener number*" or "*Wiener index*" is nowadays in standard use in chemistry and is sometimes encountered also in the mathematical literature [25, 26].

In chemistry the Wiener number is one of the most thoroughly studied, best understood and most frequently used graph–theory–based molecular–shape descriptors; for reviews on chemical aspects of W and further references see [18, 27]. W found numerous applications in the modelling of physico–chemical, pharmacological and biological properties of organic molecules. To give an idea about the versatility of the applications of the Wiener number, we mention its use in the study of ultrasonic sound velocities in alkanes and alcohols [30], rates of electroreduction of chlorobenzenes [3], cytostatic and antihistaminic activities of certain drugs [24], protonation constants of derivatives of salicylhydroxamic acid and their fungicidal activities [22], and isomerism in fullerenes [28]. The success of W was long thought to lie in its (putative) capability of measuring molecular volumes, surfaces and/or surface–to–volume ratios. It was shown quite recently [16] that, indeed, W is proportional to molecular surface areas. On the other hand, contrary to earlier expectations, no relation between W and molecular volumes could be established [16].

A graph G is called a *partial binary Hamming graph*, if each vertex $v \in V(G)$ can be labelled by a word of fixed length, $\ell(v)$, defined on a two–letter alphabet, say on the alphabet $\{0,1\}$, such that for all $u, v \in V(G)$ the number of positions in which $\ell(u)$ and $\ell(v)$ differ equals $d_G(u, v)$, cf. [21]. The labeling ℓ is called a *binary Hamming labeling*. Partial binary Hamming graphs can also be described as isometric subgraphs of hypercubes. We refer to [2, 5, 7, 20, 21, 34, 35] for many results and aspects of partial (binary) Hamming graphs.

In the next section we introduce the Wiener number, $W(G, w)$, of a vertex-weighted graph (G, w), and give a formula for computing $W(G, w)$ in the case when G is a partial binary Hamming graph. In Section 3 two classes of graphs of interest in chemistry are discussed: hexagonal systems and phenylenes. In particular, a distance based definition of an elementary cut of a hexagonal system is presented. Finally, in the last section, a formula is obtained for the Wiener number of a phenylene in terms of its hexagonal squeeze.

2 The Wiener number of vertex–weighted graphs

A *vertex–weighted graph* (G, w) is a graph G together with a function $w : V(G) \to \mathbb{N}^+$. (Evidently, we could have chosen for vertex–weights (positive) real numbers. For the present considerations, however, weighting of the vertices with positive integers will

suffice.) From now on vertex–weighted graphs in which all weights are positive integers will be called simply *weighted graphs*.

The Wiener number $W(G,w)$ of a weighted graph (G,w) is defined as

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

Note that if $w(u) = 1$ holds for all vertices $u \in V(G)$, then $W(G,w) = W(G)$. More generally, if w is a constant function, say $w \equiv m$, then $W(G,w) = m^2\ W(G)$. Observe also that if the distance matrix of a graph G is given, then it is no more difficult to compute $W(G,w)$ than $W(G)$.

Wiener indices of weighted graphs, as defined above, seem not to be previously studied (in either mathematical or chemical literature). Exceptionally, one of the present authors did some work [14] on $W(G,w)$, where the weight $w(u)$ was set to be equal to the degree of the vertex u.

Let (G,w) be a weighted partial binary Hamming graph, i.e., a weighted graph (G,w) where G is a partial binary Hamming graph. Let $V(G) = \{v_1, v_2, \ldots, v_n\}$ and set

$$\widetilde{V}(G) = \{v_1^1, \ldots, v_1^{w(1)}, v_2^1, \ldots, v_2^{w(2)}, \ldots, v_n^1, \ldots, v_n^{w(n)}\}\,,$$

where the abbreviation $w(i)$ is used instead of $w(v_i)$. Let g be a binary Hamming labeling of G. We define a labeling $\widetilde{g}$ of the elements of $\widetilde{V}(G)$ by $\widetilde{g}(v_i^j) = g(v_i)$ for all i and j. We call $\widetilde{g}$ an *extended binary Hamming labeling*. For $u \in \widetilde{V}(G)$ let $\widetilde{g}_i(u)$ denote the ith coordinate of the label $g(u)$.

With the above notation we have:

Proposition 1 *Let G be a partial binary Hamming graph with a binary Hamming labeling g of length k. Let $\widetilde{g}$ be the extended binary Hamming labeling of the weighted partial binary Hamming graph (G,w). Then*

$$W(G,w) = \sum_{i=1}^{k} m_i(m - m_i)\,,$$

where $m = \sum_{u \in V(G)} w(u) = |\widetilde{V}(G)|$, and m_i is the number of vertices $u \in \widetilde{V}(G)$ with $\widetilde{g}_i(u) = 1$, for $i = 1, 2, \ldots, k$.

Proof. Let $V = V(G)$. For $u, v \in V$, let $\delta_i(u,v)$ be 0 if $g_i(u) = g_i(v)$, and 1 otherwise. Since g is a binary Hamming labeling, we have:

$$W(G,w) \;\; = \;\; \frac{1}{2} \sum_{u \in V} \sum_{v \in V} w(u)w(v)d_G(u,v)$$

$$
\begin{aligned}
&= \frac{1}{2} \sum_{u \in V} \sum_{v \in V} w(u) w(v) \sum_{i=1}^{k} \delta_i(u, v) \\
&= \sum_{i=1}^{k} \left(\frac{1}{2} \sum_{u \in V} \sum_{v \in V} w(u) w(v) \delta_i(u, v) \right) \\
&= \sum_{i=1}^{k} m_i (m - m_i).
\end{aligned}
$$

□

The following special case of Proposition 1 is a previously known result [23, Proposition 3.1]:

Corollary 2 *Let G be a partial binary Hamming graph on n vertices and let g be a binary Hamming labeling of G of length k. For $1 = 1, 2, \ldots, k$ let n_i be the number of vertices u of G with $g_i(u) = 1$. Then*

$$W(G) = \sum_{i=1}^{k} n_i (n - n_i) .$$

Proposition 1 provides a simple method for the calculation of the Wiener numbers of (weighted) partial binary Hamming graphs, which is particularly suitable for the chemically very important class of hexagonal systems, described in the subsequent section.

3 Hexagonal systems and phenylenes

Hexagonal systems (or *benzenoid systems* or *benzenoid graphs*, see below) are finite connected plane graphs with no cut vertices, in which every interior region is bounded by a regular hexagon of side length 1, cf. [31, 39]. The *inner dual* of a hexagonal system G is a graph with vertices corresponding to the hexagons of G, and two vertices are adjacent if the corresponding hexagons share an edge.

Hexagonal systems provide the graph representation of the so–called benzenoid hydrocarbons, a class of substances of outstanding importance in chemistry. Therefore they are often referred to as *benzenoid graphs* or *benzenoid systems*. Details of the extensive research on these molecular graphs can be found in the book [15] and the review [13]. Recall that the number of known benzenoid hydrocarbons is well above 500; some of them play a major role in chemical industry, some are notorious pollutants; a few of them are highly carcinogenic.

Let G be a hexagonal system in which no three hexagons meet in a vertex, i.e., let G be a tree–like hexagonal system. (In chemistry these are referred to as catacondensed

benzenoid systems [15]). Then separate each pair of hexagons that share an edge uv as follows. If u', v' and u'', v'' are the corresponding vertices in the separated cycles, join u' with u'' and v' with v'', and repeat this for all pairs of adjacent hexagons of G. The graph obtained in this way is called a *phenylene* and the graph G is called the *hexagonal squeeze* of the respective phenylene. An example of a phenylene, its hexagonal squeeze as well as the inner dual of the hexagonal squeeze are shown in Fig. 1.

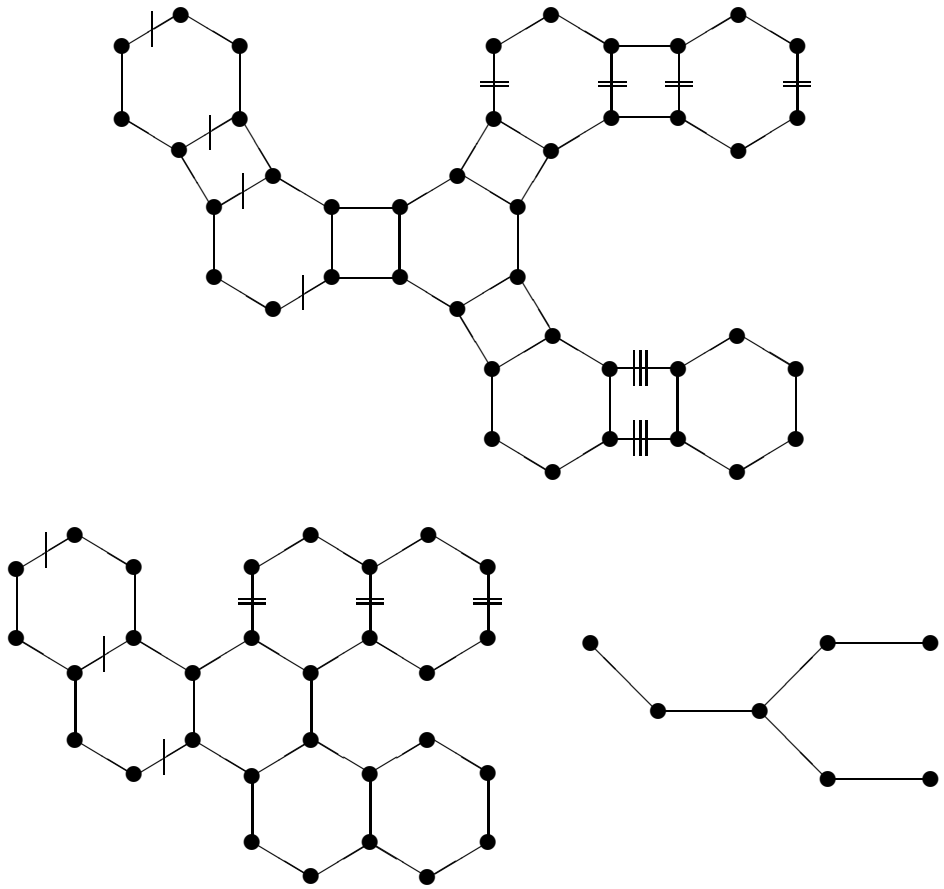

Figure 1: A phenylene, its hexagonal squeeze and the inner dual of the squeeze

The graphs described above provide the graph representation of another class of polycyclic hydrocarbons, which are known in chemistry under the name *phenylenes*. (Using the same name for both a chemical compound and the respective molecular graph should cause no confusion whatsoever.) Phenylenes are very attractive from the point of view of theoretical chemistry because they consist of six-membered cycles (known to stabilize the molecule) and four-membered cycles (known to destabilize the

molecule). The (experimental) chemistry of phenylenes is nowadays in rapid expansion (see [32]). It should be mentioned that the number of phenylenes (hydrocarbons) known at present is around 10, much below the number of known benzenoids. Of the theoretical results on phenylenes (which are not numerous either) we mention the following [12]: If PH is a phenylene and HS is its hexagonal squeeze, then the determinant of the adjacency matrix of PH is equal to (plus or minus) the square of the number of perfect matchings of HS. No result on phenylenes (graphs) seems to have ever been reported in the mathematical literature.

4 The Wiener number of phenylenes

Let G be a connected graph. Then the relation Θ on $E(G)$, which was introduced by Djoković [7] in a somewhat different form (see also [10, 20, 21, 35]), is defined as follows. If $e = xy \in E(G)$ and $f = uv \in E(G)$, then $e\Theta f$ if $d(x,u) + d(y,v) \neq d(x,v) + d(y,u)$. The relation Θ is reflexive and symmetric, yet it need not be transitive. We denote its transitive closure by Θ^* and call the equivalence classes of Θ^* the *cuts* of G. Hence, cuts of G are pairwise disjoint subsets of the edge set $E(G)$.

In Fig. 1 two cuts of the hexagonal squeeze are indicated, as well as the corresponding cuts of the phenylene. In addition to this, one more cut of the phenylene is marked. This cut consists of two opposite (outer) edges of a square. Such cuts will be referred to as *square cuts*. It is well-known that if we remove the edges of a cut from a partial binary Hamming graph (in particular from a hexagonal system or from a phenylene) then the remaining graph consists of two connected components.

Winkler [35] proved that a connected graph G is a partial binary Hamming graph if and only if G is bipartite and $\Theta^* = \Theta$. Since hexagonal systems are partial binary Hamming graphs ([23, Theorem 2.1]), it follows that cuts of hexagonal systems coincide with the so–called (elementary, orthogonal) cuts of hexagonal systems, cf. [23, 31, 38]. The same holds for the cuts of phenylenes since as a part of the proof of Theorem 3 we show that phenylenes are partial binary Hamming graphs as well.

Let HS denote the hexagonal squeeze of a phenylene PH. Define the weighted graph $\widetilde{HS} = (HS, w)$ by setting $w(u) = 2$, if u is a vertex of degree 3, and $w(u) = 1$, otherwise. We say that $\widetilde{HS}$ is the *weighted hexagonal squeeze* of the phenylene PH. For our purpose we can view $\widetilde{HS}$ as a graph which we obtain from HS by replacing each vertex of degree 3 by a pair of vertices at distance 0, cf. Fig. 2.

We are now prepared to state the following result.

Theorem 3 *Let PH be a phenylene, let $\widetilde{HS}$ be its weighted hexagonal squeeze and let ID be the inner dual of the hexagonal squeeze. Then*

$$W(PH) = W(\widetilde{HS}) + 36\, W(ID).$$

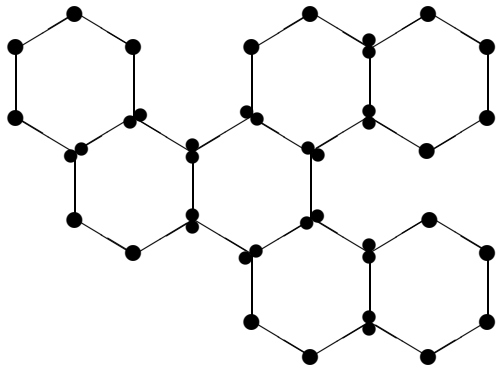

Figure 2: Another way of representing $\widetilde{HS}$

Proof. Let $|V(PH)| = n$ and let $\{C_1, C_2, \ldots, C_s, C_{s+1}, C_{s+2}, \ldots, C_{s+t}\}$ be the set of cuts of PH, where the cuts C_i, $s+1 \leq i \leq t$, correspond to the square cuts and the cuts C_i, $1 \leq i \leq s$, to the other cuts. Note that t is equal to the number of edges of ID and s is the number of cuts in HS.

For $i = 1, 2, \ldots s+t$, let G_i^0 and G_i^1 be the connected components of $PH \setminus C_i$. Define the ith component of the mapping $g : V(PH) \to \{0,1\}^{s+t}$ as follows:

$$g_i(u) = \begin{cases} 0; & u \in G_i^0, \\ 1; & u \in G_i^1. \end{cases}$$

Hence, $g(u) = (g_1(u), g_2(u), \ldots, g_s(u), g_{s+1}(u), \ldots, g_{s+t}(u))$. Let u and v be any two vertices of PH and let Q be a shortest path in PH between u and v. Clearly, if $xy \in C_j$ is an edge of Q, then $g_j(x) \neq g_j(y)$ and this is the only coordinate in which $g(x)$ and $g(y)$ differ. In addition, no two edges of Q belong to the same cut, for otherwise Q would not be a shortest path. It follows that the distance between u and v is equal to the number of coordinates in which $g(u)$ and $g(v)$ differ. Thus g is a binary Hamming labeling of a partial binary Hamming graph PH. Then by Corollary 2

$$W(PH) = \sum_{i=1}^{s+t} n_i \, (n - n_i) \, ,$$

where n_i is the number of vertices u of PH with $g_i(u) = 1$. This equation can be rewritten as

$$W(PH) = \sum_{i=1}^{s} n_i \, (n - n_i) + \sum_{i=s+1}^{s+t} n_i \, (n - n_i) \, . \tag{1}$$

Consider the hexagonal squeeze HS of PH and let $C_1', C_2', \ldots, C_s'$ be the cuts of HS corresponding to the cuts $C_1, C_2, \ldots, C_s$ of PH. Let H_i^0 and H_i^1 be the connected

components of $HS \setminus C_i'$. By [23, Theorem 2.1] HS is a partial binary Hamming graph. Moreover, a binary Hamming labeling $g' : V(HS) \to \{0,1\}^s$ can be defined analogously as the labeling g for PH, as defined above. Let u be a vertex of PH and let u' be the corresponding vertex of HS. Then by the definitions of g and g' we get that $g'(u')$ is equal to the first s coordinates of $g(u)$. Also, a vertex of HS of degree 3 corresponds to two vertices in PH with identical first s coordinates. By Proposition 1 we hence get

$$\sum_{i=1}^{s} n_i(n - n_i) = W(\widetilde{HS})\,. \tag{2}$$

Consider now the inner dual ID of HS. Recall that ID has t edges, say e_{s+1}, e_{s+2}, ..., e_{s+t}, where for $i = s+1, s+2, \ldots, s+t$, the edge e_i corresponds to the cut C_i of PH. By a classical result of Wiener [33] (or by Corollary 2) we have

$$W(ID) = \sum_{i=s+1}^{s+t} n_1(e_i)n_2(e_i)\,,$$

where $n_1(e_i)$ denotes the number of vertices closer to one end vertex of e_i and $n_2(e_i)$ the number of remaining vertices of ID. Let C_i be a cut of PH where $i \in \{s+1, s+2, \ldots, s+t\}$. Then the number of vertices in G_i^0 is equal to $6n_1(e_i)$ and the number of vertices in G_i^1 is $6n_2(e_i)$, or vice versa. Therefore $n_i\,(n - n_i) = 36n_1(e_i)n_2(e_i)$ and hence

$$\sum_{i=s+1}^{s+t} n_i(n - n_i) = 36 \sum_{i=s+1}^{s+t} n_1(e_i)n_2(e_i) = 36W(ID)\,. \tag{3}$$

Combining (1) with (2) and (3) completes the proof. □

To illustrate Theorem 3 consider the phenylene from Fig. 1. Then $t = 6$ (the number of square cuts) and $s = 15$ (the number of all the other cuts). By Proposition 1 we have

$$W(\widetilde{HS}) = 6 \cdot (3 \cdot 39) + 3 \cdot (6 \cdot 36) + 3 \cdot (9 \cdot 33) + 3 \cdot (18 \cdot 24) = 3537.$$

Furthermore, $W(ID) = 48$ and by Theorem 3 we conclude that $W(PH) = 3537 + 36 \cdot 48 = 5265$.

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