Wiener Dimension: Fundamental Properties and (5,0)-Nanotubical Fullerenes

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Abstract

The Wiener dimension of a connected graph is introduced as the number of different distances of its vertices. For any integer D and any integer k, a graph of diameter D and of Wiener dimension k is constructed. An infinite family of non-vertex-transitive graphs with Wiener dimension 1 is presented and it is proved that a graph of dimension 1 is 2-connected. It is shown that the $(5,0)$-nanotubical fullerene graph on $10k$ ($k \geq 3$) vertices has Wiener dimension k. As a consequence the Wiener index of these fullerenes is obtained.

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1   Introduction

The distance considered in this paper is the usual shortest path distance. We assume throughout the paper that all graphs are connected unless stated otherwise. For terms not defined here we refer to [21].

Let G be a graph and $u \in V(G)$. Then the *distance* of u is

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

In location theory, sets of vertices with the minimum (or maximum) distance in a graph play a special role because they form target sets for locations of facilities. The set of vertices of a graph G that minimizes the distance is called the median set of G. The framework can be made more general (at least) in two ways: by considering the sum of distances to a specified multiset of vertices (such multisets are referred to as profiles) and by considering weighted graphs. For more information in this direction of research see [2, 3, 17, 22].

The *Wiener index* of a graph G is defined as

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

This graph invariant has been extensively investigated in the last decades and continues to be an utmost active research area; see the recent papers [12, 13, 14, 16] and references therein. In particular, in the latter paper the so-called semi-cartesian product of graphs is introduced in order to simplify the computation of the Wiener index of chemical graphs such as carbon nanotubes and nanotori.

Suppose now that $\{d_G(u) \mid u \in V(G)\} = \{d_1, d_2, \ldots, d_k\}$. Assume in addition that G contains t_i vertices of distance d_i, $1 \le i \le k$. Then the Wiener index of G can be expressed as

$$W(G) = \frac{1}{2} \sum_{i=1}^{k} t_i d_i \,. \tag{1}$$

We therefore say that the *Wiener dimension* $\dim_W(G)$ of G is k. That is, in this paper we introduce the Wiener dimension of a graph as the number of different distances of its vertices.

The paper is organized as follows. In the next section the Wiener dimension is given for some classes of graphs. Then, in Section 3, we construct for any integer D and any integer k a graph of diameter D and of Wiener dimension k. In Section 4 we consider graphs of Wiener dimension 1. An infinite family of non-vertex-transitive graphs with Wiener dimension 1 is constructed and it is proved that a graph of dimension 1 is 2-connected. In the final section we determine the Wiener dimension of $(5, 0)$-nanotubical fullerene graphs and as a consequence obtain their Wiener index.

2 The Wiener dimension of cyclic phenylenes

It is easy to see that $\dim_W(K_n) = \dim_W(C_n) = \dim_W(P) = 1$, where P is the Petersen graph, the intrinsic reason being that all these graphs are vertex-transitive, cf. Section 4. It is also clear that $\dim_W(K_{n,m}) = 2$ as soon as $n \neq m$, and it is not difficult to infer that $\dim_W(P_n) = \lceil n/2 \rceil$ for any $n \geq 1$. For a sporadic example of a graph G with $\dim_W(G) = 4$ see Fig. 1, where the graph G is shown together with the distances of its vertices.

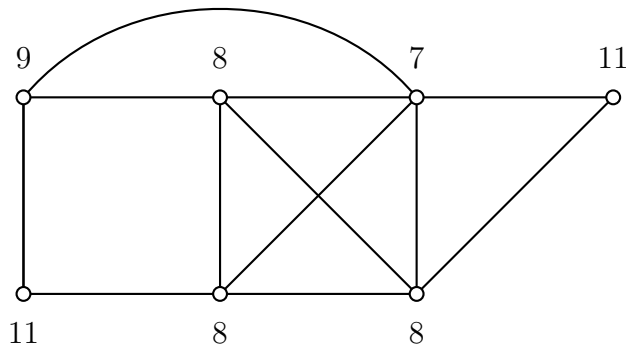

Figure 1: An asymmetric graph G with $\dim_W(G) = 4$

For a slightly more elaborate example consider the family of cyclic phenylenes, a class of graphs arising in mathematical chemistry [4, 24]. These graphs are composed of cyclically attached hexagons and squares, as shown in Fig. 2 for the cyclic phenylene R_5. The definition of R_k, $k \geq 3$, should be clear from this example.

Let u, v, w be vertices of R_h, where u is a vertex of the inner long cycle, v a vertex of degree 3 on the outer long cycle, and w a vertex of degree 2. Then it is not
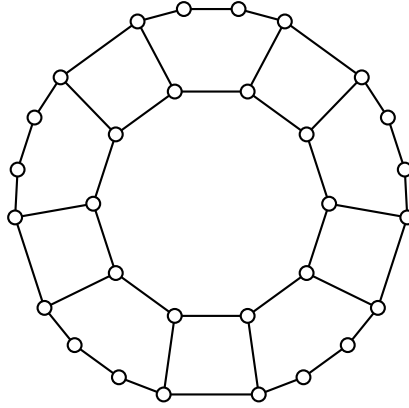
Figure 2: The cyclic phenylene R_5

difficult to see that for any $k \geq 3$, $d_{R_k}(u) = 3k^2 + 6k$, $d_{R_k}(v) = 3k^2 + 12k - 12$, and $d_{R_k}(w) = 3k^2 + 18k - 24$. Since $d_{R_k}(u) < d_{R_k}(v) < d_{R_k}(w)$ holds for $k \geq 3$, we have $\dim_W(R_k) = 3$, $k \geq 3$.

Using (1), we thus also get:

$$
\begin{aligned}
W(R_k) &= \frac{1}{2} 2k \left((k^2 + 6k) + (3k^2 + 12k - 12) + (3k^2 + 18k - 24) \right) \\
&= 9k^3 + 36k^2 - 36k \,.
\end{aligned}
$$

3 Graphs with given diameter and Wiener dimension

The *inverse Wiener index problem* is to find a graph from a certain class of graphs with a given value of the Wiener index. The inverse Wiener index problem was solved for general graphs by Goldman et al. [9]: for every positive integer n except 2 and 5 there exists a graph G such that the Wiener index of G is n. Lepovič and Gutman [15] conjectured that all but 49 positive integers are Wiener indices of trees. The conjecture was independently proved in [18] and [19]. Later, Fink et al. [7] showed that there are semi-exponential number of trees with given Wiener index. For some recent developments on the inverse Wiener problem see [20, 23].

In this section we start the inverse Wiener dimension problem. As the first result in this direction we prove that for any integer D and any integer k there exists a

graph of diameter D and of Wiener dimension k. The corresponding construction uses two main ingredients, graphs of diameter 2 and Cartesian products of graphs. We begin with the following:

Lemma 3.1. *Let G be a graph of order n, diameter 2, and let $v \in V(G)$. Then $d_G(v) = 2n - \deg(v) - 2$. In particular, $\dim_W(G) = |\{\deg(u) \mid u \in V(G)\}|$.*

Proof. Since $\mathrm{diam}(G) = 2$, we have $d_G(v) = \deg(v) + 2(n - \deg(v) - 1) = 2n - \deg(v) - 2$. Therefore, $d_G(u) = d_G(w)$ if and only if $\deg(u) = \deg(w)$. $\square$

The Cartesian product $G \square H$ of graphs G and H has vertex set $V(G \square H) = V(G) \times V(H)$, and (g, h) is adjacent to (g', h') if $g = g'$ and $hh' \in E(H)$, or $h = h'$ and $gg' \in E(G)$. This graph operation is associative, hence we may consider powers of graphs with respect to it. Powers of K_2 are known as hypercubes, the d-tuple power is denoted with Q_d.

Let $(g, h), (g', h') \in V(G \square H)$, then it is well-known (cf. [8, Proposition 5.1]) that $d_{G \square H}((g, h), (g', h')) = d_G(g, g') + d_H(h, h')$. Note that this fact in particular implies that $\mathrm{diam}(G \square H) = \mathrm{diam}(G) + \mathrm{diam}(H)$. Moreover,

$$
\begin{aligned}
d_{G \square H}((g, h)) &= \sum_{(g', h') \in V(G \square H)} d_{G \square H}((g, h), (g', h')) \\
&= \sum_{(g', h') \in V(G \square H)} (d_G(g, g') + d_H(h, h')) \\
&= |V(H)| \sum_{g' \in V(G)} d_G(g, g') + |V(G)| \sum_{h' \in V(H)} d_H(h, h') \\
&= |V(H)| d_G(g) + |V(G)| d_H(h). \qquad (2)
\end{aligned}
$$

Equation (2) has several consequences. First of all,

$$
\dim_W(G \square H) = |\{|V(H)| \, d_G(g) + |V(G)| \, d_H(h) \mid g \in V(G), h \in V(H)\}|.
$$

Consequently,

$$
\max\{\dim_W(G), \dim_W(H)\} \leq \dim_W(G \square H) \leq \dim_W(G)\dim_W(H).
$$

For our purposes, we apply Equation (2) as follows:

Corollary 3.2. *Let G be a graph and let H be a graph with $\dim_W(H) = 1$. Then $\dim_W(G \square H) = \dim_W(G)$.*

Proof. Since $\dim_W(H) = 1$, there exists a constant s such that $d_H(h) = s$ for any $h \in V(H)$. Then by (2), $d_{G \square H}((g,h)) = |V(H)|d_G(g) + |V(G)|s$ for any vertex $(g,h) \in V(G \square H)$. The conclusion is then clear. $\square$

Now everything is ready for the main result of this section. Since the only graphs of diameter one are complete graphs, their Wiener dimension is not interesting. However, for diameter at least two we have:

Theorem 3.3. *For any $D \geq 2$, and any $k \geq 1$ there exists a graph G such that* $\mathrm{diam}(G) = D$, *and* $\dim_W(G) = k$.

Proof. For $d \geq 2$ and $k = 1$ note that $\mathrm{diam}(C_{2D}) = D$ and $\dim_W(C_{2D}) = 1$. Hence it remains to prove the theorem for any $D \geq 2$ and any $k \geq 2$.

Let G_k, $k \geq 2$, be the graph defined as follows: $V(G_k) = \{1, 2, \ldots, k+1\}$ and $ij \in E(G_k)$ whenever $i + j \leq k + 2$. The vertex 1 of G_k is of degree k, and since G_k is not a complete graph we first get that $\mathrm{diam}(G_k) = 2$. Moreover, the degree sequence of G_k is $k, k-1, \ldots, k/2+1, k/2, k/2, k/2-1, \ldots, 2, 1$ when k is even and $k, k-1, \ldots, (k+1)/2+1, (k+1)/2, (k+1)/2, (k+1)/2-1, \ldots, 2, 1$ when k is odd. In any case, Lemma 3.1 implies that for any $k \geq 2$, $\dim_W(G_k) = k$.

So G_k, $k \geq 2$, is a graph with $\mathrm{diam}(G_k) = 2$, and $\dim_W(G_k) = k$. Let now $D \geq 3$, and let H be an arbitrary vertex-transitive graph of diameter $D-2$. (Say, $H = Q_{D-2}$.) Then since $\mathrm{diam}(G \square H) = \mathrm{diam}(G) + \mathrm{diam}(H)$, we have $\mathrm{diam}(G_k \square H) = 2 + (D-2) = D$ and by Corollary 3.2, $\dim_W(G_k \square H) = k$. $\square$

4 Graphs with Wiener dimension 1

In this section we consider graphs with Wiener dimension 1. Examples of such graphs are vertex-transitive graphs, but there are other examples as well. We construct an infinite family of non-vertex-transitive graphs with Wiener dimension 1. We also show that a graph of dimension 1 is 2-connected.

Let $\mathrm{Aut}(G)$ denote the automorphism group of the graph G. Let $u, v \in V(G)$ and

$\alpha \in \text{Aut}(G)$ be such that $\alpha(u) = v$. Then, since α preserves distances, we have

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

This means that vertices of the same orbit of the automorphism group of a graph G have the same distance; in particular, $\dim_W(G) = 1$ holds for vertex-transitive graphs G. Using (1) again we thus have:

Corollary 4.1. ([25]) *Let G be a vertex-transitive graph and $u \in V(G)$. Then $W(G) = |V(G)| d_G(u)/2$.*

Zhang and Li [25] extended this result by considering a subgroup of $\text{Aut}(G)$ and its orbits. The approach using Corollary 4.1 (and its edge-transitivity variation) was applied in [6].

On the other hand, $d_G(u) = d_G(v)$ does not necessarily imply that u and v are in the same orbit of $\text{Aut}(G)$ as we have already observed in Fig. 1. Note in addition that the graph G from the figure is asymmetric.

Theorem 4.2. *There exists a family of graphs $\{G_k\}_{k \geq 0}$ such that G_k is non-vertex-transitive and $\dim_W(G_k) = 1$.*

Proof. Set G_0 to be the Tutte 12-cage. It is well-known that it is not vertex-transitive and we checked (using computer) that $\dim_W(G_0) = 1$. Set now $G_k = G_0 \,\square\, Q_k$, $k \geq 1$, where Q_k is the k-dimensional cube. Since a Cartesian product has transitive automorphism group if and only if every factor has transitive automorphism group, cf. [8, Theorem 6.17], we get that G_k, $k \geq 1$, is not vertex-transitive. On the other hand, since Q_k is vertex-transitive, $\dim_W(Q_k) = 1$ and hence by Corollary 3.2, $\dim_W(G_k) = 1$. $\square$

It is clear from the above proof that the same effect could also be obtained by considering Cartesian powers of the Tutte 12-cage, that is, G_0^k, $k \geq 1$, are not vertex-transitive but have Wiener dimension 1.

The Tutte 12-cage is an example of a semisymmetric graph, where a graph G is called *semisymmetric* if G is regular, edge-transitive but not vertex-transitive [5]. Of course, $1 \leq \dim_W(G) \leq 2$ holds for any semisymmetric graph G. We have checked the Wiener dimension of the four smallest cubic semisymmetric graphs. Interestingly,

two of them, namely the Gray graph and the Ljubljana graph have Wiener dimension 2, while the other two—the 110-Iofinova-Ivanov graph and the Tutte 12-cage—have Wiener dimension 1. It seems an interesting problem to characterize semisymmetric graphs with Wiener dimension 2.

We conclude with the following structural property of graphs of dimension 1:

Proposition 4.3. *If* $\dim_W(G) = 1$*, then* G *is 2-connected.*

Proof. Suppose on the contrary that x is a cut-vertex of G. Let G_1 be an arbitrary connected component of $G - x$ and let G_2 be the remaining graph of $G - x$. Let $|G_1| = n_1$ and $|G_2| = n_2$, so that $|G| = n_1 + n_2 + 1$. Let y be a neighbor of x from G_1. Denote by $\bar{d}_{G_1}(x)$ and $\bar{d}_{G_2}(y)$ the sum of the distances between the vertex x (resp. y) and all the vertices from G_1 (resp. G_2), i.e.

$$\bar{d}_{G_1}(x) = \sum_{v \in G_1} d_G(x, v) \ \text{ and } \ \bar{d}_{G_2}(y) = \sum_{v \in G_2} d_G(y, v) \, .$$

Then

$$\begin{aligned} \bar{d}_{G_1}(x) &\leq \bar{d}_{G_1}(y) + n_1 \, , \\ \bar{d}_{G_2}(y) &= \bar{d}_{G_2}(x) + n_2 \, . \end{aligned}$$

Summing up these inequalities we get

$$\bar{d}_{G_1}(x) + \bar{d}_{G_2}(x) + n_2 \leq \bar{d}_{G_1}(y) + \bar{d}_{G_2}(y) + n_1 \, .$$

Since $d_G(x) = \bar{d}_{G_1}(x) + \bar{d}_{G_2}(x)$ and $d_G(y) = \bar{d}_{G_1}(y) + \bar{d}_{G_2}(y) + 1$ if follows that

$$d_G(x) + n_2 \leq (d_G(y) - 1) + n_1 \, .$$

Therefore, $n_2 < n_1$. On the other hand, selecting a neighbor of x in G_2, an analogous argument gives $n_1 < n_2$, a contradiction. $\qquad\square$

As cycles show, in the above proposition 2-connectivity cannot be improved to 3-connectivity. We next show that there are other examples of graphs with Wiener dimension 1 which are 2-connected but not 3-connected.

Let $G_{2k+1,b}$ be a graph constructed from $2k + 1$ copies of the complete graph K_b, and $2k + 1$ isolated vertices. Connect each isolated vertex to all the vertices from two
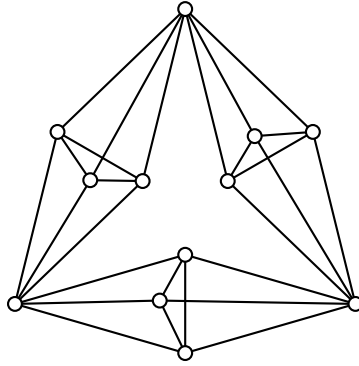
Figure 3: The graph $G_{3,3}$

copies of K_b in such a way that each vertex from K_b is connected to precisely two isolated vertices. Fig. 3 depicts the graph $G_{2k+1,b}$ for $k = 1$ and $b = 3$.

Graphs $G_{2k+1,b}$ are not 3-connected, but $\dim_W(G_{2k+1,b}) = 1$. Due to the symmetry of the graph we only need to consider two types of vertices. Let x be an arbitrary vertex connected with two different subgraph K_b, and let y be an arbitrary inner vertex of some K_b. Then by a simple calculation we find that

$$d_{G_{2k+1,b}}(x) = 2k(1+k) + b(1 + 2k + 2k^2) = d_{G_{2k+1,b}}(y),$$

hence $\dim_W(G_{2k+1,b}) = 1$.

5 The Wiener dimension of $(5,0)$-nanotubes

A *fullerene graph* is a 3-connected 3-regular planar graph with only pentagonal and hexagonal faces. By Euler's formula, the number of pentagonal faces is always twelve. Grűnbaum and Motzkin [11] showed that fullerene graphs with n vertices exist for all even $n \geq 24$ and for $n = 20$. Although the number of pentagonal faces is negligible compared to the number of hexagonal faces, their layout is crucial for the shape of fullerene graphs.

Nanotubical graphs or simply *nanotubes* are cylindrical fullerene graphs with each of the two ends capped by a subgraph containing six pentagons and possibly some hexagons called *caps*, and a "cylindrical" part.

The cylindrical part of the nanotube is determined by the (p_1, p_2)-vector that de-

fines the way an infinite hexagonal grid is wrapped in order to get the cylindrical part (the tube). The numbers p_1 and p_2 denote the coefficients of the linear combination of the unit vectors $\vec{a}_1$ and $\vec{a}_2$ such that the vector $p_1\vec{a}_1 + p_2\vec{a}_2$ joins pairs of identified points, i.e. the integers p_1 and p_2 denote the number of unit vectors along two directions in the honeycomb lattice. We can always assume that $p_1 \geq p_2$ since we want to avoid the mirror effect. Fig. 4 shows the construction of the cylindrical part of a $(4,3)$-nanotube.
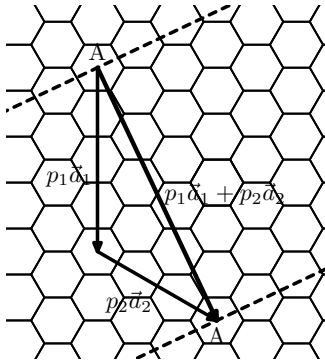

Figure 4: Construction of the cylindrical part of a $(4,3)$-nanotube. The hexagons with the same name overlap.

Here we will consider the $(5,0)$-nanotubes, such nanotubes belong to the family of zig-zag nanotubes. More precisely, *zig-zag nanotubes* are nanotubes with $p_2 = 0$. The two caps of a $(5,0)$-nanotube are identical, and comprised only from six pentagons, one of which is central. Due to this fact the $(5,0)$-nanotubes can be represented as shown in Fig. 5. Such a fullerene has $10k$, $k \geq 2$, vertices and will be denoted in the rest with C_{10k}.

From [1] we recall the following result on the diameter of $(5,0)$-nanotubes:

Theorem 5.1. *If $k \geq 5$, then* $\operatorname{diam}(C_{10k}) = 2k - 1$.

Let p be the central pentagon in one of the caps of C_{10k}, that is, p is the pentagon adjacent to five other pentagons. Let the central pentagon in the other cap be denoted by p'. We define L_0 to be the set of all incident vertices to p as an initial layer and $F_0 = \{p\}$. Inductively, having defined the sets L_{i-1} and F_{i-1}, L_i is the set of vertices incident with F_{i-1}, not contained in L_{i-1}. Furthermore, F_i is the set of faces incident with L_i that are not contained in F_{i-1}. For an edge $e = uw$, where $u, w \in V(G)$, we
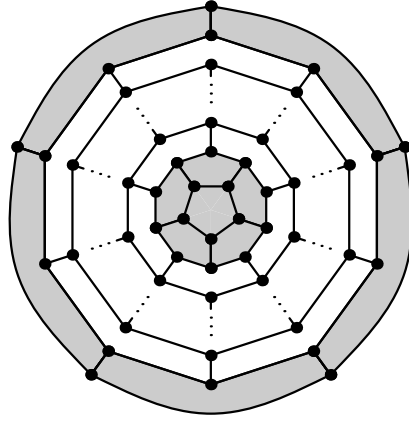
Figure 5: A $(5, 0)$-nanotube. The shaded faces are pentagons including the outer face.

say that it is an *incoming* edge to L_i if $u \in L_{i-1}$ and $w \in L_i$. If e is an incoming edge to L_i, then we also say that e is an *outgoing* edge from L_{i-1}. The vertex u is an *outgoing* vertex, and w is an *incoming* vertex, respectively. Notice that a vertex cannot be outgoing and incoming at the same time; all the vertices in the last layer are incoming, and those in the first layer are outgoing vertices.

The vertices of C_{10k} are grouped into $k + 1$ layers $L_0, L_1, \ldots, L_k$, such that L_0 and L_k have five vertices, while the remaining layers have 10 vertices each. The vertices of C_{10k} can also be grouped into layers with respect to the other central pentagon p'. Let the i-th layer with respect to the pentagon p' be denoted by L_i', $0 \le i \le k$. Observe that $L_i = L_{k-i}'$. Even more, if v is an incoming vertex for the layer L_i, then the vertex v is an outgoing vertex for L_{k-i}' and vice versa. Similarly holds for incoming and outgoing edges.

The smallest $(5, 0)$-nanotube is the dodecahedron C_{20} created only by the two caps. This fullerene has full icosahedral symmetry, and therefore its Wiener dimension is one. Using the powers of the adjacency matrix [10] of C_{30}, C_{40}, and C_{50}, we calculate that $\dim_W(C_{30}) = 3$, $\dim_W(C_{40}) = 4$, and $\dim_W(C_{50}) = 5$. Even more, we find the following:

- For C_{30}, i.e. $k = 3$, the vertices from L_0 and L_3 have distance 99, the incoming vertices from L_1 and outgoing vertices from L_2 have distance 95, and the outgoing vertices from L_1, as well as incoming vertices from L_1 have distance 93.

- For C_{40}, i.e. $k = 4$, we find 4 classes of vertices: vertices from $L_0 \cup L_4$ with distance 166, incoming vertices from layer L_1 and outgoing vertices from layer L_3 with distance 155, outgoing vertices from L_1 and incoming vertices from L_2 have distance 148, and vertices from L_2 with distance 138.

- For C_{50}, i.e. $k = 5$, there are 5 different classes of vertices, each of them having 10 vertices. The first class contains all the vertices from the first and last layer. These vertices have distance 251. The incoming vertices from L_1 and outgoing from L_4 are in the second class of vertices with distance 231. The outgoing vertices from L_2 and incoming vertices from L_4 have distance 218, and they form the third class. The remaining vertices from $L_2 \cup L_4$ have distance 198. The vertices from the layer L_3 are in the last class with distance 193.

These computations motivated the following result:

Theorem 5.2. *If $k \geq 3$, then* $\dim_W(C_{10k}) = k$.

Proof. The assertion is true for $k = 3, 4, 5$ by the above computations. In what follows we assume that $k \geq 6$.

From the fullerene's structure and its symmetry it follows that all the incoming (resp. outgoing) vertices from the same layer have the same distance. Even more, an outgoing (resp. incoming) vertex from the layer L_i has the same distance as an incoming (resp. outgoing) vertex from the layer L_{k-i}. Observe that with this, we divide the vertices into k classes (each containing ten vertices) such that the vertices in the same class have the same distance. This observation gives the upper bound $\dim_W(C_{10k}) \leq k$.

In the sequel we show that vertices from different classes have different distances, which will establish the theorem. More precisely, we will show that the distance of the vertices is decreasing when the vertices are "farther" from the central pentagon. Because of the symmetry we only consider vertices from "one half" of C_{10k}, i.e. layers $L_0, L_1, \ldots, L_{\lfloor k/2 \rfloor}$. Also from each layer we take only two representatives: one incoming, and one outgoing vertex. Notice that if k is even, all of the vertices from $L_{k/2}$ have equal distances (belong to the same class).

Denote by

$$d_i^{out}(u) = \sum_{w \in L_0 \cup \cdots \cup L_i} d(u, w),$$

the sum of all the distances between an outgoing vertex $u \in L_i$ to the vertices from the layers L_j, where $0 \le j \le i$, and

$$d_i^{in}(v) = \sum_{w \in L_0 \cup \cdots \cup L_{i-1}} d(v, w),$$

the sum of all the distances between an incoming vertex $v \in L_i$ to the vertices from the previous layers L_j, $0 \le j < i$.

Let u be a vertex from layer L_i, $0 < i < k$. Then

$$d_{C_{10k}}(u) = \sum_{v \in V(C_{10k})} d(u, v) = \begin{cases} d_i^{in}(u) + d_{k-i}^{out}(u) & u \text{ is incoming,} \\ d_i^{out}(u) + d_{k-i}^{in}(u) & u \text{ is outgoing.} \end{cases} \tag{3}$$

If a vertex belongs to L_0 or L_k, then the following claim holds.

Claim 1. If $u \in L_0 \cup L_k$, then $d_{C_{10k}}(u) = 26 + 5k(2k - 1)$.

Using the adjacency matrix of C_{60}, we find that $d_{C_{60}}(u) = 356$, and that confirms the claim for $k = 6$. Let assume that the claim holds for C_{10k}, $k \ge 6$. The fullerene $C_{10(k+1)}$ can be constructed when 5 outgoing vertices are added in L_k, and new layer L_{k+1} of 5 incoming vertices is formed, in a way that the new graph is still a $(5, 0)$-nanotube. Notice that the distance between u and the new outgoing vertices in L_k is $\operatorname{diam}(C_{10(k+1)}) - 1$, and the distance between u and the vertices from the new layer L_{k+1} is $\operatorname{diam}(C_{10(k+1)})$. By induction and Theorem 5.1, we have

$$\begin{aligned} d_{C_{10(k+1)}}(u) &= 26 + 5k(2k - 1) + 5[2(k + 1) - 2 + 2(k + 1) - 1] \\ &= 26 + 5(k + 1)(2k + 1), \end{aligned}$$

which proves Claim 1.

In the following we will simplify the notations $d_i^{out}(u)$ and $d_i^{in}(u)$ to d_i^{out} and d_i^{in} respectively.

Claim 2. If $5 \le i < k$, then

$$d_i^{out} = 40 + 5i(2i + 1). \tag{4}$$

To prove the claim we again proceed by induction in a similar way as for Claim 1. The basis of it is for $k = 5$ in which case we have $d_5^{out} = 315$. The values of d_i^{out}, $i \le 5$, are given in Table 1.

i	0	1	2	3	4	5
d_i^{out}	6	39	84	144	220	315
d_i^{in}		36	79	134	204	290

Table 1: The values of d_i^{out} and d_i^{in} for $i \le 5$.

Let $v \in L_i$ be an incoming vertex, and let u be the adjacent vertex to v such that $u \in L_{i-1}$. Clearly, u is an outgoing vertex, and a shortest path from v to any vertex from L_j, $0 \le j < i$ goes through the vertex u, i.e. $d(v, x) = d(u, x) + 1$, where $x \in L_j$ and $0 \le j < i$. This observation gives us the following

$$d_i^{in} = d_{i-1}^{out} + |L_0 \cup \cdots \cup L_{i-1}| = d_{i-1}^{out} + 5 + 10(i-1) = d_{i-1}^{out} + 10i - 5.$$

After plugging this relation in (4), for $6 \le i < k$ we get

$$d_i^{in} = 40 + 5i(2i - 1). \tag{5}$$

The values of d_i^{in} for $i \le 5$ are also given in Table 1.

Now we can determine the distance of each vertex of C_{10k}. If $u \in L_i$ for $6 \le i \le k - 6$, then

$$d_{C_{10k}}(u) = \begin{cases} 80 + 5[i(2i - 1) + (k - i)(2k - 2i + 1)] & u \text{ is incoming,} \\ 80 + 5[i(2i + 1) + (k - i)(2k - 2i - 1)] & u \text{ is outgoing.} \end{cases} \tag{6}$$

The distances for $u \in L_i$, $0 \le i \le 5$ (resp. $k - 5 \le i \le k$) are calculated using Equations (3), (4), and (5), and Table 1; the results are presented in Table 2.

Let u, v be two adjacent vertices. In order to conclude the proof of the theorem we consider the following two cases:

Case 1. u and v belong to the same layer L_i, $0 < i \le \lfloor k/2 \rfloor$ (in the first half of the tube).

Let u be an incoming vertex, and v be an outgoing vertex. If k is even and $i = k/2$, then u, v belong to the layer $L_{k/2}$. From the symmetry of the $(5, 0)$-nanotube, as mention above $d_{C_{10k}}(u) = d_{C_{10k}}(v)$, i.e. u and v belong to the same class.

i	u is incoming vertex	u is outgoing vertex
0		$26 + 5k(2k - 1)$
1	$51 + 5(k - 1)(2k - 1)$	$79 + 5(k - 1)(2k - 3)$
2	$94 + 5(k - 2)(2k - 3)$	$124 + 5(k - 2)(2k - 5)$
3	$149 + 5(k - 3)(2k - 5)$	$184 + 5(k - 3)(2k - 7)$
4	$219 + 5(k - 4)(2k - 7)$	$260 + 5(k - 4)(2k - 9)$
5	$305 + 5(k - 5)(2k - 9)$	$355 + 5(k - 5)(2k - 11)$

Table 2: The distance of the vertex $u \in L_i$ for $i \leq 5$. Knowing that an incoming (resp. outgoing) vertex from L_i has the same distance as an outgoing (resp. incoming) vertex from L_{k-i}, this table also gives the distance of the vertex $u \in L_i$ for $k - 5 \leq i \leq k$.

Now, it remains to consider the cases $i \leq \lfloor (k - 1)/2 \rfloor$. From the results presented in Table 2, for $i \leq 5$ we find that $d_{C_{10k}}(u) - d_{C_{10k}}(v) = C_i + 10(k - i)$, where $C_1 = -28$, $C_2 = -30$, $C_3 = -35$, $C_4 = -41$, and $C_5 = -50$. Since $i \leq \lfloor (k-1)/2 \rfloor$, one can easily deduce that $C_i + 10(k - i) > 0$, i.e. $d_{C_{10k}}(u) > d_{C_{10k}}(v)$. For $i > 5$ we use (6), and find $d(u) - d(v) = 10(k - 2i) > 0$. Observe that the distance between L_0 and v (the smallest distance between a vertex from L_0 and v) is greater than the distance between L_0 and u.

Case 2. u and v belong to different layers, say $v \in L_i$ and $u \in L_{i-1}$.
Clearly v is an incoming, and u is an outgoing vertex. Notice that a shortest path between v and any vertex x from the layers $L_0 \cup \cdots \cup L_{i-1}$ traverses the vertex u, and vice versa the shortest path between u and any vertex y form the layers $L_i \cup \cdots \cup L_k$ passes trough v. Therefore we have $d(x, v) = d(x, u) + 1$, and $d(y, u) = d(x, v) + 1$. Now,

$$
\begin{aligned}
d_{C_{10k}}(u) - d_{C_{10k}}(v) &= \sum_{w \in V(C_{10k})} [d(u, w) - d(v, w)] \\
&= |L_i \cup \cdots \cup L_k| - |L_0 \cup \cdots \cup L_{i-1}| \\
&= 10(k - 2i) + 5,
\end{aligned}
$$

which is nonnegative since $i \leq \lfloor k/2 \rfloor$. Notice that in this case as well, the distance between v and L_0 is greater than the distance between u and L_0. $\square$

Combining Eq. (1) with the above computations we conclude the paper with the following corollary already obtained by Graovac et al [10].

Corollary 5.3. $W(C_{20}) = 500$, $W(C_{30}) = 1435$, $W(C_{40}) = 3035$, *and for $k \geq 5$,*

$$W(C_{10k}) = \frac{100}{3}k^3 + \frac{1175}{3}k - 670 \,.$$

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