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On Diameter of Nanotubical Fullerene Graphs

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Abstract

Fullerene graphs are 3-connected cubic planar graphs with only pentagonal and hexagonal faces. Nanotubes are special type of fullerene graphs determined by a vector (p, q). We show that the diameter of a (p, q)-nanotubical fullerene graph is essentially $n/(p+q)$. In addition, we determine the diameter of $(9, 0)$-isolated pentagon nanotubes.

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1 Introduction

Fullerenes [1] are polyhedral molecules made of carbon atoms arranged in pentagonal and hexagonal faces. The wide variety of fullerenes, and possible applications made the them a subject of intense experimental and theoretical investigation. One of the most important aims was to determine the structural properties of stable fullerenes. In order to achieve these goals, graph theoretical methods were applied to mathematically model fullerene molecules as fullerene graphs.

Fullerene graphs are 3-connected, cubic planar graphs with only pentagonal and hexagonal faces. Due to Euler's formula, the number of pentagonal faces in a fullerene graph is always twelve. Grűnbaum and Motzkin [2] showed that fullerene graphs with n vertices exist for all even $n \geq 24$ and for $n = 20$, i.e., there exists a fullerene graph with α hexagons where α is any non-negative integer distinct from 1. Although the number of pentagonal faces is negligible compared to the number of hexagonal faces, their layout is crucial for the shape of a fullerene graph.

If the pentagonal faces are "uniformly" distributed, we obtain fullerene graphs of icosahedral symmetry, whose smallest representative is the dodecahedron. On the other end of the spectrum, if the pentagons are grouped into two rather compact patches, we obtain a class of fullerene graphs of tubular shapes, called *nanotubes*. Carbon nanotubes were discovered by Iijima in 1991 [3].

There are fullerene graphs where no two pentagons are adjacent, i.e., each pentagon is surrounded by five hexagons. Those fullerene graphs satisfy the *isolated pentagon rule* or shortly IPR, and they are the most stable fullerenes [4], in the sense that all experimentally observed fullerenes so far are IPR. The smallest such fullerene has 60 vertices, and IPR fullerenes on n vertices exist for all even values of $n \geq 70$ [5]. The smallest isolated pentagon fullerene, also known as C_{60} or Buckminsterfullerene, has full icosahedral symmetry.

A number of graph-theoretical invariants were examined as potential stability predictors with various degrees of success. Among them are the number of pentagon adjacencies, bipartivity, independence number, the smallest eigenvalue, separator and others [6–12]. Among other graph invariants that are on the list of possible stability predictors are the number of (perfect) matchings, the saturation number, the diameter [13, 14], etc. More results and questions on fullerenes can be found in [15–18].

In [20] it was remarked that the diameter can be considered as a measure of fullerene stability. Here we are concerned with the bounds on the diameter of nanotubical fullerenes. For general fullerenes the problem was solved in [19], while the special case of highly symmetric icosahedral fullerenes was settled in [20]. The icosahedral fullerenes are defined by the Goldberg vector $\overrightarrow{G} = (i, j)$ which determines the position of the pentagons in the fullerene graph [21, 22]

Theorem 1.1. [19] *Let G be a fullerene graph with n vertices. Then,*

$$\frac{\sqrt{24n-15}-3}{6} \leq \mathrm{diam}(G) \leq \frac{n}{5}+1\,.$$

Theorem 1.2. [20] *Let G be a $(0,i)$-icosahedral fullerene graph with $i > 0$. Then* $\mathrm{diam}(G) = 6i - 1 = \sqrt{\frac{9}{5}n} - 1\,.$

Theorem 1.3. [20] *Let G be an (i,i)-icosahedral fullerene graph with $i > 0$. Then* $\mathrm{diam}(G) = 10i - 1 = \sqrt{\frac{5}{3}n} - 1.$

In the next sections we show that the diameter of a (p,q)-nanotubical fullerene F on n vertices is essentially $\dfrac{n}{p+q}$. Then, we show that the diameter of a $(9,0)$ isolated pentagon nanotube on n vertices is at most $(n+21)/9$.

2 Definitions and preliminaries

Before we determine the diameter of (p,q)-nanotubes and the diameter of isolated pentagon fullerenes, we introduce some basic definitions as well as some new notation and notions [19].

The *diameter* of graph G is the length of the shortest path between the most distanced vertices. A *patch* is a 2-connected plane graph with only pentagonal or hexagonal faces, except maybe one (the unbounded) face. All interior vertices of a patch are of degree 3, and all vertices of the exceptional face, which we consider as the *outer* face, are of degree 2 or 3. Let P be a patch with h hexagons and p pentagons. All the vertices incident to the outer face – the *boundary* of P, $b(P)$ – are of degree two or three; let the number of vertices of degree two and three on the border of P be denoted by $n_{2,b}(P)$ and $n_{3,b}(P)$, respectively. Clearly for the size of the border $|b(P)|$ holds $|b(P)| = n_{2,b}(P) + n_{3,b}(P)$. Bornhöft et al. [23] give the following relation between the number of vertices on the border and the number of pentagons in the patch.

Lemma 2.1. *Let P be a patch with p pentagons. Then $n_{2,b}(P) - n_{3,b}(P) = 6 - p$, and $|b(P)| = 2n_{3,b}(P) + 6 - p$.*

The degrees of the vertices on the boundary can be regarded as a sequence of length $|b(P)|$ whose elements are 2 and 3. An edge incident to the outer face is said to be an *i-j* edge, if it is adjacent to vertices of degrees i and j.

Inserting a face (pentagon or hexagon) to a patch P means creating a new patch from P with one face more than P such that the new face is incident to at least one edge from the outer face of P. *Removing* a face is an inverse operation of addition.

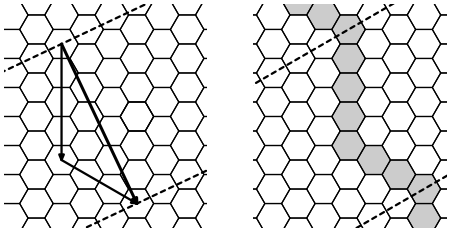

Figure 1: Construction of the cylindrical part of a $(4,3)$-nanotube (left). Ring of a $(4,3)$-infinite (hexagonal) tube (right). The shaded hexagons on the dashed lines are overlapping.

An *infinite (hexagonal) tube* is obtained from a planar hexagonal grid by identifying objects (vertices, edges, faces) lying on two parallel lines. The way the grid is wrapped is represented by a pair of integers (p, q). The numbers p and q denote the coefficients of the linear combination of the unit vectors $\vec{a}_1$ and $\vec{a}_2$ such that the vector $p\vec{a}_1 + q\vec{a}_2$ joins pairs of identified points, i.e., the integers p and q denote the number of unit vectors along two directions in the hexagonal lattice, see Figure 1 (left). We can always assume that $p \geq q$ since we want to avoid the mirror effect.

Denote by $\mathrm{Tran}_{\vec{a}}A$ a translation of an object A for a vector $\vec{a}$. Let h_0 be a hexagon of the infinite (hexagonal) tube. The set $\{h_0, h_1, \ldots, h_{p+q-1}\}$ of hexagons with $h_i = \mathrm{Tran}_{\vec{b}_i} h_0$, where $\vec{b}_i = i\vec{a}_1$ for $0 \leq i \leq p$ and $\vec{b}_i = p\vec{a}_1 + (i-p)\vec{a}_2$ for $p < i \leq p+q$, is called *ring*. See Figure 1 (right) for an illustration of a $(4,3)$-nanotube ring. Let a *tube* be a union of a series of consecutive rings. The *circumference* of a (p,q)-(nano)tube is the sum $p+q$.

Nanotubical graphs or simply *nanotubes* are cylindrical fullerene graphs with each of the two ends capped by a patch with six pentagons and possibly some hexagons – called *caps* – and a "cylindrical" part – which is actually a tube. The cylindrical part of the

nanotube is a subgraph of some (p, q)-infinite hexagonal tube, and therefore the nanotube fullerene is also called a (p, q)-nanotube.

Notice that the caps are not well defined. One can find infinitely many caps for a (p, q)-nanotube by inserting or removing a hexagonal face from a patch with six pentagons that is a subgraph of the nanotube. On the other side Brinkmann et al. [24] showed that from all possible caps for a (p, q)-nanotube, we can always choose a "nice" cap. We call a cap P *nice* if it boundary can be represented by the sequence $(23)^p(32)^q$, and at least one pentagon is incident to the boundary of P. Observe that if $p \geq q > 0$ the boundary of a nice cap has precisely one 2-2 edge and one 3-3 edge. If $q = 0$, all the edges on the boundary are 2-3 edges. Starting with any cap, and inserting or removing a hexagon finitely many times we can construct a nice cap. If the number of vertices of the nanotube is large enough compared to p and q, we can always choose the two caps such that they are nice and disjoint. Thus, as a consequence of [24], we have the following result.

Theorem 2.1. *Let F be a (p, q)-nanotube on n vertices, n large enough compared to p and q. Then, the caps P_1 and P_2 can be chosen such that they are nice and disjoint.*

Let $\mathcal{P}_{(p,q)}$ be the set of all possible nice caps for a (p, q)-nanotube. Notice that here, a cap is a patch containing six pentagon and a boundary which can be represented by the sequence $(23)^p(32)^q$, but does not have whole ring(s) of hexagons. The definition of a cap in [24] is a bit more rigorous, there a cap is the minimal fullerene patch containing six pentagons, and a boundary which can be represented by the sequence $(23)^p(32)^q$. A nice cap according to Brinkmann et al. can be transformed in to a nice cap according to current definition by inserting less than $p + q$ hexagons. Brinkmann et al. in [24, 25] give a method for constructing all possible nice caps for a (p, q)-nanotubes. Due to this result we have that $\mathcal{P}_{(p,q)}$ is a finite set.

3 Diameter of (p, q)-nanotube

In this section we determine the bounds on the diameter of (p, q)-nanotubes on n vertices. We show that the diameter od these nanotubes is essentially $n/(p + q)$.

Let F be a fullerene graph, and let P be a patch (i.e., a 2-connected subgraph) of F. We define L_1^P to be the set of vertices on the border of P as an initial layer, and F_1^P as a set of faces incident with vertex from $b(P)$ not belonging to P. The inner vertices of

P form the layer L_0^P. Inductively, having defined the sets L_{i-1}^P and F_{i-1}^P, L_i^P is the set of vertices incident with F_{i-1}^P, not contained in L_{i-1}^P. Furthermore, F_i^P is the set of faces incident with L_i^P that are not contained in F_{i-1}^P.

Let e be the edge uw, where $u, w \in V(F)$ and $u \in L_{i-1}^P$ and $w \in L_i^P$. We say that 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, and also that the vertices in the end-layer(s) are never outgoing (it may also happen that such a vertex is neither incoming).

Let v be an arbitrary vertex in F, and let P be a patch composed by the three faces incident to v. In the same manner as before we can define layers L_i^v and F_i^v with respect to the vertex v. When there is no possibility of confusion we denote the k-th layer with respect to a patch or a vertex simply by L_k.

Observe that an incoming vertex to L_k is a vertex of degree 3 on the border of the patch induced by $\cup_{i=0}^k L_i$, and the vertices of degree 2 are outgoing vertices from L_k.

The next lemma determines the distance between two consecutive layers [19].

Lemma 3.1. *For every vertex $x \in L_{i+1}^v$, $i \geq 1$, there exists a vertex $y \in L_i^v$ such that $d(x, y) \leq 2$.*

The inequality in Lemma 3.1 is tight only when x is an outgoing vertex, otherwise there is a vertex $y \in L_i^v$ adjacent to x.

Observe that the previous lemma holds when layers are defined with respect to a patch P as well.

Theorem 3.1. *Let F be a (p, q)-nanotube, $p, q \in \mathbb{N}$, on n vertices. Then, there are constants $C'_{p,q}$ and $C''_{p,q}$ such that*

$$\frac{n}{p+q} + C'_{p,q} \leq \operatorname{diam}(F) \leq \frac{n}{p+q} + C''_{p,q}\,.$$

Proof. From the structure of nanotubes it is clear that the most distanced vertices are the vertices from different caps. First, we consider the case when the number of vertices is n large enough compared to p and q. By Theorem 2.1, we can choose two nice caps.

Let the two nice caps of F be denoted by P_1 and P_2, and let T denote the cylindrical part – the tube of F. Since P_1 and P_2 are nice caps, their boundaries of can be represented as $(23)^p(32)^q$, hence, $|b(P_1)| = |b(P_2)| = 2(p+q)$, $V(T) \cap V(P_1) = b(P_1)$ and $V(T) \cap$

$V(P_2) = b(P_2)$. Let k be the number of rings in the tube T – all the rings between $b(P_1)$ and $b(P_2)$. Then the number of layers (counting $b(P_1)$ and $b(P_2)$ as layers as well) of the tube is $k+1$. Observe that the layers of T with respect to the cap P_1 (and the cap P_2) have the same size $|b(P_1)| = |b(P_2)| = 2(p+q)$.

Let $v \in L_0^{P_1}$. We claim that: *for i large enough the vertex v is equally distanced from all outgoing (resp. incoming) vertices from layer L_i with respect to the cap P_1.* Let u be one of the closest outgoing (resp. incoming) vertices from $L_0^{P_1}$. Due to the hexagonal tube properties, there are at least two closest outgoing vertex from $L_1^{P_1}$ to the vertex v, at least three from $L_2^{P_1}$, at least four from $L_3^{P_1}$, etc. As the number of the closest outgoing (resp. incoming) vertices increases in the next layer, and each layer has $p+q$ outgoing (resp. incoming) vertices, all the outgoing (resp.incoming) vertices from layer $L_{p+q-1}^{P_1}$ are equally distanced from the vertex v. In some cases this can happen even for $i < p+q-1$. This establishes the claim.

Let $\bar{d}(P)$ be the largest distance between an inner vertex of a cap P and its closest vertex of degree 2 from $b(P)$. Let $\bar{n}(P)$ be the number of inner vertices of a cap P.

Now, it is clear that $\operatorname{diam}(F) = \bar{d}(P_1) + \bar{d}(P_2) + 2(k-1) + 1$. At the same time

$$n = \bar{n}(P_1) + \bar{n}(P_2) + 2(p+q)(k+1)\,,$$

i.e.

$$k = \frac{n - \bar{n}(P_1) - \bar{n}(P_2)}{2(p+q)} - 1\,. \tag{1}$$

Plugging in (1) into the expression for the diameter we find that

$$\operatorname{diam}(F) = \bar{d}(P_1) + \bar{d}(P_2) + \frac{n}{p+q} - \frac{\bar{n}(P_1) + \bar{n}(P_2)}{p+q} - 3\,.$$

Set

$$C'_{p,q} = 2\min_{P\in\mathcal{P}}\left\{\bar{d}(P) - \frac{\bar{n}(P)}{p+q}\right\} - 3 \quad \text{and} \quad C''_{p,q} = 2\max_{P\in\mathcal{P}}\left\{\bar{d}(P) - \frac{\bar{n}(P)}{p+q}\right\} - 3\,. \tag{2}$$

As $\mathcal{P}$ is a finite set of all possible nice caps for a (p,q)-nanotube, the constants $C'_{p,q}$ and $C''_{p,q}$ are well defined. Now we have the bounds of the diameter of F

$$\frac{n}{p+q} + C'_{p,q} \le \operatorname{diam}(F) \le \frac{n}{p+q} + C''_{p,q}, \tag{3}$$

and the constants $C'_{p,q}$ and $C''_{p,q}$ are determined by (2).

Now, let consider the case when the number of vertices of F is not large enough (compared to p and q). Recall that for i not large enough (compared to p and q), some vertices from the layer L_i are closer to the vertex $v \in L_0^{P_1}$ than the others. Since P_1 and P_2 are nice caps, the boundary of P_2, $b(P_2)$, is also a layer with respect to the cap P_1. As the number of vertices is small, at least one vertex from the boundary of P_2 is closer to v. Denote this vertex by u. Additionally $\bar{d}(P_2)$ is defined as the largest distance between an inner vertex and its closer vertex of degree 2 from $b(P_2)$. We denote the corresponding vertex from $b(P_2)$ by w. As the vertices of $b(P_2)$ induce a cycle, the distance between u and v is at most half of $|b(P_2)|$, i.e., $p+q$.

If we can not choose P_1 and P_2 such that they are nice and disjoint caps, then there are no rings of hexagons. This means that the tube does not exist, and the nanotube is comprised only by the two caps with boundaries of size $2(p+q)$. Again the previous discussion holds.

Now it clear that (p,q)-nanotubes with small number of vertices (compared to p and q) will have larger diameter, and the constant $C''_{p,q}$ can increase at most $p+q$. □

In [19], the constants $C'_{p,q}$ and $C''_{p,q}$ are determined for $(5,0)$-nanotubes, i.e. nanotubes with the smallest circumference.

Theorem 3.2. *Let F be a $(5,0)$-nanotube on n vertices. Then*

$$\frac{n}{5} - 1 \leq \operatorname{diam}(F) \leq \frac{n}{5} + 1\,.$$

Next, we give the bound of the diameter of $(6,0)$-nanotubes, and hence the constants $C'_{6,0}$ and $C''_{6,0}$ for these nanotubes.

Example 3.1. *Let F be a $(6,0)$-nanotube on n vertices. There are four possible caps for a $(6,0)$-nanotube as shown of Figure 2. Each layer with respect to one of the caps on Figure 2 has precisely 12 vertices. The number of inner vertices of the cap (A), $\bar{n}_A = 6$ and the distance from from a vertex of degree two on the boundary to the most distanced inner vertex for the cap (A) is $\bar{d}_A = 2$. From Figure 2 we find that $\bar{n}_B = 8$, $\bar{n}_C = 10$, $\bar{n}_D = 12$, $\bar{n}_E = 16$, $\bar{d}_B = 3$, $\bar{d}_C = 4$, $\bar{d}_D = 4$, and $\bar{d}_E = 4$. Since $\mathcal{P} = \{A, B, C, D, E\}$, we find that $C'_{6,0} = -1$, and $C''_{6,0} = \frac{5}{3}$. With respect to Theorem 3.1 we have the following.*

Let F be a $(6,0)$-nanotube on n vertices, n large enough. Then

$$\frac{n}{6} - 1 \leq \operatorname{diam}(F) \leq \frac{n}{6} + \frac{5}{3}\,.$$

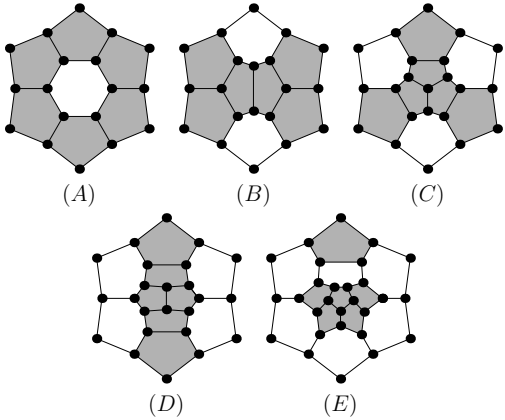

Figure 2: All possible caps for a $(6,0)$-nanotube.

If F is a $(6,0)$-nanotube with both caps (A), then $n = 12(k+2)$, where the integer k is the number of hexagonal rings. For the diameter of F the following holds:

- *if* $n \leq 36$ *then,* $\mathrm{diam}(F) = n/6 + 1 = 2k + 5$*;*
- *if* $36 < n \leq 60$ *then,* $\mathrm{diam}(F) = n/6 = 2k + 4$*;*
- *if* $n > 60$ *then,* $\mathrm{diam}(F) = n/6 - 1 = 2k + 3$*,*

what confirms the theorem.

4 Diameter of isolated pentagon $(9,0)$-nanotubes

Next we determine the diameter of isolated pentagon $(9,0)$-nanotubes as IPR nanotubes with the smallest circumference. Observe that the Buckminsterfullerene can be considered as an isolated pentagon $(9,0)$-nanotube on 60 vertices, as nanotube with no hexagonal rings. The diameter of C_{60} is 9, i.e. it holds $\mathrm{diam}(C_{60}) = \dfrac{n+21}{9}$.

Theorem 4.1. *Let F be an isolated pentagon $(9,0)$-nanotube on n vertices. Then,*

$$\mathrm{diam}(F) = \begin{cases} \dfrac{n+21}{9}, & n \in \{60, 78\} \\ \dfrac{n+12}{9}, & n \in \{96, 114, 132\} \\ \dfrac{n+3}{9}, & n > 132\,. \end{cases}$$

Proof. Observe that the isolated pentagon $(9,0)$-nanotube has uniquely determined nice cap on 39 vertices on both sides, which structure is shown in Figure 3. Aside of this, the $(9,0)$-isolated pentagon nanotube is not uniquely determined. Depending on the position of the caps (with respect to each other) and the parity of the number of rings, there are two possibilities as shown in Figures 4 and 5.

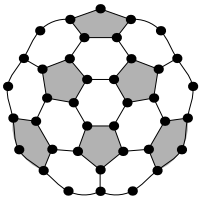

Figure 3: Nice cap of a $(9,0)$-isolated pentagon nanotube. Observe that the fullerene C_{60} is comprised only by two such, so the vertices on boundary count only once.

The cap has 21 inner vertices, 18 vertices on the border, and each layer of the tube has 18 vertices. So the total number of vertices in an isolated pentagon $(9,0)$-nanotube with k rings is $n = 2 \cdot 21 + 18(k+1) = 42 + 18(k+1)$. The number $\ell = k+1$ equals the number of layers of size 18 with respect to one of the caps (P_1), i.e., the number of layers in fullerene's tube.

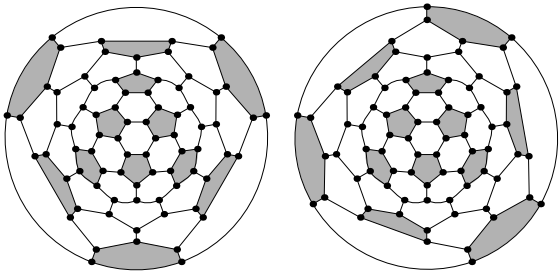

Figure 4: The only two $(9,0)$-isolated pentagon nanotubes on 78 vertices.

Let F_k be an isolated pentagon $(9,0)$-nanotube with k rings between the caps. The diameter of the graph is the distance between the most distanced vertices, in this case they belong to the different caps, and are incident to the central hexagon.

We use induction to prove the statement of the theorem. It is not difficult to determine that $\mathrm{diam}(F_1) = 10$, $\mathrm{diam}(F_2) = 12$, $\mathrm{diam}(F_3) = 14$, $\mathrm{diam}(F_4) = 16$ and $\mathrm{diam}(F_5) = 17$,

and therefore for $k = 1, 2, 3, 4, 5$ the theorem holds. Assume that the theorem holds for F_k, $k \geq 6$.

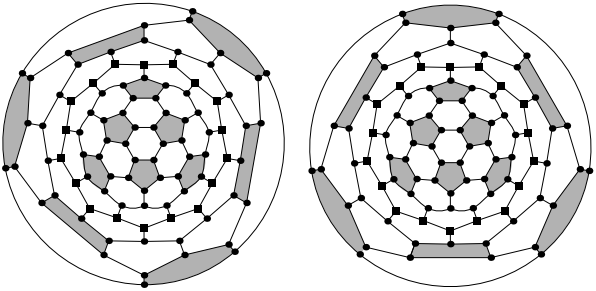

Figure 5: The only two $(9, 0)$-isolated pentagon nanotubes on 96 vertices. In each fullerene the vertices from one layer of size 18 are marked by squares.

The fullerene F_{k+1} can be easily constructed from F_k by adding one extra ring (layer) between the caps, and $|V(F_{k+1})| = |V(F_k)| + 18$. (Note that there are two isomers of F_{k+1}.) Now, we have that

$$\mathrm{diam}(F_{k+1}) = \mathrm{diam}(F_k) + 2\,,$$

i.e.

$$\mathrm{diam}(F_{k+1}) = \frac{|V(F_k)| + 3}{9} + 2 = \frac{|V(F_k)| + 18 + 3}{9} = \frac{|V(F_{k+1})| + 3}{9}\,,$$

and that completes the proof. □

Alternatively, the diameter can be calculated using the number of rings in the tube. Let F be a $(9, 0)$-isolated pentagon nanotube with k rings. As we saw in the proof of the theorem, each layer of the tube has 18 vertices, i.e., for the number of vertices of F holds $n = 42 + 18(k + 1)$. Now, the diameter of the nanotube is determined by the following:

$$\mathrm{diam}(F) = \begin{cases} 2k + 9, & k \leq 1 \\ 2k + 8, & 1 < k \leq 4 \\ 2k + 7, & k > 4. \end{cases}$$

As isolated pentagon $(9, 0)$-nanotube has the smallest circumference among all isolated pentagon nanotubes on n vertices, from Theorem 3.1 follows that among all isolated pentagon nanotubes on n vertices, $(9, 0)$-nanotube has the largest diameter. This observation gives us the upper bound on the diameter for isolated pentagon nanotubes. Notice that this bound is tight only for isolated pentagon fullerenes on 60 and 78 vertices [26].

Corollary 4.1. *Let F be an IPR nanotube on n vertices. Then*

$$\mathrm{diam}(F) \leq \frac{n+21}{9}\,.$$

We end this paper with a conjecture that the upper bound on the diameter of isolated pentagon fullerenes on n vertices is essentially $n/10$.

Conjecture 4.1. *Let F be an isolated pentagon fullerene on n vertices. If F is not a $(9,0)$-nanotube, then,*

$$\mathrm{diam}(F) \leq \frac{n}{10} + C\,,$$

for some constant C.

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