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Embeddability of open-ended carbon nanotubes in hypercubes ☆

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A graph that can be isometrically embedded into a hypercube is called a partial cube. An open-ended carbon nanotube is a part of hexagonal tessellation of a cylinder. In this article we determine all open-ended carbon nanotubes which are partial cubes.

1. Introduction

Since Iijima's original report [18], carbon nanotubes have been recognized as fascinating materials with nanometer dimensions promising exciting new areas of carbon chemistry and physics. From the viewpoint of fullerene science, carbon nanotubes are forms of giant fullerenes [23]. In 1996 Smalley group at Rice university successfully synthesized the aligned single-walled nanotubes [28], which are carbon nanotubes with the almost alien property of electrical conductivity and super-steel strength. Carbon nanotubes have attracted great attention in different research fields such as chemistry physics, artificial materials, and so on. For the details, see [14,15].

Each open-ended single-walled nanotube can be viewed as a mapping of a graphene sheet onto the surface of a cylinder [24]. In fact, open-ended nanotubes (tubules) are the basis for many research problems in physics and chemistry. For example, it has been shown that recognizing the metallic carbon nanotubes and semiconducting nanotubes depends on the size and geometry of the tubule [15].

For a graph G, let $V(G)$ and $E(G)$ denote its vertex set and edge set, respectively. The *distance* $d_G(u,v)$ between two vertices u and v of G is the length of a u,v-geodesic (i.e. a shortest path between u and v). If the graph G is clear from the context, then we will simply use $d(u,v)$. For a connected graph G, d_G is a distance function on G. For a given positive integer λ, a mapping $\phi : V(G) \to V(H)$ is called a *λ-embedding* from connected graphs G into H if, for any two vertices x, y of G, we have $d_H(\phi(x),\phi(y)) = \lambda d_G(x,y)$. If $\lambda = 1$, then ϕ is called an *isometric embedding* of G into H.

The *Cartesian product* $G \square H$ of graphs G and H is the graph with vertex set $V(G) \times V(H)$ such that the vertex (a,x) is adjacent to the vertex (b,y) whenever $ab \in E(G)$ and $x = y$, or $a = b$ and $xy \in E(H)$.

An *n-dimensional hypercube* or *n-cube* Q_n is defined as follows: The vertex set consists of all n-tuples $b_1b_2\cdots b_n$ with $b_i \in \{0,1\}$, and two vertices are adjacent if and only if the corresponding n-tuples differ in precisely one place. A graph G is called a *partial cube* (*binary Hamming graph*) [19], if G admits an isometric embedding into Q_n for some positive integer n. A connected graph G is called an *l_1-graph* if it allows a λ-embedding into a cube Q_k for some λ and k [1]. Shpectorov

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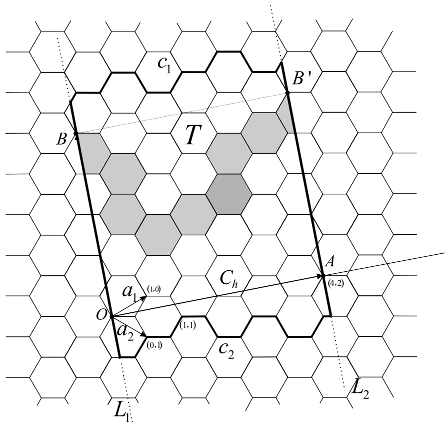


Fig. 1. Illustration for a $(4,2)$-type nanotube T. $\vec{a_1}$ and $\vec{a_2}$ are the basic lattice vectors. $\overrightarrow{OA} = 4\vec{a_1} + 2\vec{a_2}$ is the chiral vector of T and $\overrightarrow{OB}$ indicates the direction of the axis of T.

[27] showed that a graph is an l_1-graph if and only if it is isometrically embeddable into the Cartesian product of complete graphs, half-cubes, and cocktail party graphs. Deza and Laurent [9] (even Blake and Gilchrist [4] had showed earlier) showed that if G is a connected bipartite graph, then G is a partial cube if and only if G is an l_1-graph. Hence bipartite l_1-graphs coincide with partial cubes.

Many topological indices of molecules based on the distances, such as the Wiener index, the Szeged index, the PI index, etc., are related closely to their physico-chemical properties [3,25,30]. Distance between any two vertices in a hypercube is the Hamming distance, i.e. the number of different places of the two tuples [19]. If a graph is a partial cube, we can easily calculate the distances between any two vertices of the graph. So it is interesting to determine whether a graph is a partial cube. The l_1-embeddability of some chemical relevant graphs have been considered extensively.

A *benzenoid system* [17] (alias *benzenoid graph* or *hexagonal system*), is a finite connected plane graph with no cut vertices in which every interior face is bounded by a regular hexagon of side length 1. For benzenoid systems, Klavžar, Gutman and Mohar [22] showed that any benzenoid system is a partial cube. Deza and Shtogrin [10] generalized the above result to all poly-6-cycles (i.e. graphs in the plane with the vertices being of degrees 2 or 3, all the internal vertices of degree 3, and all interior faces hexagons). Zhang and Xu [32] showed that none of the coronoid system (i.e. benzenoid systems with holes) is a partial cube. Deza et al. [7] investigated the list of l_1-embeddable fullerenes and conjectured it consisting of $F_{20}(I_h)$, $F_{26}(D_{3h})$, $F_{44}(T)$, and $C_{80}(I_h)$. Here a fullerene is a 3-connected planar trivalent graph whose faces are pentagons and hexagons. Recently, Deza and Shpectorov [11] determined all finite closed polyhexes (trivalent surface graphs with hexagonal faces) which are l_1.

In this article, we consider open-ended single-walled nanotubes (nanotubes for short), which can be formed by rolling up a two-dimensional hexagonal sheet. More precisely, we define nanotubes as follows. Choose any lattice point in the plane hexagonal lattice as the origin O. Let $\vec{a_1}$ and $\vec{a_2}$ be the two basic lattice vectors (see Fig. 1). Choose a vector $\overrightarrow{OA} = n\vec{a_1} + m\vec{a_2}$ such that n and m are two integers and at least one of them is not zero. Draw two straight lines L_1 and L_2 passing through O and A perpendicular to OA, respectively. By rolling up the hexagonal strip between L_1 and L_2 and gluing L_1 and L_2 such that A and O superimpose, we can obtain a hexagonal tessellation $\mathcal{H}$ of the cylinder. L_1 and L_2 indicate the direction of the axis of the cylinder. Using the terminology of graph theory, a nanotube is defined to be the finite graph induced by all the hexagons of $\mathcal{H}$ that lie between c_1 and c_2, where c_1 and c_2 are two vertex-disjoint cycles of $\mathcal{H}$ encircling the axis of the cylinder, denoted by T. The vector $\overrightarrow{OA}$ is called the chiral vector of T, usually denoted by C_h. The cycles c_1 and c_2 are the two open-ends of T.

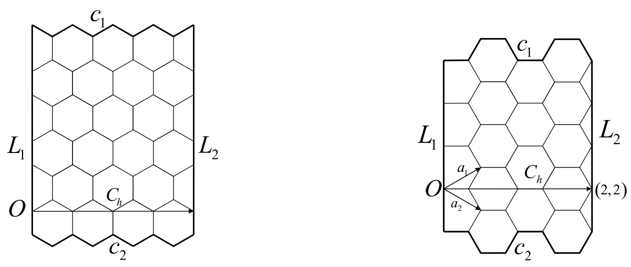
For any nanotube T, if its chiral vector is $C_h = n\vec{a_1} + m\vec{a_2}$, T will be called an (n,m)-*type* nanotube. For example, a $(4,2)$-type nanotube is shown in Fig. 1. A zigzag nanotube is an $(n,0)$ or $(0,m)$-type nanotube (see Fig. 2(a)). An armchair nanotube is an (n,n)-type nanotube (see Fig. 2(b)).

In this article, we show that all nanotubes are not partial cubes except the $(1,0)$-type, $(0,1)$-type and $(1,1)$-type nanotubes. Our main theorem is described as follows.

Theorem 1.1. *Let T be an open-ended nanotube. Then T is a partial cube if and only if T is one of the nanotubes of the following three types*: $(1,0)$-*type,* $(0,1)$-*type and* $(1,1)$-*type* (*refer to Figs.* 11(a) *and* 12(a)).

Since open-ended nanotubes are bipartite graphs [26], combining with Theorem 1.1, we can easily obtain that among all the open-ended nanotubes only the $(1,0)$-type, $(0,1)$-type and $(1,1)$-type nanotubes are l_1-graphs.

The Wiener index of a graph G is defined as the sum of all distances between pairs of vertices, denoted by $W(G)$. From this definition, John et al. [20] and Diudea et al. [12] derived explicit formulas for the Wiener indices of zigzag nanotubes and armchair nanotubes, respectively. In [21], Klavžar obtained a general method to calculate $W(G)$ of any



(a) A (4, 0)-type or (0, 4)-type nanotube. (b) A (2, 2)-type nanotube.

Fig. 2. Two special type nanotubes.

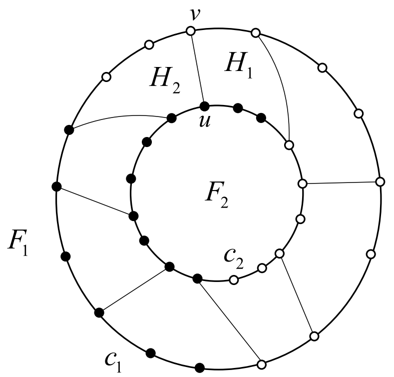


Fig. 3. A cyclic chain H is drawn on the plane with vertices in W_{uv} colored black and vertices in W_{vu} colored white.

connected graph G according to the canonical metric representation of G. If G is a partial cube, the computation of $W(G)$ can be greatly simplified. For example, as an application of partial cubes the Wiener index of a benzenoid system can be computed in linear time [6]. We have known that $W(P_n) = \frac{n^3-n}{6}$ and $W(G \,\Box\, H) = W(G) \cdot |V(H)|^2 + W(H) \cdot |V(G)|^2$ [16]. From these, the Wiener indices of (1, 0)-type, (0, 1)-type and (1, 1)-type can be easily obtained as $W(P^*_{2m}) = \frac{8m^3-2m}{6}$ and $W(P_m \,\Box\, K_2) = \frac{2}{3}m^3 + m^2 - \frac{2}{3}m$. If a molecular graph is not a partial cube, the calculation of the Wiener index will be more complicated. For general (n,m)-type nanotubes, there is no result on the Wiener index.

2. Cyclic chains

In this section we introduce the concept of a cyclic chain and explore some properties of cyclic chains. For convenience, we assume that a nanotube T is drawn in such a way that its (central) axis is vertical.

Definition 2.1. A cyclic chain of a nanotube consists of some cyclically concatenated hexagons with each hexagon adjacent to exactly two other hexagons, and encircles the axis of the nanotube. For example, see the graph shown shaded in Fig. 1.

It is easy to see that a cyclic chain of a nanotube T always exists.

Since any hexagonal tessellation of the cylinder is an infinite bipartite graph [26,31], and a cyclic chain H is its subgraph, H is also a finite bipartite graph. Let c_1 and c_2 be the top and bottom perimeter of H. We draw H in the plane such that the face F_1 surrounded by c_1 is infinite and the face F_2 surrounded by c_2 is an inner face (see Fig. 3).

For an edge uv of G, let W_{uv} be the set of vertices of G that are closer to u than to v. In symbols,

$$W_{uv} = \{x \mid d(u,x) < d(v,x)\}.$$

Notice that for any edge uv of a bipartite graph G, the set $\{W_{uv}, W_{vu}\}$ is a partition of $V(G)$. Now we color the vertices in W_{uv} black and the vertices in W_{vu} white.

An edge $e = uv$ of H is called *transversal* if $u \in c_i$ and $v \in c_j$ such that $\{i, j\} = \{1, 2\}$. Obviously, if H has at least two hexagons, then each hexagon of H has two transversal edges and each transversal edge is shared by exactly two hexagons. A transversal edge both of whose ends are colored white (black) is called a *white* (*black*) *transversal edge*.

A hexagon f of H is called *I-type* (resp. *III-type*) if $|f \cap c_1 = 1|$ and $|f \cap c_2| = 3$ (resp. $|f \cap c_1 = 3|$ and $|f \cap c_2| = 1$), otherwise it is called *II-type*.

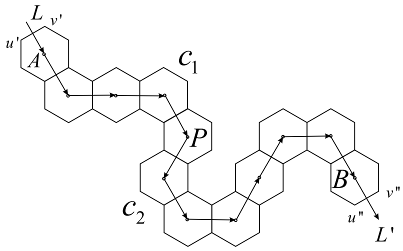


Fig. 4. A cyclic chain drawn on the plane being cut along one transversal edge uv.

The *inner dual* of a plane graph: place a vertex in the center of each interior face, and connect the centers of two interior faces by an edge when they share an edge.

Proposition 2.2. *For any cyclic chain H of a nanotube T, $|E(c_1)| = |E(c_2)|$.*

Proof. Suppose that H is a cyclic chain of a nanotube T with n hexagons. It is evident for $n = 1$. So suppose that $n \geqslant 2$. For any transversal edge uv of H, let A and B be the two hexagons of H sharing the edge uv. If H is cut along uv, then it can be unrolled onto the plane and it becomes a part of some benzenoid system **B**. Let $u'v'$ and $u''v''$ be the two edges corresponding to uv with $u'v' \in A$ and $u''v'' \in B$. Then $u'v'$ is parallel to $u''v''$ in **B** (see Fig. 4).

Draw a radial L with tail at the center of A orthogonal to $u'v'$ and draw a radial L' with head at the center of B orthogonal to $u''v''$. Since $u'v'$ and $u''v''$ are parallel, L and L' have the same direction. The inner dual of the part of **B** corresponding to H is a path P (see Fig. 4).

If we have no turns from L to L' along P, the number of edges in c_1 is $2n$ and the number of edges in c_2 is also $2n$.

If there are some turns from L to L' along P, the angle of each turn is $\frac{\pi}{3}$. Then the number of clockwise turns must be equal to the number of anticlockwise turns from L to L'. Only in this way can we arrive at L'. Without loss of generality, assume that at every clockwise turn the hexagon has three edges of c_1 and one edge of c_2, then at every anticlockwise turn the hexagon has one edge of c_1 and three edges of c_2. Each of the other hexagons has two edges of c_1 and two edges of c_2. By direct calculations, $|E(c_1)| = |E(c_2)|$. $\square$

From the proof of Proposition 2.2, it is immediate to induce the following corollary.

Corollary 2.3. *For any cyclic chain of a nanotube, the number of I-type hexagons equals that of III-type hexagons.*

Define the *length* of a cyclic chain to be the number of hexagons of it. A connected subgraph H of a graph G is said to be *isometric*, if $d_H(u, v) = d_G(u, v)$ for every pair of vertices u and v of H.

Theorem 2.4. *Each cyclic chain with minimum length in a nanotube T is an isometric subgraph of T.*

Proof. Suppose that T is a nanotube and H is a cyclic chain of T with minimum length. If H itself is the nanotube T, we are done.

Suppose, to the contrary, that H is not an isometric subgraph of T. Then there exist two vertices x and y of H such that $d_H(x, y) > d_T(x, y)$.

Let $S := \{(x, y) \in V(H) \times V(H) \mid d_H(x, y) > d_T(x, y)\}$. Choose $(u, v) \in S$ such that $d_T(u, v) = \min_{(x,y)\in S}\{d_T(x, y)\}$. Then the vertices u and v lie on the same perimeter of H. If not, assume that u and v lie in two different perimeters of H and P is a shortest path between u and v in T. Then uv cannot be an edge of T. If u and v are adjacent in T, by our choice, uv is a transversal edge of H. So $d_H(u, v) = d_T(u, v)$, which contradicts that $(u, v) \in S$. Further there exists a vertex $w \in V(P \cap H)\backslash\{u, v\}$ such that

$$d_H(u, w) + d_H(w, v) \geqslant d_H(u, v) > d_T(u, v) = d_T(u, w) + d_T(w, v). \tag{1}$$

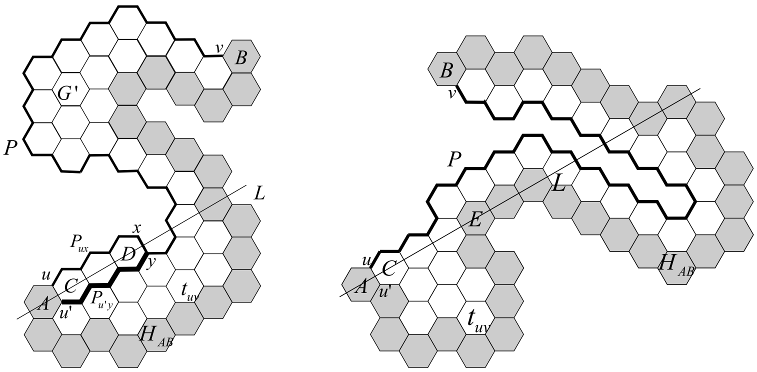
Since

$$d_H(u, w) \geqslant d_T(u, w), \tag{2}$$

and

$$d_H(w, v) \geqslant d_T(w, v), \tag{3}$$

inequality (1) induces that at least one inequality of (2) and (3) strictly holds. Without loss of generality, assume that $d_H(u, w) > d_T(u, w)$. This indicates that $(u, w) \in S$, but $d_T(u, w) < d_T(u, v)$, which contradicts the minimality of $d_T(u, v)$ in S.



(a) L first meets an edge of P in G''.

(b) L first passes through one center of a hexagon of H_{AB} in G''.

Fig. 5. Illustration for the proof of Theorem 2.4.

Without loss of generality, assume that both u and v lie on the top perimeter of H. Similarly we can show that

($*$) Every shortest path P connecting u and v in T intersects H only at u and v.

Otherwise, we can choose a common vertex w of P and H not coinciding with u and v satisfying that

$$d_H(u,w)+d_H(w,v)\geqslant d_H(u,v)>d_T(u,v)=d_T(u,w)+d_T(w,v).$$

As above discussed, either $d_H(u,w)>d_T(u,w)$ or $d_H(w,v)>d_T(w,v)$. This contradicts the minimality of $d_T(u,v)$ in S.

Then u and v must be two vertices of degree 2 in H and they lie in two certain hexagons. Without loss of generality, suppose that u lies in A and v lies in B.

Denote by t the top perimeter of H. We know that t is an even cycle [26]. Hence u and v divide t into two paths t_{uv} and t'_{uv}. Since $P\cap t=\{u,v\}$, one of the two cycles $P\cup t_{uv}$ and $P\cup t'_{uv}$ (say $P\cup t_{uv}$) is a cycle not encircling the axis of T. Let G' be the subgraph formed by the vertices and edges of hexagons lying on $P\cup t_{uv}$ and in its interior. Denote by H_{AB} the set of hexagons of H that contains at least one edge of t_{uv} (the graph shaded in Fig. 5). Since $P\cup t_{uv}$ contains no open-end of T, G' is homeomorphic to a benzenoid system. Therefore $G''=G'\cup H_{AB}$ is also homeomorphic to a benzenoid system. In the following, both G' and G'' are considered to be benzenoid systems.

Denote the hexagon of G' which contains u by C. Suppose that uu' is the edge shared by A and C. Draw a straight line L across the centers of A and C. Then the edges of G'' intersecting with L form an edge-cut of G'' [5]. So some edges of P lie on one side of L and some hexagons of H_{AB} lie on the other side of L.

Since G'' is a finite benzenoid system, along the direction of AC, L first meets an edge of P or first passes through some hexagon's center of H_{AB}.

If L first meets one edge, say xy, of P with x lying on the same side of L as u, as shown in [5], there is a unique shortest path P_{ux} in G'' connecting u and x along L (see Fig. 5(a)). And there is a unique shortest path $P_{u'y}$ in G'' connecting u' and y along L. Since $uP_{ux}xy$ is a part of P, it is a shortest path connecting u and y in G''. Obviously, $d(u,x)+d(x,y)=d(u,u')+d(u',y)$. So $uu'P_{u'y}y$ is also a shortest path connecting u and y in G''. Hence $P-(P_{ux}+xy)+(uu'+P_{u'y})$ is also a shortest path connecting u and v in T. This contradicts statement ($*$) above.

If L first passes through one center of some hexagon E of H_{AB} (see Fig. 5(b)), replace the hexagons of H_{AB} from A to E by the hexagons from A to E whose centers are passed through by L. Then we obtain a cyclic chain shorter than H, a contradiction.

So there is no such vertices u and v in S that $d_H(u,v)>d_T(u,v)$ and S is empty. This indicates that for any two vertices x and y in H, $d_H(x,y)=d_T(x,y)$ and the proof is complete. □

Proposition 2.5. *Let T be a nanotube and H a shortest cyclic chain of T with length at least three. Then every hexagonal face of H is isometric in H. Furthermore, it is isometric in T.*

Proof. By the contrary, suppose that $C=abcdefa$ is a hexagon of H which is not isometric. There exist such two vertices of C that the distance between them in H is less than that in C. Since H is bipartite, these two vertices must be the two vertices of the cycle whose distance is three in C, say a and d, which satisfy that $d_C(a,d)>d_H(a,d)$. Hence there is an edge connecting a and d in H. But except C there are at least two hexagons in H. It is impossible to connect a and d by an edge. □

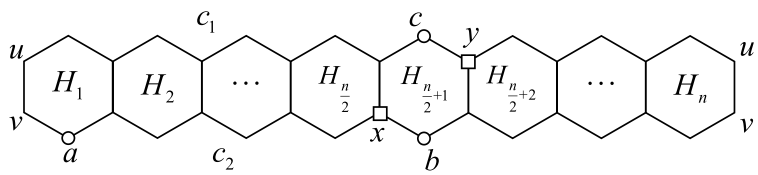


Fig. 6. A shortest cyclic chain with all hexagons of II-type and n even.

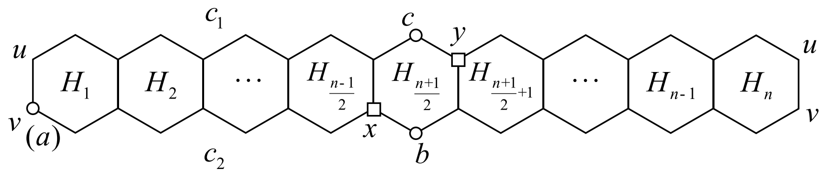


Fig. 7. A shortest cyclic chain with all hexagons of II-type and n odd.

Remark 2.6. The condition "the length of H is at least three" in Proposition 2.5 is necessary. For example, in the graph in Fig. 12(a), the vertices $u_2, v_2 \in H_2$, and $d_{H_2}(u_2, v_2) = 3$, but $d_H(u_2, v_2) = 1$.

3. Proof of the main theorem

For a graph G, if it is an l_1-graph, d_G must satisfy the following 5-gonal inequality [8]: For any five vertices x, y, a, b, c of G,

$$d(x,y) + \bigl(d(a,b) + d(a,c) + d(b,c)\bigr) \leqslant \bigl(d(x,a) + d(x,b) + d(x,c)\bigr) + \bigl(d(y,a) + d(y,b) + d(y,c)\bigr).$$

A further characterization of partial cube was obtained by Avis in 1981.

Lemma 3.1. *(See [2].) A graph G is a partial cube if and only if it is bipartite and d_G satisfies the 5-gonal inequality.*

Lemma 3.2. *Let H be a shortest cyclic chain of a nanotube T with at least two hexagons. If all the hexagons of H are II-type, then H is not a partial cube.*

Proof. Denote the hexagons of H by $H_1, H_2, \dots, H_n$ ($n \geqslant 2$) with H_i being adjacent to H_{i-1} and H_{i+1}, where i is taken modulo n. Suppose that H_1 and H_n share an edge uv with $u = H_1 \cap H_n \cap c_1$ and $v = H_1 \cap H_n \cap c_2$. Next we will show that H is not a partial cube.

Case 1. n is even. Let a be the vertex of $H_1 \cap c_2$ with $d_H(a) = 2$. Let x be the vertex of $H_{\frac{n}{2}} \cap H_{\frac{n}{2}+1} \cap c_2$, b the neighbor of x in $H_{\frac{n}{2}+1} \cap c_2$, y the vertex of $H_{\frac{n}{2}+1} \cap H_{\frac{n}{2}+2} \cap c_1$, and c the neighbor of y in $H_{\frac{n}{2}+1} \cap c_1$ (see Fig. 6).

By the symmetry of H, we can obtain that: $d(a,b) = n$, $d(b,c) = 3$, $d(a,c) = n+1$, $d(x,y) = 3$; $d(x,a) = n-1$, $d(x,b) = 1$, $d(x,c) = 2$, $d(y,a) = n$, $d(y,b) = 2$, and $d(y,c) = 1$.

So $d(a,b)+d(b,c)+d(a,c)+d(x,y) = n+3+(n+1)+3 = 2n+7$, and $d(x,a)+d(x,b)+d(x,c)+d(y,a)+d(y,b)+d(y,c) = (n-1)+1+2+n+2+1 = 2n+5$. Clearly, $d(a,b)+d(b,c)+d(a,c)+d(x,y) > d(x,a)+d(x,b)+d(x,c)+d(y,a)+d(y,b)+d(y,c)$. These five vertices violate the 5-gonal inequality.

Case 2. n is odd. Choose v as our a in the first hexagon. Let x be the vertex of $H_{\frac{n-1}{2}} \cap H_{\frac{n+1}{2}} \cap c_2$, b the neighbor of x in $H_{\frac{n+1}{2}} \cap c_2$, y the vertex of $H_{\frac{n+1}{2}} \cap H_{\frac{n+1}{2}+1} \cap c_1$ and c the neighbor of y in $H_{\frac{n+1}{2}} \cap c_1$ (see Fig. 7).

By simple calculations as Case 1, we can obtain that $d(a,b)+d(b,c)+d(a,c)+d(x,y) = n+3+(n+1)+3 = 2n+7$, and $d(x,a)+d(x,b)+d(x,c)+d(y,a)+d(y,b)+d(y,c) = (n-1)+1+2+n+2+1 = 2n+5$.

It is easy to see that these five vertices violate the 5-gonal inequality.

By Lemma 3.1, H is not a partial cube in both of the cases. □

A connected subgraph H of a graph G is said to be *convex* if each shortest path in G between any two vertices of H lies entirely in H. Let $\langle S \rangle$ denote the subgraph induced by the vertex subset S. Recall that for an edge uv of G, W_{uv} is the set of vertices of G that are closer to u than to v. Djoković characterized partial cubes in the following lemma.

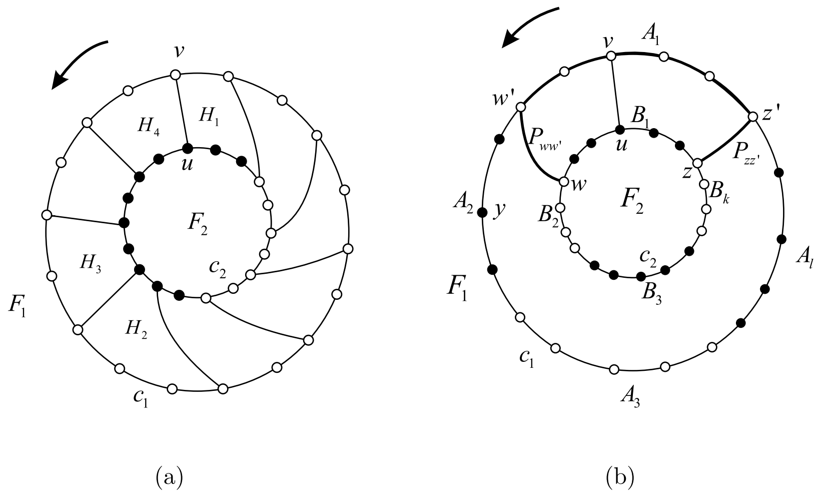


Fig. 8. Illustration for the proof of Claim 2.

Lemma 3.3. *(See [13].) Let G be a bipartite graph. Then G is a partial cube if and only if for every edge uv of G, $\langle W_{uv}\rangle$ and $\langle W_{vu}\rangle$ are convex subgraphs of G.*

Lemma 3.4. *Let H be a shortest cyclic chain with length at least three of a nanotube T. If not all the hexagons of H are II-type, then H is not a partial cube.*

Proof. In the following, H is considered to be drawn in the plane with one infinite face F_1 surrounded by c_1 and one inner face F_2 surrounded by c_2. Since not all the hexagons of H are II-type and there is at least three hexagons in H, by Corollary 2.3, there must be at least one I-type hexagon H_1 and one III-type hexagon H_2 in H. Let $d(H_1, H_2) = \min\{d_H(x, y) \mid x \in H_1,\ y \in H_2\}$. We choose a I-type hexagon H_1 and a III-type hexagon H_2 such that $d(H_1, H_2)$ is minimum. In the following, we will define the direction along c_1 from H_1 to H_2 as our direction. Without loss of generality, we assume that the direction is anticlockwise (see Fig. 8(a)). Next we will show that H is not a partial cube by the contrary. Assume that H is a partial cube. For the second transversal edge uv of H_1 with $u \in c_2$ and $v \in c_1$, by Lemma 3.3, $\langle W_{uv}\rangle$ and $\langle W_{vu}\rangle$ are convex subgraphs of H. Color the vertices in W_{vu} by white and the vertices in W_{uv} by black. It is clear that $u \in W_{uv}$ and u is colored by black.

Claim 1. *If two diametrical vertices u and u′ of a hexagon C in H (i.e., $d_C(u, u') = 3$) are colored by one color, then all the vertices of the hexagon are colored by the same color as u.*

Let $C = abcdefa$ be a hexagon of H. Suppose that a and d are colored black, i.e. a and d lie in W_{uv}. By Proposition 2.5, $d_H(a, d) = d_C(a, d) = 3$. Then $abcd$ and $afed$ are two shortest paths connecting a and d in H. Since $\langle W_{uv}\rangle$ is a convex subgraph of H, the vertices b, c, e and f all lie in W_{uv} and they must be colored black. This completes the proof of Claim 1.

Claim 2. *$\langle W_{uv} \cap c_1\rangle$ and $\langle W_{uv} \cap c_2\rangle$ are two paths in H, so are $\langle W_{vu} \cap c_1\rangle$ and $\langle W_{vu} \cap c_2\rangle$.*

Firstly we show that there are white vertices and black vertices in both c_1 and c_2. If H_1 and H_2 are adjacent, it is easy to see that there are white vertices and black vertices in both c_1 and c_2 (see Fig. 3).

If H_1 and H_2 are not adjacent, according to the choice of H_1 and H_2, the hexagons from H_1 to H_2 must be II-type. It is easy to see that there are white vertices and black vertices in c_2 (see Fig. 8(a)). If all the vertices in c_1 are white, by Claim 1 we know that H_2 has two diametrical white vertices. So all the vertices in H_2 are white. The vertices of the hexagon H_3 previous to H_2 must be all white (since H_3 is II-type). Doing this way we will find that the vertices of the hexagon H_4 (possibly identify with H_3) successive to H_1 are all white. But u and the neighbor of u in H_4 are colored black, a contradiction. Hence there are black and white vertices in both c_1 and c_2.

Secondly, we show that $\langle W_{uv} \cap c_1\rangle$ and $\langle W_{uv} \cap c_2\rangle$ are two paths in H, so are $\langle W_{vu} \cap c_1\rangle$ and $\langle W_{vu} \cap c_2\rangle$. If c_1 is divided into l ($\geqslant 2$) black and white segments denoted by $A_1, A_2, \ldots, A_l$ and c_2 into k ($k \geqslant 4$) black and white segments $B_1, B_2, \ldots, B_k$ anticlockwise (see Fig. 8(b)). Suppose that $v \in A_1$ and $u \in B_1$, then the vertices in A_1 and B_i (i even) are all white and the vertices in A_2 are black. Denote by w the first vertex of B_2, w' the last vertex of A_1, z' the first vertex of A_1 and z the last vertex of B_k. Note that w, w', z' and z are white vertices. Since $\langle W_{vu}\rangle$ is convex, the vertices of any shortest path $P_{ww'}$ connecting w and w' and the vertices of any shortest path $P_{zz'}$ connecting z and z' are all white. For any black

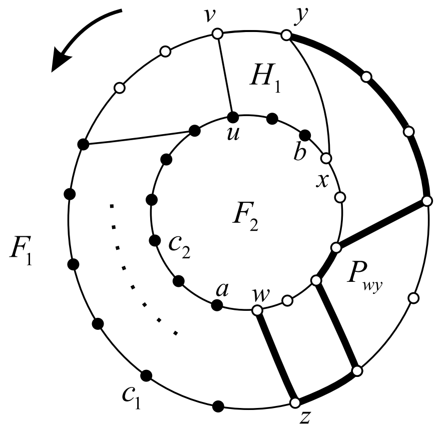


Fig. 9. Illustration for Case 1.

vertex $y \in c_1$, any shortest path P_{yu} joining y to u must intersect $P_{ww'} \cup P_{zz'} \cup \langle A_1 \rangle$ at some white vertex. This contradicts the convexity of $\langle W_{uv} \rangle$.

If c_2 is divided into at least two segments and c_1 into at least four segments, the contradiction is similar. Hence c_1, as well as c_2, consists of one path with all of whose vertices being black and the other path with all of whose vertices being white. This proves Claim 2.

Claim 3. *There must be a white transversal edge and a black transversal edge in H, i.e. $\langle W_{uv} \rangle$ and $\langle W_{vu} \rangle$ are connected in H.*

Since $\langle W_{uv} \rangle$ and $\langle W_{vu} \rangle$ are convex, it is immediate for this claim.

Recall that the direction is counterclockwise. Select the first white transversal edge from uv, say wz, and the last white transversal edge, say xy, with $w, x \in c_2$ and $z, y \in c_1$. So xy and uv lie in the same hexagon H_1 and y is adjacent to v. Let a be the previous vertex of w in c_2 and b the neighbor of x in H_1 (see Fig. 9). Since $d(u, b) = 2$ and $d(v, b) = 3$, the vertex b is colored black.

Case 1. a is colored black (see Fig. 9).

Claim 4. $d(a, u) = d(w, v)$.

Since a is black and w is white, $d(a, u) = d(a, v) - 1$ and $d(w, v) = d(w, u) - 1$. We use contrary, suppose that $d(a, u) \neq d(w, v)$. If $|d(a, u) - d(w, v)| = 1$, then $P_{au} + uv + P_{vw} + wa$ is a closed odd walk, here P_{au} is a shortest a, u-path, P_{vw} is a shortest v, w-path, and "+" denotes the union of graphs. Then there is an odd cycle in H [29, Lemma 1.2.15], which contradicts the fact that H is bipartite. If $d(a, u) \geqslant d(w, v) + 2$, then $d(a, u) \geqslant d(w, v) + 2 > d(w, v) + d(w, a) \geqslant d(a, v)$. This contradicts $d(a, u) = d(a, v) - 1$. If $d(w, v) \geqslant d(a, u) + 2$, we can similarly obtain a contradiction and the proof of Claim 4 is complete.

Let P_{wy} be a shortest path joining w to y in H. Since w and y are white and $\langle W_{vu} \rangle$ is a convex subgraph of H, all of the vertices of P_{wy} are colored white. Suppose the length of P_{wy} equals p.

The vertex y lies in a shortest path between w and v. Otherwise, any shortest path connecting w and v must pass through the vertices from v to z in c_1. By the convexity of $\langle W_{vu} \rangle$, all the vertices from v to z in c_1 are white. At the same time, the vertices w, z, x and y are white, so the black vertices in c_1 cannot arrive at u by a shortest path without including white vertices. This contradicts the convexity of $\langle W_{uv} \rangle$.

By Claim 4, $d(a, u) = d(w, v) = d(w, y) + d(y, v) = p + 1$. Since a and b are black, all shortest paths between a and b must pass through u. Since $d(u, b) = 2$,

$$d(a, b) = d(a, u) + d(u, b) = (p + 1) + 2 = p + 3.$$

We are known that $aw + P_{wy} + yx + xb$ is a walk that connects a and b. Then the length of any shortest a, b-path is no more than

$$d(a, w) + d(w, y) + d(y, x) + d(x, b) = 1 + p + 1 + 1 = p + 3.$$

This indicates that we can find a shortest a, b-path with length no more than $p + 3$ passing through white vertices, which contradicts the convexity of $\langle W_{uv} \rangle$. So H is not a partial cube.

Case 2. a is colored white.

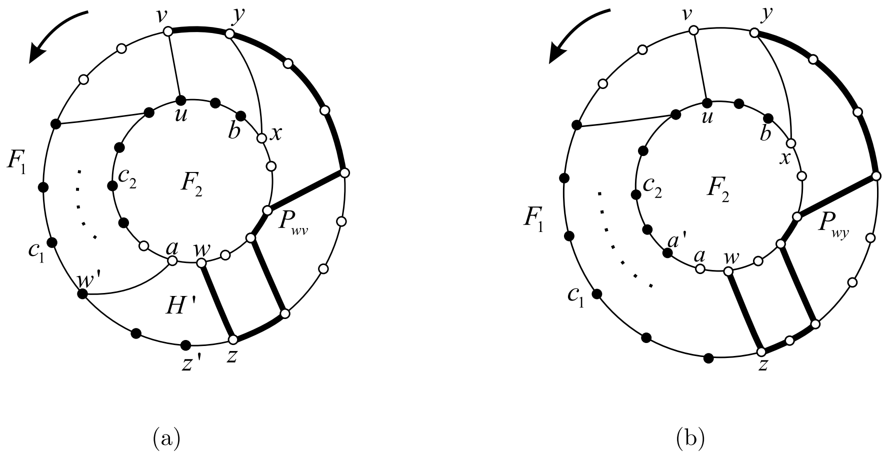


Fig. 10. (a) Illustration for the proof of Claim 5; (b) a is colored white and the previous vertex a' of a is colored black.

Claim 5. $d_H(a) = 2$.

Suppose not, then $d_H(a) = 3$ and a, w and z lie in the same hexagon H'. In H', denote the neighbor of a in c_1 by w' and the neighbor of z in c_1 by z' (see Fig. 10(b)). Then w' and z' must be black vertices. Otherwise, wz cannot be the first white transversal edge. As shown in Claim 4, $d(a, v) = d(w', u)$. Since w' is black, due to the convexity of $\langle W_{uv}\rangle$, any shortest w', u-path consists of black vertices. Because a and w are white, any shortest a, v-path must pass through the vertex w. Otherwise, there is a shortest a, v-path which does not pass through the vertex w. Then the shortest a, v-path must intersect some shortest w', u-path at a black vertex, which contradicts the convexity of $\langle W_{vu}\rangle$. Since z' is black and z is white, any shortest z', u-path must pass through w'. Therefore,

$$d\big(z', u\big) = d\big(z', w'\big) + d\big(w', u\big) = 2 + d(a, v) = 2 + \big(d(w, v) + 1\big) = d(w, v) + 3.$$

Let P_{wv} be a shortest path connecting w and v in H. Choose the walk $z'z + zw + P_{wv} + vu$ connecting z' and u. Then the length of any shortest z', u-path is no more than

$$d\big(z', z\big) + d(z, w) + d(w, v) + d(v, u) = d(w, v) + 3.$$

This illustrates that we can find a shortest z', u-path which passes through white vertices. But this contradicts the convexity of $\langle W_{uv}\rangle$ and Claim 5 is proved.

By Claim 5, the previous neighbor of a in c_2, say a', must be colored black (see Fig. 10(b)). Otherwise, wz cannot be the first white transversal edge.

It is clear that every shortest path between a and v passes through w and y, therefore $d(a, v) = d(a, w) + d(w, y) + d(y, v) = p + 2$. As shown in Claim 4, $d(a', u) = d(a, v) = p + 2$. Since a' and b are black vertices, all shortest a', b-paths must pass through u. Then

$$d\big(a', b\big) = d\big(a', u\big) + d(u, b) = p + 4.$$

Choose the walk $a'a + aw + P_{wy} + yx + xb$ connecting a' and b. Obviously, the length of any shortest a', b-path is no more than

$$d\big(a', a\big) + d(a, w) + d(w, y) + d(y, x) + d(x, b) = p + 4.$$

This indicates that we can find a shortest a', b-path with length no more than $p + 4$ which passes through some white vertices. So $\langle W_{uv}\rangle$ is not convex.

Summarizing the above two cases, we know that $\langle W_{uv}\rangle$ is not convex. By Lemma 3.3, H is not a partial cube. □

Since l_1-graphs allow multiple edges, our definition does not exclude multiple edges in G. Let P_m be the path of order m and K_2 the complete graph on two vertices. Denote by P^*_{2m} the graph obtained from P_{2m} by adding multiple edges from the very beginning of P_{2m} on every second edge (see Fig. 11(b)).

A graph is a *median graph* if there exists a unique vertex x to every triple of vertices u, v, and w such that x lies simultaneously on a shortest u, v-path, a shortest u, w-path, and a shortest w, v-path.

Lemma 3.5. *(See [19, Propositions 1.26, 1.38 and 2.22].)*

1. *Trees are median graphs.*

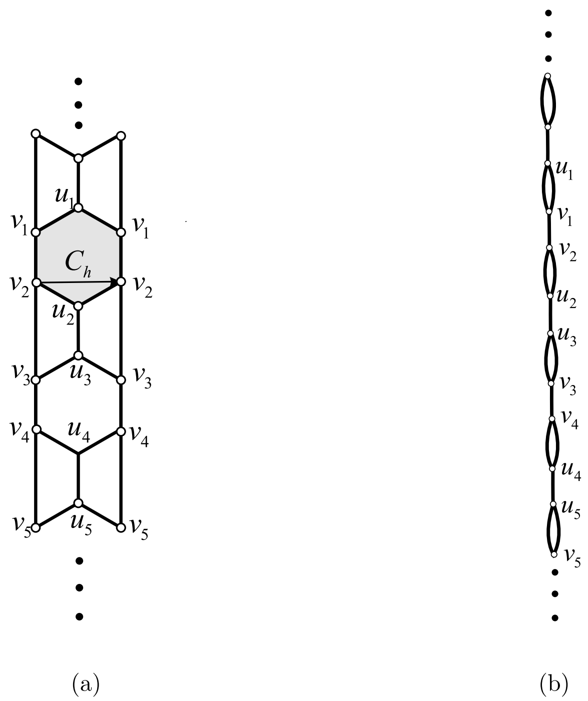


Fig. 11. (a) A $(1,0)$-type or $(0,1)$-type nanotube. The vertices with the same label are identified; (b) P^*_{2m}.

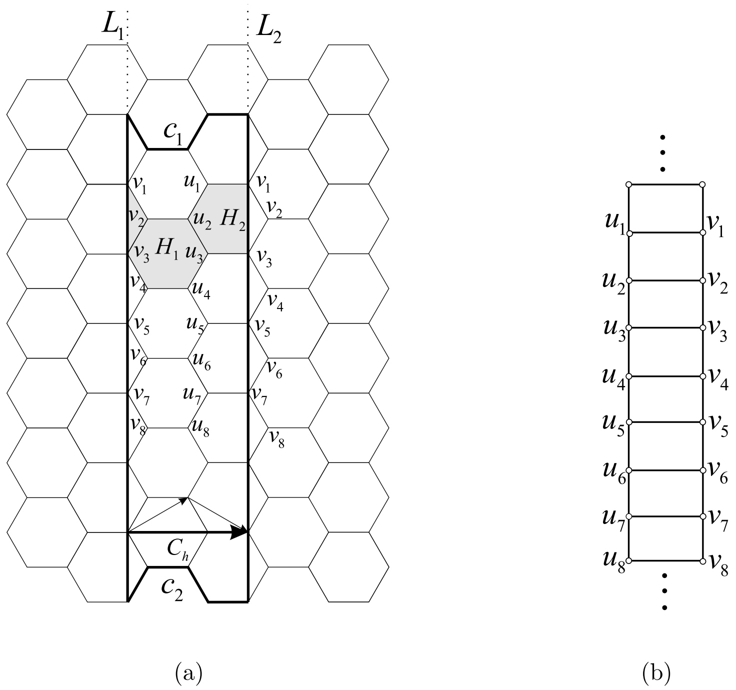


Fig. 12. (a) A $(1,1)$-type nanotube whose shortest cyclic chain has exactly one I-type hexagon and one III-type hexagon; (b) $P_m \,\square\, K_2$.

2. *Cartesian products of median graphs are median graphs.*
3. *Median graphs are partial cubes.*

Proof of Theorem 1.1. Suppose that T is an open-ended nanotube and H is a cyclic chain of T with minimum length. Suppose that H has exactly n hexagons. By Theorem 2.4, H is an isometric subgraph of T. There are two cases to consider:

Case 1. All hexagons of H are II-type.

If $n = 1$, cut T along a straight line parallel to its axis, then T is turned into the graph as indicated in Fig. 11(a). Since T is finite, if all the vertices of T are labeled, it is easy to see that it is the graph P^*_{2m} for some integer m. Suppose that $P^*_{2m} = v_1 v_2 \ldots v_{2m}$ such that v_i is adjacent to v_{i+1}, $1 \leqslant i \leqslant 2m-1$. Define a mapping ϕ from $V(P^*_{2m})$ to $V(Q_{2m-1})$ such that $\phi(v_i) = (\underbrace{1, \ldots, 1}_{i-1}, \underbrace{0, \ldots, 0}_{2m-i})$. It is clear to verify that $d_{P^*_{2m}}(v_i, v_j) = |j - i| = d_{Q_{2m-1}}(\phi(v_i), \phi(v_j))$ for any $v_i, v_j \in V(P^*_{2m})$. Hence P^*_{2m} a partial cube. In the (n, m) notation of nanotubes, this nanotube is a $(1, 0)$-type or $(0, 1)$-type nanotube.

If $n \geqslant 2$, by Lemma 3.2, H is not a partial cube. Therefore, T is not a partial cube.

Case 2. Not all the hexagons of H are II-type. By Corollary 2.3, we know that H has at least two hexagons.

If $n = 2$, by Corollary 2.3, there is exactly one I-type hexagon H_1 and one III-type hexagon H_2 in H. Cut T along a straight line parallel to the axis of T and unroll it onto the plane. Then T is turned into the graph as shown in Fig. 12(a). Since T is finite, if we label all the vertices of T, it is easy to check that this graph is indeed the graph $P_m \square K_2$ for some integer m (see Fig. 12(b)). By Lemma 3.5, $P_m \square K_2$ is a partial cube. In fact, $P_m \square K_2$ is an isometric subgraph of Q_m. In the (n, m) notation of nanotubes, this nanotube is a $(1, 1)$-type nanotube.

If $n \geqslant 3$, then by Lemma 3.4, H is not a partial cube. Hence T is not a partial cube.

Cases 1 and 2 indicate that Theorem 1.1 holds. □

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