

On the Djoković–Winkler Relation and Its Closure in Subdivisions of Fullerenes, Triangulations, and Chordal Graphs

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Abstract

It was recently pointed out that certain SiO₂ layer structures and SiO₂ nanotubes can be described as full subdivisions aka subdivision graphs of partial cubes. A key tool for analyzing distance-based topological indices in molecular graphs is the Djoković–Winkler relation Θ and its transitive closure Θ^* . In this paper we study the behavior of Θ and Θ^* with respect to full subdivisions. We apply our results to describe Θ^* in full subdivisions of fullerenes, plane triangulations, and chordal graphs.

1 Introduction

Partial cubes, that is, graphs that admit isometric embeddings into hypercubes, are of great interest in metric graph theory. Fundamental results on partial cubes are due to Chepoi [8], Djoković [13], and Winkler [32]. The original source for their interest however goes back to the paper of Graham and Pollak [18]. For additional information on partial

cubes we refer to the books [12, 16], the semi-survey [26], recent papers [1, 7, 24], as well as references therein.

Partial cubes offer many applications, ranging from the original one in interconnection networks [18] to media theory [16]. Our motivation though comes from mathematical chemistry where many important classes of chemical graphs are partial cubes. In the seminal paper [21] it was shown that the celebrated Wiener index of a partial cube can be obtained without actually computing the distance between all pairs of vertices. A decade later it was proved in [20], based on the Graham-Winkler's canonical metric embedding [19], that the method extends to arbitrary graphs. The paper [21] initiated the theory under the common name "cut method," while [23] surveys the results on the method until 2015 with 97 papers in the bibliography. The cut method has been further developed afterwards, see [6, 9, 25, 30, 31] for some recent results on it related to partial cubes.

Now, in a series of papers [3–5] it was observed that certain SiO_2 layer structures and SiO_2 nanotubes that are of importance in chemistry can be described as the full subdivisions aka subdivision graphs of relatively simple partial cubes. (The paper [29] can serve as a possible starting point for the role of SiO_2 nanostructures in chemistry.) The key step of the cut-method for distance based (as well as some other) invariants is to understand and compute the relation Θ^* . Therefore in [4] it was proved that the Θ^* -classes of the full subdivision of a partial cube G can be obtained from the Θ^* -classes of G . Note that in a partial cube the latter coincide with the Θ -classes.

The above developments yield the following natural, general problem that intrigued us: Given a graph G and its Θ^* -classes, determine the Θ^* -classes of the full subdivision of G . In this paper we study this problem and prove several general results that can be applied in cases such as in [3–5] in mathematical chemistry as well as elsewhere. In the next section we list known facts about the relations Θ and Θ^* as well as the distance function in full subdivisions needed in the rest of the paper. In Section 3, general properties of the relations Θ and Θ^* in full subdivisions are derived. These properties are then applied in the subsequent sections. In the first of them, Θ^* is described for fullerenes (a central class of chemical graph theory, see e.g. [2, 15, 17, 27, 28, 33, 34]) and plane triangulations. In Section 5 the same problem is solved for chordal graphs.

2 Preliminaries

If R is a relation, then R^* denotes its transitive closure. The distance $d_G(x, y)$ between vertices x and y of a connected graph G is the usual shortest path distance. If $x \in V(G)$ and $e = \{y, z\} \in E(G)$, then let

$$d_G(x, e) = \min\{d_G(x, y), d_G(x, z)\}.$$

Similarly, if $e = \{x, y\} \in E(G)$ and $f = \{u, v\} \in E(G)$, then we set

$$d_G(e, f) = \min\{d_G(x, u), d_G(x, v), d_G(y, u), d_G(y, v)\}.$$

Note that the latter function does not yield a metric space because if e and f are adjacent edges then $d_G(e, f) = 0$. To get a metric space, one can define the distance between edges as the distance between the corresponding vertices in the line graph of G . But for our purposes the function $d_G(e, f)$ as defined is more suitable.

Edges $e = \{x, y\}$ and $f = \{u, v\}$ of a graph G are in relation Θ , shortly $e\Theta f$, if $d_G(x, u) + d_G(y, v) \neq d_G(x, v) + d_G(y, u)$. If G is bipartite, then the definition simplifies as follows.

Lemma 2.1 *If $e = \{x, y\}$ and $f = \{u, v\}$ are edges of a bipartite graph G with $e\Theta f$, then the notation can be chosen such that $d_G(u, x) = d_G(v, y) = d_G(u, y) - 1 = d_G(v, x) - 1$.*

The relation Θ is reflexive and symmetric. Hence Θ^* is an equivalence relation, its classes are called Θ^* -classes. Partial cubes are precisely those connected bipartite graph for which $\Theta = \Theta^*$ holds [32]. In partial cubes we may thus speak of Θ -classes instead of Θ^* -classes. In the following lemma we collect properties of Θ to be implicitly or explicitly used later on.

Lemma 2.2 (i) *If P is a shortest path in G , then no two distinct edges of P are in relation Θ .*

(ii) *If e and f are edges from different blocks of a graph G , then e is not in relation Θ with f .*

(iii) *If e and f are edges of an isometric cycle C of a bipartite graph G , then $e\Theta f$ if and only if e and f are antipodal edges of C .*

(iv) If H is an isometric subgraph of a graph G , then Θ_H is the restriction of Θ_G to H .

If G is a graph, then the graph obtained from G by subdividing each edge of G exactly once is called the *full subdivision* (graph) of G and denoted with $S(G)$. We will use the following related notation. If $x \in V(G)$ and $e = \{x, y\} \in E(G)$, then the vertex of $S(G)$ corresponding to x will be denoted by \bar{x} and the vertex of $S(G)$ obtained by subdividing the edge e with \overline{xy} . Two edges incident with \overline{xy} will be denoted with $e_{\bar{x}}$ and $e_{\bar{y}}$, where $e_{\bar{x}} = \{\bar{x}, \overline{xy}\}$ and $e_{\bar{y}} = \{\bar{y}, \overline{xy}\}$. See Fig. 1 for an illustration.

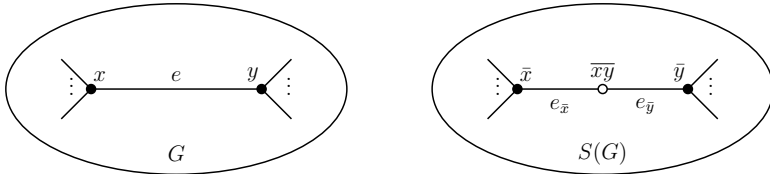


Figure 1. Notation for the vertices and edges of $S(G)$.

The following lemma is straightforward, cf. [22, Lemma 2.3].

Lemma 2.3 *If G is a connected graph, then the following assertions hold.*

- (i) *If $x, y \in V(G)$, then $d_{S(G)}(\bar{x}, \bar{y}) = 2d_G(x, y)$.*
- (ii) *If $x \in V(G)$ and $\{y, z\} \in E(G)$, then $d_{S(G)}(\bar{x}, \overline{yz}) = 2d_G(x, \{y, z\}) + 1$.*
- (iii) *If $\{x, y\}, \{u, v\} \in E(G)$, then $d_{S(G)}(\overline{xy}, \overline{uv}) = 2d_G(\{x, y\}, \{u, v\}) + 2$.*

3 Θ^* in full subdivisions

Lemma 3.1 *If G is a connected graph and $e_{\bar{x}} \Theta_{S(G)} f_{\bar{u}}$, then $e \Theta_G f$.*

Proof. Let $e = \{x, y\}$ and $f = \{u, v\}$. If $\bar{x} = \bar{u}$ and $\bar{y} = \bar{v}$, then $e_{\bar{x}} = f_{\bar{u}}$ and $e = f$, so there is nothing to prove. If $\bar{x} = \bar{v}$ and $\bar{y} = \bar{u}$, then $e_{\bar{x}}$ and $f_{\bar{u}}$ are adjacent edges which cannot be in relation $\Theta_{S(G)}$ because $S(G)$ is triangle-free. For the same reason the situation $\bar{x} = \bar{u}$ and $\bar{y} \neq \bar{v}$ is not possible. Assume next that $\bar{x} = \bar{v}$ and $\bar{y} \neq \bar{u}$. Then $d_{S(G)}(\bar{u}, \overline{xy}) = 3$ by Lemma 2.3, and hence $\overline{xy}, \bar{x}, \overline{uv}, \bar{u}$ is a geodesic containing $e_{\bar{x}}$ and $f_{\bar{u}}$, contradiction the assumption $e_{\bar{x}} \Theta_{S(G)} f_{\bar{u}}$. In the rest of the proof we may thus assume that $\{x, y\} \cap \{u, v\} = \emptyset$.

Since $S(G)$ is bipartite, in view of Lemma 2.1 we need to consider the following two cases, where, using Lemma 2.3(i), we can assume that the distances $d_{S(G)}(\bar{x}, \bar{u})$ and $d_{S(G)}(\bar{xy}, \bar{uv})$ are even. Based on the assumption $e_{\bar{x}} \Theta_{S(G)} f_{\bar{u}}$, we have $d_{S(G)}(\bar{x}, \bar{u}) + d_{S(G)}(\bar{xy}, \bar{uv}) = d_{S(G)}(\bar{x}, \bar{uv}) + d_{S(G)}(\bar{xy}, \bar{u})$ in a bipartite graph, thus the following cases.

Case 1. $d_{S(G)}(\bar{x}, \bar{u}) = d_{S(G)}(\bar{xy}, \bar{uv}) = 2k$ and $d_{S(G)}(\bar{x}, \bar{uv}) = d_{S(G)}(\bar{xy}, \bar{u}) = 2k + 1$.

In the following, Lemma 2.3 will be used all the time.

By $2k = d_{S(G)}(\bar{xy}, \bar{uv}) = 2d_G(\{x, y\}, \{u, v\}) + 2$, we get

$$k - 1 \leq d_G(y, v), d_G(x, u), d_G(x, v), d_G(y, u),$$

where the lower bound is attained at least once.

Since $d_{S(G)}(\bar{x}, \bar{u}) = 2k$, we have $d_G(x, u) = k$. Because $d_{S(G)}(\bar{x}, \bar{uv}) = 2k + 1$, we find that $d_G(x, \{u, v\}) = k$ and hence in particular $d_G(x, v) \geq k$. Similarly, as $d_{S(G)}(\bar{xy}, \bar{u}) = 2k + 1$ we have $d_G(u, \{x, y\}) = k$ and hence in particular $d_G(u, y) \geq k$. With the first observation this yields $k - 1 = d_G(y, v)$. In summary,

$$d_G(x, u) + d_G(y, v) = k + (k - 1) \neq k + k \leq d_G(x, v) + d_G(y, u),$$

which means that $e \Theta_G f$.

Case 2. $d_{S(G)}(\bar{x}, \bar{u}) = d_{S(G)}(\bar{xy}, \bar{uv}) = 2k$ and $d_{S(G)}(\bar{x}, \bar{uv}) = d_{S(G)}(\bar{xy}, \bar{u}) = 2k - 1$.

Again, $d_{S(G)}(\bar{x}, \bar{u}) = 2k$ implies $d_G(x, u) = k$. The assumption $d_{S(G)}(\bar{x}, \bar{uv}) = 2k - 1$ yields $d_G(x, \{u, v\}) = k - 1$ and consequently $d_G(x, v) = k - 1$. The condition $d_{S(G)}(\bar{xy}, \bar{u}) = 2k - 1$ implies $d_G(u, \{x, y\}) = k - 1$ and so $d_G(u, y) = k - 1$. Finally, the assumption $d_{S(G)}(\bar{xy}, \bar{uv}) = 2k$ gives us $d_G(\{x, y\}, \{u, v\}) = k - 1$, in particular, $d_G(y, v) \geq k - 1$. Putting these facts together we get

$$d_G(x, u) + d_G(y, v) \geq k + (k - 1) > (k - 1) + (k - 1) = d_G(x, v) + d_G(y, u),$$

hence again $e \Theta_G f$. ■

Lemma 3.1 implies the following result on the relation Θ^* .

Corollary 3.2 *If $e_{\bar{x}} \Theta_{S(G)}^* f_{\bar{u}}$, then $e \Theta_G^* f$.*

Proof. Suppose $e_{\bar{x}} \Theta_{S(G)}^* f_{\bar{u}}$. Then there exists a positive integer k such that

$$e_{\bar{x}} \Theta_{S(G)} f_{\bar{x}_1}^{(1)}, f_{\bar{x}_1}^{(1)} \Theta_{S(G)} f_{\bar{x}_2}^{(2)}, \dots, f_{\bar{x}_k}^{(k)} \Theta_{S(G)} f_{\bar{u}}.$$

Then, by Lemma 3.1, we have

$$e \Theta_G f^{(1)}, f^{(1)} \Theta_G f^{(2)}, \dots, f^{(k)} \Theta_G f,$$

implying that $e \Theta_G^* f$. ■

The next lemma is a partial converse to Lemma 3.1.

Lemma 3.3 *If $e \in \Theta_G f$, then there is a pair of edges $e_{\bar{x}}, f_{\bar{u}}$ in $S(G)$ such that $e_{\bar{x}} \Theta_{S(G)} f_{\bar{u}}$. Moreover, if G is bipartite, then there are two (disjoint) such pairs.*

Proof. Let $e = \{x, y\}$, $f = \{u, v\}$, and let $k = d_G(x, u)$. Since $e \in \Theta_G f$, we may without loss of generality assume that $d_G(x, u) + d_G(y, v) < d_G(y, u) + d_G(x, v)$ and that $d_G(x, u) \leq d_G(y, v)$. We distinguish the following cases.

Case 1. $d_G(y, v) = k$.

In this case, $\{d_G(x, v), d_G(y, u)\} \subseteq \{k - 1, k, k + 1\}$. Moreover, our assumption about the sum of distances implies that $\{d_G(x, v), d_G(y, u)\} \subseteq \{k, k + 1\}$. Since $e \in \Theta_G f$, the two distances cannot both be equal to k . Hence, up to symmetry, we need to consider the following two subcases.

Suppose $d_G(x, v) = d_G(y, u) = k + 1$. Then $d_{S(G)}(\bar{x}, \bar{v}) = 2k + 2$, $d_{S(G)}(\overline{xy}, \overline{uv}) = 2k + 2$, $d_{S(G)}(\bar{x}, \overline{uv}) = 2k + 1$, and $d_{S(G)}(\overline{xy}, \bar{v}) = 2k + 1$. Hence $e_{\bar{x}} \Theta_{S(G)} f_{\bar{v}}$.

Suppose $d_G(x, v) = k$ and $d_G(y, u) = k + 1$. Then $d_{S(G)}(\bar{y}, \bar{u}) = 2k + 2$, $d_{S(G)}(\overline{xy}, \overline{uv}) = 2k + 2$, $d_{S(G)}(\bar{y}, \overline{uv}) = 2k + 1$, and $d_{S(G)}(\overline{xy}, \bar{u}) = 2k + 1$. Hence $e_{\bar{y}} \Theta_{S(G)} f_{\bar{u}}$. A similar situation occurs when $d_G(x, v) = k + 1$ and $d_G(y, u) = k$.

Case 2. $d_G(y, v) = k + 1$.

Again, $\{d_G(x, v), d_G(y, u)\} \subseteq \{k - 1, k, k + 1\}$, but since $d_G(x, u) + d_G(y, v) < d_G(y, u) + d_G(x, v)$ it must be that $d_G(x, v) = d_G(y, u) = k + 1$. Then $d_{S(G)}(\bar{y}, \bar{v}) = 2k + 2$, $d_{S(G)}(\overline{xy}, \overline{uv}) = 2k + 2$, $d_{S(G)}(\bar{y}, \overline{uv}) = 2k + 3$, and $d_{S(G)}(\overline{xy}, \bar{v}) = 2k + 3$. Hence $e_{\bar{y}} \Theta_{S(G)} f_{\bar{v}}$.

Case 3. $d_G(y, v) = k + 2$.

In this case the fact that $\{d_G(x, v), d_G(y, u)\} \subseteq \{k - 1, k, k + 1\}$ implies that $d_G(x, u) + d_G(y, v) \geq d_G(y, u) + d_G(x, v)$. As this is not possible, the first assertion of the lemma is proved.

Assume now that G is bipartite. Combining Lemma 2.1 with the above case analysis we infer that the only case to consider is when $d_G(x, u) = d_G(y, v) = k$ and $d_G(x, v) = d_G(y, u) = k + 1$. Then, just in the first subcase of the above Case 1 we get that $e_{\bar{x}} \Theta_{S(G)}^* f_{\bar{v}}$ and, similarly, $e_{\bar{y}} \Theta_{S(G)}^* f_{\bar{u}}$. ■

We say that cycles C and C' of G are *isometrically touching* if $|E(C) \cap E(C')| = 1$ and $C \cup C'$ is an isometric subgraph of G . Note that isometrically touching cycles are isometric.

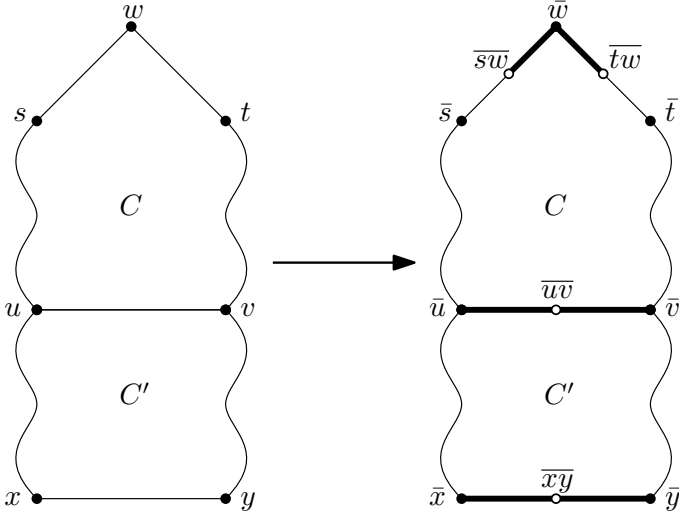


Figure 2. Isometrically touching cycles and their subdivisions.

Lemma 3.4 *Let C and C' be isometrically touching cycles in G with $E(C) \cap E(C') = \{e\}$. Then in $S(G)$ both edges corresponding to e are in the same $\Theta_{S(G)}^*$ -class. Moreover, this class contains the edges thickened in Fig. 2.*

Proof. We take the notation from Fig. 2 and content ourselves with only providing the proof for the case where C is odd and C' is even. The other cases go through similarly. From Lemma 2.2(iii) we get that $\{\bar{u}, \bar{u}\bar{v}\} \Theta_{S(G)} \{\bar{w}, \bar{t}\bar{w}\}$ and $\{\bar{u}, \bar{u}\bar{v}\} \Theta_{S(G)} \{\bar{y}, \bar{x}\bar{y}\}$. However, note now that $d(\bar{y}, \bar{w}) = d(\bar{x}\bar{y}, \bar{s}\bar{w}) = d(\bar{y}, \bar{s}\bar{w}) - 1 = d(\bar{x}\bar{y}, \bar{w}) - 1$. Thus we also have $\{\bar{w}, \bar{s}\bar{w}\} \Theta_{S(G)} \{\bar{y}, \bar{x}\bar{y}\}$. Since $\{\bar{w}, \bar{s}\bar{w}\}$ is also in relation with $\{\bar{v}, \bar{v}\bar{w}\}$ we obtain the claim for $\Theta_{S(G)}^*$ by taking the transitive closure. ■

For the full subdivision $S(G)$ of G denote by $S(\Theta_G^*)$, the relation on the edges of $S(G)$, where $\{\bar{x}, \bar{x}\bar{y}\}$ and $\{\bar{u}, \bar{u}\bar{v}\}$ are in relation $S(\Theta_G^*)$ if and only if $\{x, y\} \Theta^* \{u, v\}$. In particular, $\{\bar{x}, \bar{x}\bar{y}\}$ and $\{\bar{x}\bar{y}, \bar{y}\}$ are always in relation.

Lemma 3.5 *We have $\{\bar{x}, \bar{x}\bar{y}\} \Theta_{S(G)}^* \{\bar{x}\bar{y}, \bar{y}\}$ for all $\{x, y\} \in G$ if and only if $\Theta_{S(G)}^* = S(\Theta_G^*)$.*

Proof. The backwards direction holds by definition. Conversely, by Lemma 3.1 we have that if $\{\bar{x}, \bar{xy}\} \Theta_{S(G)}^* \{\bar{uv}, \bar{v}\}$, then $\{x, y\} \Theta^* \{u, v\}$. Therefore, $\Theta_{S(G)}^* \subseteq S(\Theta_G^*)$. On the other hand, Lemma 3.3 assures that if $\{x, y\} \Theta^* \{u, v\}$, then there is a pair $\{\bar{x}, \bar{xy}\} \Theta_{S(G)}^* \{\bar{uv}, \bar{v}\}$, but then by our assumption also $\{\bar{y}, \bar{xy}\} \Theta_{S(G)}^* \{\bar{uv}, \bar{v}\}$ and so on. Thus, $\Theta_{S(G)}^* \supseteq S(\Theta_G^*)$. ■

Lemma 3.4 and 3.5 immediately yield:

Proposition 3.6 *If every edge of G is in the intersection of two isometrically touching cycles, then $\Theta_{S(G)}^* = S(\Theta_G^*)$.*

4 Θ^* in subdivisions of fullerenes and plane triangulations

In this section we study relation Θ^* in full subdivisions of fullerenes and plane triangulations, for which Proposition 3.6 will be essential. We begin with fullerenes. Recall that a *fullerene* is a 3-connected, cubic, planar graph all of whose faces are of length 5 or 6.

A cycle C of a connected graph G is *separating* if $G \setminus C$ is disconnected. A *cyclic edge-cut* of G is an edge set F such that $G \setminus F$ separates two cycles. To prove our main result on fullerenes we need the following result.

Lemma 4.1 *Given a fullerene graph G , every separating cycle of G is of length at least 9. Moreover, the only separating cycles of length 9, are the cycles separating a vertex incident only to 5-faces, see the left of Fig. 3.*

Proof. Let C be separating cycle of length at most 9. Since G is cubic, there are $|C|$ edges of G incident to C which are not in C . Thus, without loss of generality, we may assume at most four of them are in the inner side of C . As they form an edge cut, and since fullerenes are cyclically 5-edge-connected [14], the subgraph induced by vertices in the inner part of C is a forest, say F . If F consists of one vertex, say v , then we have three edges connecting v to C which form three faces G . As each of these faces is of length at least 5, they are exactly 5-faces. Otherwise, F contains at least two vertices u and v each of which is either an isolated vertex of F or a leaf. As they are of degree 3 in F , each of them must be connected by two edges to C . And since there at most four such edges, it follows that u and v are of degree 1 in F and that every other vertex of F is of degree 3 in F , which means there no other vertex and u is adjacent to v . Thus inside C we have

five edges and four faces. But C itself is of length at most 9 and thus one of these four faces is of length at most 4, a contradiction with the choice of G . ■

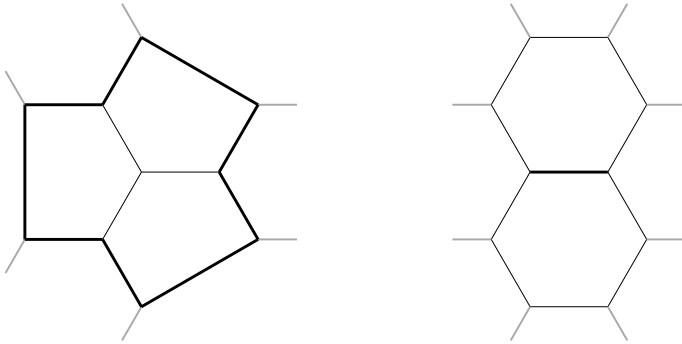


Figure 3. A separating 9-cycle and isometrically touching 6-cycles.

Theorem 4.2 *If G is a fullerene, then $\Theta_{S(G)}^* = S(\Theta_G^*)$.*

Proof. We claim that every edge e of G is the intersection of two isometrically touching cycles. For this sake consider the cycles C and C' that lie on the boundary of the faces containing e . We have to prove that the union $C \cup C'$ is isometric. Assume on the contrary that this is not the case, that is, there exist vertices $u, v \in C \cup C'$ such that there is a shortest u, v -path P (in G) interiorly disjoint from $C \cup C'$, that is shorter than any shortest path P' from u to v in $C \cup C'$.

Consider the cycle C'' obtained by joining P and a shortest path P' from u to v in $C \cup C'$. Since C and C' are of length at most 6, the graph $C \cup C'$ is of diameter at most 5, thus the cycle C'' is of length at most 9. We will prove that there is a separating cycle contradicting Lemma 4.1.

First, note that if $e \in P'$, then C'' separates the graph $C \cup C'$. Thus, by Lemma 4.1 C'' is of length at most 9, so the endpoints of P' must be at distance 5 on $C \cup C'$, i.e., one is in C and the other in C' . Thus, both sides of C'' contain more than one vertex, contradicting Lemma 4.1.

Hence, P' is on the boundary of $C \cup C'$. Suppose that C'' is not induced. Then since the girth of fullerenes is 5, there is a single chord from P to P' which splits C'' into a 5-cycle A and into a 5- or a 6-cycle B . In particular, $|C''| \geq 8$ and P' has at least five vertices on C'' . Thus, one vertex of P' has degree 2 in $C \cup C'$ and is not incident to the

chord. Thus, this vertex has a neighbor in the interior of A or B , that is, one of them is separating, contradicting Lemma 4.1.

If C'' is induced, it follows from the fact that C and C' are faces and $|C''| \geq 5$, that C'' is not a face, i.e., it is separating. Thus, $|C''| = 9$ and the patch Q consisting of C'' and its interior is a single vertex surrounded by three 5-faces, see Lemma 4.1. Moreover, C and C' are 6-faces so that their union can have diameter 5. Note that any path P' on the boundary of $C \cup C'$ of length 5 uses only one vertex of degree 3, see the right of Fig. 3. But any path P' of length 5 on the boundary Q uses at least two vertices of degree 2, see the left of Fig. 3. Thus, P' cannot be in both boundaries simultaneously – contradiction.

We have shown the claim from the beginning and Proposition 3.6 yields the result.

■

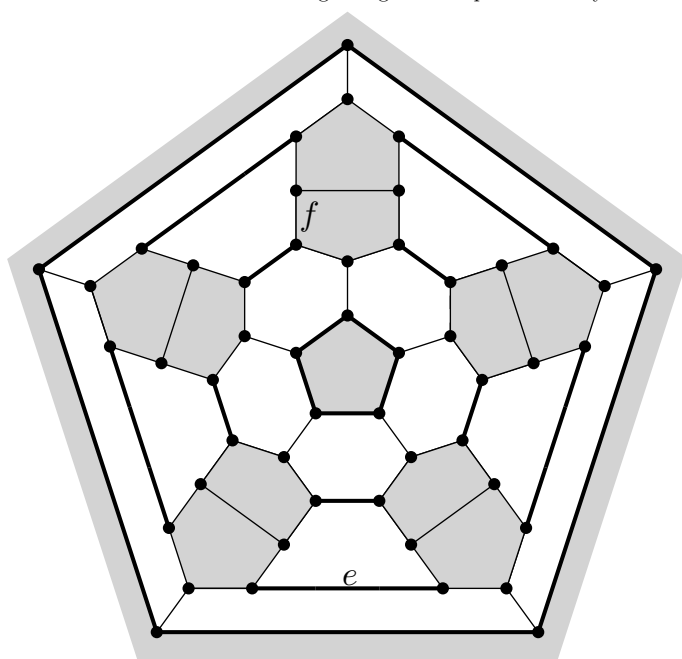


Figure 4. A fullerene G which has two $\overline{\Phi}^*$ -classes (bold and normal edges), but only one Θ_G^* -class since $e\Theta_G f$.

We have proved how Θ_G^* of a fullerene behaves with respect to subdivision. What can we say about Θ_G^* itself? If G is a fullerene, then we define a relation Φ on $E(G)$ as follows: $e\Phi f$ if e and f are opposite edges of a facial C_6 . Relation Φ falls into cycles and paths, that have been called *railroads* [11]. In particular, it has been shown that cycles

can have multiple self-intersection. We denote by $\overline{\Phi}$ the relation where additionally any two non-incident edges of a facial C_5 are in relation. Finally, recall that $\overline{\Phi}^*$ denotes the transitive closure of $\overline{\Phi}$. Since faces are isometric subgraphs, it is easy to see that $\overline{\Phi}$ is a refinement of Θ_G as well as $\overline{\Phi}^*$ is a refinement of Θ_G^* . One might believe that the converse also holds, but the example in Fig. 4 shows that this is not always the case. We believe that determining Θ_G^* in fullerenes is an interesting problem.

We now turn our attention to plane triangulations. It is straightforward to verify that if G is a plane triangulation, then Θ^* consists of a single class. On the other hand, Θ^* on the full subdivision of a plane triangulation has the following non-trivial structure.

Theorem 4.3 *Let $G \neq K_4$ be a plane triangulation. Then $\Theta_{S(G)}^*$ consists of one global class γ , plus one class γ_x for every degree three vertex x . Here, if $N(x) = \{y_1, y_2, y_3\}$, then $\gamma_x = \{\{\overline{y_1}, \overline{y_1x}\}, \{\overline{y_2}, \overline{y_2x}\}, \{\overline{y_3}, \overline{y_3x}\}\}$. If $G = K_4$ the same holds, except that there is no global class γ .*

Proof. Recall that $S(K_4)$ is a partial cube, cf. [22], its Θ -classes (= Θ^* -classes) are shown in Fig. 5. Hence the result holds for K_4 .

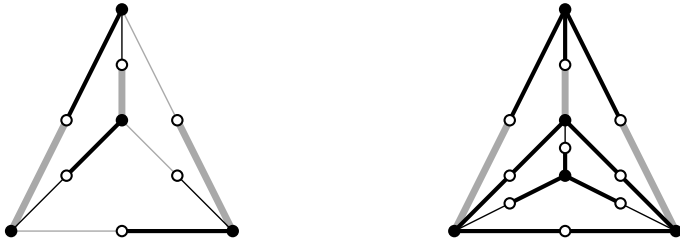


Figure 5. The relation Θ^* in $S(K_4)$ and the full division of the graph obtained by stacking into one face.

We proceed by induction on the number of vertices. Let G have minimum degree at least 4, and let $e = \{x, y\}$ be an edge shared by triangles C and C' bonding faces of G . If $C \cup C'$ is isometric, then by Lemma 3.4 we have $\{\overline{x}, \overline{xy}\} \Theta_{S(G)}^* \{\overline{xy}, \overline{y}\}$. Otherwise, $C \cup C'$ induces a K_4 , but since the minimum degree of G is at least 4, the other two triangles of the K_4 cannot be faces. An easy application of Lemma 3.4 on the other edges of this K_4 implies $\{\overline{x}, \overline{xy}\} \Theta_{S(G)}^* \{\overline{xy}, \overline{y}\}$. Since in a triangulation there is only one Θ^* -class, Proposition 3.6 implies the result, that is, there is only one global class γ in $S(G)$.

Now suppose that G contains a vertex v of degree 3. The graph $G' = G \setminus \{v\}$ is a plane triangulation, thus our claim holds for G' by induction. In particular, if $G' = K_4$, see Fig. 5 again. Otherwise, since $S(G')$ is an isometric subgraph of $S(G)$, Lemma 2.2(iv) says that $\Theta_{S(G')}$ is the restriction of $\Theta_{S(G)}$ to $S(G')$.

Consider an edge $e = \{x, y\}$ of the triangle of G that contains v . Note that the facial triangles C, C' containing e have an isometric union, so by Lemma 3.4 we have $\{\bar{x}, \overline{xy}\}\Theta_{S(G)}^*\{\overline{xy}, \bar{y}\}$, which corresponds to our claim, since neither x or y can be of degree 3. If one of them—say x —was of degree 3 in G' , then now only the class γ_x and γ where merged. Since $G' \neq K_4$, not both x and y are of degree 3. Note furthermore that by Lemma 3.4 the edges incident to v will all be in the class γ .

Finally, all the edges of the form $f = \{\bar{x}, \overline{v\bar{x}}\}$ are in relation Θ with each other. In order to see that they are the only constituents of the class γ_v it suffices to notice that $d(\overline{v\bar{x}}, z) = d(\bar{x}, z) + 1$ for all $z \in S(G')$. The result then follows by Lemma 2.2 (i). ■

5 Θ^* in subdivisions of chordal graphs

Recall that a graph is *chordal* if all its induced cycles are of length 3. As in fullerenes we define relation Φ on the edges of $S(G)$, by $e\Phi f$ if e, f are opposite edges of a C_6 .

Lemma 5.1 *If G is a chordal graph, then $\Phi_{S(G)}^* = \Theta_{S(G)}^*$.*

Proof. Let $e\Theta_{S(G)}f$, where e and f are edges created by subdividing $\{a, b\}, \{c, d\} \in E(G)$, respectively. Then by Lemma 3.1 we have $\{a, b\}\Theta\{c, d\}$. Similarly as in the proof of Lemma 3.3, we have (up to symmetry) two options.

Case 1. $d_G(a, c) = d_G(b, d) = k$.

We can assume that $d_G(a, d) \in \{k, k + 1\}$ and $d_G(b, c) = k + 1$. Let $P = p_0p_1 \dots p_k$ and $P' = p'_0p'_1 \dots p'_k$ be shortest a, c - and b, d -paths, respectively. Clearly, P and P' must be disjoint since otherwise it cannot hold $d_G(a, d) \in \{k, k + 1\}, d_G(b, c) = k + 1$. The cycle C formed by $\{a, b\}, P', \{d, c\}, P$ must have a chord. Inductively adding chords we can show that there is a chord of C incident with a or b . Since P and P' are shortest paths and the assumptions on distances hold, it follows that the latter chord must be incident with a and the vertex p'_1 of P' . In particular, $d_G(a, d) = k$. Similarly, one can show that there must be a chord between p'_1 and p_1 , and inductively between every $p_i p'_{i+1}$ for $0 \leq i < k$ and every $p_{i+1} p'_{i+1}$ for $0 \leq i < k - 1$.

By the assumption on the distances, the only pair of subdivided edges of $\{a, b\}, \{c, d\}$, that is in relation $\Theta_{S(G)}$, is $\{\bar{b}, \overline{ba}\}\Theta_{S(G)}\{\bar{c}, \overline{cd}\}$, i.e., $e = \{\bar{b}, \overline{ba}\}$ and $f = \{\bar{c}, \overline{cd}\}$. Then

$$\{\bar{b}, \overline{ba}\}\Phi_{S(G)}\{\bar{a}, \overline{ap'_1}\}\Phi_{S(G)}\{\bar{p}_1, \overline{p_1p'_1}\}\Phi_{S(G)} \cdots \Phi_{S(G)}\{\bar{c}, \overline{cd}\}.$$

Case 2. $d_G(a, c) = k, d_G(b, d) = k + 1$.

Then we have $d_G(a, d) = d_G(b, c) = k + 1$. Similarly as above, shortest a, c - and b, d -paths, say $P = p_0p_1 \dots p_k$ and $P' = p'_0p'_1 \dots p'_{k+1}$, cannot intersect. Using the same notation as above, C must have a chord incident with a or b . By similar arguments, there must be a chord between every $p_i p'_{i+1}$ and $p_{i+1} p'_{i+1}$ for $0 \leq i < k$.

By the assumption on the distances, the only pair of subdivided edges of $\{a, b\}, \{c, d\}$, that is in relation $\Theta_{S(G)}$, is $\{\bar{b}, \overline{ba}\}\Theta_{S(G)}\{\bar{d}, \overline{dc}\}$, i.e., $e = \{\bar{b}, \overline{ba}\}$ and $f = \{\bar{d}, \overline{dc}\}$. Then

$$\{\bar{b}, \overline{ba}\}\Phi_{S(G)}\{\bar{a}, \overline{ap'_1}\}\Phi_{S(G)}\{\bar{p}_1, \overline{p_1p'_1}\}\Phi_{S(G)} \cdots \Phi_{S(G)}\{\bar{d}, \overline{dc}\}.$$

We have proved that $\Theta_{S(G)} \subset \Phi_{S(G)}^*$, thus $\Theta_{S(G)}^* = \Phi_{S(G)}^*$. ■

An edge of a graph G is called *exposed* if it is properly contained in a single maximal complete subgraph of G . This concept was recently introduced in [10], where it was proved that G is a connected chordal graph if and only if G can be obtained from a complete graph by a sequence of removal of exposed edges. Denote by G^{-ee} the graph obtained from G by removing all its exposed edges. We will denote by $c(G^{-ee})$ the number of connected components of G^{-ee} . The singletons of G^{-ee} include the simplicial vertices of G , and if G is 2-connected, its simplicial vertices coincide with singletons of G^{-ee} . It is easy to verify that if G is a chordal graph, then Θ^* consists of a single class. However, on the full subdivision of a chordal graph Θ^* has the following structure.

Theorem 5.2 *Let G be a 2-connected, chordal graph. Then the coloring, that for an edge $\{a, b\}$ with a being in the i -th connected component of G^{-ee} colors edge $\{\overline{ab}, b\}$ with color i , corresponds to the $\Theta_{S(G)}^*$ -partition. In particular, $|\Theta_{S(G)}^*| = c(G^{-ee})$.*

Proof. We first prove that the above coloring of edges is a coarsening of $\Theta_{S(G)}^*$. Let a be a vertex of G and b, c its neighbors. Since G is 2-connected, there is a b, c -path P that avoids a . Pick P such that it is shortest possible. Then since G is chordal, a is adjacent to every vertex on P , otherwise there exists a shorter path. Denote $P = p_0p_1 \dots p_k$, where $p_0 = b$ and $p_k = c$. Then $\{\overline{p_1a}, \overline{p_1}\}\Theta_{S(G)}\{\overline{p_{i+1}a}, \overline{p_{i+1}}\}$, proving that $\{\overline{ba}, \overline{b}\}\Theta_{S(G)}^*\{\overline{ca}, \overline{c}\}$.

Furthermore, if ab is not an exposed edge in G , then ab lies in two maximal cliques. In particular, it lies in two isometrically touching triangles. By Lemma 3.4, $\{\overline{ab}, \overline{b}\} \Theta_{S(G)}^* \{\overline{a}, \overline{ab}\}$. By transitivity, and the above two facts, all the edges $\{\overline{ab}, \overline{b}\}$, with a being in the same connected component of G^{-ee} , are in relation $\Theta_{S(G)}^*$.

Finally, we prove that no other edge besides the asserted is in $\Theta_{S(G)}^*$. Assume otherwise, and let $\{\overline{a}, \overline{ab}\} \Theta_{S(G)}^* \{\overline{c}, \overline{cd}\}$ be such that b and d do not lie in the same connected component of G^{-ee} . By Lemma 5.1, we can assume that $\{\overline{a}, \overline{ab}\} \Phi_{S(G)} \{\overline{c}, \overline{cd}\}$. But then the edges lie on a 6-cycle, implying that $b = d$. This cannot be. ■

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References

- [1] M. Albenque, K. Knauer, Convexity in partial cubes: the hull number, *Discr. Math.* **339** (2016) 866–876.
- [2] V. Andova, F. Kardoš, R. Škrekovski, Mathematical aspects of fullerenes, *Ars Math. Contemp.* **11** (2016) 353–379.
- [3] M. Arockiaraj, S. Klavžar, J. Clement, S. Mushtaq, K. Balasubramanian, Edge distance-based topological indices of strength-weighted graphs and their application to coronoid systems, carbon nanocones and SiO₂ nanostructures, *Mol. Inf.* **38** (2019) #1900039.
- [4] M. Arockiaraj, S. Klavžar, S. Mushtaq, K. Balasubramanian, Distance-based topological indices of nanosheets, nanotubes and nanotori of SiO₂, *J. Math. Chem.* **57** (2019) 343–369.
- [5] M. Arockiaraj, S. Klavžar, S. Mushtaq, K. Balasubramanian, Topological indices of the subdivision of a family of partial cubes and computation of SiO₂ related structures, *J. Math. Chem.* **57** (2019) 1868–1883.
- [6] S. Brezovnik, N. Tratnik, General cut method for computing Szeged-like topological indices with applications to molecular graphs, *Int. J. Quantum Chem.* (2020) #e26530.
- [7] J. Cardinal, S. Felsner, Covering partial cubes with zones, *El. J. Comb.* **22** (2015) #3.31.

- [8] V. Chepoi, Isometric subgraphs of Hamming graphs and d -convexity, *Cybernetics* **1** (1988) 6–9.
- [9] M. Črepnjak, N. Tratnik, The Szeged index and the Wiener index of partial cubes with applications to chemical graphs, *Appl. Math. Comput.* **309** (2017) 324–333.
- [10] J. Culbertson, D. P. Guralnik, P. F. Stiller, Edge erasures and chordal graphs, arXiv:1706.04537v2 [math.CO] (14 Aug 2018).
- [11] M. Deza, M. Dutour, P. W. Fowler, Zigzags, railroads, and knots in fullerenes, *J. Chem. Inf. Comput. Sci.* **44** (2004) 1282–1293.
- [12] M. Deza, M. Laurent, *Geometry of Cuts and Metrics*, Springer–Verlag, Berlin, 1997.
- [13] D. Djoković, Distance preserving subgraphs of hypercubes, *J. Comb. Theory Ser. B* **14** (1973) 263–267.
- [14] T. Došlić, Cyclical edge–connectivity of fullerene graphs and $(k, 6)$ -cages, *J. Math. Chem.* **33** (2003) 103–112.
- [15] T. Došlić, Nice pairs of odd cycles in fullerene graphs, *J. Math. Chem.* **58** (2020) 2204–2222.
- [16] D. Eppstein, J.-C. Falmagne, S. Ovchinnikov, *Media Theory*, Springer–Verlag, Berlin, 2008.
- [17] F. Foucaud, H. Hocquard, S. Mishra, N. Narayanan, R. Naserasr, É. Sopena, P. Valicov, Exact square coloring of subcubic planar graphs, arXiv:2009.00843, 2020.
- [18] R. L. Graham, H. Pollak, On the addressing problem for loop switching, *Bell System Tech. J.* **50** (1971) 2495–2519.
- [19] R. L. Graham, P. M. Winkler, On isometric embeddings of graphs, *Trans. Amer. Math. Soc.* **288** (1985) 527–536.
- [20] S. Klavžar, On the canonical metric representation, average distance, and partial Hamming graphs, *Eur. J. Comb.* **27** (2006) 68–73.
- [21] S. Klavžar, I. Gutman, B. Mohar, Labeling of benzenoid systems which reflects the vertex–distance relations, *J. Chem. Inf. Comput. Sci.* **35** (1995) 590–593.
- [22] S. Klavžar, A. Lipovec, Partial cubes as subdivision graphs and as generalized Peters graphs, *Discr. Math.* **263** (2003) 157–165.
- [23] S. Klavžar, M. J. Nadjafi–Arani, Cut method: update on recent developments and equivalence of independent approaches, *Curr. Org. Chem.* **19** (2015) 348–358.

- [24] T. Marc, Classification of vertex-transitive cubic partial cubes, *J. Graph Theory* **86** (2017) 406–421.
- [25] K. P. Narayankar, A. T. Kahsay, S. Klavžar, On peripheral Wiener index: line graphs, Zagreb index, and cut method, *MATCH Commun. Math. Comput. Chem.* **83** (2020) 129–141.
- [26] S. Ovchinnikov, Partial cubes: structures, characterizations, and constructions, *Discr. Math.* **308** (2008) 5597–5621.
- [27] J. Qian, H. Liang, F. Bai, The lower bound of Kekulé count of fullerenes, *MATCH Commun. Math. Comput. Chem.* **84** (2020) 239–248.
- [28] P. Schwerdtfeger, L. N. Wirz, J. Avery, The topology of fullerenes, *WIREs Comp. Mol. Sci.* **5** (2015) 96–145.
- [29] W. Tian, S. Liu, L. Deng, N. Mahmood, X. Jian, Synthesis and growth mechanism of various SiO₂ nanostructures from straight to helical morphologies, *Compos. Part B-Eng.* **149** (2018) 92–97.
- [30] N. Tratnik, A method for computing the edge-hyper-Wiener index of partial cubes and an algorithm for benzenoid systems, *Appl. Anal. Discr. Math.* **12** (2018) 126–142.
- [31] N. Tratnik, Generalized cut method for computing the edge-Wiener index, *Discr. Appl. Math.* **282** (2020) 222–233.
- [32] P. Winkler, Isometric embeddings in products of complete graphs, *Discr. Appl. Math.* **7** (1984) 221–225.
- [33] L. Zhao, H. Zhang, On resonance of (4, 5, 6)-fullerene graphs, *MATCH Commun. Math. Comput. Chem.* **88** (2018) 227–244.
- [34] L. Zhao, H. Zhang, On the anti-Kekulé number of (4, 5, 6)-fullerenes, *Discr. Appl. Math.* **283** (2020) 577–589.