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 SiO_2 layer structures and SiO_2 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.

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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 [7], Djoković [12], and Winkler [27]. The original source for their interest however goes back to the paper of Graham and Pollak [15]. For additional information on partial cubes we refer to the books [11, 14], the semi-survey [22], recent papers [1, 6, 21], as well as references therein.

Partial cubes offer many applications, ranging from the original one in interconnection networks [15] to media theory [14]. Our motivation though comes from mathematical chemistry where many important classes of chemical graphs are partial cubes. In the seminal paper [18] 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 [17], based on the Graham-Winkler's canonical metric embedding [16], that the method extends to arbitrary graphs. The paper [18] initiated the theory under the common name "cut method," while [20] surveys the results on the method until 2015 with 97 papers in the bibliography. The cut method has been further developed afterwards, see [8, 25, 26] 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 [24] 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, 23]) 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 thus an equivalence, its classes are called Θ^*-classes. Partial cubes are precisely those connected bipartite graph for which $\Theta = \Theta^*$ holds [27]. 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 each 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.

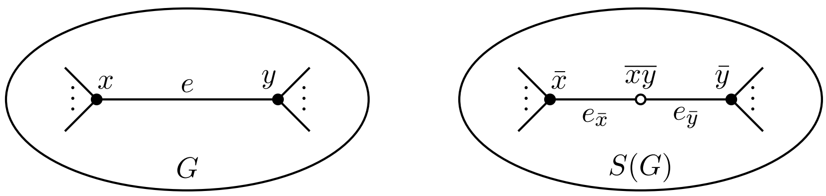

Figure 1: Notation for the vertices and edges of $S(G)$.

The following lemma is straightforward, cf. [19, 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 $d_{S(G)}(\overline{xy}, \overline{uv})$ are even. Based on the assumption $e_{\bar{x}} \,\Theta_{S(G)}\, f_{\bar{u}}$, we have $d_{S(G)}(\bar{x}, \bar{u}) + d_{S(G)}(\overline{xy}, \overline{uv}) = d_{S(G)}(\bar{x}, \overline{uv}) + d_{S(G)}(\overline{xy}, \bar{u})$ in a bipartite graph, thus the following cases.

Case 1. $d_{S(G)}(\bar{x}, \bar{u}) = d_{S(G)}(\overline{xy}, \overline{uv}) = 2k$ and $d_{S(G)}(\bar{x}, \overline{uv}) = d_{S(G)}(\overline{xy}, \bar{u}) = 2k+1$.
In the following, Lemma 2.3 will be used all the time.

By $2k = d_{S(G)}(\overline{xy}, \overline{uv}) = 2d_G(\{x,y\}, \{u,v\}) + 2$, 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 $d_{S(G)}(\bar{x}, \overline{uv}) = 2k+1$, we find that $d_G(x, \{u,v\}) = k$ and hence in particular $d_G(x,v) \geq k$. Similarly, as $d_{S(G)}(\overline{xy}, \bar{u}) = 2k+1$ 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. $d_{S(G)}(\bar{x}, \bar{u}) = d_{S(G)}(\overline{xy}, \overline{uv}) = 2k$ and $d_{S(G)}(\bar{x}, \overline{uv}) = d_{S(G)}(\overline{xy}, \bar{u}) = 2k-1$.
Again, $d_{S(G)}(\bar{x}, \bar{u}) = 2k$ implies $d_G(x,u) = k$. The assumption $d_{S(G)}(\bar{x}, \overline{uv}) = 2k-1$ yields $d_G(x, \{u,v\}) = k-1$ and consequently $d_G(x,v) = k-1$. The condition $d_{S(G)}(\overline{xy}, \bar{u}) = 2k-1$ implies $d_G(u, \{x,y\}) = k-1$ and so $d_G(u,y) = k-1$. Finally, the assumption $d_{S(G)}(\overline{xy}, \overline{uv}) = 2k$ 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 $e\,\Theta_G\,f$. $\square$

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

$$e_{\bar{x}}\,\Theta_{S(G)}\,f^{(1)}_{\overline{x_1}},\, f^{(1)}_{\overline{x_1}}\,\Theta_{S(G)}\,f^{(2)}_{\overline{x_2}},\ldots,\, f^{(k)}_{\overline{x_k}}\,\Theta_{S(G)}\,f_{\bar{u}}\,.$$

Then, by Lemma 3.1, we have

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

implying that $e\Theta^*_G f$. $\square$

The next lemma is a partial converse to Lemma 3.1.

Lemma 3.3 *If $e\,\Theta_G\,f$, 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 $e\,\Theta_G\,f$, 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 $d_G(x,u) \le d_G(y,v)$. 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 $e\,\Theta_G\,f$, 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 $d_G(x,u) + d_G(y,v) \ge d_G(y,u) + d_G(x,v)$. 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, $e_{\bar{y}}\, \Theta^*_{S(G)}\, f_{\bar{u}}$. $\square$

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.

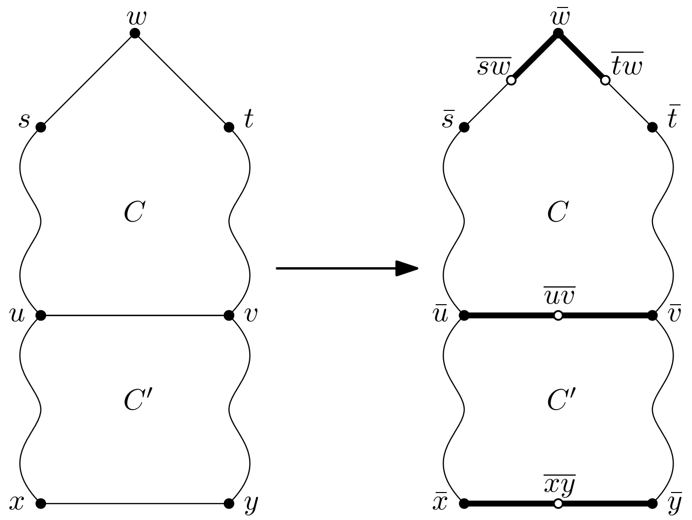

Figure 2: Isometrically touching cycles and their subdivisions.

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 $\{\bar{u}, \overline{uv}\}\Theta_{S(G)}\{\bar{w}, \overline{tw}\}$ and $\{\bar{u}, \overline{uv}\}\Theta_{S(G)}\{\bar{y}, \overline{xy}\}$. However, note now that $d(\bar{y}, \bar{w}) = d(\overline{xy}, \overline{sw}) = d(\bar{y}, \overline{sw}) - 1 = d(\overline{xy}, \bar{w}) - 1$. Thus we also have $\{\bar{w}, \overline{sw}\}\Theta_{S(G)}\{\bar{y}, \overline{xy}\}$. Since $\{\bar{w}, \overline{sw}\}$ is also in relation with $\{\bar{v}, \overline{uv}\}$ we obtain the claim for $\Theta^*_{S(G)}$ by taking the transitive closure. $\square$

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

Lemma 3.5 *We have $\{\bar{x}, \overline{xy}\}\Theta^*_{S(G)}\{\overline{xy}, \bar{y}\}$ 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 $\{\bar{x}, \overline{xy}\}\Theta^*_{S(G)}\{\overline{uv}, \bar{v}\}$, 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 $\{\bar{x}, \overline{xy}\}\Theta^*_{S(G)}\{\overline{uv}, \bar{v}\}$, but then by our assumption also $\{\bar{y}, \overline{xy}\}\Theta^*_{S(G)}\{\overline{uv}, \bar{v}\}$ 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 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 and that 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 [13], 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. □

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

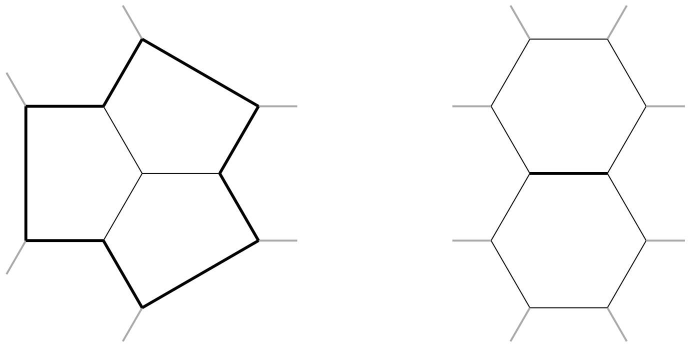

Figure 3: A separating 9-cycle and two isometrically touching 6-cycles in a fullerene.

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. □

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

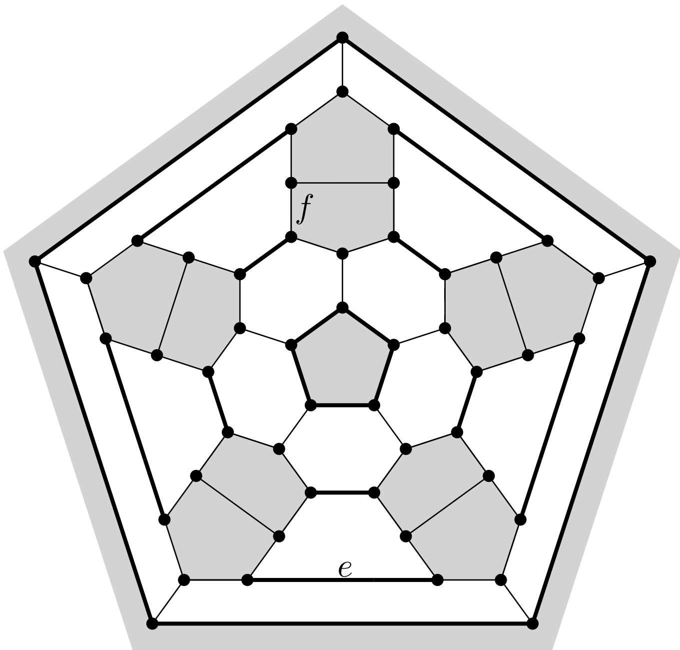

Figure 4: A fullerene G which has two $\overline{\Phi}^*$-classes (bold and normal edges), but only one Θ_G^*-class since $e\Theta_G f$.

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* [10]. 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 $\gamma_x = \{\{\bar{y}_1, \overline{y_1x}\}, \{\bar{y}_2, \overline{y_2x}\}, \{\bar{y}_3, \overline{y_3x}\}\}$. 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. [19], its Θ-classes ($= \Theta^*$-classes) are shown In Fig. 5. Hence the result holds for K_4.

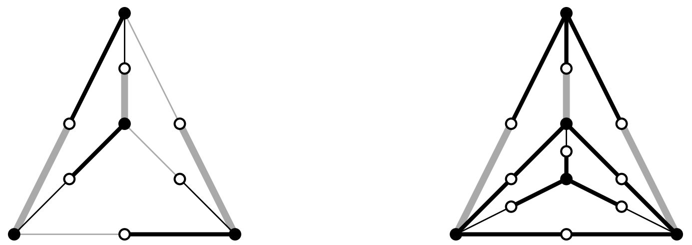

Figure 5: The relation Θ^* in $S(K_4)$ and the full division of the graph obtained by stacking into one face.

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 $\{\bar{x}, \overline{xy}\}\Theta^*_{S(G)}\{\overline{xy}, \bar{y}\}$. 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 $\{\bar{x}, \overline{xy}\}\Theta^*_{S(G)}\{\overline{xy}, \bar{y}\}$. 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 $f = \{\bar{x}, \overline{vx}\}$ 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 $d(\overline{vx}, z) = d(\overline{x}, z) + 1$ for all $z \in S(G')$. The result then follows by Lemma 2.2 (i). $\square$

5 Θ^* in subdivisions of chordal graphs

Recall that a graph is *chordal* if all its induced cycles are of length 3. Similarly as in fullerenes we shall 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 $p_ip'_{i+1}$ for $0 \le i < k$ and every $p_{i+1}p'_{i+1}$ for $0 \le i < k-1$.

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 $\{\overline{b},\overline{ba}\}\Theta_{S(G)}\{\overline{c},\overline{cd}\}$, i.e., $e = \{\overline{b},\overline{ba}\}$ and $f = \{\overline{c},\overline{cd}\}$. Then

$$\{\overline{b},\overline{ba}\}\Phi_{S(G)}\{\overline{a},\overline{ap'_1}\}\Phi_{S(G)}\{\overline{p_1},\overline{p_1p'_1}\}\Phi_{S(G)} \ \cdots \ \Phi_{S(G)}\{\overline{c},\overline{cd}\}\,.$$

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 $p_ip'_{i+1}$ and $p_{i+1}p'_{i+1}$ for $0 \le i < k$.

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 $\{\overline{b},\overline{ba}\}\Theta_{S(G)}\{\overline{d},\overline{dc}\}$, i.e., $e = \{\overline{b},\overline{ba}\}$ and $f = \{\overline{d},\overline{dc}\}$. Then

$$\{\overline{b},\overline{ba}\}\Phi_{S(G)}\{\overline{a},\overline{ap'_1}\}\Phi_{S(G)}\{\overline{p_1},\overline{p_1p'_1}\}\Phi_{S(G)} \ \cdots \ \Phi_{S(G)}\{\overline{d},\overline{dc}\}\,.$$

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 [9], where it was proved that a 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}, for a chordal graph G, the graph obtained from G by removing all its exposed edges. We will denote by $\mathrm{c}(G^{-ee})$ the number of connected components of G^{-ee}. Note that 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 straightforward to verify that if G is a chordal graph, then Θ^* consists of a single class. On the other hand, Θ^* on the full subdivision of a chordal graph has the following non-trivial 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 exists a b,c-path P that does not cross 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 $\{\overline{p_ia}, \overline{p_i}\}\Theta_{S(G)}\{\overline{p_{i+1}a}, \overline{p_{i+1}}\}$, 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 $\{\bar{a}, \overline{ab}\}\Theta^*_{S(G)}\{\bar{c}, \overline{cd}\}$ 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 $\{\bar{a}, \overline{ab}\}\Phi_{S(G)}\{\bar{c}, \overline{cd}\}$. But then the edges lie on a 6-cycle, implying that $b = d$. This cannot be. □

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