

ENCODING FULLERENES AND GEODESIC DOMES*

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Abstract. Coxeter’s classification of the highly symmetric geodesic domes (and, by duality, the highly symmetric fullerenes) is extended to a classification scheme for all geodesic domes and fullerenes. Each geodesic dome is characterized by its signature: a plane graph on twelve vertices with labeled angles and edges. In the case of the Coxeter geodesic domes, the plane graph is the icosahedron, all angles are labeled one, and all edges are labeled by the same pair of integers (p, q) . Edges with these “Coxeter coordinates” correspond to straight line segments joining two vertices of Λ , the regular triangular tessellation of the plane, and the faces of the icosahedron are filled in with equilateral triangles from Λ whose sides have coordinates (p, q) .

We describe the construction of the signature for any geodesic dome. In turn, we describe how each geodesic dome may be reconstructed from its signature: the angle and edge labels around each face of the signature identify that face with a polygonal region of Λ and, when the faces are filled by the corresponding regions, the geodesic dome is reconstituted. The signature of a fullerene is the signature of its dual. For each fullerene, the separation of its pentagons, the numbers of its vertices, faces, and edges, and its symmetry structure are easily computed directly from its signature. Also, it is easy to identify nanotubes by their signatures.

Key words. fullerenes, geodesic domes, nanotubes

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1. Introduction. By a fullerene, we mean a trivalent plane graph $\Phi = (V, E, F)$ with only hexagonal and pentagonal faces. It follows easily from Euler’s formula that each fullerene has exactly 12 pentagonal faces. In this paper, we work with the duals to the fullerenes: geodesic domes, i.e., triangulations of the sphere with vertices of valence 5 and 6. It is in this context that Coxeter [3], Caspar and Klug [2], and Goldberg [7] parameterized the geodesic domes/fullerenes that include the full rotational group of the icosahedron among their symmetries. These highly symmetric geodesic domes are obtained by filling in each face of the icosahedron with a fixed equilateral triangle inscribed in Λ , the regular triangular tessellation of the plane. Coxeter’s classification boils down to classifying the equilateral triangles of Λ .

Our plan is to extend Coxeter’s approach to other plane graphs with 12 vertices, filling in their faces with regions from Λ such that the original 12 vertices are the vertices of valence 5 in the resulting geodesic dome. These special planar graphs with 12 vertices will be called signature graphs. The signature graph along with the labeling of the edges and angles that determines just how the faces are to be filled in will be called the signature of the resulting geodesic dome.

Let $\Phi = (V, E)$ be any graph with a set of edge weights, $\omega : E \rightarrow \mathbb{R}^+$. The *structure graph* of the weighted graph Φ, ω is the union of all shortest spanning trees of Φ . Now let $\Gamma = (V, E, F)$ be a geodesic dome and let P denote the set of the 12, 5-valent vertices of Γ . The first step in constructing the signature graph of Γ is to construct the complete graph on the vertex set P and assign to each of its edges the distance between its endpoints, as vertices in Γ . This weighted graph is called the *first auxiliary graph* of Γ and is denoted by $\mathcal{A}_1(\Gamma)$. The second step is to construct

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the structure graph of $\mathcal{A}_1(\Gamma)$. This graph is called the *second auxiliary graph* of Γ and is denoted by $\mathcal{A}_2(\Gamma)$. This graph, $\mathcal{A}_2(\Gamma)$, has a natural drawing on the sphere but may admit crossing edges. To eliminate any crossings, we make a slight alteration in the weight function and construct the structure graph of $\mathcal{A}_2(\Gamma)$ with this new weight function to get a third graph. This third graph also has a natural drawing on the sphere and it admits no crossings. The plane graph consisting of this third graph and its natural planar embedding is called the *signature graph* of Γ and is denoted by $\mathcal{S}(\Gamma)$. Each edge of $\mathcal{S}(\Gamma)$ may be identified with a line segment joining two vertices in Λ . This identification leads to a labeling system for the edges and angles of $\mathcal{S}(\Gamma)$. The signature graph of Γ along with this labeling is called the *signature* of Γ . We should note that Coxeter's approach has been generalized to some other triangulations of the sphere by Fowler, Cremona, and Steer [4] and by Fowler and Cremona [5] using an entirely different labeling system.

Each geodesic dome Γ is completely determined by its signature. Using the signature of Γ as a blueprint, one can construct a polygonal region or a set of polygonal regions in Λ with sides corresponding to the edges of $\mathcal{S}(\Gamma)$ and then glue them together to reconstruct Γ . Since all signature graphs of geodesic domes have exactly 12 vertices and since any planar graph admits only a finite number of distinct planar embeddings, there are only a finite number of plane graphs which could be the signature graph of a geodesic dome. This leads to a partition of the collection of all geodesic domes into a finite number of classes each corresponding to a different signature graph. We may label the angles of a given signature graph in a finite number of ways and we may label the edges with variables in a finite number of ways. Hence, within each class, we have a finite number of families. Each family corresponds to a signature graph with labeled angles and with variable labels on the edges. Each choice of the variables, satisfying an included set of equalities and inequalities, will then yield the signature of a specific geodesic dome or fullerene. The geodesic domes described by Coxeter form such a family.

We develop the signature in a more general setting defining it for each *plane triangulation*, that is for each plane graph with only triangular faces. To carry out these tasks, we will need several tools. We start our investigation with a short section on the basic properties of structure graphs followed by an extensive development of the "geometry" of Λ .

2. Structure graphs.

LEMMA 1. *Let Θ be the structure graph of the weighted graph Φ, ω .*

- i. *If u, v, w are vertices of a 3-circuit in Φ with $\omega(\{u, w\}) < \omega(\{v, w\})$ and $\omega(\{u, v\}) < \omega(\{v, w\})$, then the edge $\{v, w\}$ is not in Θ .*
- ii. *Deleting the edges of maximum weight from Θ disconnects Θ .*
- iii. *If the edges of Θ of maximum weight are deleted from Θ , then each of the resulting components is the structure graph of the corresponding vertex induced weighted subgraph of Φ .*
- iv. *If Ω is any connected subgraph of Θ , then deleting the edges of maximum weight from Ω disconnects Ω .*

Proof. Let $\Phi = (V, E)$ and $\Theta = (V, F)$.

Part i. Suppose that the edge $e = \{v, w\}$ is in Θ and let (V, T) be a shortest spanning tree of Φ containing e . Delete e from (V, T) . The vertex u is either in the component of $(V, T - e)$ which contains v or in the component which contains w . If it is in the component containing v , then $(V, T - e + e')$, where $e' = \{u, w\}$, is a shorter spanning tree; if u is in the component containing w , then $(V, T - e + e'')$, where

$e'' = \{u, v\}$, is a shorter spanning tree. Since both possibilities contradict the fact that (V, T) is a shortest spanning tree, our supposition must be false.

Part ii. Let m denote the maximum among the weights of the edges of Θ and let $e = \{v, w\}$ be an edge of Θ with weight m . Let (V, T) be a shortest spanning tree of Φ which contains e . Delete e from (V, T) . We show that each edge in the cutset of the edges of Θ joining the two components of $(V, T - e)$ has weight m . Let e' be any edge of Θ with an endpoint in each of the two components. Thus $(V, T - e + e')$ is also a spanning tree of Φ . This new tree has weight $\omega(T) - m + \omega(e')$, where $\omega(T)$ denotes the sum of the weights of the edges in T . Since (V, T) is a shortest spanning tree $\omega(T) \leq \omega(T) - m + \omega(e')$ or $m \leq \omega(e')$. But, $\omega(e') \leq m$; hence e' has weight m .

Part iii. Let m denote the maximum weight of the edges in Θ and let U be the vertex set of a component of the subgraph of Θ obtained by deleting all edges of weight m . Let $\Phi' = (U, G)$ and $\Theta' = (U, H)$ be the subgraphs of Φ and Θ induced by U . We show that Θ' is the structure graph of Φ' . Let (V, T) be a shortest spanning tree of Φ and let (U, T') be the subgraph of this tree induced by U . We assert that (U, T') is a shortest spanning tree of Φ' .

Suppose that (U, T') is not connected. If e is any edge of Θ' joining two components of (U, T') and e' is any edge in $T - T'$ incident to one of these components, we have that $\omega(e) < m = \omega(e')$ and that $(V, T - e' + e)$ is a shorter spanning tree of Φ . Thus (U, T') is a spanning tree of Φ' . Let (U, T'') be any shortest spanning tree of Φ' . Then $(V, T - T' + T'')$ is a spanning tree of Φ and $\omega(T'') \leq \omega(T')$. It follows that $\omega(T'') = \omega(T')$, that (U, T') is a shortest spanning tree of Φ' and that $(V, T - T' + T'')$ is a shortest spanning tree of Φ . Thus Θ' is the union of the shortest spanning trees of Φ' .

Part iv. We proceed by induction on the number of vertices of Φ . Let Ω be any connected subgraph of Θ . If the maximum weight of the edges in Ω equals the maximum weight of the edges in Θ , then, by part ii, deleting the edges of this maximum weight disconnects Ω . If the maximum weight of the edges in Ω is less than the maximum weight of the edges in Θ , then Ω is a subgraph of the structure graph of the smaller weighted graph Φ' induced by the vertex set of the component containing Ω of the graph obtained by deleting all edges of maximum weight from Θ . We may now apply the induction hypothesis. \square

3. The regular triangular tessellation of the plane. Consider Λ , the regular triangular tessellation of the plane. We think of Λ as the infinite plane graph with all vertex valences 6 and all face valences 3. The automorphisms of this graph correspond with the congruences of Λ as a geometric object in the plane: the translations, rotations, reflections, and glide reflections that map Λ onto Λ . Two vertex sets of Λ are said to be *congruent* if there is an automorphism of Λ which maps one onto the other. By a *segment* of Λ we simply mean a pair of vertices of Λ and we visualize a segment as the straight line segment joining the two vertices. To each segment which does not coincide with a "line" of the tessellation, we assign *Coxeter coordinates* (p, q) as follows: select one endpoint of the segment to be the origin; take the edge of the graph to the right of the segment as the unit vector in the p direction; take the edge of the graph to the left of the segment as the unit vector in the q direction; finally, assign to the segment the coordinates of its other endpoint in this coordinate system. If the segment coincides with a "line" of the tessellation, that segment is assigned the single Coxeter coordinate (p) , where p is the number of edges of Λ in the segment. In Figure 1, we illustrate this definition by giving the Coxeter coordinates assigned to the sides of several different regions in Λ . The *length* of a segment σ with endpoints

v and w is defined to be the graph-theoretic distance between the endpoints in the graph Λ ; it is denoted by $\delta(v, w)$ or $|\sigma|$. Collected in the next lemma are several observations about this labeling of segments. The proofs are straightforward.

LEMMA 2. Let σ denote a segment with endpoints v and w and let (p, q) [or (p)] denote its Coxeter coordinates as computed from v .

- i. The Coxeter coordinates of σ computed from w are also (p, q) [(p)].
- ii. p and q are positive integers (p is a positive integer).
- iii. $|\sigma| = p + q$ ($|\sigma| = p$).
- iv. The segments σ , with Coxeter coordinates (p, q) , and σ' , with Coxeter coordinates (p', q') , are congruent if and only if either $p' = p$ and $q' = q$ or $p' = q$ and $q' = p$. Furthermore, $p' = p$ and $q' = q$ if and only if σ' is the image of σ under a rotation or translation of the tessellation and $p' = q$ and $q' = p$ if and only if σ' is the image of σ under a reflection or glide reflection of the tessellation.
- v. The segments σ , with Coxeter coordinate (p) , and σ' , with Coxeter coordinate (p') , are congruent if and only if $p' = p$. Furthermore, any two segments with coordinates (p) are images of one another under both a translation or rotation and a reflection or glide reflection.

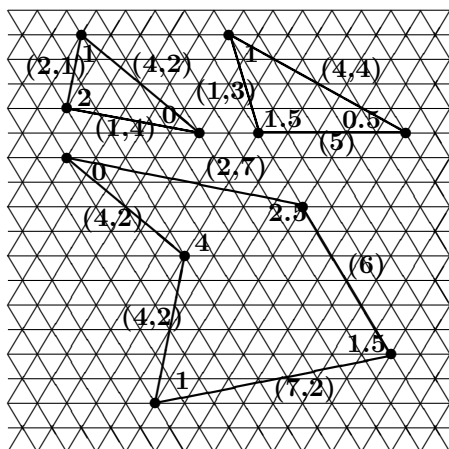


FIG. 1.

We are particularly interested in angles. Much of the information about an angle is coded in the Coxeter coordinates of its sides, but not all. Suppose that we have two segments forming an angle at a common endpoint v ; denote them, in clockwise order, by σ and σ' , denoting their Coxeter coordinates by (p, q) and (p', q') , respectively. The missing information is the multiple of 60 degrees between the edge from v along which p is measured and the edge along which p' is measured. This multiple is easily seen to be the number of edges from v which lie between the two segments. Hence, we define the *type* of the angle between two segments with a common endpoint v to be the number of edges from v which lie between the two segments. Segments with Coxeter coordinates of the form (p) coincide with an edge; in this case, the edge contributes $\frac{1}{2}$ to each of the types of the angles on either side of the segment. These definitions are illustrated in Figure 1 and the next lemma lists some useful properties of angle type.

LEMMA 3.

- i. Given segments α , β , and γ in clockwise order around a common endpoint,

the type of the angle between α and γ is the sum of the types of the angles between α and β and between β and γ .

- ii. Given segments $\sigma_1, \sigma_2, \dots, \sigma_n$ with a common endpoint, the sum of the types of the angles between them is 6.
- iii. Given an n -gon with angle types A_1, A_2, \dots, A_n , we have $A_1 + \dots + A_n = 3n - 6$.

Proof. Part i follows directly from the definition of angle type, and part ii follows directly from part i.

Turning to part iii, consider a triangle with vertices labeled v_A, v_B, v_C in clockwise order with corresponding angle types A, B , and C . Let α denote the segment opposite v_A ; β , the segment opposite v_B ; and γ , the segment opposite v_C . For any segment σ with Coxeter coordinates (p, q) , let θ_σ denote the measure, in degrees, of the angle between the segment and the lattice edge in the direction along which p is measured; note that θ_σ is independent of the endpoint of σ at which it is measured. For a segment with Coxeter coordinate (p) , define θ_σ to be 30° . We observe that, in degrees, the measure of the angle at v_A is $60A - \theta_\beta + \theta_\gamma$; see Figure 2. Similarly, the measure of the angle at v_B is $60B - \theta_\gamma + \theta_\alpha$ and the measure of the angle at v_C is $60C - \theta_\alpha + \theta_\beta$. Summing the measures of these three angles gives $60A + 60B + 60C = 180$ or $A + B + C = 3$.

Since each n -gon can be partitioned into $n - 2$ triangles, the result follows from this special case and part i. \square

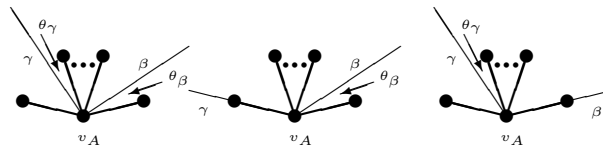


FIG. 2.

Our next task is to explore the structure of Λ in the neighborhood of a segment. We start by characterizing shortest paths in Λ and certain shortest paths in an arbitrary plane triangulation Γ . To do this, we introduce some additional terminology. Let $v = v_0, v_1, \dots, v_n = w$ be any path from v to w in Λ or any v, w -path in Γ such that v_1, \dots, v_{n-1} are 6-valent. Consider the vertex $v_i, i = 1, \dots, n - 1$, and consider the vertices adjacent to v_i clockwise from v_{i-1} . If v_{i+1} is in the first position, we say the path takes a *sharp left turn* at v_i ; v_{i+1} in the second position corresponds to a *left turn*; v_{i+1} in the fourth position corresponds to a *right turn*; v_{i+1} in the fifth position corresponds to a *sharp right turn*; otherwise we say the path continues *straight on* at v_i .

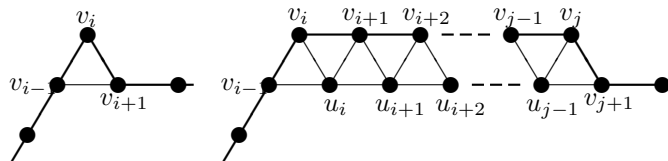


FIG. 3.

First, observe that if there is a sharp right (sharp left) turn at v_i , then $v = v_0, v_1, \dots, v_{i-1}, v_{i+1}, \dots, v_n = w$ is a shorter v, w -path. This is pictured at the left in Figure 3. Next, suppose that the path takes a right (left) turn at v_i , then continues straight on to v_j , where it takes another right (left) turn, pictured at the right in

Figure 3. Let u_i be the vertex adjacent to v_{i-1}, v_i, v_{i+1} ; then let u_k be the vertex adjacent to u_{k-1}, v_k, v_{k+1} , for $k = i + 1, \dots, j - 1$ (see Figure 3). Again we see that we have a shorter v, w -path:

$$v = v_0, v_1, \dots, v_{i-1}, u_i, \dots, u_{i-1}, v_{i+1}, \dots, v_n = w.$$

Now suppose that we have a v, w -path Π in Λ which makes no sharp turns and in which the turns alternate between left and right. One easily verifies that this is a shortest v, w -path. We have the following lemma.

LEMMA 4. *Let Π denote a shortest path in Λ or a shortest path in a plane triangulation Γ that has only 6-valent interior vertices. Then Π makes no sharp turns and consecutive turns alternate between left and right. Furthermore, a path in Λ which makes no sharp turns and in which the turns alternate between left and right is a shortest path between its endpoints.*

Consider a segment σ in Λ with endpoints v and w and Coxeter coordinates (p, q) . From this lemma, we easily see that all shortest paths from v to w lie in the parallelogram with antipodal vertices v and w and with sides parallel to the p and q directions. Furthermore, all v, w -paths in this parallelogram using only edges in the p or q directions are shortest v, w -paths. We call these the *family of shortest paths associated with the segment σ* and denote this family of paths and the parallelogram containing them by G_σ .

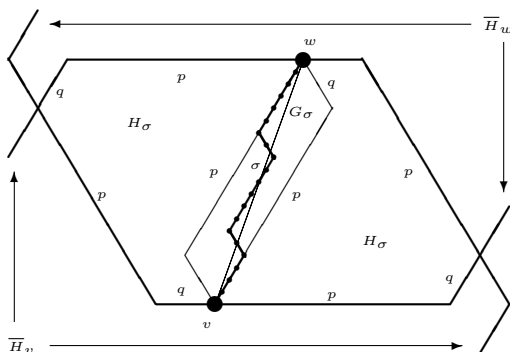


FIG. 4.

Now construct the hexagonal circuit \overline{H}_v about v spanned by the vertices at a distance of $p + q$ from v and let H_v denote the finite subgraph of Λ bounded by \overline{H}_v . Define \overline{H}_w and H_w similarly. Let $H_\sigma = H_v \cap H_w$ and denote its bounding circuit by \overline{H}_σ . We have pictured the various regions and boundaries of this construction in Figure 4. In drawing this picture, we have made some assumptions, namely that $0 < q < p$. If $q = p$, the picture is the same but with the segment vertical and, if $q > p$, the picture is the mirror image of this picture with the p and q labels reversed. \overline{H}_σ is a hexagon with opposite sides parallel and equal in length. The points v and w are antipodal on this boundary dividing the sides containing them into segments of length p and q . If σ has Coxeter coordinate (p) , H_σ consists of the union of two equilateral triangles with the given segment as the common side. In this case, \overline{H}_σ is a rhombus with sides of length p and may be visualized by letting $q = 0$ in Figure 4. Some easily checked but useful properties of this configuration are listed in the next lemma.

LEMMA 5.

- a. Let the segment σ , with endpoints v and w and Coxeter coordinates (p, q) , be given and let $G_\sigma, H_\sigma, \overline{H}_\sigma, \overline{H}_v$, and \overline{H}_w be defined as above.
 - (i) The collection of shortest v, w -paths in Λ is the collection of all v, w -paths in the parallelogram G_σ using only edges in the p or q directions.
 - (ii) For any vertex $u \in H_\sigma$, $\delta(u, v) \leq |\sigma|$ and $\delta(u, w) \leq |\sigma|$ with strict inequality in both cases whenever $u \in H_\sigma - \overline{H}_\sigma$.
- b. Let the segment σ , with endpoints v and w and Coxeter coordinate (p) , be given and let $G_\sigma, H_\sigma, \overline{H}_\sigma, \overline{H}_v$ and \overline{H}_w be defined as above.
 - (i) $G_\sigma = \sigma$, i.e., σ is the only shortest v, w -path in Λ .
 - (ii) For any vertex $u \in H_\sigma$, $\delta(u, v) \leq |\sigma|$ and $\delta(u, w) \leq |\sigma|$ with strict inequality in both cases whenever $u \in H_\sigma - \overline{H}_\sigma$.

While the graph distance function δ plays an important role in our development, a second distance function will be needed. If the segment σ has Coxeter coordinates (p, q) , we define the *refined length* of σ to be $p + q + \frac{|p-q|}{p+q+1}$ and denote it by $\|\sigma\|$; if σ has Coxeter coordinate (p) , we define $\|\sigma\| = p + \frac{p}{p+1}$. For example, the Coxeter coordinates of a segment which has length 5 must be one of (5), (4, 1), (3, 2), (2, 3), or (1, 4) and the refined length of this segment will be $5\frac{5}{6}, 5\frac{1}{2}, 5\frac{1}{6}, 5\frac{1}{6}$, or $5\frac{1}{2}$, respectively.

Let σ have Coxeter coordinates (p, q) $[(p)]$; then $\|\sigma\| = |\sigma| + \frac{|p-q|}{p+q+1}$ ($\|\sigma\| = |\sigma| + \frac{p}{p+1}$). Since $0 \leq \frac{|p-q|}{p+q+1} < 1$ ($0 < \frac{p}{p+1} < 1$), $|\sigma| \leq \|\sigma\| < |\sigma| + 1$. It follows that $|\sigma| = \lfloor \|\sigma\| \rfloor$. And from this we can conclude that if $\|\sigma\| = \|\sigma'\|$, then $|\sigma| = |\sigma'|$. Finally, suppose that σ' has Coxeter coordinates (p', q') and that $\|\sigma\| = \|\sigma'\|$. Then $p + q = p' + q'$ and $|p - q| = |p' - q'|$. It follows that either $p' = p$ and $q' = q$ or $p' = q$ and $q' = p$. We conclude that if $\|\sigma\| = \|\sigma'\|$, then σ and σ' are congruent segments. The converse is clearly true. Leaving the special case that σ and σ' have Coxeter coordinates (p) and (p') to the reader, we have the following lemma.

LEMMA 6. For segments σ and σ' ,

- i. $|\sigma| \leq \|\sigma\| < |\sigma| + 1$;
- ii. $|\sigma| = \lfloor \|\sigma\| \rfloor$;
- iii. if $\|\sigma\| = \|\sigma'\|$, then $|\sigma| = |\sigma'|$;
- iv. if $|\sigma| < |\sigma'|$, then $\|\sigma\| < \|\sigma'\|$;
- v. σ and σ' are congruent if and only if $\|\sigma\| = \|\sigma'\|$.

4. The signature of a plane triangulation. Let Γ be a finite plane triangulation and let P denote the set of all vertices of Γ with valence different from 6. Define the *first auxiliary graph* of Γ to be the complete graph $\mathcal{A}_1(\Gamma) = (P, K)$ and, for each $\{v, w\} \in K$, define $\omega_1(\{v, w\})$ to be the distance between v and w in Γ . Let $\mathcal{A}_2(\Gamma) = (P, E)$ be the structure graph of $\mathcal{A}_1(\Gamma), \omega_1$. $\mathcal{A}_2(\Gamma)$ is called the *second auxiliary graph* of Γ . We wish to investigate the geometry of Γ in the neighborhood of an edge of $\mathcal{A}_2(\Gamma)$. Let $\{v, w\}$ be an edge in $\mathcal{A}_2(\Gamma)$ and select a shortest path from v to w in Γ . By Lemma 1, part i, we conclude that there is no vertex $u \in P$ so that both the distance from u to v and the distance from u to w are less than $\omega_1(\{v, w\})$. In particular, all of the vertices (other than v and w) on this or any shortest path joining v and w have valence 6. Now consider this path as a subgraph of Γ . Since every vertex interior to this path has valence 6, we can trace a copy of this path in Λ such that the turns at each interior vertex are the same on the path and its copy. Label the corresponding ends of the copy by v and w . Then, by Lemma 4, this copy is a shortest v, w -path in Λ and may be identified with a segment σ in Λ as pictured in Figure 4.

Now consider the mapping from our path in Γ into Λ . We wish to extend this mapping to as large a region of Γ as is possible. Since both Λ and Γ are triangulations, we can extend this map to all vertices and edges which complete a triangle with one edge on the path or are adjacent to one vertex interior to the path. We continue to extend the domain of this map outward from the path by including adjacent vertices of degree 6. In view of Lemma 1, part i and Lemma 5, parts a(ii) and b(ii), we see that this mapping may be extended to a region of Γ which is mapped onto H_σ . We may think of the hexagonal region H_σ , pictured in Figure 4, as a region in Γ with the understanding that some of the vertices on the boundary may belong to P . We will call such a region a *hexagonal region of Γ* and we will use the same notation for this region and its various subsets as is used for their images in Λ .

Using this construction, each edge $\{v, w\}$ of $\mathcal{A}_2(\Gamma)$ may be identified with a segment in a hexagonal region of Γ . However, this identification depends on the choice of a shortest v, w -path in Γ . If σ is the segment associated with a given v, w -path, then any of the paths in G_σ will give the same hexagonal region. But Γ is a finite planar graph and perhaps there is another shortest v, w -path running “around the back.” This can indeed happen, in which case we would have another segment σ' associated with the edge $\{v, w\}$ in $\mathcal{A}_2(\Gamma)$ and another hexagonal region $H_{\sigma'}$ in Γ with v and w on its boundary. When this occurs we will add another v, w -edge to $\mathcal{A}_2(\Gamma)$ associated with σ' . Thus $\mathcal{A}_2(\Gamma)$, as amended, is a multigraph and we label each edge with the Coxeter coordinates of the segments associated with that edge. Note, if σ and σ' are the segment associated with multiple edges, then $|\sigma| = |\sigma'|$.

We may actually draw this amended $\mathcal{A}_2(\Gamma)$ on the sphere by superimposing it on the given drawing of Γ : for each edge of $\mathcal{A}_2(\Gamma)$, draw in the associated segment σ as it appears in H_σ . If these segments do not cross, this will be a planar embedding of $\mathcal{A}_2(\Gamma)$. Unfortunately, some of the edges of this drawing of $\mathcal{A}_2(\Gamma)$ may cross. We solve this problem by replacing the weight function ω_1 with the weight function ω_2 : for each edge e in $\mathcal{A}_2(\Gamma)$, let σ_e denote its associated segment and let $\omega_2(e) = \|\sigma_e\|$. The structure graph of $\mathcal{A}_2(\Gamma)$ with weight function ω_2 is called the *signature graph* of Γ and is denoted by $\mathcal{S}(\Gamma)$. We must keep in mind that $\mathcal{S}(\Gamma)$ could actually be a multigraph. However, we will continue to abuse notation and call it simply the signature graph of Γ . Since $\mathcal{S}(\Gamma)$ is obtained from $\mathcal{A}_2(\Gamma)$ by simply deleting some of its edges, $\mathcal{S}(\Gamma)$ inherits a natural drawing in the plane, and conveniently we have deleted enough edges to eliminate all crossings.

LEMMA 7. *For a plane triangulation Γ , the drawing of $\mathcal{S}(\Gamma)$ on the sphere described above is a planar embedding.*

Proof. Let Γ be a plane triangulation and consider the drawing of $\mathcal{S}(\Gamma)$ described above. Suppose that, in this drawing, the segments σ and σ' with endpoints $\{v, w\}$ and $\{v', w'\}$, respectively, cross. Denote the Coxeter coordinates of the segments by (p, q) and (p', q') , respectively. (We leave to the reader the similar but simpler cases where one or both of the segments have a single Coxeter coordinate.) Assume that $\|\sigma\| \geq \|\sigma'\|$; hence, $|\sigma| \geq |\sigma'|$ as well. We have drawn the hexagonal region of Γ about σ in Figure 5.

Since they belong to P , the vertices v' and w' cannot lie in the interior of H_σ . Select a shortest v', w' -path associated with the segment σ' and consider the intersection of this path with H_σ . This intersection contains a subpath which crosses σ . Let r and s denote the endpoints of this subpath, so that the clockwise order of the four points around \bar{H}_σ is v, r, w , and s .

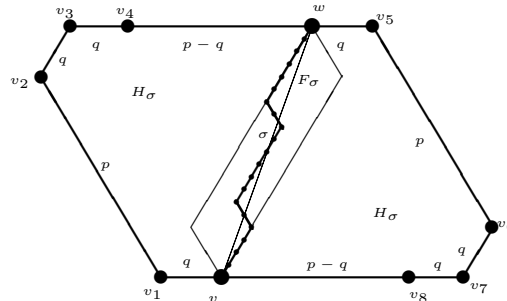


FIG. 5.

First, suppose that r lies on the section of the boundary from v_3 to w while s lies on the boundary from w to v_7 . In this case, w lies on a shortest r, s -path and, hence, on a shortest v', w' -path, which is impossible. Likewise, the possibility that r lies between v and v_3 while s lies on the boundary from v to v_7 can be eliminated.

Next, suppose that r lies on the section of the boundary from v_1 to v_3 while s lies on the boundary from v_5 to v_7 . In this case, $|\sigma| \geq |\sigma'| \geq \delta(r, s) \geq p + q = |\sigma|$ and equality must hold throughout. But equality can hold only if $\{v', w'\} = \{r, s\} = \{v_1, v_7\}$ or $\{v', w'\} = \{r, s\} = \{v_3, v_5\}$, and both options have already been excluded.

We conclude that one of r and s lies on the top boundary of H_σ and the other on the bottom boundary of H_σ . Thus we again have $|\sigma| \geq |\sigma'| \geq \delta(r, s) \geq p + q = |\sigma|$, and again equality must hold throughout. Thus $\{v', w'\} = \{r, s\}$ and we are free to assume $r = v'$ and $s = w'$.

Note that the segments joining v to v_4 and w to v_8 are reflections of σ and hence have the same refined length as σ . Now, if v' were to lie between v_4 and w , we easily see that the refined lengths from v' to v and v' to w are both less than $\|\sigma\|$, violating Lemma 1, part i. If v' were to lie between v_3 and v_4 , the refined length from v' to v would be greater than $\|\sigma\|$, and $\|\sigma'\|$ would be even larger, violating our original assumption. All that remains is the case where v' lies between v_1 and v while w' lies between w and v_5 . Again one can easily see that, in this case, $\|\sigma'\| > \|\sigma\|$, violating our original assumption. \square

We may now give the formal definition of the *signature* a plane triangulation Γ . It is the signature graph $\mathcal{S}(\Gamma)$ with the planar embedding given by the natural drawing of it superimposed on Γ , with its edges labeled by the Coxeter coordinates of the associated segments and its angles labeled by the angle types given by the drawing on Γ . We illustrate this definition with an example of a geodesic dome on 62 vertices (the dual fullerene has 120 vertices).

In Figure 6, the geodesic dome is pictured in the plane and is therefore somewhat distorted. The 5-valent vertices are circled and 6 segments of the signature are drawn in as double lines (note that two of them pass through vertices of valence 6). The remaining 14 segments of the signature all have length 1 and join adjacent 5-valent vertices. The signature graph is then redrawn on the left in Figure 7 with the segment and angle labels: the two lobes are identical and, to minimize clutter, we have included the angle labels only in the top lobe and the edge labels only in the bottom lobe.

The natural question to ask is, Does the signature of a plane triangulation uniquely determine that plane triangulation? Basically we are asking if it is true that the faces of the signature can be filled in consistent with the edge and angle labels in only one way. In the next section, we show that the answer is “yes” for geodesic domes. For

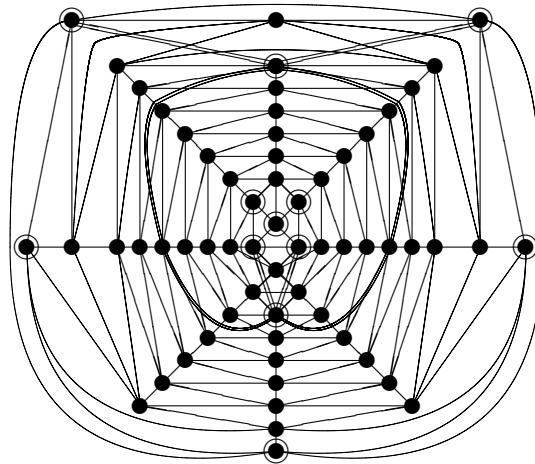


FIG. 6.

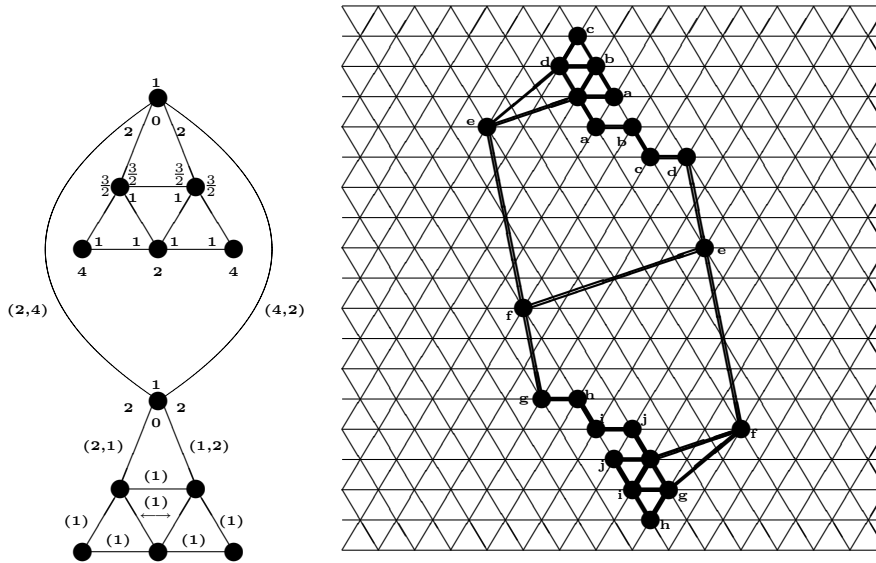


FIG. 7.

now, we simply continue with this example. On the right in Figure 7, we have drawn the faces of the signature in Λ with several of the segments identified. To build a three-dimensional model of Γ , simply cut along the unidentified segments and make the identifications indicated by the vertex labels.

5. The signature of a fullerene. The first part of the problem posed in the last section is to rebuild a plane triangulation from its signature. This boils down to filling in each face of the signature with a region from Λ that is consistent with the segment and angle labels of that face. The second part of the problem is to show that this can be done in only one way. The natural approach to filling in the faces is to select a face of the signature and then simply reconstruct its boundary in Λ

as prescribed by its segment and angle labels: denote the segments by $\sigma_1, \dots, \sigma_k$ in clockwise order around the face; draw a segment σ'_1 in Λ congruent to σ_1 ; draw in a segment σ'_2 congruent to σ_2 sharing an endpoint so that the angles between σ_1 and σ_2 and σ'_1 and σ'_2 have the same type; and so on. Ultimately this is precisely what we will do; but at the outset it is not even clear that this “dead reckoning” approach will result in a closed polygonal region of Λ . To aid in our investigation we introduce some additional notation. Following Brinkmann, Friedrichs, and Nathusius [1], we define an (m, k) -patch to be a plane graph such that

- all faces are k -gons, except for one n -gon,
- the boundary of the n -gon is an elementary circuit and is called the boundary of the patch,
- all vertices not on the boundary have valence m while those on the boundary have valence at most m .

For a simple example of a $(6, 3)$ -patch, consider any region of Λ bounded by an elementary circuit. For a more complicated example, consider a long narrow region which curves around and overlaps itself. For the $(6, 3)$ -patch, we consider the overlapping portions of the region to be distinct. Now let Γ be a geodesic dome and consider a face of $\mathcal{S}(\Gamma)$. Replace each segment σ in the boundary of this face by a shortest path joining its endpoints that lies in G_σ . If the angle between consecutive segments σ and σ' is small, G_σ and $G_{\sigma'}$ may overlap. In this case, we select the paths in $G_\sigma \cup G_{\sigma'}$ so that they do not intersect. Next, label the vertices and edges on these paths clockwise around the face; vertices and edges which lie on paths corresponding to segments that bound the face on two sides are labeled twice, once from each side. Considering doubly labeled vertices and edges as two distinct vertices or edges, we have associated a $(6, 3)$ -patch with the given face.

By a *drawing* of a $(6, 3)$ -patch, Δ , in Λ , we mean a graph homomorphism from Δ into Λ such that distinct triangular faces sharing a common edge are mapped onto distinct triangular faces sharing a common edge. Up to an automorphism of Λ , a given $(6, 3)$ -patch has a unique drawing in Λ : select any triangular face of Δ and map into Λ ; this mapping extends uniquely to its neighboring triangular faces and then to their neighbors, etc., until the entire patch is drawn. Let Δ be a $(6, 3)$ -patch with boundary Ω and let $v_0, \dots, v_{n-1}, v_n = v_0$ be the vertices of Ω in cyclic order around the patch. The cyclic sequence of valences $\rho(v_0), \dots, \rho(v_{n-1}), \rho(v_n) = \rho(v_0)$ is called the *boundary code* for Ω . Note that, by the definition of (m, k) -patch, $2 \leq \rho(v_i) \leq 6$, for each $i = 1, \dots, n$. Given the boundary code of Δ , we may inductively draw this boundary in Λ : in Λ , select any two adjacent vertices v'_0 and v'_1 to be the images of v_0 and v_1 ; once the edge $\{v'_{i-1}, v'_i\}$ has been drawn, let v'_{i+1} be the $\rho(v_i)$ th vertex adjacent to v'_i counting counterclockwise starting with v'_{i-1} and draw in $\{v'_i, v'_{i+1}\}$. At each step, the drawing of this circuit must match with the boundary of the appropriate drawing of the entire patch Δ . Thus, the drawing of Ω in Λ is unique up to an automorphism of Λ and depends only on the boundary code for Ω .

Now let Δ be a $(6, 3)$ -patch associated with a face of the signature of a geodesic dome Γ , as constructed above, and draw its boundary in Λ . The image of the boundary may then be partitioned into paths corresponding to the segments in $\mathcal{S}(\Gamma)$ from which they came. Clearly, the endpoints of each such path define a segment in Λ with the same Coxeter coordinates its corresponding segment in $\mathcal{S}(\Gamma)$. Replacing these paths by segments in Λ , results in a (perhaps overlapping) polygonal region of Λ bounded by segments corresponding to the segments bounding the given face. Furthermore, the angle labels match. We have proved the following lemma.

LEMMA 8. *Up to an automorphism of Λ , the polygonal boundary of the face of the signature of a plane triangulation has a unique drawing in Λ with the same sequence of Coxeter coordinates and angle types.*

The next question is, Is the polygonal region of a face of the signature of a geodesic dome uniquely determined by its boundary? X. Guo, P. Hansen, and M. Zheng [8] constructed two distinct (3,6)-patches with the same boundary sequence and his example is easily altered to produce two distinct (6,3)-patches with the same boundary. We say that a boundary sequence is *ambiguous* if there exist two distinct (6,3)-patches with the same boundary sequence. We say that the face of the signature of a plane triangulation is *ambiguous* if there exist two distinct polygonal regions with the boundary of that face. The next lemma follows at once from Lemma 8.

LEMMA 9. *A geodesic dome with a signature that admits no ambiguous faces is uniquely determined by its signature.*

If the drawing of the boundary of a (6,3)-patch is an elementary circuit, then its interior is uniquely determined and the patch is not ambiguous. Hence the drawing of an ambiguous (6,3)-patch in Λ must be self-overlapping. The drawings of faces of triangulations with vertices of valence more than 6 may well be self-overlapping and possibly ambiguous. In the remainder of this section, we sketch the proof that a face of the signature of a geodesic dome cannot yield a self-overlapping region when drawn in Λ thereby verifying:

THEOREM 1. *A geodesic dome is uniquely determined by its signature.*

The basic idea is that a face of the signature of a geodesic dome cannot curve back in itself far enough to overlap. Rather than looking at all possible faces of the signature of a geodesic dome, we consider the single face of a shortest spanning tree of the geodesic dome. This is the union of all of the faces of the signature and, if its drawing is not self-overlapping, none of the faces can have self-overlapping drawings. As a prototype self-overlapping face of a shortest spanning tree, consider the region pictured in Figure 8. There are several features to observe. First, since a spanning tree has 11 segments, this face is bounded by 22 segments. Second, in order to turn back on itself as pictured here, the face must have several angles of types greater than 3 (e.g., A , B , and C).

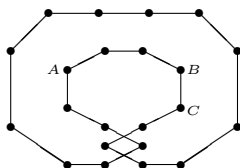


FIG. 8.

We start by eliminating the possibility of some angle types. The arguments we include here are very geometric and will be carried out in Λ . They will be valid in the geodesic dome by virtue of the fact that they will be carried out in a region of Λ corresponding to the union of overlapping hexagonal regions of signature segments in the geodesic dome.

LEMMA 10. *The signature of a geodesic dome admits no angles of types $\frac{1}{2}$ or $4\frac{1}{2}$. A shortest spanning tree of a geodesic dome admits no angles of types 0, $\frac{1}{2}$, or $4\frac{1}{2}$. Furthermore, the vertices at angles of types 4 and $3\frac{1}{2}$ in a shortest spanning tree have valence 2 while angles of type 5 occur only at pendant vertices.*

Proof. Let Γ be a geodesic dome and let segments σ with endpoints v and w and τ with endpoints u and v be segments in $\mathcal{S}(\Gamma)$. Assume that the type T of the angle between these two segments is 0 or $\frac{1}{2}$ and that $|\sigma| \geq |\tau|$. Since u cannot lie interior to the hexagonal region of σ , it must lie on the top boundary of H_σ as illustrated in Figure 9. We observe that the distance between u and w is less than the distance between v and w . Thus, both σ and τ can belong to $\mathcal{S}(\Gamma)$ only if they have the same refined length. If $T = \frac{1}{2}$, this is impossible since their Coxeter coordinates are (p, q) and $(p + q)$. Thus $\mathcal{S}(\Gamma)$ does not have an angle of type $\frac{1}{2}$. $\mathcal{S}(\Gamma)$ will include both σ and τ with $T = 0$ if τ has Coxeter coordinates (q, p) . But in this case, the segment joining u and w would be considered by the shortest spanning tree algorithm before σ and τ and at most one of σ and τ could belong to a shortest spanning tree.

Since the types of the angles at a vertex in $\mathcal{S}(\Gamma)$ or a shortest spanning tree must sum to 5, an angle of type $4\frac{1}{2}$ is excluded. In a shortest spanning tree, an angle of type 4 or type $3\frac{1}{2}$ can only occur at a vertex of valence 2 across from a vertex of type 1 or type $1\frac{1}{2}$ and an angle of type 5 is excluded from a shortest spanning tree unless it is a pendant vertex. \square

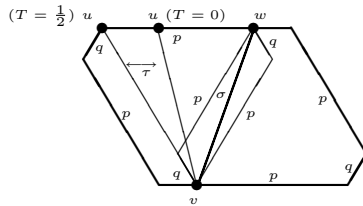


FIG. 9.

There are three basic ways in which an overlap could occur: as the result of a broad curve like that pictured in Figure 8, a broad curve in conjunction with a pendant vertex, or as the result of several pendant vertices. We consider each of these possibilities in turn.

The edges at each vertex of Λ divide the neighborhood about that vertex into six sectors. We label these sectors with the integers mod six starting with 0 at the bottom and working clockwise around the vertex; see Figure 10. Fix a shortest spanning tree and let σ_0 and σ_1 be segments of the tree with a common endpoint v_1 . Suppose that, moving clockwise around the tree (counterclockwise around the face), we encounter σ_0 followed by σ_1 . Suppose further that the type of the angle the segments make at v_1 is T_1 (an integer) and that σ_0 approaches v_1 through sector 0; then σ_1 leaves v_1 through sector T_1 . We have illustrated this with an angle of type 4 on the left in Figure 10. If T_1 were not an integer, say $3\frac{1}{2}$, then σ_1 would leave along the edge separating sectors 3 and 4 or σ_0 could enter along the edge separating sectors 0 and 1 while σ_1 leaves through sector 4. If σ_1 leaves v_1 through sector T_1 , it approaches its other endpoint through sector $T_1 - 3$. Hence, if we have a path which is a section of the boundary $\sigma_0, v_1, \dots, v_k, \sigma_k$ with angle type T_i at v_i and if σ_0 approaches v_0 through sector 0, then σ_k approaches v_{k+1} through sector $(\sum_1^k T_i) - 3k$, (if $(\sum_1^k T_i) - 3k = T + \frac{1}{2}$, σ_k approaches v_{k+1} along the edge separating sectors T and $T + 1$). This number, $(\sum_1^k T_i) - 3k$, is called the *excess* of the path. In order to yield a self-overlapping region, this section of the boundary must make a complete clockwise change of direction and approach v_{k+1} through sector 3 or higher. That is, its excess must be at least 3: $(\sum_1^k T_i) - 3k \geq 3$ or $(\sum_1^k T_i) \geq 3k + 3$. Hence we must have several angles of type 4 or $3\frac{1}{2}$ along a portion of the tree. Since angles of types $3\frac{1}{2}$ and 4 occur only at vertices of valence 2 in our shortest spanning tree, it is not surprising that the “worst case

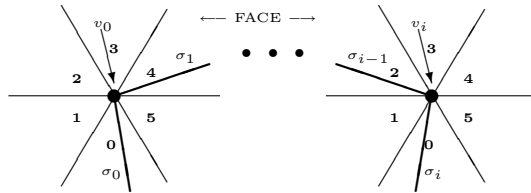


FIG. 10.

scenario” is that our shortest spanning tree is a simple path. So think of a subpath of our tree along which the angles have types 4, $3\frac{1}{2}$, and 3. We investigate this subpath by considering the angles on the other side of the path.

We are interested in constructing a path in our shortest spanning tree of length k so that the sum of the types of the angles along this path is at most $5k - (3k + 3) = 2k - 3$. In Figure 11, we have drawn an angle of type 1 at vertex v_0 . Around the vertex v_{-1} , we have constructed a hexagon; any vertex in this hexagon has its distance to v_{-1} less than $|\sigma_0|$. Thus v_1 is outside (or on) the hexagon; were it inside, the segment joining v_{-1} to v_1 would have been selected in place of σ_0 or σ_1 when constructing the shortest spanning tree. If the next segment, σ_2 (from v_1 to v_2), were to make an angle of type 1, it would either (1) force v_2 to lie in the hexagon; (2) force σ_2 to be so long that it completely crosses the hexagon; (3) force σ_2 to be so short that it never intersects the hexagon. In the first case, we have the previous contradiction. In the second case, v_2 is closer to v_{-1} than to v_1 , resulting in another contradiction. The third case is impossible since v_2 must lie outside the corresponding hexagon around v_1 . The same argument will exclude an angle of type $1\frac{1}{2}$. Thus, the angle at v_1 is of type at least 2. At this point we note that the angle at v_0 would be of type $1\frac{1}{2}$ if σ_1 were horizontal. And the above arguments would still preclude the angle at v_1 being of type 1. However, two successive angles of type $1\frac{1}{2}$ are possible. We continue considering the case of angles of integer type and simply note that our arguments can be adapted to the cases involving angles of fractional type.

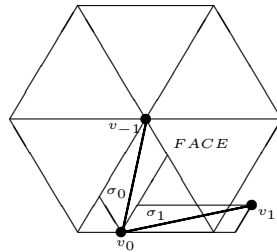


FIG. 11.

In Figure 12, we have added σ_2 with an angle of type 2 at v_1 and σ_3 with an angle of type 2 at v_2 . Neither of these aid in our goal of a path with type sum $2k - 3$. It would seem that the only way to make a sharp, type 1 turn to the left is to first pull away from the hexagon and then turn toward it but not into it. To pull away, we could include a type 3 angle; but this would nullify the initial type 1 angle in the sum. The only other option is to make a segment like σ_3 much longer than the side of the hexagon. However, this won't work either. For example, the distance between v_3 and v_{-1} must be as long or longer than $|\sigma_0|$, $|\sigma_1|$, $|\sigma_2|$, and $|\sigma_3|$; otherwise

the segment joining v_3 and v_{-1} would have been added to the shortest spanning tree before the longest of those segments. In short, adding a long segment at an angle of type 2 increases the size of the “forbidden hexagon” about v_{-1} for all subsequent vertices. We conclude that, as we move along a section of the boundary of the face in either direction from a vertex of type 1, we must encounter a vertex of type 3 or more before we may encounter a second vertex of type 1. A similar conclusion holds when fractional types are considered. Hence, we can never achieve a path with type sum at most $2k - 3$ nor one with type sum at least $3k + 3$ (excess 3 or more) using only nonpendant vertices.

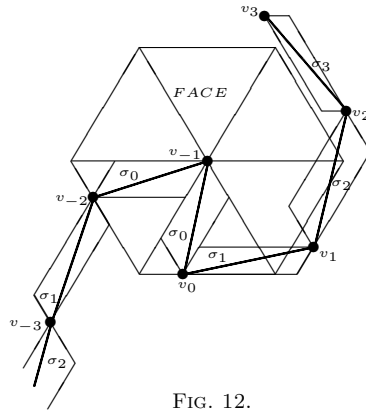


FIG. 12.

So the next question is, Can we get a little extra back curvature at a pendant vertex? The answer is “yes, but far too little for an overlap.” We illustrate this by assuming that v_{-1} has valence 5. This is also pictured in Figure 12. As one can see, the face does turn back on itself—but not sharply enough to self-intersect. Because the vertices of the spanning tree have valence 5 in Γ , we have that the outside angle at v_{-1} is of type 1. If the two copies of segment σ_1 were extended to intersect, their outside angle would be of type 2 and the two copies of σ_2 make an angle of type 3. So, at each step away from v_{-1} , the two boundary paths are pulling away from one another and we conclude that no overlapping can occur near the pendant vertices.

The only remaining question is whether several pendant vertices could yield an overlap. Here there are many cases to consider. By a *branch*, we mean a single edge along with one of the components that its deletion yields. A branch with k vertices yields a section of the boundary with $2k$ edges and $2k - 1$ vertices; see Figure 13 below. We can easily compute the excess of this entire section of the boundary path of the face: the sum of all angle types at these $2k - 1$ vertices is $5k$; so the excess along the entire path is $5k - 3(2k - 1) = 3 - k < 3$. The natural question to ask is, Could a subpath have a higher excess?

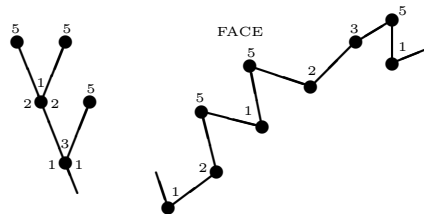


FIG. 13.

Among all possible subpaths of the face boundaries of branches, consider those with largest possible excess. Suppose that v is a pendant vertex of the branch and is interior to the subpath of the face boundary. Let $T, 5, T'$ be the angle types of the three vertices on the subpath centered at v . These three vertices contribute $T + 5 + T' - 9 = T + T' - 4$ to the excess of the path. Now delete this pendant vertex from the branch and adjust the subpath accordingly. The three vertices are replaced by a single vertex of type $T + T'$ which contributes $T + T' - 3$ to the excess. Thus the smaller branch has a subpath with a larger excess. We have carried out this reduction on the branch in Figure 13 and recorded the result in Figure 14. We conclude that the branches with a subpath having a largest possible excess have just two pendant vertices and that the subpath with largest possible excess runs from one pendant vertex to the other. Checking our examples, we see that the subpath in Figure 13 between the extreme pendant vertices has an excess of 3 while the corresponding subpath in Figure 14 has an excess of 4.

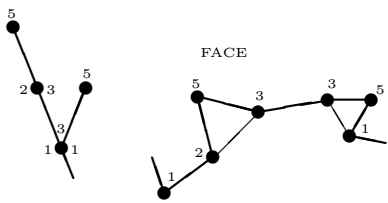


FIG. 14.

As we have noted the sum of the angle types along the entire path around a branch with k vertices is $5k$. Assume that we have a branch with just two pendant vertices. To make the excess of the subpath that runs from one pendant vertex to the other as large as is possible, we should make the sum of the types along the outside of paths from the trivalent vertex to the pendant vertices as small as possible. As we have already shown, the sum of the types along such a path will be as small as is possible when we have one angle of type 1 (or two of type $1\frac{1}{2}$) and the rest of type 2. This smallest sum is then $2(k - 2)$. So the sum of the angle types along the subpath joining the two pendant vertices is $5k - 2(k - 2) = 3k + 4$ and its excess is 4.

Finally, we note that a pendant vertex gives rise to two sides of an equilateral triangle along the face boundary. If we add the triangle to the face replacing the two edges by the third side of the triangle, we get a region of Λ that contains the face. We note further that making this substitution in the subpath results in decreasing the excess by 1. Carrying out this reduction throughout the entire face results in a region containing the face which has the property that no subpath of the boundary has excess 3 or more and hence is nonoverlapping. Hence the face is nonoverlapping.

6. Using the signature. It follows from Theorem 1 that the signature $\mathcal{S}(\Gamma)$ of a geodesic dome carries complete information about the geodesic dome Γ and its fullerene dual. It would be convenient if we could read some of this information directly from $\mathcal{S}(\Gamma)$. In *An Atlas of Fullerenes* [6], Fowler and Manolopoulos indicate that whether or not pentagonal faces are adjacent is an important feature of a fullerene. Clearly, the relative positions of the pentagonal faces can be read directly from its signature. Another feature of a geodesic dome/fullerene that can be easily deduced from its signature is its symmetry structure.

Let the geodesic dome Γ be given. Any automorphism α of Γ must permute the 5-valent vertices, and hence it induces a permutation of the vertices of $\mathcal{A}_1(\Gamma)$ which we also denote by α . Since α preserves distance, it is an automorphism of the weighted

graph $\mathcal{A}_1(\Gamma), \omega_1$. It must then map spanning trees of $\mathcal{A}_1(\Gamma)$ onto spanning trees of $\mathcal{A}_1(\Gamma)$. It follows that α must map $\mathcal{A}_2(\Gamma)$, the structure graph of $\mathcal{A}_1(\Gamma)$, onto itself. Suppose that v and w are vertices in P joined by the segment σ in $\mathcal{A}_2(\Gamma)$. Clearly, α maps the hexagonal region of Γ determined by v and w onto the hexagonal region of Γ determined by $\alpha(v)$ and $\alpha(w)$. Thus $\alpha(\sigma)$ is congruent to σ and α preserves refined length.

Applying the above arguments to $\mathcal{A}_2(\Gamma), \omega_2$, we conclude that α induces an automorphism of its structure graph, namely $\mathcal{S}(\Gamma)$. Furthermore, if the original α is an orientation preserving automorphism of Γ , the induced α is an orientation preserving automorphism of $\mathcal{S}(\Gamma)$ that maps segments onto segments with the same Coxeter coordinates and, if the original α is an orientation reversing automorphism of Γ , the induced α is an orientation reversing automorphism of $\mathcal{S}(\Gamma)$ that maps segments onto segments with reversed Coxeter coordinates. In both cases α preserves angle types. Thus we are led to define an *automorphism* of a signature to be an automorphism of the signature graph (as a plane graph) that preserves angle types and preserves or reverses the Coxeter coordinates of the edges, according to whether it is orientation preserving or orientation reversing.

Now suppose that α is an automorphism of the signature of Γ . Since the edge and angle labels around a face determine a unique region of Λ up to an automorphism of Λ , α has a natural extension to an automorphism of Γ . Thus this mapping of the automorphism group of Γ into the automorphism group of its signature is onto. Is it one-to-one? Surprisingly, the answer is “not always.” We explore these exceptional cases next.

Let α and β be automorphisms of Γ which induce the same automorphism on its signature. Since Γ is a triangulation of the plane, two automorphisms which agree on a single triangular face agree everywhere. Let v and w be any two vertices in P joined by an edge in the signature. Then α and β map the hexagonal region determined by v and w onto the hexagonal region determined by $\alpha(v) = \beta(v)$ and $\alpha(w) = \beta(w)$. If they agree on this hexagonal region, they would agree everywhere. Hence the hexagonal region must be symmetric and the two images of the v, w -hexagonal region must be reflections of one another. This is only possible if the edge is of type (p) or (p, p) . Next, suppose that u, v , and w are the vertices of a path of length two in the signature. Since the image of this path must be invariant under reflection, v has valence two in $\mathcal{S}(\Gamma)$ and the angles at v are both of type $\frac{\rho}{2}$, where ρ is the valence of v in Γ . It follows that $\mathcal{S}(\Gamma)$ is either a path or a circuit, that its edge labels are of the forms (p) and (p, p) and that the angle types are equal at each vertex. If Γ is a plane triangulation with such a signature, one easily sees that both the identity and the reflection through the line or circuit of its signature induce the identity on its signature. An example of such a geodesic dome is worked out at the end of this section. We have proved the following theorem.

THEOREM 2. *Let Γ be a plane triangulation.*

- i. *If $\mathcal{S}(\Gamma)$ is not a path or circuit with the special labeling described above, then its automorphism group and the automorphism group of its signature are isomorphic.*
- ii. *If $\mathcal{S}(\Gamma)$ is a path or circuit with the special labeling described above, then its automorphism group is isomorphic to the direct product of the automorphism group of its signature and the reflection through its signature.*

The next question we tackle is, How can we compute the number of vertices, edges and faces of a plane triangulation from its signature? To answer this question, consider

a polygonal region with vertices v_0, v_1, \dots, v_n in counterclockwise order around the region. Fix the coordinate system with v_0 at the origin, with the horizontal edge to the right at v_0 as the unit vector in the x direction and the next edge counterclockwise as the unit vector in the y direction. The x, y -coordinates of the segment directed from the point v to the point w is simply the coordinates of w minus the coordinates of v . It should be clear that the x, y -coordinates of a segment can be computed directly from its orientation and its Coxeter coordinates. Returning to our polygonal region, the orientations of the bounding segments are determined, in order, by the orientation of the previous segment and the type of the angle between them. For $i = 1, \dots, n$, let (x_i, y_i) denote the x, y -coordinates of the segment joining v_{i-1} and v_i . It follows that the coordinates of the vertex v_i are $(\bar{x}_i, \bar{y}_i) = (\sum_{j=1}^i x_j, \sum_{j=1}^i y_j)$. The standard formula for the area of such a polygonal region is $\frac{1}{2} \sum_{1 \leq i < n} (\bar{x}_i \bar{y}_{i+1} - \bar{x}_{i+1} \bar{y}_i)$. Note that a unit square in the x, y coordinate system consist of two lattice triangles and thus the area of the region is equal to the area of $\sum_{1 \leq i < n} (\bar{x}_i \bar{y}_{i+1} - \bar{x}_{i+1} \bar{y}_i)$ lattice triangles. Finally, substituting the x, y values for \bar{x}, \bar{y} in this formula gives the area, in lattice triangles, as

$$\sum_{1 \leq i < j \leq n} (x_i y_j - x_j y_i).$$

Using this formula, we compute the area of each face of the signature of a plane triangulation Γ . The sum t of these areas will then be the number of the triangles or faces of Γ and the numbers of edges and vertices will be given by the formulas $e = \frac{3t}{2}$ and $v = \frac{t+4}{2}$.

We close with one more example. This is the signature for one of the families of fullerenes that arose in our discussion of symmetry. The signature graph consists of a single path; the angle labels are 5 at the pendant vertices and 2.5 for all other angles; the segment labels are variables. See Figure 15.

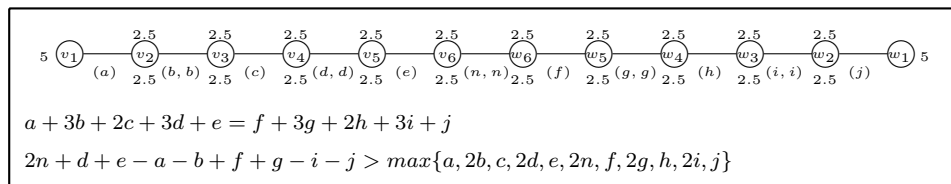


FIG. 15.

In selecting values for the parameters the conditions listed in the figure must be satisfied. The equality ensures that the face, as laid out in Λ , actually closes. If one were to carry out this construction for a given set of values, the vertices v_1 and w_1 could be quite close to one another. In that case, (v_1, w_1) would be a segment in the signature of the fullerene we construct. So, in order to make sure that the signature with which we start is the signature of the fullerene we produce, the inequality must hold.

Using the formula for area derived above, we may compute the number of triangles in the geodesic dome or the number of vertices in the fullerene. This number turns out to be a rather complicated quadratic polynomial in these 11 variables:

$$2ab + 2ac + 4ad + 2ae + 2bc + 6bd + 4be + 2cd + 2ce + 2de + 2fg + 2fh + 4fi + 2fj + 2gh + 6gi + 4gj + 2hi + 2hj + 2ij + (d + e - a - b + f + g - i - j + 4n)s, \text{ where } s = a + 3b + 2c + 3d + e = f + 3g + 2h + 3i + j.$$

One final observation: The fullerenes in this family are nanotubes. Select any fullerene in this family, i.e., select values for the parameters that satisfy the equality and the inequality and note that n can be increased without limit while keeping the remaining parameters fixed. In general, a nanotube will have a signature containing an edge cut set consisting of congruent segments that partition the vertices into two classes of six vertices each and have a parameter that may be enlarged independent of all other parameters. Our first example, pictured in Figures 6 and 7, is also a nanotube. The cut set consists of the double edges connecting the vertices labeled e and f in the right-hand picture of Figure 7. Replace their Coxeter coordinates with $(n, 4)$ and $(4, n)$; increasing n beyond 2 simply moves the top configuration (vertices a through e) up and to the right along the line of the tessellation.

REFERENCES

- [1] G. BRINKMANN, O. D. FRIEDRICHS, AND U. V. NATHUSIUS, *Numbers of faces and boundary encodings of patches*, to appear in *Graphs and Discovery, Proceedings of the DIMACS Workshop on Computer-Generated Conjectures from Graph Theoretic and Chemical Databases*.
- [2] D. L. D. CASPAR AND A. KLUG, *Physical principles in the construction of regular viruses*, *Cold Spring Harbor Symp. Quant. Biol.*, 27 (1962), pp. 1–24.
- [3] H. S. M. COXETER, *Virus macromolecules and geodesic domes*, in *A Spectrum of Mathematics*, J. C. Butcher, ed., Oxford University Press, Oxford, UK, 1971, pp. 98–107.
- [4] P. W. FOWLER, J. E. CREMONA, AND J. I. STEER, *Systematics of bonding in non-icosahedral carbon clusters*, *Theor. Chim. Acta*, 73 (1988), pp. 1–26.
- [5] P. W. FOWLER AND J. E. CREMONA, *Fullerenes containing fused triples of pentagonal rings*, *J. Chem. Soc., Faraday Trans.*, 93 (1997), pp. 2255–2262.
- [6] P. W. FOWLER AND D. E. MANOLOPOULOS, *An Atlas of Fullerenes*, Clarendon Press, Oxford, UK, 1995.
- [7] M. GOLDBERG, *A class of multi-symmetric polyhedra*, *Tôhoku Math. J.*, 43 (1937), pp. 104–108.
- [8] X. GUO, P. HANSEN, AND M. ZHENG, *Boundary Uniqueness of Fusenes*, Tech. report G-99-37, GERAD, Montreal, Quebec, Canada, 1999.