THE CLASSIFICATION OF ℓ_1-EMBEDDABLE FULLERENES

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ABSTRACT

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In Chemistry, fullerenes are molecules composed entirely of carbon atoms, in the form of a hollow sphere, ellipsoid or tube, such that each atom is bonded with three other atoms and the atoms form pentagonal or hexagonal rings. The spherical fullerenes motivated the related mathematical concept: a fullerene graph is a trivalent plane graph such that all faces are pentagons and hexagons.

The goal of this research is to prove the conjecture that there are exactly five ℓ_1-embeddable fullerenes. These are known to be the following fullerenes: $\mathcal{F}_{20}(I_h)$, $\mathcal{F}_{26}(D_{3h})$, $\mathcal{F}_{40}(T_d)$, $\mathcal{F}_{44}(T)$ and $\mathcal{F}_{80}(I_h)$ (where the group of symmetry is given in parentheses for each fullerene). We proceed in proving this result by looking at the minimal distance between the pentagonal faces of the fullerene. In the cases when the minimal distance between pentagons is greater than two we obtain a contradiction, which leads us to conclude that in an ℓ_1-embeddable fullerene there must exist at least two pentagons that either are adjacent or have a common hexagonal neighbor. For the latter cases we show that the only possibilities are the five fullerenes listed above.

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CHAPTER 1

INTRODUCTION

1.1 About ℓ_1-embeddable graphs

In recent years, a lot of research has been done around the ℓ_1-embeddability of finite or infinite graphs. The present dissertation contributes to this line of research, filling one of the existing gaps.

The main concept of this thesis is the concept of an ℓ_1-*graph*. To define it let us start with a more familiar one. A *distance space* is a set X with a function $d : X \times X \to \mathbb{R}_+$, such that d is symmetric and $d(x, y) = 0$ if and only if $x = y$. If d also satisfies the triangle inequality, *i.e.*, $d(x, z) \leq d(x, y) + d(y, z)$, for all $x, y, z \in X$, then d is called a *metric* and (X, d) becomes a *metric space*. Examples of metric spaces are abundant, but probably the most well known are the ℓ_p spaces. Given the vector space $\mathbb{R}^n$ we can define on it the metric $d_{\ell_p}(x, y) = (\sum_{i=1}^n |x_i - y_i|^p)^{\frac{1}{p}}$, thus obtaining an ℓ_p space. For $p = 2$ we get the usual Euclidean metric. When $p = \infty$ the distance function can be defined as $d_{\ell_\infty}(x, y) = max\{|x_i - y_i|, 1 \leq i \leq n\}$. The ℓ_p spaces often play the role of the standard metric spaces with which other metric spaces are compared.

In graph theory, many examples of metric spaces come from connected weighted graphs, where each edge has a certain weight—also called its *length*. Ordinary connected graphs can be viewed as having constant edge weight one, which leads to the concept of the path distance on the graph. Thus, every connected graph can be viewed as a distance space, in fact, a metric space.

Given two distance spaces, an *isometric mapping* between the two spaces is a mapping that preserves distances. These mappings are the natural morphisms in the category of distance spaces. They are always injective mappings.

Observe that with every standard distance space we can associate a class of distance spaces, namely the distance spaces isometrically embeddable into the standard space considered. Thus we can define the ℓ_p*-distance spaces* as the distance spaces isometrically embeddable into the ℓ_p spaces for a fixed p. The most prominent of these are the ℓ_1*-distance spaces*, the ℓ_2*-distance spaces* (these are actually subsets of the Euclidean space) and the ℓ_∞*-distance spaces*. This thesis will deal with the class of ℓ_1-distance spaces, specifically with the subclass of ℓ_1-graphs.

Some examples of ℓ_1-graphs are: the *complete graphs*, the *Hamming graphs*, the *Johnson graphs* $J(n, k)$. A further example is the infinite hexagonal lattice in the plane or any finite convex part of it.

The above are examples of classes of graphs where all graphs are ℓ_1-embeddable. However, not all classes of graphs have the nice property that all their members are ℓ_1-embeddable. Therefore an interesting question to pose is which of the graphs in a given class of graphs are ℓ_1-embeddable. This approach was taken in quite a few papers, among which we can cite [DFS], [DDG], [CDG], [DDS] and [DDS05]. Of particular importance is the book [DGS], where many classes of polyhedral and lattice graphs were systematically examined.

A central result in the problem of recognizing which graphs are ℓ_1-graphs was established by Assouad and Deza in [AsDe1] and [AsDe2], see Theorem 2.1.1 below. According to this result a graph is an ℓ_1-graph if and only if it is scale embeddable into a hypercube. A scale embedding is an embedding of one space into the other such that the distance in the second space is proportional with the distance in the first. The proportionality constant is called *the scale* of the embedding.

In the paper [Sh93] Shpectorov establishes, among other things, that the ℓ_1-graphs can be recognized in polynomial time which is surprising since Karzanov proved that for the general ℓ_1-distance spaces the recognition problem is NP-complete, that is, requires exponential time.

In another paper [DeSh], Deza and Shpectorov proposed a concrete algorithm for determining the ℓ_1-embeddability of graphs. This algorithm was later implemented by Pasechnik within the computer algebra programming system called GAP. Later, the algorithm has been improved by Dutour and it has been used successfully to determine the ℓ_1-embeddability of many concrete graphs. The five ℓ_1-embeddable fullerenes that we mentioned in the Abstract have been discovered via this computer program.

Deza proposed as a research project the determination of all ℓ_1-graphs that are the edge graphs of various polyhedra. Together with Grishukhin and Shtogrin, Deza systematically examined many classes of polyhedral, polytopal and lattice graphs in the book [DGS]. Along the same lines, Deza, Dutour and Shpectorov published the paper [DDS] which deals with the Archimedean Wythoff polytopes.

Another interesting class of graphs is the class m_n of trivalent plane graphs such that every face is either a hexagon or an m-gon and n represents the number of vertices if the graph is finite. The unique graph 6_n is the infinite hexagonal lattice and it is embeddable into the infinite dimensional ℓ_1-space. If $m > 6$ the graphs obtained are also infinite and drawn naturally on the Minkovski plane. They have been shown to be ℓ_1-embeddable. When $m < 6$ the graphs m_n are finite. In particular, 5_n are the fullerene graphs. The ℓ_1-embeddable 4_n graphs have been determined by Deza, Dutour and Shpectorov in [DDS05]. The ℓ_1-embeddable 3_n graphs have also been classified (only the tetrahedron is ℓ_1-embeddable among such graphs; see [DDS05] for the explanation). Thus the present dissertation completes the last open case ($m = 5$) of the classification of all m_n graphs that are ℓ_1-embeddable.

Let us mention another class of ℓ_1-embeddable graphs: the *outerplanar graphs.* These are graphs that have an embedding into the Euclidean plane such that the vertices lie on a fixed circle and the edges lie inside the disk and do not intersect. The outerplanar graphs were shown to be ℓ_1-embeddable in [CDG].

More on ℓ_1-graphs: two papers complete the classification of *complementary* ℓ_1*-graphs* ($i.e.$, of those graphs that enjoy the property that both the graph and its complement graph are ℓ_1-embeddable). These papers are by Shpectorov [Sh97] and Marcusanu [Ma02].

Research has been done also around relaxing the condition of ℓ_1-embeddability, $i.e.$, graphs have been studied that have an embedding into an ℓ_1-space which is isometric only to a limited distance t (such embeddings are called t*-embeddings*). The study of t-embeddings was started by Deza and Shpectorov in [DeSh], where they constructed the unique 7-embedding of $C_{60}(I_h)$. A comprehensive answer regarding the t-embeddings of icosahedral fullerenes and their duals (icosahedral fullerenes are fullerenes of highest attainable symmetry I_h) was obtained by Deza, Fowler and Shtogrin in [DFS].

Finally, Puharic in his PhD thesis [Puh] studied the *face consistency* of fullerenes. This condition is for most fullerenes equivalent to 3-embeddability. In particular, he directed his efforts to constructing new classes of fullerenes that are face consistent and that have as symmetry groups the groups D_{5h} or I.

1.2 About fullerenes

The fullerene geometrical structure seems to appear everywhere in nature - from the red giant stars and interstellar gas clouds to the outer shell of viruses and the neural cells in our bodies. But what exactly is a fullerene? We mentioned above that fullerenes are important in Chemistry, that they are a variety of polyhedra and can be viewed as graphs belonging to the class of graphs 5_n, but we did not give a full precise definition. In the remainder of this chapter we are going to define fullerenes (both from a chemical and a mathematical point of view) and list some interesting facts about them together with some of their applications.

So let us define fullerenes. In Chemistry, fullerenes are carbon molecules in which each carbon atom is chemically bonded to exactly three other carbon atoms and the atoms in the molecule form only pentagonal or hexagonal rings. Fullerenes were discovered (synthesized as stable molecule) relatively recently in 1985 by Sir H. Kroto (U.K.) and two researchers at Rice University (R. Curl and R. Smalley). They were named after Richard Buckminster Fuller, a famous architect who popularized the geodesic dome (which the buckminsterfullerene, one of the fullerenes with 60 vertices, resembles). The three researchers were awarded the Nobel Prize in Chemistry in 1996 for their discovery.

The applications of fullerenes in Chemistry are numerous. Carbon nanotubes constitute one application. These nanotubes are from the fullerene family but they are not spherical fullerenes, being made only of hexagons (sheets of hexagons rolled up into a cylinder). These nanotubes are characterized by high electrical conductivity, high resistance to heat, and relative chemical inactivity (being round with no exposed atoms that can be easily displaced). Another application surged when by crystallizing the buckminsterfullerene at high pressures, chemists created a material that could scratch diamond.

Fullerene chemistry is a new field of organic chemistry devoted to the chemical properties of fullerenes. Research in this field is driven by the need to functionalize fullerenes and tune their properties to the particular applications. In addition to the examples mentioned above, we can refer to the known fact that fullerenes are notoriously insoluble and thus by adding a suitable group one can enhance their solubility. By adding a polymerizable group, a fullerene polymer can be obtained. Functionalized fullerenes are divided into two classes: exohedral with substituents outside the cage and endohedral fullerenes with trapped molecules inside the cage. The latter involves the opening of fullerenes by breaking several of the double bonds with the aim of inserting small molecules through the hole, for instance hydrogen in endohedral hydrogen fullerene.

Next, let us look at applications of fullerene structures to microbiology (virology). In microbioloy it is known that small organisms have to economize upon their resources. This holds true especially for viruses. If one is facing the problem of housing a genome with as few protein as possible (in terms of coding effort) the approach may be to use one protein which self-organizes to form the required capsule. The *icosahedral viruses* do so, by generating a capsid (meaning, the outer shell of a virus) of 60 symmetry related subunits. Among the *small* icosahedral viruses are the well known human or animal pathogens causing poliomyelitis, cold (rhinovirus), hepatitis, foot and mouth disease or a variety of enteric diseases. Plant pathogens, like the rice yellow mottle virus, destroy a year's harvest in whole regions. Insect viruses or bacteriophages employ the same construction principle as well.

Molecular biology is another field in which fullerene structures appear. Clathrin is a fullerene-like protein which was discovered in 1969 by Kanaseki and Kadota. Clathrins are the major components of coated vesicles - important organelles for intracellular material transfer including synaptic neurotransmitter release. Neural cells (neurons) contain clathrin with 12 pentagons and 20 hexagons (as molecule $\mathcal{F}_{60}$), with diameters of 70-80 nm. However, liver cells contain clathrin with 30 hexagons, while fibroblasts have clathrin with 60 hexagons (like higher fullerenes).

Mathematically, a *fullerene* $\mathcal{F}_n$, n being the number of vertices, is a finite connected plane trivalent graph whose faces are pentagons and hexagons. Fullerene structures appeared first in a paper by Goldberg in 1933 and they were referred to as *medial polyhedra*.

The smallest fullerene is the dodecahedron - the unique fullerene on twenty vertices. Since the number of vertices of a fullerene is always even, it follows in particular that there are no fullerenes with 21 vertices. It has also been proven that there are no fullerenes with 22 vertices (see [Gr67], page 271). The number of fullerenes $\mathcal{F}_n$ grows with increasing n = 24, 26, 28... For instance, there are 1812 non-isomorphic fullerenes $\mathcal{F}_{60}$ (non-isomorphic fullerenes with the same number of vertices are called *isomers*). Among all fullerenes $\mathcal{F}_{60}$, only one (specifically, the buckminsterfullerene, alias truncated icosahedron) has no pair of adjacent pentagons and this is the smallest fullerene with such property. A fullerene without a pair of adjacent pentagonal faces is called a *preferable fullerene*. In Chemistry, preferable fullerenes correspond to more stable molecules.

To further illustrate the growth of the number of isomers as n increases, consider another example: there are 214,127,713 non-isomorphic fullerenes $\mathcal{F}_{200}$. Among these, only 15,655,672 have no adjacent pentagons. It was proved (Thurston, 1998) that the number of fullerenes with n vertices grows as n^9. In order to distinguish between the many isomers of a fullerene, their group of symmetries is considered. There are 28 groups of symmetries for fullerenes. For instance, the most famous fullerene (the buckminsterfullerene) has as group of symmetries I_h (the icosahedral group). Similarly, the dodecahedron (the only fullerene with 20 vertices) also admits I_h as its group of symmetries. For more details on groups of symmetries for fullerenes, see [FMRR].

Regarding the ℓ_1-embeddability of fullerenes, the ℓ_1-status of more than 4,000 small fullerenes and their duals is known. It was determined by Pasechnik and Dutour via a computer program in GAP. The conclusion of their work is that among fullerenes with less than 60 vertices, only four fullerenes, $\mathcal{F}_{20}(I_h)$, $\mathcal{F}_{26}(D_{3h})$, $\mathcal{F}_{40}(T_d)$, $\mathcal{F}_{44}(T)$ are ℓ_1-embeddable, and that among *preferable fullerenes* with less than 86 vertices, only one fullerene, $\mathcal{F}_{80}(I_h)$, is embeddable. However, for fullerenes with at least 60 vertices or for *preferable fullerenes* with at least 86 vertices, no research determined exhaustively the ℓ_1-status of all such fullerenes.

CHAPTER 2

BASIC THEORY OF ℓ_1-GRAPHS

Let Γ be a graph and u, v two of its vertices. We denote by $d_\Gamma(u, v)$ the path distance in Γ between u and v, *i.e.*, the length of a shortest path between u and v (such a path will be referred to as a *geodesic*). In particular, $d_\Gamma(u, v)$ can be infinite if u and v belong to different connected components of Γ. When Γ is connected, d_Γ is a metric on Γ which turns Γ into a metric space.

2.1 Isometric embeddings, labels, shifts

A *scale* k *embedding* between two distance spaces (Γ, d_Γ) and (Δ,d_Δ) (where k is a positive integer) is a mapping $f : \Gamma \to \Delta$ such that $d_\Delta(f(u), f(v)) = kd_\Gamma(u, v)$, for every $u, v \in \Gamma$. If $k = 1$, we say that f is an *isometric embedding.* Note that every graph is naturally a distance space (with respect to its distance function). Also note that $\mathbb{R}^n$ with the ℓ_1-distance $d(x, y) = \sum_{i=1}^{n} |x_i - y_i|$ is a metric space to which we refer to as *the standard* ℓ_1*-space.*

With these remarks, a graph is called an ℓ_1*-graph* if, as a distance space (the path distance being its metric), it has an isometric embedding into the standard ℓ_1-space $\mathbb{R}^n$ (for some n).

A nice and important example of ℓ_1-graph is the Hamming Hypercube graph H_n. Consider $\Omega = \{1, 2, \ldots, n\}$. Then we construct H_n by considering as vertices all subsets of Ω

(2^n vertices) and by joining vertices A and B if $|A \triangle B| = 1$, where the symbol $\triangle$ denotes the symmetric difference of the sets A and B (*i.e.*, the set formed with elements that belong either to A or to B but not to both). The path distance in H_n can be computed via $d_{H_n}(A, B) = |A \triangle B|$ for any pair A, B of subsets of Ω. Thus H_n can be isometrically embedded into $\mathbb{R}^n$ endowed with the ℓ_1-norm by the mapping that assigns to each vertex of H_n its characteristic vector in $\mathbb{R}^n$.

The graph $\frac{1}{2}H_n$ obtained from H_n by considering only the even size subsets of Ω is called the *half-cube graph*. In this graph, vertices are adjacent if their symmetric difference has size two and the distance between any two vertices A, B is half the cardinality of their symmetric difference. Thus the half-cube graph $\frac{1}{2}H_n$ is scale two embeddable in H_n.

Note that the set of all subsets of the set Ω considered above together with the operation of symmetric difference $\triangle$ forms an abelian group. In order to see this, the associativity and commutativity of the symmetric difference are to be verified. Indeed, from the definition of the symmetric difference it follows that it is commutative. To prove the associativity, we note that every subset of Ω is represented by its characteristic function with values in Z mod two (in the field GF(2)). Then the symmetric difference is simply the addition of the characteristic functions, which is known to be associative. The group of all subsets of Ω is the same as the (n-dimensional) GF(2)-vector space of all functions on Ω with values in GF(2). The unity in this group is the element $\emptyset$. Moreover, each subset A of Ω admits itself as inverse, given the equality $A \triangle A = \emptyset$.

The following characterization of ℓ_1-graphs from [AsDe1] and [AsDe2] will be used throughout this text:

Theorem 2.1.1. *(Assouad, Deza) A graph is an ℓ_1-graph iff it admits a scale embedding into a hypercube.*

Let Γ be an ℓ_1-graph and let it embed in a hypercube H_n with scale k via the mapping ϕ that assigns to each vertex of Γ a vertex of H_n, *i.e.*, a subset of $\{1, 2, \ldots, n\}$. The set $\phi(v)$ is referred to as a *coordinate set* (or simply, the coordinates) of the vertex v. Note that the coordinates of the vertices of Γ depend on the chosen embedding ϕ.

For each edge between two vertices $u, v \in \Gamma$ we have $d_\Gamma(u,v) = 1 = \frac{1}{k}|A \triangle B|$, where $A = \phi(u)$ and $B = \phi(v)$. The set $A \triangle B$ constitutes the *label* of the edge uv and by the equality above we see that every edge label consists of precisely k elements from $\{1, 2, \ldots, n\}$.

For a scale k embedding ϕ of Γ into H_n we define a *shift of* ϕ *by* A (where A is an arbitrary subset of $\{1, 2, \ldots, n\}$) to be the mapping $\phi_A : \Gamma \to H_n$ that assigns to a vertex v the set $\phi_A(v) = \phi(v) \triangle A$.

Lemma 2.1.2. *Any shift ϕ_A of a scale k embedding ϕ is also a scale k embedding. Moreover, ϕ_A induces exactly the same edge labels as ϕ.*

Proof: Using the commutativity and associativity of the symmetric difference and the fact that $A \triangle A = \emptyset$, we get $\phi_A(u) \triangle \phi_A(v) = (\phi(u) \triangle A) \triangle (\phi(v) \triangle A) = \phi(u) \triangle \phi(v)$, for all $u, v \in \Gamma$. In particular, $d_{H_n}(\phi_A(u), \phi_A(v)) = d_{H_n}(\phi(u), \phi(v)) = k d_\Gamma(u,v)$. Therefore, ϕ_A is a scale k embedding. Furthermore, if u and v are adjacent, the equality $\phi_A(u) \triangle \phi_A(v) = \phi(u) \triangle \phi(v)$ shows that ϕ and ϕ_A induce the same labels on the edges. □

We will consider ϕ and all its shifts ϕ_A to be equivalent embeddings. This is justified since $\phi_B = (\phi_A)_{A \triangle B}$ for all subsets A and B of Ω. So two different shifts of one scale embedding are shifts of each other.

Thus for every scale embedding ϕ and any given vertex v there is an equivalent embedding that assigns to v the coordinate set $\emptyset$, namely, the embedding $\phi_{\phi(v)}$, which indeed maps v to $\emptyset$. Then all vertices adjacent to v have coordinate sets consisting of k elements, all vertices situated at distance two from v have coordinate sets with $2k$ elements, *etc.*

2.2 Labels on geodesics and isometric cycles

Lemma 2.2.1. *Let v_0, v_n be two vertices of an ℓ_1-graph Γ and ϕ a scale k embedding of Γ into a hypercube. The following hold:*

a) For any path from v_0 to v_n, $\phi(v_0) \triangle \phi(v_n)$ is the symmetric difference of all edge labels.

b) In the case of a geodesic path, the edge labels are pairwise disjoint and $\phi(v_0)\triangle\phi(v_n)$ is the disjoint union of edge labels.

Proof: a) Consider an arbitrary path $\{v_0, v_1, \ldots, v_n\}$. Then the edge labels are the sets $E_i = \phi(v_{i-1})\triangle\phi(v_i)$, where $i = 1, ..., n$. The symmetric difference of all edge labels is $E = E_1\triangle E_2\triangle \ldots \triangle E_n$. Hence $E = (\phi(v_0)\triangle\phi(v_1))\triangle(\phi(v_1)\triangle\phi(v_2))\triangle \ldots \triangle(\phi(v_{n-1})\triangle\phi(v_n)) = \phi(v_0)\triangle\phi(v_n)$, since all other terms cancel.

b) Now consider a geodesic path $\{v_0, v_1, \ldots, v_n\}$. We then have $d_\Gamma(v_0, v_n) = n = \frac{1}{k}|\phi(v_0)\triangle\phi(v_n)|$ and thus the symmetric difference of all edge labels has cardinality kn. Given that each edge label has k elements and that there are n edge labels we deduce that these edge labels are pairwise disjoint (otherwise their symmetric difference has less than kn elements). □

A subgraph Δ of Γ is called *isometric* if for all vertices u and v of Δ we have $d_\Delta(u, v) = d_\Gamma(u, v)$. Equivalently, Δ is isometric if its identity embedding into Γ is an isometric mapping. Geodesic paths in Lemma 2.2.1, part b, are examples of isometric subgraphs. The next result shows how we can use edge labels to characterize some other isometric subgraphs of an ℓ_1-graph, specifically, the isometric cycles on five or six vertices. This result will be applied later to the faces of an ℓ_1-fullerene.

Proposition 2.2.2. *In an ℓ_1-embeddable graph the following hold:*

1) Opposite edges in a hexagonal isometric cycle have the same label. Edges that are not opposite have disjoint labels.

2) In the case of pentagonal isometric cycles, the opposite edges share half of their label (i.e., $\frac{k}{2}$ elements, k being the scale of the embedding). Edges that are not opposite have disjoint labels.

Proof: 1) Consider a hexagonal cycle with vertices $\{v_1, \ldots, v_6\}$. Denote the edge labels by $E_i = \phi(v_i)\triangle\phi(v_{i+1})$, where $i = 1, ..., 6$, $v_7 = v_1$ and ϕ is a scale k embedding. The cycle being isometric, we have that $d(v_1, v_4) = 3$. The paths $\{v_1, v_2, v_3, v_4\}$ and $\{v_1, v_6, v_5, v_4\}$

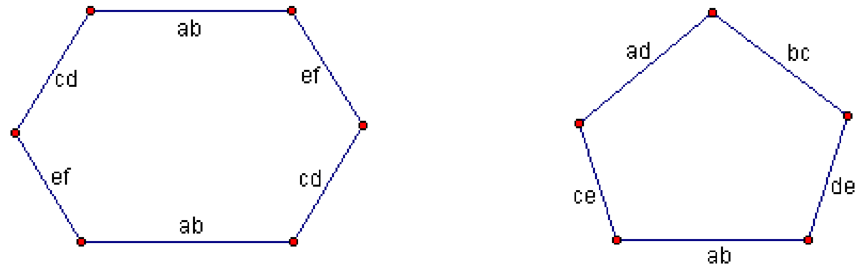

Figure 2.1: Edge labels on hexagonal and pentagonal isometric cycles

are geodesics and therefore the edge labels E_1, E_2, E_3 are pairwise disjoint and similarly for E_4, E_5, E_6. Applying the same argument to the pairs of vertices $\{v_2, v_5\}$ and $\{v_3, v_6\}$ we infer that non-opposite edges of the cycle have disjoint labels. We now turn our attention to opposite edges. Let us prove that $E_1 = E_4$. We have $d(v_2, v_4) = 2$ and by the previous lemma applied to the path $\{v_2, v_1, v_6, v_5, v_4\}$ we also get that $|E_1 \triangle E_6 \triangle E_5 \triangle E_4| = |\phi(v_2) \triangle \phi(v_4)| = 2k$. Since the sets E_1, E_6, E_5 are pairwise disjoint and E_4, E_5, E_6 are pairwise disjoint we must have that $E_1 = E_4$, otherwise the symmetric difference of the four edge labels above has more than $2k$ elements.

2) For the case of a pentagonal cycle we employ similar notation as for the hexagonal cycles (v_i denote vertices and E_i denote edge labels). We have $d(v_1, v_3) = 2$ and thus the path $\{v_1, v_2, v_3\}$ is a geodesic which implies that E_1, E_2 are disjoint. Similarly, we see that E_2, E_3 are disjoint, E_3, E_4 are disjoint, E_4, E_5 are disjoint and E_5, E_1 are disjoint *i.e.*, we proved that non-opposite edges have disjoint edge labels. Let us prove that $|E_1 \cap E_3| = k/2$. We consider the path $\{v_1, v_2, v_3, v_4\}$ and we have $|E_1 \triangle E_2 \triangle E_3| = |\phi(v_1) \triangle \phi(v_4)| = 2k$. Since E_1, E_2 are disjoint and E_2, E_3 are disjoint, we get that $|E_1 \triangle E_3| = k$. But we know that $|E_1 \triangle E_3| = |E_1| + |E_3| - 2|E_1 \cap E_3|$ and $|E_1| = |E_3| = k$. Thus it follows that $|E_1 \cap E_3| = k/2$. The argument can be applied to all pairs of opposite edges. □

2.3 Zones

For any element j ($1 \leq j \leq n$), consider the set of all edges in Γ that contain j in their label and call it the *j-zone*. The concept of a zone will be very useful in proving the main result of this paper.

We next define a cut in Γ. Consider a partition of the vertices of Γ into two parts P and $\bar{P}$. The *cut* in Γ corresponding to the partition $(P, \bar{P})$ is the set of all edges that have one end vertex in P and the other one in $\bar{P}$.

Lemma 2.3.1. *Every zone is a cut. Thus, the j-zone determines a partition of the vertex set of* Γ*.*

Proof: Let ϕ be the map via which Γ embeds into H_n. Let P be the set of vertices of Γ that contain j in their coordinate set and $\bar{P}$ be the complement of P, *i.e.*, the set of vertices that do not contain j in their coordinate set. Obviously, this constitutes a partition of the vertex set of Γ. Moreover, any edge of the zone contains j in its label which means that j must be present in exactly one of the coordinate sets of its end vertices (since the edge label is by definition the symmetric difference of the coordinate sets of the edge's end vertices). Thus every edge of the zone must have an end vertex in P and the other end vertex in $\bar{P}$ and therefore the j-zone is a cut. □

A subset C of Γ is called a *convex subset* if for any vertices $u, v \in C$ the vertices of every geodesic from u to v lie in C.

Proposition 2.3.2. *Every j-zone partitions the vertex set of* Γ *into two convex subgraphs.*

Proof: Let P and $\bar{P}$ be the partition of the vertex set of Γ as in the previous lemma. It is enough to prove that P is convex. Consider v, u in P and a geodesic path from v to u consisting of the vertices $\{v_0, v_1, \ldots, v_n\}$ in this order (with $v = v_0$, $u = v_n$ and $n = d(v, u)$). If this path is not entirely in P it follows that there exists a smallest index i and a largest index h such that v_i and v_h are not in P (i and h can be equal, $1 \leq i \leq h \leq n-1$). Then the edges $v_{i-1}v_i$ and $v_h v_{h+1}$ belong both to the geodesic path and to the j-zone, having one vertex in P and the other in $\bar{P}$. Thus, on one hand, the labels of these two edges must be disjoint (by Lemma 2.2.1) and, on the other hand, both labels contain j (the edges are in the j-zone), impossible. Thus we conclude that any geodesic path between two vertices in P must lie entirely in P, $i.e.$, P is convex. □

In what follows we will call *halves* each of the two convex subgraphs defined by a zone from Γ.

CHAPTER 3

PROPERTIES OF FULLERENES

3.1 Basic properties

The results in this section apply to fullerenes in general, no ℓ_1-embeddability being assumed.

Recall that a *fullerene* is a finite connected trivalent plane graph, whose faces are pentagons and hexagons only. By *faces* we mean all faces: the finite faces as well as the infinite face. This means that we adopt the point of view that the fullerene is drawn on a sphere, where all faces have equal status.

The next theorem establishes some of the basic properties of fullerenes.

Theorem 3.1.1. *The number of pentagons in every fullerene is exactly twelve, the number of hexagons is* $(n-20)/2$ *(where* n *is the number of vertices of the fullerene). In particular, the number of vertices of a fullerene is even.*

Proof: We apply Euler's Theorem to get $n - e + f = 2$, where e is the number of edges and f is the number of faces. Let us denote by p and h the number of pentagons and hexagons, respectively. Taking into account that a fullerene is a trivalent graph and that every edge belongs to two faces we obtain: $n = \frac{5p+6h}{3}$ and $e = \frac{5p+6h}{2}$. From the three equations we immediately see that $p = 12$, $h = \frac{n-20}{2}$ and thus the theorem is proved. $\square$

3.2 Cycles in a fullerene

In this section we study short cycles (up to length six) in a fullerene Γ. We show that such cycles are necessarily isometric and that, in fact, the only short cycles are the face cycles of Γ.

Consider $\gamma = uvw$, a path in Γ with $u \neq w$ (that is, not a return). We say that γ *makes a right turn at* v if vw immediately follows uv (no other edge in between) in the counterclockwise direction around v (we refer here to the embedding of Γ into the sphere). Similarly, the path makes a *left turn at* v if vw immediately follows vu (no other edge in between) in the clockwise direction around v.

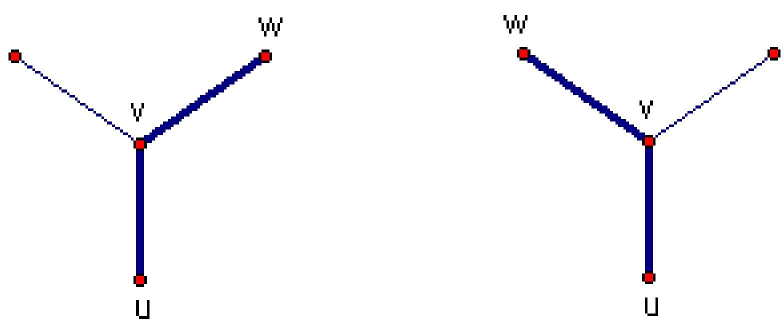

Figure 3.1: Right and left turns

Correspondingly, a path $\gamma = a_0 a_1 \ldots a_n$ without returns ($i.e.$,, $a_{i+1} \neq a_{i-1}$, $1 \leq i \leq n-1$) makes a *right turn* at a_i or a *left turn* at a_i, where $1 \leq i \leq n-1$, if so does the subpath $a_{i-1} a_i a_{i+1}$.

Note that for an ordered edge uv we can speak of the face on the *right side* and the face on the *left side* of uv. If uvw makes a right turn then on the right side of uv and vw lies the same face. Similarly, if uvw makes a left turn then on the left side of uv and vw lies the same face. This immediately yields the following lemma.

Lemma 3.2.1. *(Face Cycle Lemma) Let* $\gamma = a_0 a_1 \ldots a_n$ *be a path without returns. Then* γ *follows the boundary of a face* F *if and only if* γ *makes only right turns at each vertex*

a_i ($0 < i < n$) or makes only left turns at each vertex. In the first case γ goes around F in the clockwise direction, while in the second case it goes around F in the counterclockwise direction. □

We give a few more definitions and some comments before proceeding with the next results. If $\gamma = a_0 a_1 \dots a_n$ is a path without returns in Γ then at every a_i, $1 \leq i \leq n-1$, there is a unique edge that is not on γ. We will refer to this edge as the *side edge* at a_i. If γ makes a right turn at a_i, we say that the side edge at a_i *points left*, and similarly, if γ makes a left turn then the side edge *points right*. When γ is a cycle without returns and self-intersections, cutting the sphere through γ produces two disks, which we will call the *sides* of γ; there is the left side and the right side. Note that there is a symmetry between left and right: if we reflect the sphere in any hyperplane then we obtain another plane realization of the same graph, where all right becomes left and vise versa. Also, if we reverse the path (cycle) then again the left and the right switch.

Lemma 3.2.2. Γ *contains no 3-cycles.*

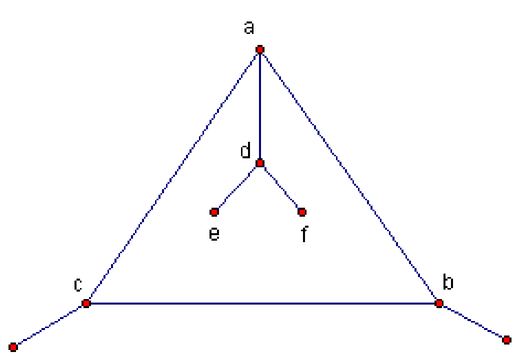

Figure 3.2: Side edge at a points left

Proof: Suppose that $\gamma = abca$ is a 3-cycle in Γ. If all side edges of γ point to one side then the other side is a face by the Face Cycle Lemma, which is impossible since Γ has no triangular faces. Thus, two of the side edges point to one side, say, right, and the remaining side edge points to the other side, that is, left. Suppose the side edge at a points right, as shown in Figure3.2, and let d be the other end of that edge. Let a, f, and e be the neighbors of d in the clockwise order. Since the path *edacbadf* makes only left turns, it must be part of a face boundary. Moreover, this path has six different vertices and is not closed ($e \neq f$) which implies that the face it goes around has more than six vertices, a contradiction. □

Corollary 3.2.3. *If abc is a path without returns in* Γ *then* $d_\Gamma(a, c) = 2$.

Proof: Since the path is without returns we have $a \neq c$. If $d(a, c) = 1$ then *abc* is a 3-cycle, which is prohibited by the previous lemma. Thus $d(a, c) = 2$. □

Lemma 3.2.4. *There is no* 4*-cycle without returns in* Γ*.*

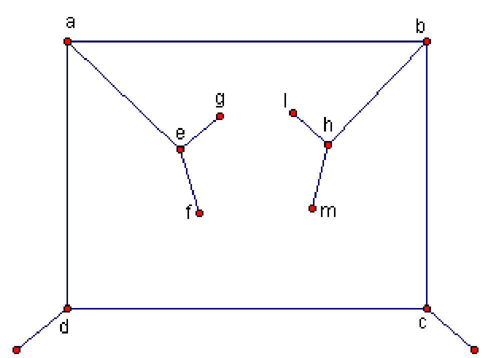

Figure 3.3: Side edges at a and b point right

Proof: Suppose $\gamma = abcda$ has no returns. If all side edges point to one side then Γ has a quadrangular face, a contradiction. Suppose one side edge points to one side (say, right) and the remaining three side edges point to the other side. By symmetry, we may assume that the side edge at a points right. Let e be the second end of that side edge and let a, g, f be the neighbors of e, read clockwise. Note that f, g cannot coincide with either of a, b, c, d because otherwise there would be either a 3-cycle or a quadrangular face in Γ, a contradiction. The path $feadcbaeg$ has seven different vertices and makes only left turns, which means that it must be part of the boundary cycle of a face with at least seven vertices, contradiction.

It remains to consider the case where two side edges point to each side. First suppose that the edges pointing right are at consecutive vertices of γ, say, at a and b. Let e, f, g

be as above, and let also h be the third neighbor of b, with b, m, l being the neighbors of h (read clockwise) as shown in Figure 3.3. The path $feadcbhm$ makes only left turns, so it goes around a face. If that face is a pentagon then $f = b$, yielding a 3-cycle, a contradiction with Lemma 3.2.2. So the face is hexagonal, which means that $f = h$ and $m = e$ (see Figure 3.4).

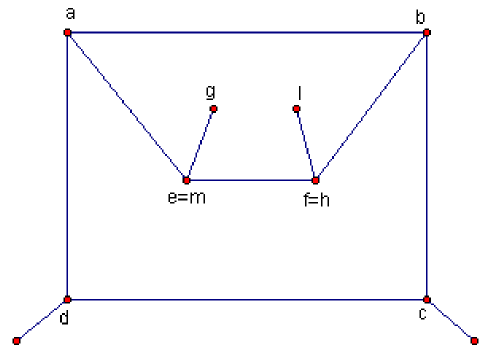

Figure 3.4: Side edges at a and b point right, iterative case

Now the 4-cycle $\gamma' = heabh$ has the side edges at two consecutive vertices pointing right, so we can iterate the above argument, constructing an infinite sequence of 4-cycles γ_i (with $\gamma_0 = \gamma$ and $\gamma_1 = \gamma'$) such that the right side of γ_{i+1} is strictly contained in the right side of γ_i. This means that all cycles γ_i are distinct, which is a contradiction with finiteness of Γ.

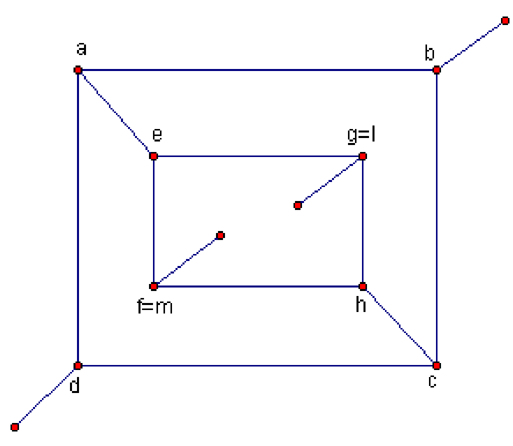

Figure 3.5: Side edges at a and c point right, iterative case

Now suppose that the side edges pointing right are at nonconsecutives vertices of γ, say at a and c. Let e, g, f be as above and let h, l, m be also as above, except h is now adjacent to c instead of b. Since the path $feadchm$ makes left turns only, we have that either $f = h$ and $e = m$, or $f = m$. Similarly, looking at $geabchl$, which makes right turns only, we have that either $g = h$ and $e = l$, or $g = l$. Since Γ has no double edges and no 3-cycles, we must in fact have that $f = m$ and $g = l$, giving raise to a 4-cycle $\gamma' = feghf$. Note that the side edges of γ' at f and g point right, since both $feadchf$ and $geabchg$ are hexagonal faces (see Figure 3.5). So we can again iterate our argument to construct an infinite array of distinct 4-cycles, contradicting the finiteness of Γ. □

Corollary 3.2.5. *Every* 5*-cycle in* Γ *has no returns and is an isometric subgraph.*

Proof: If this cycle (call it γ) would have returns then we would get a 3-cycle in Γ, contradiction. To prove the second part of the corollary, note that in γ the possible distances between vertices are either one or two. If a, b are two vertices at distance one in γ then these vertices are adjacent and thus $d_\gamma(a, b) = d_\Gamma(a, b) = 1$. If the vertices a, b are at distance two in γ then they have a common neighbor c in γ. Then acb is a path without returns and thus by the previous lemma $d_\Gamma(a, b) = 2$. □

Lemma 3.2.6. *Every* 5*-cycle is the boundary cycle of a face.*

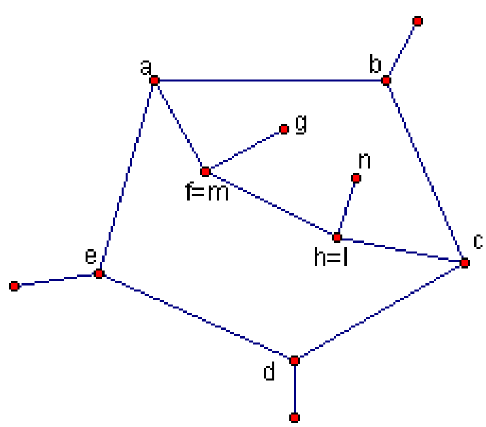

Figure 3.6: Side edges at a and c point right

Proof: We prove this lemma by contradiction, *i.e.*, we assume that there exists a 5-cycle $\gamma = abcdea$ which is not the boundary cycle of a face. By assumption, not all side edges point to the same side and therefore we have to consider only the cases: 1) one side edge points to one side (say, right), while the other four point to the other side; 2)two side edges point to one side (again, right), while the remaining three point to the other side.

In case 1), suppose the side edge of a points right, its second end vertex being f and the neighborhood of f consisting of a, g, h in the clockwise order around f. The path $hfaedcb$ makes left turns only, so it goes around a face. If the face is pentagonal then $h = c$, producing a 4-cycle without returns, a contradiction with Lemma 3.2.4. Similarly, if the face is hexagonal then $h = b$, producing a 3-cycle, again a contradiction.

In case 2), there are two subcases: either the side edges pointing right are at two consecutive vertices of γ, say, a and b, or at two nonconsecutive vertices, say, a and c. In both subcases, let f, g, h be as above.

In the first subcase, we employ exactly the same argument as in case 1). Indeed, $hfaedcb$ makes left turns only, implying that $h = c$ or $h = b$. This gives a 4-cycle without returns, or a 3-cycle, a contradiction. In the second subcase, let l be the second end of the side edge at c and let m, n be the two neighbors of l, so that c, m, n form the neighborhood of l, read clockwise. The path $hfaedclm$ makes left turns only, hence either $h = c$, producing a 4-cycle without returns, a contradiction, or $h = l$ and also $f = m$ (see Figure 3.6). Note that the 5-cycle $abclma$ has exactly two side edges pointing right, and they are at consecutive vertices of the 5-cycle. This configuration was ruled out in case 2), first subcase. □

Corollary 3.2.7. *Every* 6*-cycle in* Γ*, that has no returns, is an isometric subgraph.*

Proof: Let γ=$abcdefa$ be a 6-cycle. If two vertices are at distance one or two in γ then they are at the same distance in Γ. (For distance two we use Corollary 3.2.3 and the fact that γ has no returns.) So we just need to consider pairs of vertices at distance three in γ. By symmetry, we may assume that these vertices are a and d. So it suffices to show that $d_\Gamma(a, d) = 3$. If $d_\Gamma(a, b) = 0$ or 1 then Γ contains a 3-cycle or a 4-cycle without returns, impossible. Suppose $d_\Gamma(a, d) = 2$. Let h be the common neighbor of a and d. Then $abcdha$ and $afedha$ are 5-cycles, and so by Lemma 3.2.6 they are the boundary cycles of two faces, say F_1 and F_2. If $F_1 \neq F_2$, then they are the two faces on the two sides of the edge dh and so dha must now turn both left and right, impossible.

If $F_1 = F_2$ then the cycles must coincide, yielding $b = e$, which means that the initial cycle had a return, a contradiction. □

Lemma 3.2.8. *6-Cycles without returns in* Γ *are boundary cycles of faces.*

Proof: Let $\gamma = abcdefa$ be a 6-cycle without returns. If all side edges of γ point to one side then γ is the boundary cycle of a face. So we need to eliminate all other cases, that is, where part of the side edges point to one side and the remaining side edges point to the other side. It suffices to consider the following cases: 1) exactly one side edge points to one side (say, right), the rest of the side edges pointing to the other side; 2) two side edges point to one side (right), the remaining side edges pointing to the other side; 3) three side edges point to one side (right), the remaining side edges pointing to the other side.

For case 1) let ag be the only side edge that points right. Then $gafedcb$ is a path that makes left turns only, so it goes around a face. Depending on whether this face is a pentagon or a hexagon, we get $g = c$, leading to a 3-cycle, or $g = b$, leading to a double edge; a contradiction in both cases.

In view of symmetry, in case 2) we need to consider the following subcases: side edges at a, b point right, side edges at a, c point right or side edges at a, d point right. In the first subcase the path $gafedcb$ still makes only left turns and the argument from case 1) applies, giving a contradiction. In the second subcase, let ag and cl be the side edges that point right. Looking at the path $gafedcl$, making left turns only, we conclude that either $g = c$, leading to a 3-cycle, or $g = l$, leading to a 4-cycle without returns. None of these is possible. In the third subcase, where ag and dl are the only side edges pointing right, we look at the path $gafedl$, that makes only left turns. If the face it goes around is a pentagon then $g = l$, yielding $d_\Gamma(a, d) = 2$, a contradiction with Corollary 3.2.7. If the face is a hexagon then l and

g are adjacent and furthermore, both side edges of $dlga$ point right. However, considering now the path $gabcdl$, making right turns only, we conclude similarly that both side edges of $dlga$ point left, a contradiction.

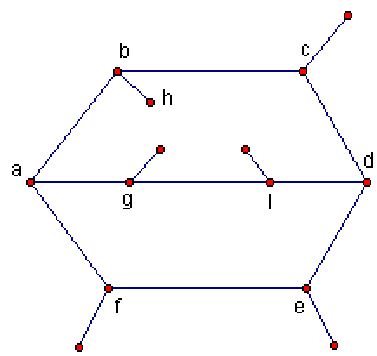

Figure 3.7: Side edges at a, b and d point right

Case 3) has three subcases, up to the symmetries of γ. First, suppose the side edges pointing right are ag, bh, and cl. Then the path $gafedcl$ makes left turns only, and so either $g = c$ or $g = l$, leading to a 3-cycle or a 4-cycle without returns; a contradiction. Secondly, suppose the side edges pointing right are ag, bh, and dl. Looking at the path $gafedl$ and arguing as in the last subcase of case 2), we either get $l = g$, giving a contradiction with Corollary 3.2.7, or that l and g are adjacent with both side edges of $dlga$ pointing right, see Figure 3.7. Consider the 6-cycle $\gamma' = lgabcdl$, which has exactly three side edges pointing right and they are at l, g, and b, so γ' is in the same subcase as γ. Iterating our argument we construct an infinite sequence of 6-cycles γ_i, such that the right side of γ_{i+1} is properly contained in the right side of γ_i. This contradicts finiteness of Γ.

Finally, suppose the side edges pointing right are ag, ch, and el and let the neighbors of these three vertices be as shown in Figure 3.8. Since the path $igabchk$ makes only right turns, we have that either $i = h$ and $g = k$, or $i = k$ and the side edge of hkg points left. Similarly, looking at $mhcdeln$, we get that either $h = n$ and $m = l$, or $m = n$ and the side edge of lnh points left. Similarly still, either $l = j$ and $p = g$, or $p = j$ and the side edge of gjl points left. Note that these equalities mean that a new cycle γ' arises in the middle of

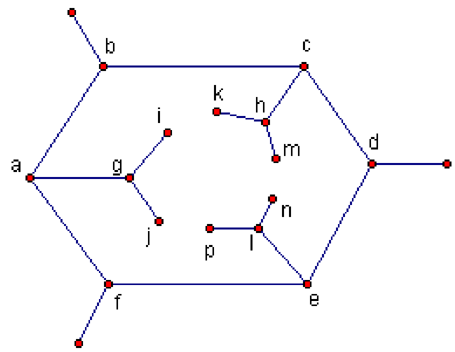

Figure 3.8: Side edges at a, c and e point right

Figure 3.8. Its length varies from three, if the first option holds for all three choices above, to six, if the second option holds for all three choices. Recall that Γ contains no 3-cycles (Lemma 3.2.2), no 4-cycles without returns (Lemma 3.2.4), and no 5-cycles with side edges pointing to both sides (Lemma 3.2.6).

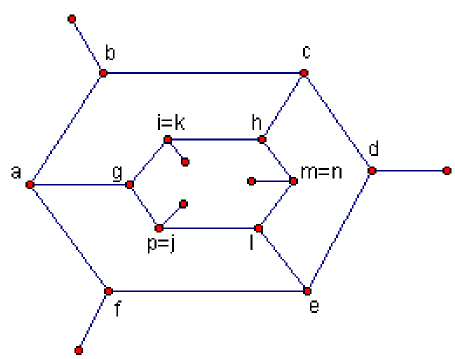

Figure 3.9: Side edges at a, c and e point right, iterative subcase

Therefore, for each of the three choices above, the second option must hold, that is, $i = k$, $m = n$, and $p = j$. Now $\gamma' = igplmhi$ is a 6-cycle that falls in the same subcase as γ, see Figure 3.9. Again, iterating the above, we construct an infinite sequence of 6-cycles such that the right side of each subsequent 6-cycle is properly contained in the right side of the preceding 6-cycle; a contradiction with finiteness of Γ. $\square$

3.3 ℓ_1-embeddable fullerenes

In the remainder of the paper we study an ℓ_1-embeddable fullerene Γ. Note that Γ is a plane graph and therefore it comes with an embedding into a sphere S.

Given a plane graph Γ we consider its *dual graph* Δ as follows: the vertices of Δ correspond to the faces of Γ, and the edges of Δ correspond to the edges of Γ. If e is an edge of Γ and E and F are the faces on the two sides of e then the edge of Δ corresponding to e connects the vertices corresponding to E and F. Note that, when Γ is a general plane graph, E and F may be the same face, in which case the edge of Δ is a loop. Also, when E and F share more than one edge, Δ may have multiple edges between vertices. However, when Γ is a fullerene, one can see that a loop in Δ leads to a loop or a multiple edge in Γ, which is impossible. So Δ has no loops. Similarly, a multiple edge in Δ yields a cycle without returns in Γ of length at most four, which is also impossible by the results of Section 3.2. Thus, Δ has no loops and no multiple edges, that is, Δ is a simple graph.

The dual graph Δ is a plane graph, namely, it can be drawn on the same sphere S. The vertices of Δ can be placed within the corresponding faces of Γ and the edges of Δ would go across the corresponding edges of Γ. Every face of Δ then has a unique vertex of Γ in it, and in fact, Γ is the dual graph of Δ. Every vertex of Δ has either five or six edges incident to it, depending on the gonality of the corresponding face of the fullerene Γ. Finally, every face of Δ is a triangle, since Γ is trivalent.

We can *label* the edges of Δ reusing the labels from the corresponding edges of Γ. Now, by the analogy with zones in Γ, we can define the *dual j-zone* as the set of edges of Δ that have j in the label. In fact, we view the dual j-zone as a subgraph of Δ, that is, for every edge we throw in its end vertices as well. Note that every vertex of the dual j-zone is adjacent to exactly two edges. This follows from Proposition 2.2.2, since Γ is an ℓ_1-graph and since its face cycles are isometric by Corollaries 3.2.5 and 3.2.7. Thus, a dual j-zone is a subgraph of valency two, *i.e.*, it is a union of cycles. Note that a dual zone goes straight through a vertex of Δ of degree six and makes just a slight left or right turn at a vertex of degree five. An illustration of dual zones can be found in the figure below which is based on Figure 2.1. The first part of the figure shows a portion of a dual zone (the dashed segments) going straight through a six degree vertex in Δ. The second part shows portions of two dual zones, one making a slight left (dual a-zone) and the other making a slight right (dual b-zone).

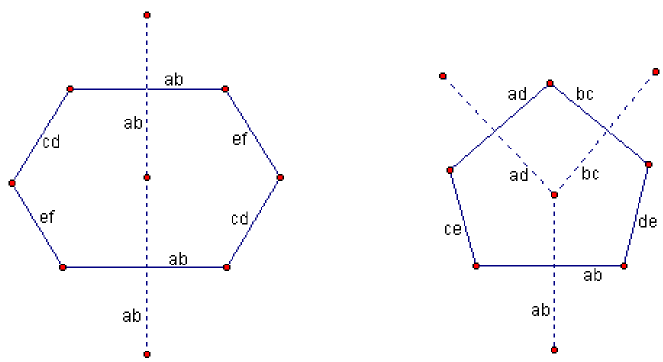

Figure 3.10: Dual zones: straight through and slightly left/right

Proposition 3.3.1. *Every dual j-zone subgraph is a simple cycle in Δ.*

Proof: Consider a dual zone subgraph in the dual graph. Specifically, this dual zone subgraph is a union of paths in Δ (it cannot contain any face of Δ due to the fact that in Γ the three edges that stem from a given vertex cannot share an element of their labels). We first prove that each of these paths (call a generic one δ) is a simple cycle and that the union actually consists of just one path (only one component). Given the fact that elements of the edge labels repeat exactly once on opposite edges inside faces of the ℓ_1 fullerene Γ, we obtain that each vertex of δ is linked with exactly two other vertices of δ. Thus δ is of degree two and must be a cycle since fullerenes are finite graphs. If δ would not be simple *i.e.*, there would exist at least one vertex of δ that is linked with at least three other vertices in the path, then this vertex would represent a face in Γ in which the same coordinate j appears on three of its edges, contradiction. Now suppose the dual zone subgraph consists of two or more such simple cycles. Then these cycles determine at least three disjoint regions (subgraphs) in the fullerene. Using the result that a zone cuts the graph Γ into two convex halves, we must have that one of the convex halves contains two or more of the disjoint disconnected regions formed by the cycles, a contradiction. □

Given the result proved above, for simplicity we will use the terminology *dual j-cycle* instead of *dual j-zone subgraph.*

We now define a *straight zone* of an ℓ_1-embeddable fullerene to be a zone that passes only trough hexagons. A *crooked zone* will be a zone that passes through at least one pentagon. Similar definitions apply to dual zones.

Recall that we called *halves* the two subgraphs of Γ obtained by removing a zone. Similarly, in the dual graph, a *hemisphere* is one of the two subgraphs obtained by *cutting* the dual graph Δ along a dual cycle *i.e.*, a hemisphere is one of the two disks obtained by cutting the sphere S (on which we draw the fullerene and its dual) by a simple cycle. Thus the halves are the subgraphs of Γ located in the corresponding hemispheres.

The next result will be used many times in this paper.

Proposition 3.3.2. *A half of an ℓ_1 fullerene is a convex subgraph. The intersection of any two halves (corresponding to different zones) is a convex subgraph. The same result holds for hemispheres in the dual graph Δ.*

Proof: We have already seen that a zone cuts the fullerene into convex parts. The *half* is by definition one of those parts. The second claim of the proposition follows from the fact that the intersection of convex sets is convex. □

We turn our attention to intersections of zones (dual zones) and to some properties of such intersections. We say that two different dual cycles *intersect* if they pass through the same vertex of Δ and do not have common edges next to this vertex. We say that two dual cycles *partially overlap* if they have a common continuous subpath such that one dual cycle comes to that subpath from the left and leaves it to the right and correspondingly, the second dual cycle comes from the right and leaves it to the left. Note that the intersection phenomenon can happen for both straight and crooked dual zones, while the partial overlapping can only happen for crooked dual zones.

Remark 3.3.3. *If two dual cycles intersect in one vertex then they intersect into exactly two vertices.*

Proof: Each of the two dual cycles (call them z_1, z_2) is a simple cycle in the dual graph Δ. Their intersection cannot consist of only one vertex, *i.e.*, a face F of the initial graph Γ, since that would imply that pairs of non-opposite edges of the face F form the two zones, contradiction. Thus for each point of intersection of the two dual cycles there exists another one, different from the first. This shows that the two dual cycles intersect in at least two points. Suppose they intersect in more than two points. Then we can find two hemispheres such that their intersection has disconnected components, contradiction with the convexity of such an intersection. □

As a final note, the definition of the dual graph allows us to talk about the distance between faces of a fullerene. Specifically, the distance between two faces of Γ will be the distance between the two corresponding vertices in the dual graph Δ.

CHAPTER 4

PREFERABLE FULLERENES

4.1 Minimal distance between pentagons ≥ 3 or of the type {1,1}

We define a *dual path* between two pentagons P_1 and P_2 of a fullerene to be a sequence of adjacent faces that starts at P_1 and ends at P_2. We can view this dual path as a path in the dual graph from the vertex corresponding to P_1 to the vertex corresponding to P_2. A *geodesic dual path* will be a shortest dual path between P_1 and P_2. Note that such a path always exists between any two pentagons of the fullerene. The *distance between two pentagons* P_1 and P_2 is the length of a geodesic dual path (and thus equal to one plus the number of faces of the geodesic, excluding P_1 and P_2).

We need a few more definitions in order to proceed with the next results. Consider two pentagons of the fullerene that are at minimal distance d^* (*i.e.*, for any other pair of pentagons the distance between them is greater or equal than d^*). Then a geodesic dual path between the two pentagons will only go through hexagonal faces (otherwise the minimality of the distance between pentagons is contradicted). If such a path makes a turn in one of the hexagonal faces we call it a *crooked dual path*, whereas if it always goes in and out of faces through opposite edges of the hexagons, we call it a *straight dual path*. A crooked dual path is said to make a *right turn* in one of the faces if the new direction it takes is to the right of the straight path it would have followed if it wouldn't have turned. Similarly, we can define a *left turn*.

Furthermore, a crooked dual path is of *type* $\{m_1, ..., m_n\}$ if the length of each subpath (before it turns) is m_i $(i < n)$ and the length of the piece after the last turn is m_n. In the next lemma we prove that a crooked dual path of type $\{m_1, ..., m_n\}$ is equivalent to a crooked dual path of type $\{m, k\}$ and also that when a crooked dual path of type $\{m, k\}$ exists then a second crooked dual path of type $\{k, m\}$ also exists and by connecting the centers of all the faces involved in both crooked paths we obtain a parallelogram π (in the dual graph).

Lemma 4.1.1. *Consider two pentagons at minimal distance such that no straight dual path exists from one to the other. The following then hold:*

a) A crooked dual path (i.e., geodesic) cannot make two consecutive left turns or two consecutive right turns;

b) A type $\{m, k\}$ *crooked dual path between the two pentagons at minimal distance is well defined, i.e., if there exists a crooked geodesic dual path (making any number of alternating left and right turns) then there exists a geodesic dual path that makes only one left turn, and also a geodesic dual path that makes only one right turn. In particular, the parallelogram* π *is well defined.*

c) The parallelogram π *can be extended to a larger one by adding two triangles.*

Proof: a) If by contradiction we assume a geodesic dual path makes two consecutive left turns, then we can find a shorter dual path between the two pentagons, which contradicts the minimality of the length of the geodesic. See Figure 4.1 (part of the thick path can be replaced by the shorter dashed path).

b) Consider a geodesic path between the two pentagons such that it makes more than one turn. By part (a) we know that the turns must alternate, *i.e.*, if one goes left the next must go right, and so on. For simplicity, assume the geodesic dual path makes exactly two turns: left, then right, as illustrated in the second drawing of Figure 4.1. Then the middle

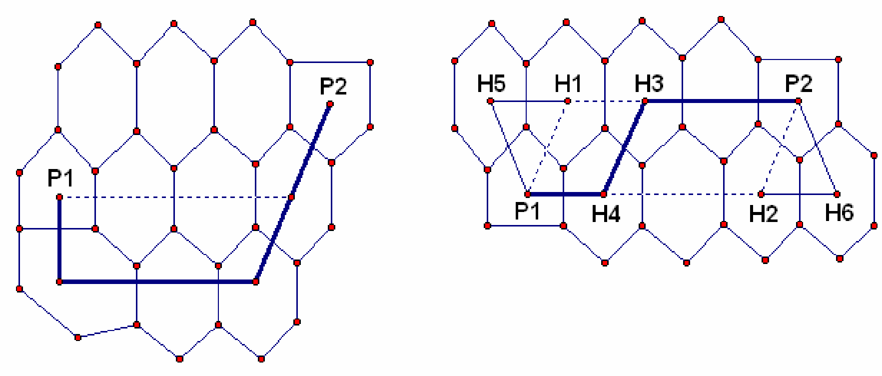

Figure 4.1: No consecutive left turns and the type $\{m, k\}$ is well defined

part (from H_3 to H_4) of the dual geodesic path can be *moved* or replaced with the path from H_1 to P_1 and similarly, with the path from P_2 to H_2. Thus we obtain two new dual geodesics - one being $P_1H_1P_2$, the other being $P_1H_2P_2$. We can now say that there is a crooked dual path of type $\{1, 3\}$ and the parallelogram π is determined by P_1, H_1, P_2, H_2. Note that all faces involved in the frontier of π and *inside* π are hexagons, otherwise the pentagons P_1, P_2 are not at minimal distance.

c) We can add to the last remark that de faces H_5, H_6 are also hexagons. In general, this translates to the fact that the faces that determine the frontier and the *inside* of the (dual) triangles with edges of length m ($m <= k$) and passing through one of P_1, P_2 and one of the other two *vertices* of π are all hexagons. Thus π can be extended by these two dual triangles. In the picture above, the extended parallelogram is $P_1H_5P_2H_6$.

□

Proposition 4.1.2. *Two pentagons at minimal distance d^* cannot allow a crooked dual path of type $\{m, k\}$ between them, where $d^* \geq 3$.*

Proof: Suppose by contradiction that there exists such crooked dual path between two pentagons P_1 and P_2 at minimal distance d^* (where $d^* = m + k$). Without loss of generality, we can also assume that $k \geq m$. Consider the parallelogram π mentioned above, having as *vertices* the faces P_1, P_2 and P_3, P_4, where P_3 and P_4 must be hexagons and the distance

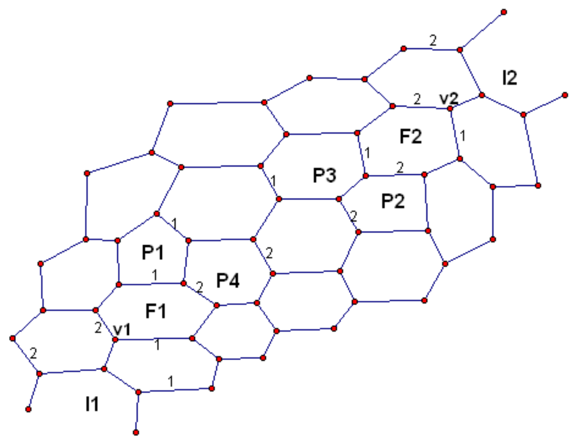

Figure 4.2: Crooked dual path of type $\{2,1\}$

between P_1 and P_3 is k, the distance between P_1 and P_4 is m. Also consider the two crooked zones z_1 and z_2 that pass through P_1, P_3 and P_4, P_2 respectively and that intersect at an acute angle in two faces F_1 and F_2, such that F_1 is at distance m from both P_1, P_4 and F_2 is at distance m from both P_2, P_3. We know that each of the two zones cuts the fullerene into two convex regions. Call these R_{11} and R_{12} (corresponding to z_1) and R_{21} and R_{22} (corresponding to z_2), such that P_1 is in R_{21} and P_2 is in R_{11}. Let v_1 be the vertex belonging to the face F_1 that lies in both R_{12} and R_{22}. The vertex v_1 is unique with such properties given our construction up to this point and the fact that z_1 and z_2 intersect at an acute angle. Similarly, consider v_2 in F_2. Now let's construct two other zones z_3 and z_4 such that these pass through faces that are adjacent to the faces of the parallelogram π, lying in the *exterior* of it. We can always consider coordinates j_1, j_2 such that $z_3 = j_1 - zone$, $z_4 = j_2 - zone$ and z_3, z_4 intersect in two faces I_1, I_2, I_1 being at distance $m+2$ from P_1 and I_2 being at distance $m+2$ from P_2. If $m+2 < d^*$ then I_1, I_2 are hexagons together with the other faces on z_3, z_4 that are adjacent to the faces of π. When $m+2 \geq d^*$ the faces I_1, I_2 can be pentagons being at distance at least d^* from P_1, P_2 (but z_3, z_4 still intersect in I_1, I_2 by carefully choosing the coordinates j_1, j_2 that determines them). With these observations, z_3 cuts the fullerene into two convex regions R_{31} and R_{32} and, similarly, z_4 cuts the fullerene into two convex regions R_{41} and R_{42}. Suppose our notations are such that R_{31} and R_{41} each contain the faces P_1 and P_2. Notice that the regions R_{12}, R_{22}, R_{31} and R_{41} are all convex and their intersection (call it C) must also be convex. Moreover, the vertices v_1, v_2 are both in C. We obtain a contradiction by noticing that there is no path from v_1 to v_2 which is contained in the convex region C. Thus the proposition is proved. □

Proposition 4.1.3. *Two pentagons at minimal distance d^* cannot allow a straight dual path, where $d^* \geq 3$.*

Proof: The proof relies on the same argument used in the previous Proposition: we construct four zones, consider the intersection of four of the regions formed by them and show that this intersection is disconnected, which contradicts the convexity of it. Let z_1 and z_2 be the two zones that pass through the hexagonal faces adjacent to the dual path between P_1 and P_2 (one zone on each side of the dual path). Then these zones intersect in two faces F_1, F_2, such that F_1 is at distance two from P_1 and F_2 at distance two from P_2. Note that the faces adjacent to the dual path together with F_1, F_2 are hexagonal, otherwise we contradict the minimality of d^*. Let's further consider z_3, z_4 passing through faces that are adjacent to the faces of z_1, z_2 just mentioned above. In the case $d^* \geq 3$, these faces are all hexagonal (by taking into account the previous proposition coupled with our assumption of P_1, P_2 being at minimal distance d^*). Furthermore, z_3, z_4 intersect in two faces I_1, I_2, situated at distance one or two from F_1, respectively F_2. Finally, we consider v_1 to be a vertex of F_1 and v_2 a vertex of F_2 such that v_1, v_2 are in the intersection of those regions formed by z_1, z_2 that do not contain P_1, P_2 in them. Then v_1, v_2 lie also in the regions formed by z_3, z_4 that contain P_1, P_2. Let C be the intersection of the four regions mentioned. Then C is convex but for the pair v_1, v_2 there is no geodesic in C, contradiction. □

We now need to deal with the cases when the minimal distance d^* between pentagons is less than three. For $d^* = 2$ we have to consider the cases of straight path or of crooked path of type $\{1, 1\}$. For $d^* = 1$ the dual path is necessarily straight, in which situation at least two pentagons of the fullerene are adjacent.

Proposition 4.1.4. *Two pentagons at minimal distance two cannot allow a crooked dual path of type* $\{1, 1\}$.

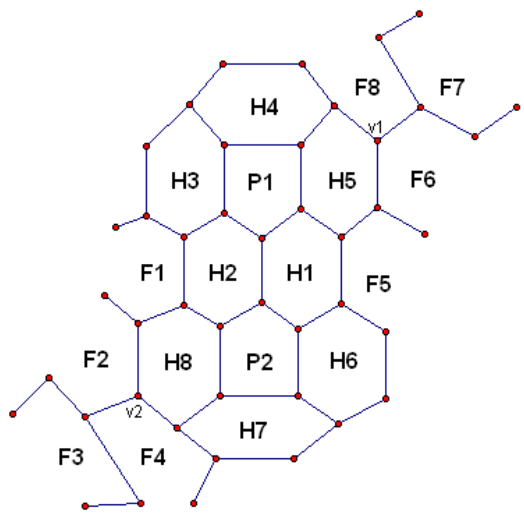

Figure 4.3: Crooked dual path of type $\{1, 1\}$

Proof: We prove this result by contradiction. Suppose P_1, P_2 are at minimal distance with crooked dual path of type $\{1, 1\}$. Note that since the minimal distance between pentagons is two, all faces adjacent with P_1 or P_2 must be hexagons (being at distance one from P_1 or P_2). Let P_1, H_1, P_2, H_2 be the *vertices* of the parallelogram π in clockwise order and let H_1, H_2, H_3, H_4, H_5 and H_2, H_1, H_6, H_7, H_8 be the hexagons adjacent with P_1 and P_2 respectively (in clockwise order). Then there is a zone z_1 that passes through H_5, P_1, H_2, H_8 and a second zone z_2 that passes through H_5, H_1, P_2, H_8. These two zones obviously intersect inside the faces H_5, H_8. Let v_1 be the vertex of H_5 and v_2 be the vertex of H_8 that lie in the intersection of the regions determined by z_1, z_2 and which do not contain π. Now construct two more zones z_3, z_4 such that z_3 passes through H_3, H_4 and z_4 passes through H_6, H_7. Let's show that these two new zones are well defined and that they intersect in two faces, each at distance ≤ 2 from H_5, respectively H_8. First, consider the faces $F_1, ..., F_8$ as shown in the Figure above. Note that out of these faces no two adjacent ones can be pentagons (since the minimal distance between pentagons is assumed to be two). If all of these faces are hexagons then zones z_3, z_4 exist indeed and intersect in F_3, F_7. If either F_2 or F_6 (or both) are pentagons, then the labels for these two zones (*i.e.*, the j, k that make z_3 be a j-zone and z_4 be a k-zone) can be chosen in such a way that z_3, z_4 intersect in F_3, F_7. Going through all possibilities we see that no matter the type of the faces $F_1, ..., F_8$ we still obtain the zones z_3, z_4 and that they intersect within F_6, F_7, F_8 on one end, and within F_2, F_3, F_4 at the other end. We note that in any of these situations, the vertices v_1, v_2 are in the intersection C of four regions determined by the four zones considered but there is no path between these vertices that lies in C, contradiction. □

4.2 Minimal distance between pentagons of type {2,0}

When the minimal distance between pentagons is two we show that all the pentagons have to be situated with respect to each other in a certain way and that any other arrangement of pentagons leads to a non-embeddable fullerene. It will straightforward to construct the only ℓ_1-embeddable fullerene with such property (which will be a fullerene on 80 vertices).

Proposition 4.2.1. *If the minimal distance between pentagons is two (with a straight dual path between them) then each pentagon is surrounded by five other pentagons, each of them at distance two from it (via straight dual paths).*

Proof: Let P_1 and P_2 be two pentagons at minimal distance two admitting a straight dual path between them (the path consisting of the faces P_1, H and P_2). Then all faces adjacent with either P_1 or P_2 must be hexagons since otherwise the minimal distance between pentagons would be one, not two. Moreover, the faces at distance two from P_1 or P_2 admitting a crooked dual path to P_1 or P_2 must also be hexagons, otherwise we contradict the previous proposition. We are left with six faces that lie at distance two from either P_1 or P_2, all of them admitting a straight dual path to one or both of these pentagons. These six faces can be either pentagons or hexagons, our goal being to show that all of them are pentagons. We consider the zone z_1 passing through four of the hexagons adjacent to the minimal dual path P_1, H, P_2 (say the ones on the *right* of the dual path) and z_2 the zone symmetric to z_1 (situated on the *left* of the dual path). Then z_1, z_2 intersect in two faces: one at distance two from P_1 (call it H_1) and the other one at distance two from P_2 (call it H_2). These zones determine four regions in the fullerene. Consider v_1 the vertex of H_1 that lies in the region not adjacent to the region containing the dual path P_1, H, P_2. Similarly, take v_2 the vertex in H_2 with the same property. We now return to the six faces at distance two from P_1 or P_2 that could be either pentagons or hexagons. Three of these faces are *to the right* of z_1, the other three being *to the left* of z_2. If at most one of the faces to the right of z_1 and at most one of the faces to the left of z_2 are pentagons, we can find two new zones z_3 and z_4 such that z_3 passes through the faces to the right of z_1 and z_4 passes through the faces to the left of z_2. Moreover, these zones will intersect such that the vertices v_1, v_2 considered above will lie in the same region as the dual path P_1, H, P_2. Thus we get that v_1, v_2 lie in the intersection of four of the regions determined by z_1, z_2, z_3, z_4, which must be convex. Since there is no path between v_1, v_2 that lies in that intersection we obtain a contradiction with its convexity. This shows that at least on one side of the dual path we must have two or more pentagons at distance two from P_1 or P_2. Suppose now that there exist two such pentagons P_3, P_4, where P_3 is adjacent to H_1 and P_4 is at distance two from both P_1, P_2 (P_3, P_4 being on the *right* side of the initial dual path P_1, H, P_2). Notice that for the pair of pentagons $\{P_1, P_4\}$ we have that P_2 is a pentagon at distance two from both, situated on the *left* of their dual path, whereas P_3 has the same property but is situated on the *right*. If there is no other pentagon at distance two from P_1, P_4 then we apply again the argument with the four zones and their convex intersection to get a contradiction. So there must exist at least one more pentagon at distance two from either P_1, P_4. Without loss of generality, we can suppose it is situated on the *right* side of dual path linking P_1, P_4. Let's denote this pentagon by P_5. Notice now that the zone z_2 will *wrap* around all of P_1, P_2, P_3, P_4, P_5 being adjacent to P_1, P_2, P_3, P_5 (not to P_4). Most of the faces through which z_2 passes are hexagons, except for one or two that we do not know what they are at this point. Denote first by P_6 the face to the right of z_1

that is at distance two from both P_2 and P_4. We show that this face is a pentagon. Suppose this is not true, *i.e.*, P_6 is a hexagon. Then there are two more faces adjacent to P_6 and such that z_2 passes through them. These two faces cannot both be pentagons (we would contradict the minimal distance of two between pentagons). Moreover, exactly one of them cannot be pentagon because it would follow that z_2 consists of several hexagons and exactly one pentagon, which would imply that two opposite faces of the pentagon carry the exact same edge label, a contradiction. Thus these two faces must be hexagons and therefore z_2 is a straight zone. We obtain a contradiction by noting that z_2 involves non-opposite edges of one of the hexagons, which is not possible. Thus P_6 must be a pentagon. In conclusion, we proved that if for a pair of pentagons at straight dual distance two there exist two pentagons such that both are on the same side of the dual path and at distance two from each other, then there is a third pentagon situated on the same side. We can apply this finding to the pair P_1, P_4, thus obtaining P_7 (on the same side as P_3, P_5). We repeat this argument to other pairs of pentagons and in the end we obtain the desired result that for each pentagon there are other five pentagons at straight distance two from it.

The last case that remains to be proved is when P_1, P_2 admit two pentagons P_3, P_4 such that both of these are situated on the same side (say, to the right) of $\{P_1, P_2\}$ and P_3 is at distance two from P_1, whereas P_4 is at distance two from P_2 and neither P_3 or P_4 are at distance two from both $\{P_1, P_2\}$. Denote by F the face which is on the same side as P_3, P_4 and which is at distance two from both P_3, P_4 (and also from P_1, P_2). Suppose that F is not a pentagon. Then construct the zone z that passes through the faces adjacent to and to the right of the faces P_3, H_1, F, H_3, P_4, such that z does not coincide with the zone z_1 considered at the beginning of the proof. We will next look at the vertices v_1, v_2 as defined at the beginning of the proof. This two vertices are the only ones that can be found in the intersection of three of the regions determined by the zones z_1, z_2, z. No edge exist though between these vertices that lies in the intersection of the regions, contradiction with the convexity of the intersection. Thus F must be a pentagon and for each pair of pentagons there exist at least three more pentagons at distance two from one or both of the pentagons of the pair and such that all three are on the same side of the dual path between the two pentagons of the pair. Applying this result to different (carefully chosen) pairs of pentagons we obtain the needed result. □

Proposition 4.2.2. *There exists exactly one ℓ_1-embeddable fullerene such that the minimal distance between pentagons is greater than or equal to two.*

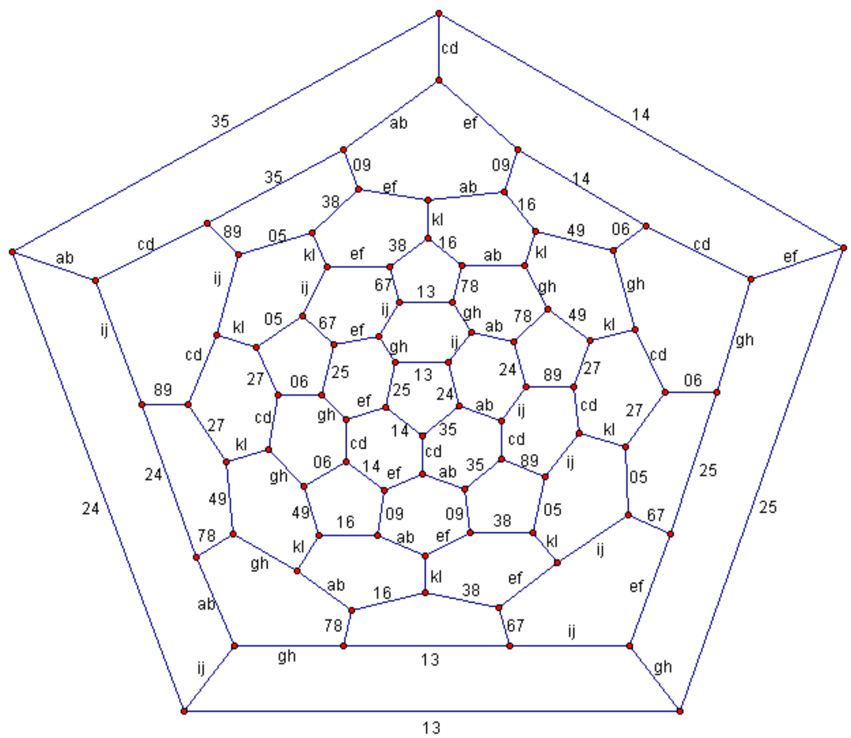

Figure 4.4: Embedding of $\mathcal{F}_{80}(I_h)$ into $\frac{1}{2}H_{22}$

Proof: We know that if in the fullerene there are two pentagons at distance two then there must be a straight path between them and we can find other six pentagons at distance two from one or both of them, such that three of these pentagons are on one side of the straight dual path and the other three on the other side. Thus we already have the position of eight of the twelve pentagons of the fullerene. Taking other pair of pentagons from the eight we have, we see that we can quickly construct the whole fullerene in this way. We obtain an

80 vertices fullerene with 30 hexagonal faces (and twelve pentagonal ones, obviously). This fullerene is unique by construction and we can put edge labels on each of its edges as shown in Figure 4.4. This fullerene is ℓ_1-embeddable. □

It remains to deal with the cases when the minimal distance between pentagons is one. We will consider subcases based on the maximum number of pentagons that are adjacent to a pentagon in the fullerene.

CHAPTER 5

ADJACENT PENTAGONS: THE CLUSTER CASE

In the case of adjacent pentagons, there are four known ℓ_1-embeddable fullerenes. We show that these are the only ones possible.

5.1 Labels on a three pentagons cluster

Lemma 5.1.1. *The labeling of the edges of the three pentagons cluster cannot follow the example in figure A, but must be as shown in figure B,i.e., the label* 1 *does not split on the vertical edge starting from* v_2 *but on the horizontal one.*

Proof: Suppose the edge label $\{13\}$ splits as shown in Figure A. Then the distance between the vertices v_1, v_2 must be three. Indeed, the path from v_1 to v_2 consisting of the edges labeled $12, 45, 67, 1x$ has the property that the symmetric difference of these labels has size six, which implies that $d(v_1, v_2) = \frac{1}{2}6 = 3$. Thus there must exist two vertices in the fullerene such that together with v_1, v_2 they form a geodesic from v_1 to v_2. There are two cases to consider. One is when a geodesic does not go through any of the vertices of the cluster of pentagons (which is shown in Figure A, the geodesic being v_1, B, C, v_2). The other case is

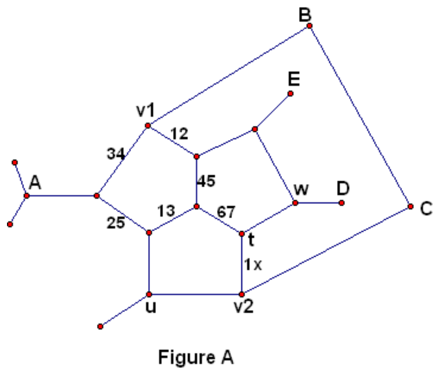

Figure 5.1: Labels on a three pentagons cluster

when there exists a geodesic that goes through one more vertex of the cluster besides v_1, v_2. Let's disprove the first case. If the third edges of B and of C (not shown in Figure A) are both going *inside* the shape formed by v_1, B, C, v_2 then starting from A, we obtain a path that makes only left turns, has no returns and has length ≥ 7, contradiction. If the third edges of B and of C (not shown in Figure A) are both going *outside* the shape formed by v_1, B, C, v_2 then starting from D, we obtain a path that makes only left turns, has no returns and has length ≥ 7, contradiction. The only possibility remaining is when one of the third edges of B and of C goes *outside* (say for B) and the other (for C) goes *inside*. Then starting at the third edge of C and making only left turns we see that the vertices C, E must be linked by an edge, otherwise we obtain a contradiction. Further, consider the third edge of E (which must go towards D). Starting at this edge and making only right turns (passing through E, C, v_2, etc) we obtain a path that has length six and ends at D. Since D, E cannot be linked by an edge (otherwise, a 4-cycle is formed, impossible in a fullerene) we deduce that the path obtained can be augmented, *i.e.*, it has length ≥ 7, contradiction.

Thus, we have shown that any geodesic between v_1, v_2 must pass through at least one more vertex of the cluster. Suppose a geodesic passes through the vertices t, w. This can happen only if v_1, w are linked by an edge. Then we consider E and one of its third edges, such that starting at that third edge and making only right turns (through E, v_1, w, E again, etc) we obtain a path of length eight, contradiction. Suppose now that a geodesic goes through u and another vertex (say F, not shown in Figure A). We assume F to be at the *left* of the cluster. If F has a third edge that does not go towards the cluster then we obtain a contradiction by paths (right turns only) using one of the third edges of A. If F goes towards the cluster then we still obtain contradictions by using paths arguments, specifically paths that start from the third edge of F and make either only left turns or only right turns. □

5.2 Six pentagons cluster case

Lemma 5.2.1. *a) The labeling of a cluster of six pentagons consisting of one central pentagon P surrounded by five other pentagons P_1, P_2, P_3, P_4, P_5 in clockwise order around P, is as shown in Figure 5.2.*

b) In an ℓ_1-embeddable fullerene a cluster of six pentagons (one of them surrounded by the others) cannot be surrounded by a layer of five hexagons.

Proof:

a) Using the previous lemma, we first label the cluster of three pentagons P, P_1, P_2, then proceed in labeling the cluster P, P_2, P_3 and so on until all six pentagons are labeled. We see that the decagon obtained using the outer edges of the pentagons P_1, P_2, P_3, P_4, P_5 has the property that its *opposite* edges have the same label.

b) If the cluster of six pentagons would be surrounded by five hexagons then in the new decagon formed by the outer edges of this layer of hexagons, edge labels would be repeated on non-opposite edges. Turning our attention to the faces surrounding this layer of hexagons, we note that two such adjacent faces (no matter their type) would share a vertex that admits non-disjoint labels on two of the three edges that stem from it, contradiction. □

Proposition 5.2.2. *There exists exactly one ℓ_1-embeddable fullerene such that one pentagon is adjacent to other five pentagons.*

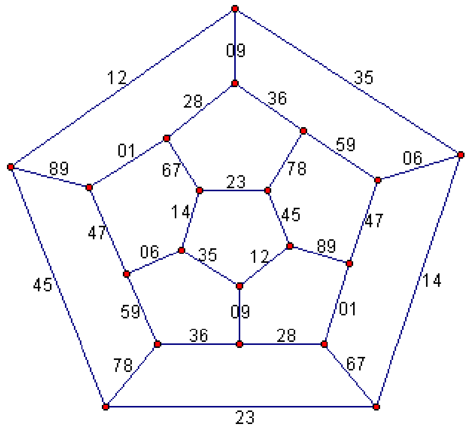

Figure 5.2: Embedding of $\mathcal{F}_{20}(I_h)$ into $\frac{1}{2}H_{10}$

Proof: Denote by P the pentagon having only pentagons as neighbors (call these neighbors P_1, P_2, P_3, P_4, P_5, in clockwise order). Notice that there exist five other faces F_1, F_2, F_3, F_4, F_5 (also in clockwise order) in the fullerene that *surround* the 6-pentagon cluster. If all these faces are pentagons then the only fullerene which can be constructed with this property is a fullerene on 20 vertices which is ℓ_1-embeddable (see Figure 5.2 above). If four of these faces are pentagons (say, F_1, F_2, F_3, F_4) and only one is hexagon (F_5) then F_5 has a vertex v not belonging to F_1, F_2, F_3, F_4 (call this vertex *the sixth vertex* of F_5) and there is a third edge vw which is not part of F_5. Then there is a path starting with wv that makes only right turns, going around the faces $F_5, F_4, F_3, F_2, F_1, F_5$ and ending at w. Since this path has more than six edges and has no returns we obtain a contradiction. Suppose, next, that three of the F_i faces are pentagons and the other two are hexagons. The first possibility is that the two hexagonal faces are adjacent (say that they are F_4 and F_5). Then a similar argument using paths can be applied to obtain a contradiction (by considering the sixth vertex of F_4 and of F_5 and their third edges). The second possibility is when the two hexagonal faces are not adjacent. Thus suppose F_3, F_5 are hexagons and F_1, F_2, F_4 are pentagons. Let v be the sixth vertex of F_5 and w be the sixth vertex of F_3. Note that v, w cannot be linked by an edge since we would obtain a 4-cycle consisting of this edge and three more edges from

F_5, F_4, F_3. On the other hand, if v and w are not part of the neighborhood of a vertex u, then we find a path of more than six edges making only left turns, contradiction. Thus there exists a vertex u adjacent with both v and w. Let t be its third neighbor. In the case that t, w, v are in clockwise order around u, the path through t, u, v making a right turn towards F_4, then F_3 and ending with w, u, t makes only right turns and has seven edges, contradiction. Similar argument if t, v, w are in clockwise order around u. In conclusion, in an ℓ_1-embeddable fullerene three of the faces surrounding the cluster cannot be pentagons. Suppose now that two of these faces are pentagons. Consider first the case when the two faces are adjacent, *i.e.*, say that F_1, F_2 are pentagons, the other three faces being hexagons. Assume that P_1 is the pentagon of the cluster that is adjacent to both F_1, F_2. Let e_1 be the edge in between P_1, F_1, let e_2 be the edge in between P_1, F_2 and e_3 be the edge in between F_1, F_2. Let also ab be the edge label of the edge between F_1, F_5. This label is carried on the opposite edge in each of the hexagons F_5, F_4, F_3. Inside the pentagons F_1, F_2 half of this label goes to e_3 and half to e_1 and e_2. Therefore two of the edges e_1, e_2, e_3 must contain one of a, b in their label which leads to contradiction (since then one of the faces F_1, F_2, P_1 would have two adjacent edges with nondisjoint labels). We look now at the case when F_1, F_3 are pentagons (non adjacent) and F_2, F_4, F_5 are hexagons. Let v be the sixth vertex of F_5, u the sixth vertex of F_2 and w the sixth vertex of F_4. Let also vv_1, uu_1, ww_1 be the third edges of v, u, w respectively. If v_1, w_1 coincide we obtain a 4-cycle in the fullerene (via the vertices v_1, v, w and a fourth vertex belonging to both F_4, F_5), impossible. If $w_1 = u_1$ then using the third neighbor of w_1 (besides u and w, let's call it t) we consider the cases when w, t, u are in clockwise or counterclockwise order. In one of these cases we obtain a more than seven edge path that makes only right turns, impossible. The other case leads to the fact that t and v_1 must coincide, and further, to contradictions based on the third neighbor of v_1 and on its position relative to the other two neighbors of v_1. If all three u_1, v_1, w_1 are different, then u_1, v_1 must be linked by an edge and the same holds for u_1, w_1. Then the label of the edge uu_1 is carried on a pair of opposite edges of F_5 and also on a pair of opposite edges of F_4, ending on two adjacent edges of the pentagon in the cluster that is adjacent to both F_4, F_5, a contradiction. Thus the case of two non adjacent pentagons and three hexagons is not possible. The next case is when there is only one pentagon and four hexagons. Say F_1 is the only pentagon. This case can be disproved by looking at the labels of the edges in between the faces F_i. The label on the edge between F_1, F_2 will be carried on the edge between F_2, F_3, then between F_3, F_4, F_4, F_5 and finally, between F_5, F_1. Thus F_1 (a pentagon) will have two opposite edges with exactly the same edge label, contradiction with the fact that in a pentagon the labels of opposite edges share only half of their digits. The last case is when all F_1, F_2, F_3, F_4, F_5 are hexagons. The previous lemma (part b) showed that such a subgraph is not possible in an ℓ_1-embeddable fullerene. □

5.3 Four pentagons cluster case

We now turn our attention to four-pentagon clusters which consist of two *central* pentagons (these are the pentagons adjacent to other three pentagons in the cluster) and two *noncentral* ones (pentagons adjacent to only two other pentagons in the cluster). We can draw such cluster starting from the central pentagons P_1, P_2 - say these two faces share a horizontal edge. Then P_3 is at the *left* of P_1, P_2, adjacent to both, whereas P_4 is at the *right* of P_1, P_2. Denote by A the face that is adjacent to P_3 but not to the central pentagons; continue clockwise to label the faces around the cluster by C, D, B, F, E.

Lemma 5.3.1. *If P_1, P_2, P_3, P_4 is a cluster of pentagons (P_1, P_2 being central and P_3, P_4 noncentral) and no pentagon inside the fullerene is adjacent with five pentagons, then the following hold:*

a) All of the faces C, D, E, F cannot be hexagons if Γ is an ℓ_1-embeddable fullerene;

b) There is no ℓ_1-embeddable fullerene such that exactly one of the faces C, D, E, F is a pentagon, the remaining three being hexagons;

c) Thus exactly one of C, D and one of E, F must be pentagons;

Proof: a) Suppose C, D, E, F are hexagons. Further suppose that A is a pentagon. Let cd be the label on the edge between A and M. Without loss of generality, suppose c is carried onto the edge between A, E and thus, ultimately, also on the edge between F, B. But c will also be on the edge between B, D (via the hexagons C, D) which implies that B is a pentagon and that there exists a c-zone (call it z). Consider two other zones: one going through D, P_4, F and the other through C, P_3, E. Let v_1 be the vertex that belongs to C, D but not to the cluster and v_2 the vertex that belongs to E, F but not to the cluster. Then v_1, v_2 are the only vertices in a convex intersection of regions determined by the three zones considered above, contradiction.

Thus A, B must both be hexagons. Then we obtain a zone z_1 through A, C, D, B and a zone z_2 through A, E, F, B. Let v_1, v_2 be the two vertices of A that are not in C or E and let u_1, u_2 be the two vertices of B that are not in D or F. Consider also the face M adjacent to both A, E and continue in counterclockwise order to label the faces on the second layer around the cluster by N, P, Q, R, S, T, U. We show that if M is a pentagon then P must be a pentagon too. Let cd be the label on the edge between A and M. Then this label is carried (by virtue of opposite edges in hexagonal faces) to the edge between B, P. Moreover, half of this label, say c, is carried to the edge between M, N (since M is a pentagon). If c would further go on the edge between N, F, then inside F two non-opposite edges would share c in their labels, contradiction. Thus c goes on the edge between N, P and therefore P must be a pentagon. This also shows that if M is a hexagon then P is also a hexagon (otherwise, P being pentagon will imply M is pentagon by the argument above). If all M, P, T, R are hexagons then we can find two more zones (z_3 through U, M, N, P, Q and z_4 through U, T, S, R, Q) such that v_1, v_2 and u_1, u_2 will be in different connected components of a convex intersection of regions formed by the zones z_1, z_2, z_3, z_4, contradiction. Note also that if N is a hexagon then z_3 still exists, no matter what type of faces M, P are. To see this, consider ab the label on the edges between N, M and N, P. Suppose that in M, a goes on the edge between U, M. Then in P, a must go on the edge between P, Q since otherwise, it goes between P, B and further, through the hexagons B, D, C, A, labeling the edge between A, M. Then M has two adjacent edges sharing a digit of their label, contradiction.

Thus the only scenario in which we may not be able to construct z_3 is when all three faces M, N, P are pentagons. In this case, there is a face F adjacent with all these three faces and F must be a pentagon since the edges between M, F and P, F share d in their label. Furthermore, F and U are adjacent faces. If U is a pentagon, then Q is a hexagon (otherwise F is a pentagon surrounded by five other pentagons). Let w_1 the third vertex in the neighborhood of v_1 and such that it is not part of the face A. Similarly, let y_1 in the neighborhood of u_1. Then w_1, y_1 are linked by an edge (since Q is a hexagon). Let s be the third vertex in the neighborhood of y_1. Then the path starting with s, y_1, w_1, going along the face T makes only left turns and is too long, contradiction.

Thus U is a hexagon, Q is a hexagon and U, Q are adjacent. If T, S, R are all three pentagons then all the vertices in the picture have valency three and we obtain a fullerene on 36 vertices which was listed in [DGS] (at page 26) as non-ℓ_1. The case when S is hexagon but T, R are pentagons is impossible (due to the sixth vertex of S). If T, R are hexagons then their sixth vertices must be adjacent (say their third edges meet in a vertex v) otherwise there is a seven edges path that makes only right turns, contradiction. Then considering the neighborhood of v and applying the argument with paths that make only right (or only left) turns we obtain a 3-cycle or a 4-cycle, *i.e.*, not a fullerene.

b) Suppose C is a pentagon and D, E, F are hexagons. If A, B are both hexagons let ab be the edge label on the edge between the faces A, E. Since A, E, F, B are hexagons, this label is carried on the edges between E, F, between F, B, between B, R and between A, S (where S is the face adjacent to faces A, C, D and R is adjacent to faces S, D, B). If S is a hexagon, then ab is also carried on the edge between S, R and we obtain a contradiction because two edges of R have the same label and have just one edge in between them (so R cannot be a pentagon and neither a hexagon). Thus S must be a pentagonal face. Hence the label ab splits on the two opposite edges in S. Suppose, without loss of generality, that

a goes onto the edge in between S and D. But D is a hexagon and therefore carries A on the edge between D, P_4. P_4 is a pentagon so we have two choices of edges that can carry a in their label. But a cannot go on the edge between P_4, F since ab already labels two opposite edges of F. Thus a goes on the edge between P_4, P_2 and further (with a similar argument) on the edge between P_2, P_3. From P_3 it can either go into the faces A or C but in both those cases we obtain contradictions. This proves that the faces A, B cannot be both hexagons. The case when one of A, B is a pentagon and the other a hexagon can also be shown to be impossible. Indeed, assume A is a pentagon and B a hexagon. Let again ab be the label on the edge between A, E. So ab will also label the edges between E, F, between F, B and between B, R. But A is a pentagon so the label ab splits onto the opposite edges. Say that a goes onto the edge between A, C. Then since C is also a pentagon, a will go either on the edge between faces C, P_1 or between faces C, D. We continue to follow a and in the same manner as above we reach to a contradiction. Thus the only possible case remaining is when both A, B are pentagons. Our assumption then is that A, B, C are pentagons and D, E, F are hexagons. We split this case into two subcases based on the type of the face S. First suppose that S is a hexagon. Let ab be again the label on the edge between A, E, and suppose a goes on the edge between A, C and that bm is the label on the edge between A, S. Then a is carried onto the edge between C, D (all other choices are impossible) and thus also on the edge between D, B (D being a hexagon). Let ax be the full label on the edge between C, D (and D, B too). Since S is a hexagon, bm will label the edge between S, R. But b already labels the edge between B, R and thus R must be a pentagon. Moreover, m will label the edge between R, P. We prove that P is also a pentagon by showing that m labels the edge between F, P. In A, m is carried onto the edge between A, P_3 and from P_3 the only possible way is that it goes onto the edge between P_3, P_2 and further, on the edge between P_2, F, thus also on the edge between F, P. So P is a pentagon. Let's look now at the label x which is on the edge between B, P and must go onto the edge between N, P. But x must also be on the edge between C, P_3 and on the edge between P_3, E (otherwise, if it goes in P_2 we would get contradictions in either of the faces P_4, F) and thus also between E, N. This shows that the face N must be a pentagon. The last face that remains to look at and that belongs to the second layer of faces around our initial four pentagons cluster, is M. If M would be a hexagon there would exist a vertex v in M, but not in S, N and there would be a path starting from the third neighbor of v such that this path makes only right turns and has at least seven edges, contradiction. Thus M must also be a pentagon and now our fullerene is complete (all vertices have valency three). This fullerene has 28 vertices and is not ℓ_1-embeddable, as was stated in [DGS] (see page 26).

We are left with the case when S is a pentagon. In this case we again have that a is carried on edges between A, C; C, D; D, B; B, F; E, F and E, A. The label of the edge between A, S is bm and in S, b must be carried on the edge between S, R (otherwise if it goes between S, D it would go inside P_4 and from there it would land in either of the faces A, F, E, S, in which we would obtain contradictions). Using the element x of the label ax of the edge between C, D and using the same argument employed above regarding x we get that both P, N are pentagons. Let v be the vertex of N that does not belong to either of E, F, P. Let w be its third neighbor, w not in N. Then starting at w and going through v we find a path that makes only right turns and has length ≥ 7, contradiction. Thus part (b) of the lemma is completely proved *i.e.*, there is no ℓ_1-embeddable fullerene such that exactly one of C, D, E, F is a pentagon.

c) From parts (a) and (b) we infer that at least two of the faces C, D, E, F are pentagons. Since we assumed in the beginning that there is no pentagon having all five neighbors pentagons, we must have that C, D cannot both be pentagons and, similarly, E, F cannot both be pentagons. Thus one of C, D must be a hexagon and one of E, F must be a hexagon. □

Lemma 5.3.2. *If P_1, P_2, P_3, P_4 is a cluster of pentagons (P_1, P_2 being central and P_3, P_4 noncentral) and no pentagon inside the ℓ_1 fullerene is adjacent with five pentagons, then the following hold:*

a) The faces A, B cannot both be pentagons;

b) The faces A, B cannot both be hexagons;

c) Thus exactly one of C, D, exactly one of E, F and exactly one of A, B must be pentagons;

Proof: a) Given the previous result, and the assumption that both A, B are pentagons we can only have the case that C, F are pentagons (thus D, E are hexagons) or the symmetrical case when D, E are pentagons (C, F being hexagons). It is enough to consider one of these situations. Suppose C, F are pentagons. Let ab be the label on the edge between A, E and suppose inside A it splits as follows: a goes between A, C and b goes between A, S (S being the face adjacent to all of A, C, D).

If, in C, a is carried on the edge between C, D we show that we obtain a fullerene on 24 vertices which was shown in [DGS] (see pages 25-26) not to be ℓ_1-embeddable. Indeed, let ay be the label on the edge between C, D. Then ay also labels the edge between D, B (D is a hexagon). Furthermore, inside the face B, a cannot go on the edge between B, N (where N is the face adjacent with E, F, B). This is because if it would, then inside the face F, a would have to split on the edge between F, P_4 , then between P_1, P_4, between P_3, P_1 and from P_1 it would go into either A or E on edges adjacent to the edge labeled ab, contradiction. Thus a goes between B, F and b goes between P_4, F. Moreover, b must continue between P_4, D and thus also between D, S. This shows that S is a pentagon. In the same way (but using y) we prove that N is a pentagon (y is part of the label of the edge between B, N and of the edge between E, N). It follows that the faces R (adjacent with all S, D, B, N) and M (M is adjacent with all S, A, E, N) must also be pentagons because otherwise, using the sixth vertex of R we would find a path that makes only right (or only left) turns and that has length ≥ 7. With R, M being pentagons we obtain a complete fullerene (all vertices considered have valency three) with 24 vertices. We know that no fullerene with 24 vertices is ℓ_1-embeddable (see [DGS]).

It remains to deal with the case when a is carried on the edge between C, P_1. Then a goes also between P_1, P_4, between P_4, F (all other choices ending in a contradiction). On the other hand, b is carried between S, R (otherwise it ends up in either of the faces A, E, F, on an edge adjacent to other edge already labeled with b, impossible) and between B, R. Thus R is a pentagon. A similar argument involving x shows that M is a pentagon too. If S is a pentagon, we can draw the complete fullerene and obtain 24 vertices *i.e.*, not an ℓ_1-embeddable fullerene (this is the same fullerene we obtained above). If S is a hexagon, then the face N is also a hexagon and the graph obtained has a four cycle as the *outer* face, which is prohibited in a fullerene.

b) We assume A, B are hexagons.

If C, E are pentagons (and D, F hexagons), we let ab be the label of the edge between A, E, cd the label between A, C, dx the label between C, D and by the label between E, F. Note that x, y cannot be the same because they lie on non-opposite edges of the hexagon B. Inside C, x goes between C, P_3, and further on, between P_3, E (if it would have gone between P_3, P_2 then it would have ended in either of D, B, F on edges adjacent to edges already labeled by x). On the other hand, y must go between E, P_3, then P_3, P_1, then P_1, P_4 and then in either B or F on an edge adjacent to the edge labeled by, contradiction.

By symmetry, it only remains to consider the case when C, F are pentagons (thus D, E are hexagons). Using again label arguments as employed above, we deduce that both S, N are pentagons. Moreover, M, R are also pentagons. We obtain a fullerene on 28 vertices such that all faces on the second layer of faces surrounding the cluster P_1, P_2, P_3, P_4 are pentagons. This fullerene is not ℓ_1-embeddable, as we know from [DGS].

c) This part follows from (a), (b) and from the previous lemma. □

Proposition 5.3.3. *There exists exactly one ℓ_1-embeddable fullerene such that there is a four-pentagon cluster but no pentagon is adjacent to five other pentagons.*

Proof: Without loss of generality, assume first that A is a pentagon and B is a hexagon. Note that since no pentagon in the fullerene is adjacent to five other pentagons, we cannot have the case when both C, E are pentagons (P_3 would be adjacent with pentagons only). Then given the previous two lemmas we only have two cases to consider. one case is when

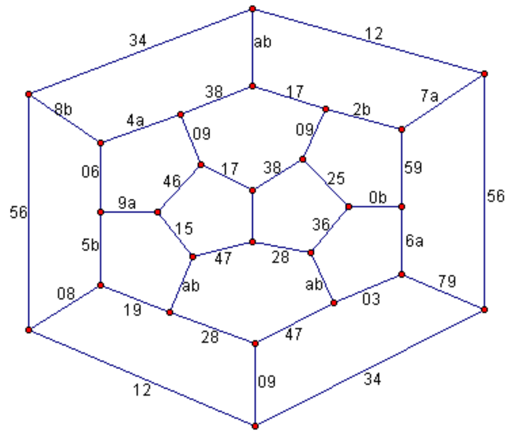

Figure 5.3: Embedding of $\mathcal{F}_{26}(D_{3h})$ into $\frac{1}{2}H_{12}$

C, F are hexagons and D, E are pentagons; the second case is when C, E are hexagons and D, F are pentagons. Consider the first case and let ab be the label on the edge between E, F and therefore also between F, B and between B, R (where R is the face adjacent to all of C, D, B). Inside E the label ab splits on opposite edges. Say that b goes between E, P_3 and a between A, E. Inside P_3, b cannot go on the edge between P_3, P_1 since it would end up in D or P_4 on an edge adjacent to an edge already admitting b in its label, contradiction. Thus b goes between C, P_3 and since C is a hexagon, it further goes between C, R. This shows that R is a pentagon. With a similar argument we get that a goes between A, S (where S is the face adjacent to A, C, R). Moreover, in R, a goes between S, R (the edge of R labeled ab splits such that b goes between R, C which means a must go on the other opposite edge, *i.e.*, between S, R). Thus S must also be a pentagon. Now, if the face M (adjacent to A, E, F) is a pentagon, then all vertices in the picture have valency three except one, which belongs to the face B but is not in either of F, P_4, D, R. This vertex must have a third neighbor, say v. Starting at v we find a path that makes only right turns and has more than six edges, contradiction. Thus M must be a hexagon. Looking at the face N (adjacent to F, B, M) we see that no matter if N is a pentagon or a hexagon we can apply the paths argument and obtain a contradiction. Thus the first case does not lead to an ℓ_1-embeddable fullerene.

Next, consider the second case (C, E are hexagons). Let ab be the label on the edge between A, E (so also between E, F). Without loss of generality, suppose a goes (inside A) between A, C, while b goes between A, S. Let the full label of the edge between A, C be ax. Then ax also labels the edge between C, D (since C is a hexagon). Moreover, a cannot go between D, B since any choice would lead to a contradiction (if a would go between D, B it would also go on the edge between B, N; then consider the face F in which the label ab splits on the opposite edges; a would go between F, P_4, then P_1, P_4, etc). So a labels the edge between D, P_4 and between P_4, F. In R (the face adjacent to C, D, B), b cannot label the edge between R, C because then it would go inside P_3 and from there, either in P_2 or E, which already have edges labeled by it. Thus b goes between S, R which shows that S is a pentagon. Using x we can prove in a similar fashion that M (adjacent to S, A, E) is a pentagon. Finally, we turn our attention to the faces N, R. If both are hexagons or if one is a hexagon and the other a pentagon, then we can find a path that makes only right (or only left) turns and that has length ≥ 7, contradiction. Thus both R, N are pentagons and we obtain a complete fullerene on 26 vertices. This fullerene is ℓ_1-embeddable as was verified in GAP (the algebra software). □

5.4 Three pentagons cluster case (no four cluster)

In order to find the ℓ_1-embeddable fullerenes possessing a cluster of three pentagons (but no cluster of four or more pentagons) we look at the first and second layers of faces surrounding the three pentagons cluster. The next lemma shows that the first layer of faces surrounding the cluster consists of hexagons only. On the second layer, there are nine faces. We note that six of these faces are adjacent to two hexagons of the first layer, whereas three of these faces are adjacent to only one hexagon of the first layer. Let's call the six faces *degree two faces* and the remaining three faces *degree one faces*. We split the discussion of three pentagons cluster into subcases based on the type (hexagonal or pentagonal) of the *degree two faces*. The second lemma that follows will be used throughout the proofs of the subcases. It essentially says that two adjacent pentagons in an ℓ_1-embeddable fullerene cannot be *surrounded by too many* hexagons, unless these pentagons are part of a cluster of three pentagons.

Lemma 5.4.1. *Consider an ℓ_1-embeddable fullerene such that no pentagon has all neighbors pentagons and also no four-pentagon cluster exists. Then if a three-pentagon cluster is present, it follows that this cluster is surrounded by a layer of hexagons.*

Proof: Let P_1, P_2, P_3 be the three-pentagon cluster in clockwise order. Since no four-pentagon cluster exists, we must have that the other face adjacent with both P_1, P_2 (besides P_3) is a hexagon (call it H_1). Similarly, we can consider the hexagon H_2 adjacent with P_2, P_3 and the hexagon H_3 adjacent with P_3, P_1. Let F_1 be the face adjacent to H_1, P_2, H_2, let F_2 be adjacent to H_2, P_3, H_3 and F_3 be adjacent to H_3, P_1, H_1. We need to show that all three faces F_1, F_2, F_3 are hexagons.

Suppose F_1 ia a pentagon. Let x be part of the edge label of both the edge between H_1, F_1 and the edge between H_2, F_1. Thus x is in the label of the edge between H_1, F_3 and of the edge between H_2, F_2. Consider the vertex v_1 belonging to both H_1, F_3 but not to P_1, and v_2 belonging to both H_2, F_2 but not to P_3.

Suppose further that F_2, F_3 are both hexagons. Then we consider the zone z consisting of the edges that contain x in their label. We also consider the zone z_1 going through the edges in between H_1, P_2 and P_2, H_2 and the zone z_2 going through the edges between F_3, H_3 and H_3, F_2. Then v_1, v_2 is the intersection of three of the regions determined by the three zones above, contradiction (since there is no edge in between v_1, v_2, *i.e.*, the intersection of regions is disconnected).

Thus F_2, F_3 cannot be both hexagons. Suppose F_2 is a pentagon, F_3 is a hexagon. We consider again the three zones defined above and obtain a contradiction.

This shows that F_2, F_3 must be pentagons, *i.e.*, we are in the case when all three of F_1, F_2, F_3 are pentagons. With x being part of the edge label of both the edge between

H_1, F_1 and the edge between H_2, F_1, we see that x also labels the edges in between H_1, F_3 and H_2, F_2 (since H_1, H_2 are hexagons).

Suppose that x also labels the edge between F_2, J_5 and thus also between F_3, J_6 (see Figure below).

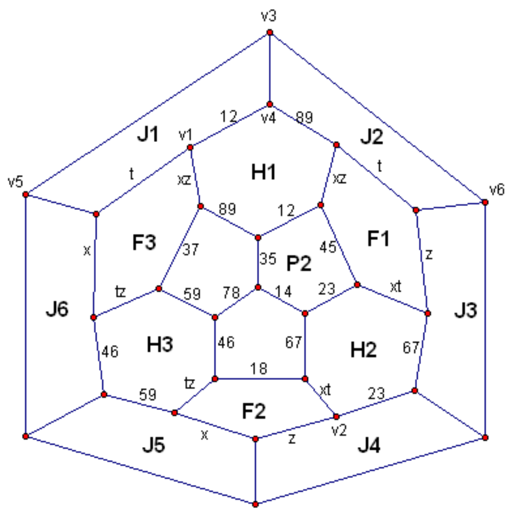

Figure 5.4: First layer lemma

Then we claim that all faces J_i, $i = 1, ..., 6$ are pentagons. Indeed, consider v_3 a vertex shared by the faces J_1, J_2 (as shown above). Inside J_1 (where J_1 can be either pentagon or hexagon), the label t will go on one of the edges going through v_3. Similarly, the label t inside J_2 goes on v_3v_4 or on v_3v_6. If at least one of the faces J_1, J_2 are hexagons then two different edges starting from v_3 share t in their label, which cannot happen in an ℓ_1-embeddable fullerene. Thus J_1, J_2 are both pentagons and t goes on the edge v_3v_4. In the same manner, J_3, J_4 are pentagons and J_5, J_6 are pentagons. We obtain a complete fullerene on 28 vertices, which is not ℓ_1-embeddable (as stated in [DGS]).

It remains to examine the case when x labels the edge between H_3, F_2. Then x also labels the edge between H_3, F_3 (since H_3 is a hexagon). Let xy be the full label of the edge between H_3, F_2 and between H_3, F_3. Consider the zone z_1 determined by y (*i.e.*, z_1 goes through the edges between J_1, F_3, F_3, H_3, H_3, F_2 and F_2, J_4, where the J_is are the faces on the second layer around the cluster and they are not necessarily pentagons). Let also z_2 be the zone determined by x (so it goes through the faces of the first layer around the cluster). Finally, let z_3 be the zone determined by the label digit 2, *i.e.*, z_3 goes through J_1, H_1, P_2, H_2, J_4. The vertices v_1, v_2 will then constitute the intersection of three of the regions formed by these three zones. Since in this intersection, v_1, v_2 are disconnected, we contradict the convexity of regions in an ℓ_1-embeddable fullerene. In conclusion, the assumptions that at least one of the faces F_1, F_2, F_3 is a pentagon leads to contradictions or to non-embeddable fullerenes, which proves that all of these faces must be hexagons. □

Lemma 5.4.2. *There exists no ℓ_1-embeddable fullerene that has a subgraph consisting of two adjacent pentagons P_1, P_2, such that the two faces adjacent with both these pentagons are hexagons and that one of these hexagons is also adjacent to two more hexagons, one of them adjacent to P_1, the other to P_2.*

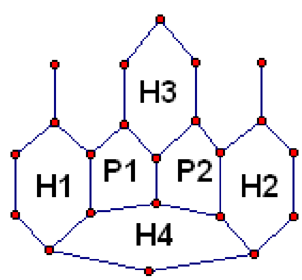

Figure 5.5: Two pentagons path

Proof: Suppose by contradiction that we have such subgraph. Let H_1, P_1, P_2, H_2 be the faces of the path, where P_1, P_2 are the two adjacent pentagons of the path. We call H_3, H_4 the hexagons adjacent to both P_1, P_2 (these are the faces above and below the two adjacent pentagons). Let H_1 be the face adjacent to both P_1 and H_4 and let H_2 be the face adjacent to P_2 and H_4. We consider the zones z_1 through H_3, P_1, H_4 and z_2 through H_3, P_2, H_4. We can also consider the two zones z_3 *parallel* to z_1 and passing through H_1 and z_4 in a similar way (*parallel* to z_2 and passing through H_2). Then in the intersection of four of the regions formed by these four zones we find one vertex from H_3 and another from H_4 though no path between them exists in this intersection, contradiction. □

In the next results we will use the following notations for the faces surrounding the cluster of three pentagons. We denote by $F_1, ..., F_6$ the six *degree two faces* in clockwise order, by A_1, A_2, A_3 the three *degree one faces* also in clockwise order, such that A_1 is adjacent to F_1, F_6, A_2 to F_2, F_3 and A_3 to F_4, F_5. Consider G_1 the face adjacent to F_1, F_2 that is not part of the first layer surrounding the cluster of three pentagons and similarly, consider G_2 adjacent to F_3, F_4 and G_3 adjacent to F_5, F_6. Also let $H_1, ..., H_6$ be the hexagons in the first layer, in clockwise order and such that H_1 is adjacent to both F_1, F_2.

Lemma 5.4.3. *Suppose all six degree two faces are pentagons. There exists exactly one ℓ_1-embeddable fullerene that has this property. This fullerene has forty vertices and is drawn below (Figure 5.6).*

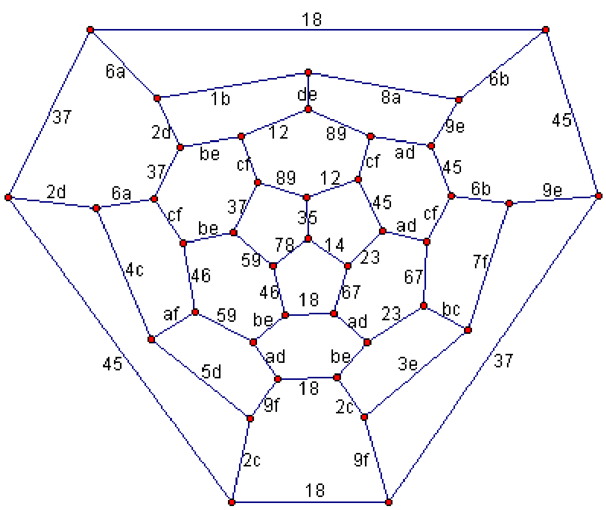

Figure 5.6: Embedding of $\mathcal{F}_{40}(T_d)$ into $\frac{1}{2}H_{15}$

Proof: With the notations above, and by applying the lemma 5.4.2 to the subgraph formed by $H_6, F_1, F_2, H_2, H_1, G_1$ we see that in order for the fullerene to be ℓ_1-embeddable we must have that G_1 is not a hexagon, *i.e.*, G_1 is a pentagon. With the same argument, G_2, G_3 are also pentagons. Then it follows that A_1, A_2, A_3 are hexagons, because otherwise the fullerene would have four pentagons cluster (e.g. A_1, F_1, F_2, G_1), contradiction. With these properties, we see that the fullerene is completely constructed (all vertices have valency three). It has 40 vertices and its edge labeling is shown in Figure 5.6. It is known that this fullerene is ℓ_1-embeddable. □

Lemma 5.4.4. *Suppose exactly five of the degree two faces are pentagons. There exists no ℓ_1-embeddable fullerene in this case.*

Proof: Consider $F_1, ..., F_5$ to be pentagons and F_6 to be hexagon. By the same arguments employed above, we have that G_1, G_2 are pentagons and that A_1, A_2, A_3 are hexagons. Let v_1 be the vertex of A_1 that is not in any of the faces F_6, H_6, F_1, G_1 and let u_1 be its third neighbor (u_1 not in A_1). In a similar way, let v_3 be the vertex of A_3 that is not in F_4, H_4, F_5, G_2 and let u_3 be its third neighbor. Then we see that $u_1 = v_3$ and $u_3 = v_1$, *i.e.*, v_1, v_3 are adjacent. Indeed, otherwise the path starting at u_1, through v_1 and the outer edges of A_1, G_1, A_2, G_2, A_3, ending with v_3, u_3, makes only left turns and its length is ≥ 7, contradiction. At this moment all the vertices that are part of the faces considered until now have valency three except one vertex of F_6 (the one not in A_1, H_6, H_5, F_5). Denote it by w and denote its third neighbor by t. Then consider the path starting at t, through w, making only right turns, going (among other vertices) through v_3, v_1 and ending at t. This path has length eight, contradiction. □

Lemma 5.4.5. *Suppose exactly four of the degree two faces are pentagons. There exists no ℓ_1-embeddable fullerene in any of the following possible cases:*

a) two sets of adjacent degree two faces are pentagons;

b) one set of adjacent degree two faces are pentagons; the other two degree two faces that are pentagons are not adjacent and the subgraph consisting of the cluster and the first two layers surrounding it is asymmetric;

c) one set of adjacent degree two faces are pentagons; the other two degree two faces that are pentagons are not adjacent and the subgraph consisting of the cluster and the first two layers surrounding it is symmetric;

Proof: a) Suppose $F_1, ..., F_4$ are pentagons and F_5, F_6 are hexagons. We then have that G_1, G_2 are pentagons and that A_1, A_2, A_3 are hexagons. Consider as in the previous proof v_1 the sixth vertex of A_1 and v_3 the sixth vertex of A_3, v_1, v_3 being adjacent by the same argument used in the previous lemma. Let w_5 be the sixth vertex of F_5 (*i.e.*, not in any of the labeled faces) and let t_5 be its neighbor that does not lie in F_5. Similarly, consider w_6 in F_6 and t_6 its neighbor that is not in F_6. Take the path starting at t_5, w_5 that makes only right turns, going through v_3, v_1 and ending at t_6. This path has length seven, contradiction.

b) Suppose F_1, F_2, F_3, F_5 are pentagons and F_4, F_6 are hexagons. We then have that G_1 is a pentagon and that A_1, A_2 are hexagons (to prevent having a four pentagons cluster). Let L_1 be the face adjacent to A_1, G_1, A_2. Then L_1 is a hexagon since it is part of the first layer surrounding the three pentagons cluster F_1, F_2, G_1. Note also that G_2 cannot be a pentagon, otherwise we contradict lemma 5.4.2 (which we apply to the adjacent pentagons F_3, G_2, using also the hexagons H_2, L_1, A_2, F_4). Thus G_2 is a hexagon. Suppose A_3 is a pentagon. Then we must have that F_5, A_3 are part of a three pentagons cluster, and thus G_3 is a pentagon. Moreover, the faces surrounding this cluster must be hexagons. Drawing these faces we see that in the graph obtained all vertices have valency three but the outer face is a four cycle, *i.e.*, the graph is not a fullerene. This shows that A_3 must be a hexagon.

If G_3 (adjacent to F_5, F_6, A_3) is a pentagon then also the face F, which is adjacent to A_1, F_6, G_3, L_1, is a pentagon (if it were a hexagon, we would get two adjacent pentagons surrounded by too many hexagons, which we showed to be impossible in an ℓ_1 fullerene). Then let v be the vertex of A_3 that is not in any of the previously labeled faces and let u be its neighbor with the same property. Also let w be the vertex of G_2 that is not in any other labeled faces and let t be its neighbor not lying in G_2. The path starting with u, v that makes only left turns and traces the outer edges of A_3, G_3, F, L_1, G_2 ending in w, t has length seven, contradiction. Thus G_3 must be a hexagon.

Now suppose the face F (adjacent to L_1, A_1, F_6, G_3) is a pentagon. Then the face adjacent to F, L_1, G_3 must be a hexagon , otherwise we contradict lemma 5.4.2. This means that t

is linked by an edge with the vertex x of G_3, where x does not belong to either of the faces A_3, F_5, F_6, F. Let y be the third neighbor of t, x, y, t being in clockwise order. Then either u, y are adjacent or they coincide. If they are adjacent, the path that starts with y, t, w, that makes only left turns and ends at a neighbor of u (possibly y) has length ≥ 7, contradiction. If $y = u$ then depending on the location of the third neighbor of u (besides v, t) we obtain contradictions via arguments with paths that make only left (or only right) turns. Thus F must be a hexagon.

Now let S be the face adjacent to F, G_3 (S is not part of the second layer of faces) and R adjacent to S, F, L_1. If both S, R are pentagons, we focus on the only two vertices that do not have all three neighbors in the faces labeled (one such vertex belongs to S, the other one is v). Using the third edges of these two vertices, we obtain a path that makes only right turns and has length seven (say, by starting with u, v), contradiction. Thus S, R cannot be both pentagons.

Suppose that S is a pentagon, R a hexagon. Let T be the face adjacent to R, S. Then T cannot be pentagon because it would follow that R is such. Thus T is a hexagon. Consider the vertex p of T that is adjacent to the edge between R, T and that does not belong to S. Also consider the third edge of p (not belonging to the face R). Then the path starting with this edge, making only left turns and ending at u has length seven, contradiction.

If R is a pentagon and S is a hexagon, then T is a hexagon and the vertex of T and S that does not belong to R must be adjacent to v. We get a contradiction by paths by using the third edge of the only vertex of S that does not belong to a face that we already considered. Thus both S, R must be hexagons.

Consider now V to be the face adjacent to A_3, F_4. Both cases : V a hexagon or a pentagon end up with a contradiction by paths. In conclusion, the scenario in part (b) does not lead to ℓ_1 fullerene.

c) Suppose F_1, F_2, F_3, F_6 are pentagons and F_4, F_5 are hexagons. We then have that G_1 is a pentagon and that A_1, A_2 are hexagons. Let L_1 be the face adjacent to A_1, G_1, A_2. Then, as proved for part (b), L_1 is a hexagon and G_2, G_3 are hexagons. If A_3 is a pentagon then we have several cases to consider based on the type of the two faces adjacent to A_3 that are not already labeled or considered by us. If both of those are pentagons then the outer face must also be a pentagon and we obtain a fullerene with a cluster of four pentagons, which case is ruled out by our assumption that no cluster involving four or more pentagons is present in the fullerenes of this subsection. If one of those faces is a pentagon and the other is a hexagon, then using the sixth vertex of the face that is a hexagon, we obtain a path that makes only right turns and that has length at least seven, contradiction. If both of those faces are hexagons, then the outer face is a hexagon and thus we obtain a 3-cycle, which is impossible in a fullerene. □

Lemma 5.4.6. *Suppose exactly three of the degree two faces are pentagons. The following cases are possible:*

a) two adjacent degree two faces are pentagons; say F_1, F_2 *and* F_3 *are pentagons,* F_4, F_5, F_6 *are hexagons (same proof when besides* F_1, F_2 *any one of the other degree two faces is a pentagon). There exists no* ℓ_1*-embeddable fullerene in this case.*

b) among the degree two faces, pentagons and hexagons alternate (i.e., F_1, F_3, F_5 *are pentagons,* F_2, F_4, F_6 *are hexagons). In this case we can find an* ℓ_1*-embeddable fullerene with 44 vertices.*

c) non-adjacent and non-alternating case, when say F_1, F_3, F_6 *are pentagons and* F_2, F_4, F_5 *are hexagons. There exists no* ℓ_1*-embeddable fullerene in this case.*

Proof: a) We have that G_1 is a pentagon, A_1, A_2 are hexagons. Consider the zone z_1 consisting of the edges between $F_4, H_4, H_5, H_6, F_1, F_2, A_2$ (note that this zone doesn't go through H_2 instead of A_2 because if it would, the hexagonal face H_4 will end up with non-opposite edges sharing a digit of their labels, impossible). Similarly, consider z_2 going through $F_5, H_4, H_3, H_2, F_2, F_1, A_1$. Also take z the zone through all of $A_3, F_4, F_3, A_2, G_1, A_1, F_6, F_5, A_3$. This is a zone because let's say we start with the edge between A_3, F_5. Since F_5, F_6, A_1 are hexagons, the labels of the considered edge repeat on the edges between these faces. G_1 being a pentagon, the label on the edge between A_1, G_1 will split - half of it will go on the edge between G_1, A_2. This part of the label will then define the zone z. It will go on the edge between A_2, F_3 and from there into F_4, A_3 (it cannot go from F_3 into H_3 because then it will go P_3, H_5, F_6 and thus the hexagonal face F_6 will have non-opposite edges with non-disjoint edge labels, impossible). Using these three zones we easily find three regions such that their intersection contains precisely three vertices (two from A_3, one from G_1) which lie in disconnected components, contradiction.

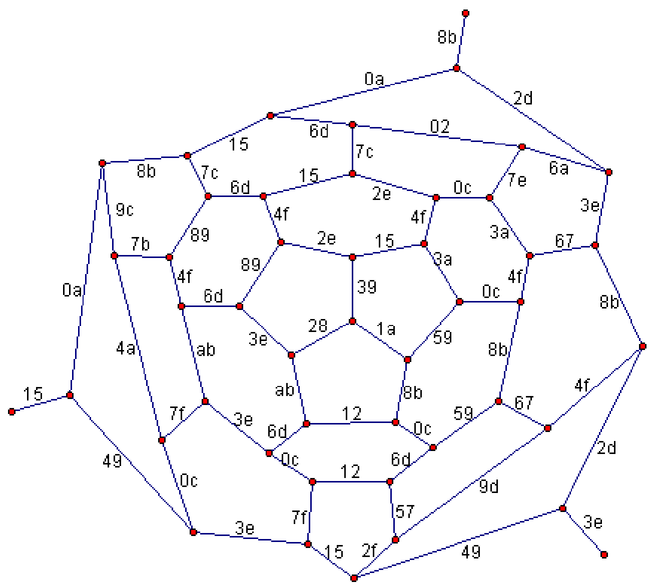

Figure 5.7: Embedding of $\mathcal{F}_{44}(T)$ into $\frac{1}{2}H_{16}$

b) Suppose that at least two of the faces A_1, A_2, A_3 are hexagons, specifically A_1, A_2 are such. Then we obtain a contradiction by considering the zones z_1, z_2 (as in part (a)) that intersect in the faces F_2 and H_4 and also the zone z_3 through F_5, F_6, A_1, G_1 and z_4 through F_4, F_3, A_2. Let L_1 be the face adjacent to G_1, F_2, A_2. Note that G_1 is a hexagon, otherwise together with F_1, it should be part of a three pentagons cluster, impossible (since A_1 is supposed to be hexagonal). Given this observation, we see that z_3 and z_4 either coincide or are different zones intersecting in the faces H_1 and A_3. In either case we can find two vertices from F_2 and two vertices from A_3 that are disconnected but must also be part of a convex intersection of regions, contradiction. This proves that at most one of the faces A_1, A_2, A_3 is a hexagon.

Suppose A_1, A_3 are pentagons and A_2 is a hexagon. Then G_1, G_3 are pentagons and G_2 is a hexagon, L_1 is a hexagon (being on the first layer of faces surrounding the cluster F_1, G_1, A_1). Similarly, the face R adjacent to L_1, G_1, A_1 is a hexagon. Then the vertices v, u must be adjacent, where v is the vertex that belongs to L_1 but not to R, G_1, F_2, A_2 and it is adjacent with a vertex of R; u is the vertex of F_4 that does not belong to any other face on the first or second layer of faces. We obtain a contradiction by paths by using the third edges of the sixth vertices of L_1 and A_2.

The last subcase remaining is when all three of A_1, A_2, A_3 are pentagons. Then G_1, G_2, G_3 are pentagons and the vertices v_1 (of G_1), v_2 (of G_2) and v_3 (of G_3) must be in the neighborhood of a vertex v, otherwise we obtain contradiction by paths. The graph obtained is a complete fullerene and we see that it is ℓ_1-embeddable by using appropriate edge labels. This fullerene has 44 vertices.

c) Suppose A_1 is a pentagon. Then at least one of G_1, G_3 must be a pentagon (otherwise, if both are hexagons, we contradict lemma 5.4.2 when trying to find an ℓ_1-embeddable fullerene). Both G_1, G_3 cannot be pentagons because in that case we obtain a five pentagons cluster, which contradicts the assumption of this subsection. Thus one of G_1, G_3 is a pentagon, the other a hexagon. Assume G_1 is the pentagon. Then looking at the cluster A_1, F_1, G_1 we see that not all faces on the first layer surrounding this cluster are hexagons (F_6 is a pentagon), contradiction. Thus G_1 must be a hexagon, G_3 a pentagon. Then the cluster A_1, F_6, G_3 has the pentagon F_1 on the first layer, contradiction.

This discussion shows that the face A_1 must be a hexagon in order to stand a chance of finding an ℓ_1-embeddable fullerene. This implies G_1 is a hexagon. Now suppose A_2 is a pentagon. Thus G_2 is a pentagon. As was have done in part (b), we can construct zones z_1, z_2 and zones z_3, z_4 such that we obtain a contradiction (note that by the Lemma 6.7, the labeling of the cluster of pentagons A_2, F_3, G_2 allows the existence of z_4). With this argument we see that A_2 must be a hexagon. Once again we consider the four zones and obtain a contradiction as above. □

Lemma 5.4.7. *Suppose exactly two of the degree two faces are pentagons. There exists no ℓ_1-embeddable fullerene in any of the following possible cases:*

a) two adjacent degree two faces are pentagons (say F_1, F_2, all other degree two faces being hexagons);

b) nonadjacent case (say F_1, F_3 are pentagons and F_2, F_4, F_5, F_6 are hexagons);

Proof: a) In this case, G_1 is a pentagon and A_1, A_2 are hexagons. As in the previous lemma, consider the zone z_1 containing the edges between $F_4, H_4, H_5, H_6, F_1, F_2, A_2$ (note that this zone doesn't go through H_2 instead of A_2 because if it would, the hexagonal face H_4 would end up with non-opposite edges sharing a digit of their labels, impossible). Similarly, consider z_2 containing the edges in between the faces $F_5, H_4, H_3, H_2, F_2, F_1, A_1$. Also consider the zone through $F_5, F_6, A_1, G_1, A_2, F_3, F_4$ (except G_1, all of these faces are hexagons and thus such zone exists). Let v be the vertex common to the faces G_1, F_1, F_2, let u be the vertex common to F_5, H_4, A_3 and w the vertex common to F_4, H_4, A_3. Then the disconnected set v, u, w is the intersection of three of the regions determined by the three zones considered, contradiction with the convexity of such intersection.

b) We consider zones z_1, z_2 as for part (a) and zones z_3, z_4 as in the proof of the previous lemma. We readily obtain a contradiction by intersecting four of the regions obtained. Thus no ℓ_1-embeddable fullerene exists in this case. □

Lemma 5.4.8. *Suppose exactly one of the degree two faces is a pentagon. There exists no ℓ_1-embeddable fullerene in this case.*

Proof: Suppose F_1 is a pentagon, $F_2, ..., F_6$ being hexagons.

If A_1 is a pentagon then A_1, F_1 must be part of a cluster of three pentagons and thus G_1 is a pentagon. Moreover, the face L_1 (adjacent to G_1, F_2) is a hexagon, since it is in the first layer of faces around the cluster. Consider the zone z_1 through $A_2, F_2, F_1, H_6, H_5, H_4, F_4$, z_2

through $G_1, F_2, H_2,\ H_3, H_4, F_5$. Further consider the zones z_3 through $A_3, F_5, F_6,\ A_1, G_1, L_1$ and z_4 through $L_1, A_2, F_3,\ F_4, A_3$. Then one vertex from F_2 and two vertices from H_4 will be in the disconnected intersection of four regions determined by the four zones, contradiction.

Thus A_1 cannot be a pentagon, so it must be a hexagon. Then G_1 must be a hexagon and using the same argument with zones, we get a contradiction. □

Lemma 5.4.9. *Suppose none of the degree two faces is a pentagon. There exists no ℓ_1-embeddable fullerene in this case.*

Proof: Same argument with the four zones can be applied, leading to a contradiction. □

Proposition 5.4.10. *There exists exactly two ℓ_1-embeddable fullerenes (with 40 and 44 vertices, respectively) such that at least one three pentagons cluster is present but no larger cluster of pentagons exists.*

Proof: Putting together the results of this subsection, we see that this proposition holds true. □

CHAPTER 6

ADJACENT PENTAGONS: NO CLUSTER CASE

6.1 Subpaths of pentagons

In this chapter we assume that the fullerenes have no cluster of three or more pentagons, *i.e.*, no three pentagons are such that each is adjacent with the other two pentagons. We have seen in the previous chapter that in an ℓ_1-embeddable fullerene there cannot exist two adjacent pentagons *surrounded* by four hexagons appropriately situated with respect to the two pentagons. In particular, this can be reformulated as: there does not exist a *path* of faces consisting of a hexagon followed by two pentagons, followed by a hexagon such that these four faces are all adjacent to a face (hexagon) of the fullerene. In the next lemmas we explore the cases of similar paths involving three, four or more pentagons, *i.e.*, cases when the path of faces (counting also the hexagons at the beginning and at the end of the path) is longer than four.

Lemma 6.1.1. *There exists no ℓ_1-embeddable fullerene that has a subgraph consisting of a simple path of faces H_1, P_1, P_2, P_3, H_2, such that H_1, H_2 are hexagons, P_1, P_2, P_3 are pentagons and all these five faces are adjacent to one face of the fullerene.*

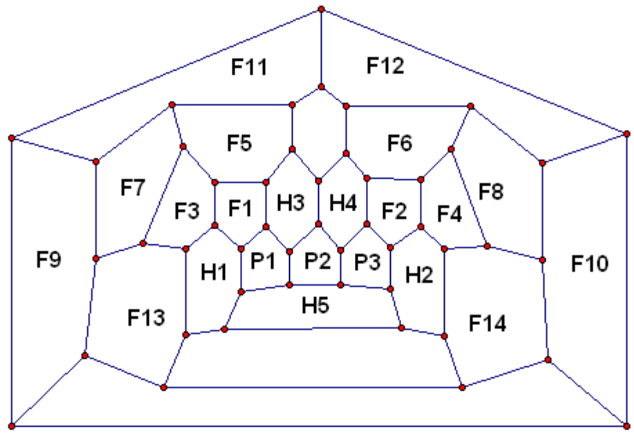

Figure 6.1: Three pentagons path

Proof: Let H_3 be the face adjacent to P_1, P_2 (above them), H_4 the face adjacent to P_2, P_3 (above them and adjacent to H_3) and H_5 the face adjacent to all three pentagons (below the pentagons) and to H_1, H_2. Since the fullerenes in this subsection are assumed to have no cluster of three or more pentagons, we deduce that H_3, H_4, H_5 are all hexagons. Let also F_1 be the face adjacent to H_1, P_1, H_3 and, symmetrically, F_2 be the face adjacent to H_4, P_3, H_2. Then F_1 is a pentagon, otherwise we apply the second lemma of the previous subsection to the pentagons P_1, P_2 together with the faces F_1, H_4, H_3, H_5 and obtain a non-embeddable fullerene. In the same manner, F_2 is a pentagon. Let F_3 be the face adjacent to F_1, H_1. Then F_3 is a pentagon, by the same argument applied to the path F_3, F_1, P_1, H_5. Let F_5 be the face adjacent to F_1, H_3. Then F_5 is a hexagon, otherwise F_3, F_1, F_5 is a cluster of three pentagons. Further, let F_7 be the face adjacent to F_3, F_5. Then F_7 is a pentagon, otherwise we consider the subgraph including the faces H_3, F_1, F_3, F_7. Finally, let F_9 be the face adjacent to F_7 but not to F_5. Then F_9 is also a pentagon, otherwise consider H_1, F_3, F_7, F_9. Let F_11 be the face adjacent to F_9, F_7, F_5. We must have that F_11 is a hexagon, otherwise we get a three pentagons cluster. In the same manner, F_13 (the face adjacent to F_9, F_7, F_3, H_1) is a hexagon. With similar arguments we can *label* the right side of the picture and obtain the faces $F_4, F_6, F_8,$ F_{10}, F_{12}, F_{14} such that F_4, F_8, F_{10} are pentagons, the other being hexagons.

The only two vertices that do not have valency three are in F_9 and F_{10}, respectively. Unless these vertices are linked by an edge we obtain a path that makes only right turns and that has length ≥ 7. Thus we must have that there exists an edge between these two vertices and we obtain a fullerene on 48 vertices, which by [DGS] is not ℓ_1-embeddable. □

Lemma 6.1.2. *There exists no ℓ_1-embeddable fullerene that has a subgraph consisting of a simple path of faces $H_1, P_1, P_2, P_3, P_4, H_2$, such that H_1, H_2 are hexagons, P_1, P_2, P_3, P_4 are pentagons and all these six faces are adjacent to one face of the fullerene.*

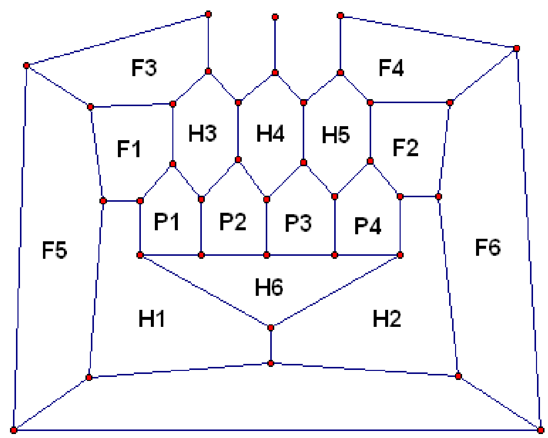

Figure 6.2: Four pentagons path

Proof: Let H_3 be the face adjacent to P_1, P_2; H_4 the face adjacent to P_2, P_3; H_5 the face adjacent to P_3, P_4; H_6 the face adjacent to all of $H_1, P_1, P_2, P_3, P_4, H_2$. Then H_3, H_4, H_5, H_6 are all hexagons (otherwise a cluster of three or more pentagons is formed). Also let F_1 be the face adjacent to H_1, P_1, H_3. Then F_1 is a pentagon, otherwise F_1, P_1, P_2, H_4 is a path of faces that was discarded in one of the previous lemmas. Similarly, consider the face F_3 adjacent to F_1, H_3. Then F_3 must also be a pentagon. Furthermore, let F_5 be adjacent to H_1, F_1, F_3. Then using the path of faces H_6, P_1, F_1, F_5 we see that F_5 is also a pentagon. We thus obtain a cluster of three pentagons (F_1, F_3, F_5), contradiction. □

Lemma 6.1.3. *There exists no ℓ_1-embeddable fullerene that has a subgraph consisting of* *a cycle of faces $H_1, P_1, P_2, P_3, P_4, P_5, H_1$, such that H_1 is a hexagon, P_1, P_2, P_3, P_4, P_5 are pentagons and all these six faces are adjacent to one face of the fullerene.*

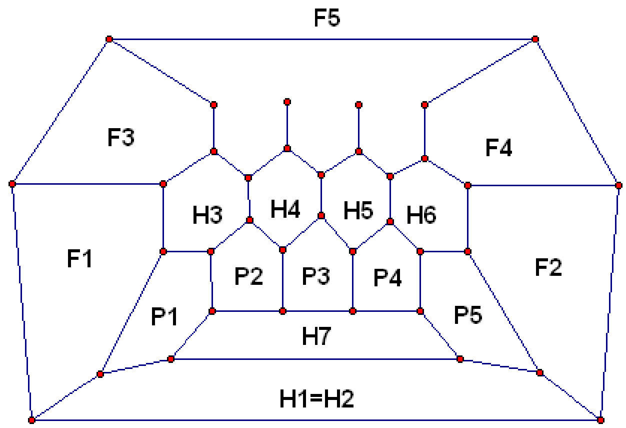

Figure 6.3: Five pentagons path

Proof: Let H_3 be adjacent to P_1, P_2, H_4 be adjacent to P_2, P_3, H_5 be adjacent to P_3, P_4 and H_6 be adjacent to all of P_4, P_5. Also let H_7 be the face adjacent to all of P_1, P_2, P_3, P_4, P_5 and to H_1. Then H_3, H_4, H_5, H_6, H_7 are all hexagons. Consider F_1 adjacent to H_1, P_1, H_3, which must be a pentagon (otherwise we contradict one of the previous lemmas). Similarly, F_3, which is adjacent to F_1, H_3, must be a pentagon. Symmetrically, we consider F_2 adjacent to H_6, P_5, H_1 and F_2 adjacent to H_6, F_2. Both of these are pentagons. Then the face F_5 adjacent to H_1, F_1, F_2, F_3, F_4 has to be a hexagon (having six different vertices). This leads to the existence of the path of faces H_7, P_5, F_2, F_5 which starts at a hexagon, goes through two pentagons and ends at a hexagon, contradiction. □

Lemma 6.1.4. *There exists no ℓ_1-embeddable fullerene that has a subgraph consisting of a cycle of six pentagons $P_1, P_2, P_3, P_4, P_5, P_6$ (no three or more pentagons cluster), such that all these pentagons are adjacent to one face of the fullerene.*

Proof: Let the cycle of pentagons be labeled $P_1, P_2, P_3, P_4, P_5, P_6$. These are all adjacent with (surround) a hexagonal face H. Since no cluster of three pentagons exist, it follows that

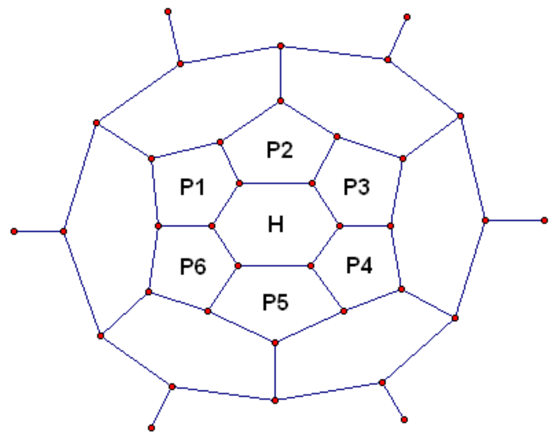

Figure 6.4: Six pentagons path

the subgraph formed by these seven faces is surrounded by a layer of hexagons. Then we can consider two of these hexagons together with two of the pentagons (say P_1, P_2) such that we obtain a path of faces starting at a hexagon, going through two pentagons and ending at a hexagon, contradiction with the lemma in the previous subsection. □

Proposition 6.1.5. *There exists no ℓ_1-embeddable fullerene with adjacent pentagons and such that no cluster of three or more pentagons is present.*

Proof: Consider two adjacent pentagons. They may or may not be adjacent with other pentagons but in any case, they form one of the *paths of faces* considered in the previous lemmas. Each of these paths though cannot exist as subgraph of an ℓ_1-embeddable fullerene (as we have shown for each such path), which proves this proposition. □

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