Spherical Fullerenes

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1 Defining Fullerenes and the Buckyball

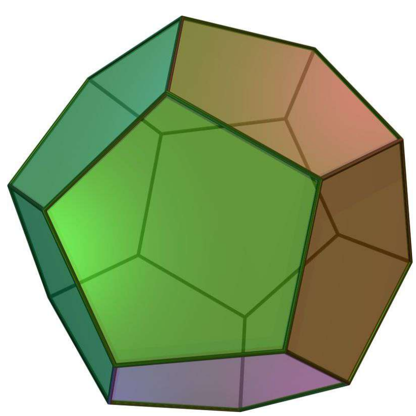
Allotropes are different physical forms in which an element can exist. Each element has a different number of allotropes. Because a carbon atom can make up to four covalent bonds with other atoms, it has a very large number of allotropes.

Some of these allotropes are well known. Diamond is an incredibly hard carbon allotrope in which all carbon atoms in the substance are connected by covalent bonds. Graphite is a very weak allotrope in which carbon atoms are bonded together in hexagonal sheets, which are loosely attracted to each other.

Some are less well known. Graphene is an allotrope consisting of one hexagonal sheet of carbon. Double bonds scattered around the sheet allow each carbon atoms to have four bonds, making this allotrope incredibly strong. Nanotubes are another strong carbon allotrope in which a hexagonal sheet is wrapped into a tube. Fullerenes are yet another carbon allotrope in which this network of carbon atoms is wrapped into a ball. That is the allotrope which I will be focusing on.

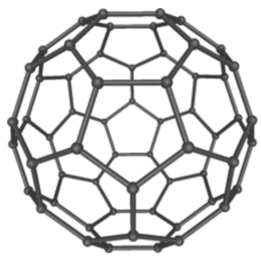
Fullerenes can vary in size. However, all fullerenes have a few features in common. Every carbon in the fullerene is bonded to three other carbons (with one covalent bond connecting to each carbon, to give each carbon four covalent bonds in total). The gaps between the carbons will form pentagons or hexagons, and there will always be exactly twelve pentagons.

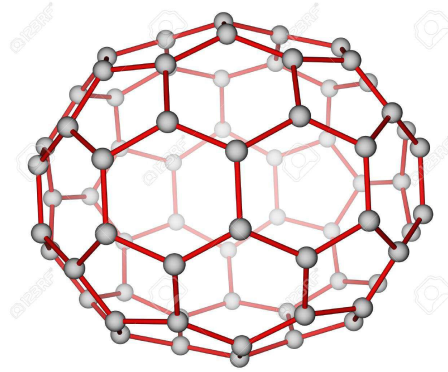
The smallest possible fullerene contains twenty carbons, and is therefore called C_{20}. The gaps between the carbons form twelve pentagons and zero hexagons. This shape is also known as a dodecahedron. However, this fullerene is extremely unstable. It is difficult to synthesize and it does not last long. This is because of the bond positions. The ideal positions for the three bonds emanating from each carbon would be 120 degrees from each other on the same plane. However, since this fullerene is small, these bonds are forced much closer to each other than they want to be, creating extreme instability.



Some other small and uncommon fullerenes are C_{28} with 28 carbons, C_{36} with 36 carbons, and C_{50} with 50 carbons. The first common fullerene is C_{60} with 60 carbons. This is the smallest fullerene in which no pentagons are touching each other, which makes it more stable than the others previously listed. This

specific fullerene is also known as a buckyball. It can be recognized as the pattern on the surface of a soccer ball.
Another quite common fullerene is C_{70}, with 70 carbons.





2 Spherical Fullerenes

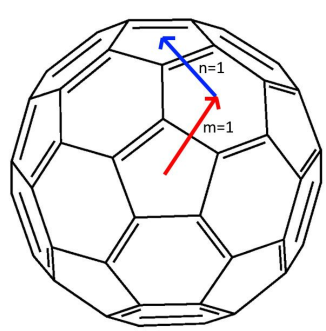
I focused specifically on spherical fullerenes. These are fullerenes that are symmetrical about each pentagonal face; if a spherical fullerene was drawn two times, once with one pentagonal face facing upward and once with some other pentagonal face facing upward, the two drawings would look identical. These pentagonal faces are also spaced equally apart on the fullerene.

The smallest spherical fullerene is C_{20}, the dodecahedron. The second smallest spherical fullerene is C_{60}, the buckyball. There are infinitely many fullerenes, but all of the rest are larger in size.

2.1 Classifying Spherical Fullerenes

(This proof is attributed to the MathILy summer program)

Consider a pathway drawn along the surface of a spherical fullerene. Define a step to be moving across a side from one hexagon/pentagon to another hexagon/pentagon. Then, consider how many steps you will have to take to get from one pentagon to the closest pentagon (any pentagon on a spherical fullerene will have five pentagons which are equidistant to it, and any of those five can be used) by taking m steps in one direction, and then turning left 60 degrees and taking n steps in that direction. You can then call that shape an (m, n) spherical fullerene. An example for C_{60} is pictured below. Using this technique, C_{60} can be determined to be the $(1, 1)$ spherical fullerene.



However, an (m, n) spherical fullerene is the same as an (n, m) spherical fullerene, so to simplify things, both can be called a $(\max(m, n), \min(m, n))$ spherical fullerene.

Examples:

- Dodecahedron: $(0, 0)$ spherical fullerene
- C60/Buckyball: $(1, 1)$ spherical fullerene
- C80: $(2, 0)$ spherical fullerene

3 Hypothesis

Given an (m, n) spherical fullerene, a line, known as a Hamiltonian Cycle, can always be drawn along the edges of the spherical fullerene, which is a loop, which doesn't cross itself, and which goes through every vertex of the spherical fullerene exactly once.

4 Determining The Number of Vertices, Edges, Faces, Hexagons, Pentagons

- By Euler's Formula: $F + V = E + 2$, where:
  - F: number of faces
  - V: number of vertices
  - E: number of edges

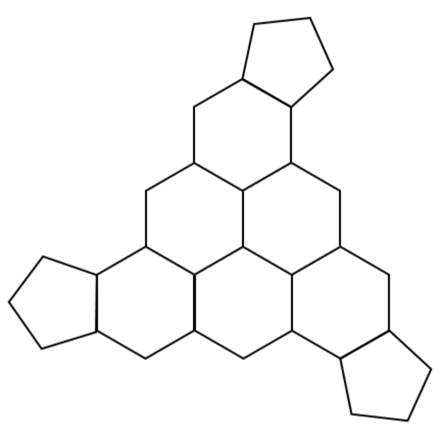
4.1 Proof

(This proof is attributed to the MathILy summer program)

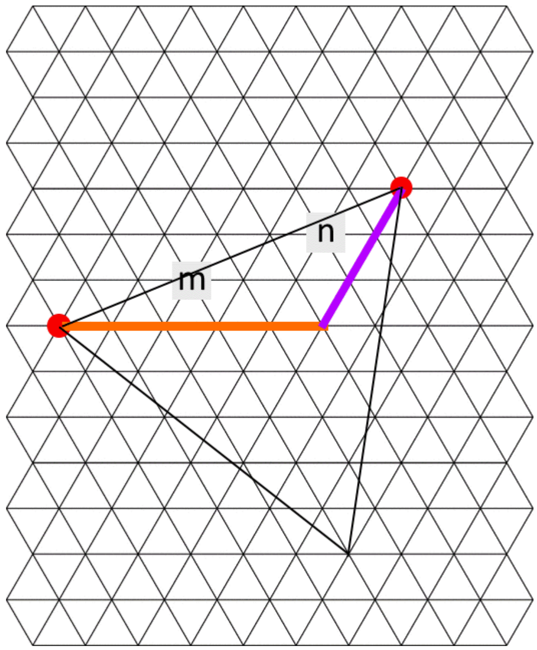
One can start by trying to find how many vertices there are. A good way to do this is to break up the surface of the spherical fullerene. This can be done by drawing points at the center of each pentagon and connecting them. This creates a polyhedron with 12 vertices, 30 edges, and 20 triangular faces: an icosahedron. I'll find how many vertices are in each icosahedron, and multiply by 20 to get the total.

Each triangular face is bounded by one pentagon at each vertex. Therefore, each triangular face can be "flattened out" into a region of hexagons with three pentagons on the edges.

Example:



As except for the three pentagons on the corners, these are all hexagons of equal size, the centers of these pentagons and hexagons can be drawn as the intersection points of an isometric grid. The shortest path between any two pentagons on the grid is shown in the image below. There is a pentagon at each end of the orange and purple path. A path between them can be drawn by going m units forward from a pentagon, then turning left and moving n units.



As the three pentagons surrounding this triangular face are equidistant from each other, the third pentagon will be centered at one of the vertices on this plane such that it would create an equilateral triangle with the other two pentagons.

Each triangle represents the thing that is surrounded by three hexagons or pentagons: a vertex. Therefore, if I find how many triangles there are in each triangular face, I can find how many vertices are in each face, on average.

Each small triangle has an area $\frac{\sqrt{3}}{4}$ and our larger equilateral triangle has an area $\frac{s^2\sqrt{3}}{4}$, where s is the distance between two pentagons. Therefore, there are s^2 little triangles in the large triangle.

$s^2 = (m + \frac{n}{2})^2 + (\frac{n\sqrt{3}}{2})^2$
$s^2 = m^2 + mn + \frac{n^2}{4} + \frac{3n^2}{4}$
$s^2 = m^2 + mn + n^2$
There are $m^2 + mn + n^2$ vertices in each triangular face, which means there are $20(m^2 + mn + n^2)$ vertices on an (m, n) spherical fullerene.

3 edges connect to each vertex, and each edge connects 2 vertices. Therefore, there are $\frac{3}{2} \cdot 20(m^2+mn+n^2) = 30(m^2 + mn + n^2)$ edges on an (m, n) spherical fullerene.

By Euler's formula, for a polyhedron $F + V - E = 2$. This can be rewritten as $F = E - V + 2$. Therefore, there are $10(m^2 + mn + n^2) + 2$ faces. We already know that 12 of these faces are pentagons. Therefore, there are $10(m^2 + mn + n^2) - 10 = 10(m^2 + mn + n^2 - 1)$ hexagons on a (m, n) spherical fullerene.

In summary:

- Number of vertices: $20(m^2 + mn + n^2)$
- Number of edges: $30(m^2 + mn + n^2)$

- Number of faces: $10(m^2 + mn + n^2) + 2$
- Number of hexagons: $10(m^2 + mn + n^2 - 1)$
- Number of pentagons: 12

5 Proof Part 1: Rephrasing Into Another Form

I claim that my hypothesis is equivalent to the following statement:

5.1 Equivalent Statement

A shape consisting of a series of connected hexagons and pentagons with $20(m^2 + mn + n^2)$ sides can be drawn on the surface of a spherical fullerene, with its edges being the edges of the spherical fullerene, such that no vertex is contained entirely within said shape, and no vertex or edge is used twice to form the shape.

5.2 Explanation

The perimeter of this shape forms a line along the edges of the spherical fullerene, which is a loop and doesn't cross itself. It contains $20(m^2 + mn + n^2)$ sides, which means it goes through $20(m^2 + mn + n^2)$ vertices, as it cannot go through any vertex or side more than once, by definition. This is equal to the number of vertices in the spherical fullerene, which means it goes through every vertex in the spherical fullerene. This satisfies all of the conditions in the hypothesis; therefore, if such a shape always exists, its perimeter would always satisfy the hypothesis, meaning the hypothesis would always be true.

Note that the condition that no vertex can be contained entirely within this shape is redundant, because all of the vertices must be on the perimeter under the other conditions, which means none can be stuck in the middle.

I am not aware for a name for this shape. Therefore, I decided to call it a Hamiltongon, after the Hamiltonian Cycle which surrounds it.

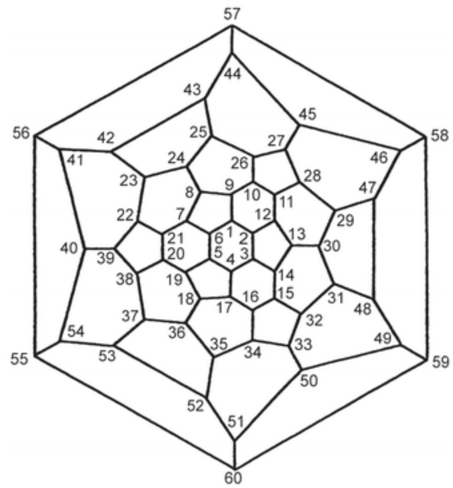
5.3 The Existence of two Hamiltongons

If a Hamiltongon is drawn on a spherical solid, like a sphere or a spherical fullerene, the exterior, or the region outside the Hamiltonian Cycle forming its perimeter, will form another shape made up of pentagons and hexagons. This shape will also have a perimeter that passes through every vertex. No vertex or edge is used twice to form the shape because it has the same perimeter as the Hamiltongon. No vertex is contained entirely within this shape because the perimeter must go through every vertex. This shape satisfies all the conditions of a Hamiltongon, so it is a Hamiltongon. This means if a Hamiltongon is drawn on a spherical fullerene, its exterior is another Hamiltongon. These two Hamiltongons will cover the entire polygon mesh of the spherical fullerene.

6 Schlegel Diagrams

It can be difficult to visualize spherical fullerenes, as they are 3D solids. A solution is to use Schlegel diagrams, which are 2D representations of the faces of 3D solids. Distances are distorted, but all edges, faces, and vertices correspond. Edges are represented as lines and vertices are represented as their intersections. Faces are represented as the spaces between the lines. The exterior represents an additional face.

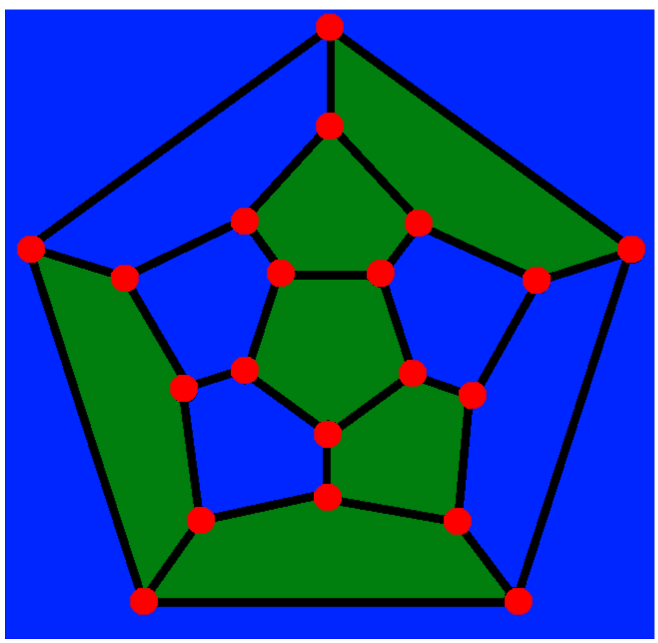
Here's an example for the (1,1) spherical fullerene (C60). All vertices are numbered.



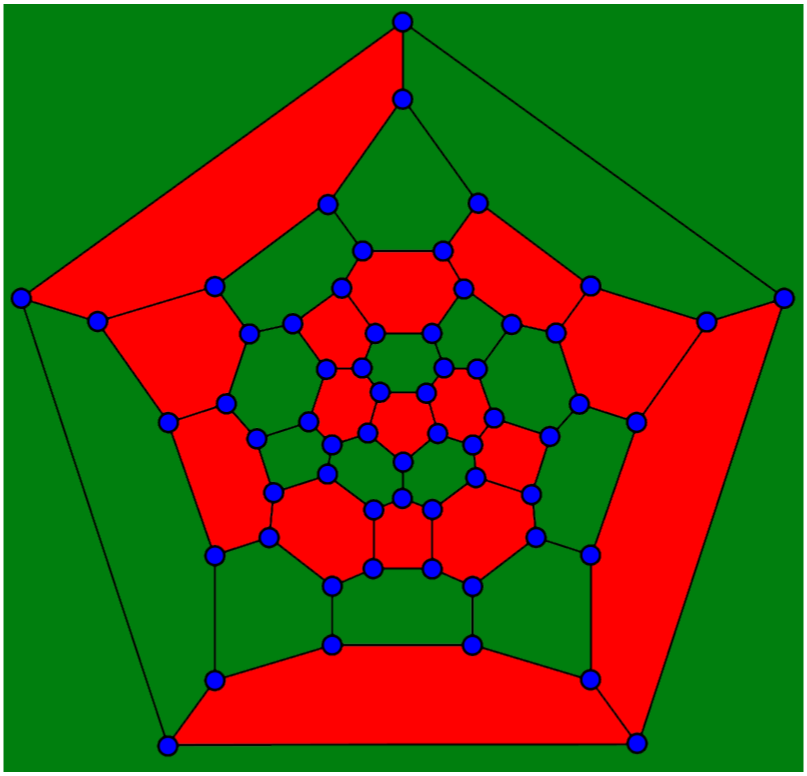
7 Schlegel Diagrams of Hamiltongons

Here are some examples of pairs of Hamiltongons for the three smallest spherical fullerenes. The two colors correspond to the two Hamiltongons, and the loop that I am looking for runs along the perimeter between the two colors.

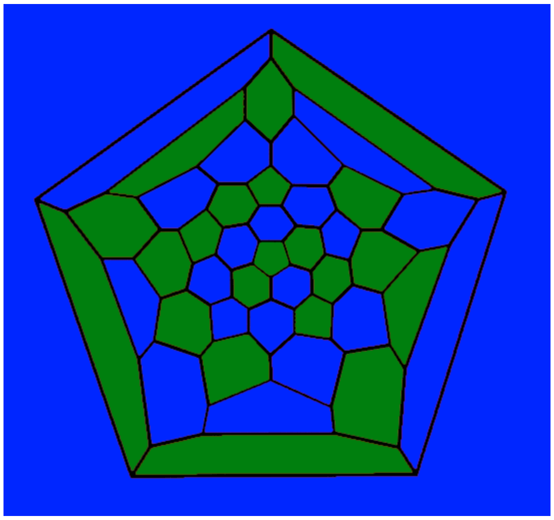
For the (1,0) spherical fullerene (C20):



For the (1,1) spherical fullerene (C60):



For the (2,0) spherical fullerene (C80):



8 Proof Part 2: Separating Pentagons and Hexagons by Rings

Pentagons and hexagons can be separated by rings based on their distance from a chosen pentagon, which can be called Pentagon P.

The distance from pentagon/hexagon Q to pentagon P can be defined in the following manner: The distance is the minimum number of edges a line traced along the exterior of the spherical fullerene, which does not pass through any vertices, must cross to get from pentagon P to pentagon/hexagon Q.

Pentagon P is a distance 0 from itself.

Because the pentagons are spaced symmetrically on the spherical fullerene as far apart as possible, there will be a diametrically opposed pentagon to pentagon P, as the 3D shape for which twelve centers of faces are spaced as far apart as possible is the dodecahedron, and that shape has diametrically opposed pentagons. This diametrically opposed pentagon will be the farthest pentagon/hexagon on the shape from pentagon P. It can be said to be in ring d. This means every other pentagon or hexagon is some distance from 1 to $d-1$ away from pentagon P. It also means that there are $d+1$ rings.

When I continue the proof, I will break the spherical fullerenes into two cases: those for which d is odd (and the number of rings is even), and those for which d is even (and the number of rings is odd).

9 Potential Hamiltongon Constructions

After defining hamiltongons and rings, I searched for methods which could be used to construct hamiltongons.

9.1 Definitions

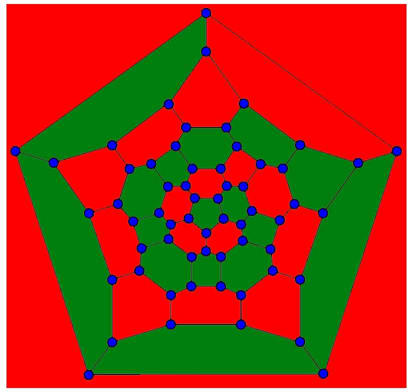
Although hamiltongons always come in pairs on a spherical fullerene, these processes will involve adding one pentagon or hexagon at a time to one of these hamiltongons. The one that these polygons are being added to will be called the **+hamiltongon**. The other hamiltongon will be called the **-hamiltongon**.

9.2 Single Spiral Method

Steps for Construction

1. Start by choosing a pentagon on the spherical fullerene. Call it P. Group the pentagons and hexagons in the figure into rings based on their distance from P.
2. Add P to the +hamiltongon.
3. Add one of the polygons in ring 1 to the +hamiltongon.
4. There will be one or more polygons adjoining the polygon that was just added in ring 2. Add the one that is clockwise of the rest.
5. Continue adding polygons in a clockwise direction in ring 2 until adding one would break a rule.
6. Add the polygon of the adjoining ones in the ring above that is clockwise of the rest and keep adding polygons clockwise of it until you would break a rule.
7. Repeat step 6 until you are forced to stop. If this works, you should be forced to stop on the diametrically opposed pentagon to P or one of the five polygons adjoining it, and you should have two hamiltongons on the spherical fullerene.

9.2.1 Example



9.2.2 Problems

This process can fail when you are moving to the next ring. This is because sometimes there is only one polygon bordering the polygon you are moving up from into the next ring, and that polygon is also bordering the polygon just counterclockwise of the one you are moving up from, creating a group of three polygons in the hamiltongon surrounding the same vertex. This is bad as the perimeter would not go through that vertex, breaking a rule.

9.2.3 Potential Solution: Switchable Single Spiral

A potential way to solve this problem is to allow switching to the opposite direction. In this method, if you reach a point of failure when adding in the clockwise direction, you can switch directions and start adding polygons in a counterclockwise direction and choosing the polygon farthest in the counterclockwise direction to move up to (starting from the polygon in the current ring which is farthest counterclockwise).

9.3 Double Spiral Method

Steps for Construction

1. Start by choosing a pentagon on the spherical fullerene. Call it P. Group the pentagons and hexagons in the figure into rings based on their distance from P.

2. Add P to the +hamiltongon.

3. Add two of the polygons that are not bordering each other in ring 1 to the +hamiltongon.

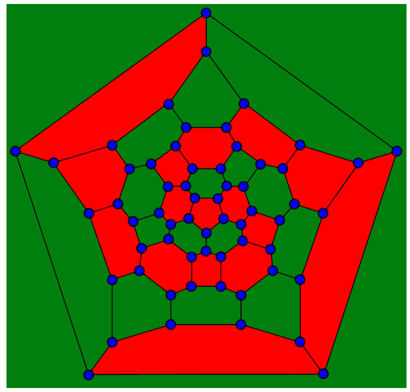
4. There will be one or more polygons adjoining the each of the polygons that was just added in ring 2. Add the one that is clockwise of the rest.

5. Continue adding polygons in a clockwise direction in ring 2 from both of the origins until adding one would break a rule.

6. Then, for each of the two ends of the spiral, add the polygon of the adjoining ones in the ring above that is clockwise of the rest and keep adding polygons clockwise of it until you would break a rule.

7. Repeat step 6 until you are forced to stop, for both ends. If this works, you should be forced to stop on two of the five polygons adjoining the diametrically opposed pentagon to P, and you should have two hamiltongons on the spherical fullerene.

9.3.1 Example



9.3.2 Problems

This process faces the same problem as the single spiral method.

9.4 Where Do These Methods Work?

Method	Which Does It Work in C20, C60, C80
Single Spiral	C20, C60
Modified Single Spiral	C20, C60, C80
Double Spiral	C20, C60

10 Next Steps

To prove my hypothesis, I will have to show that at least one of these constructions works for every spherical fullerene.

11 References

Credits to MathILy for the problem and solutions in parts 2.1 and 4.1.

My other sources were:

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