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Extended Goldberg polyhedra

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Abstract. A new methodology for understanding the construction of Extended Goldberg polyhedra has been developed on the basis of Goldberg polyhedra by using our methods of the ‘spherical rotating’ and the ‘spherical stretching’. The spherical rotating describes the deformation of rotating polygons on a sphere; the spherical stretching depicts the deformation of stretching spaces between polygons on a sphere. Our results show that these Extended Goldberg polyhedra are a kind of novel geometrical objects of icosahedral symmetry and are considered to explain some viral capsids.

1. Introduction

Goldberg polyhedra [1-3] are a kind of ‘multi-symmetric’ Fullerene polyhedra, having 12 pentagonal faces and all other hexagonal faces. Since, the discovery of the famous fullerene C_{60} [4], a new field has been opened for research of different potentially possible fullerene structures from the geometry, graph theory or topology point of view. Fulleroids, the most important fullerene-like structures have been proposed and defined [5, 6], and their symmetry has been discussed by Stanislav Jendrol[7] and František Kardoš [8, 9]. It clears that polyhedra in the world of science are mysterious and there are more novel polyhedral solids waiting for us to explore.

Goldberg polyhedra are also good models of icosahedral viral capsids which abide by Caspar-Klug (CK) ‘‘quasi-equivalence’’ theory [10, 11], that is, their pentagonal and hexagonal faces simulate pentagonal and hexagonal capsomeres, respectively. However, some spherical viral capsids which are not covered by Goldberg polyhedra have been obtained. The surface of herpes virus capsid [12] contains not only 12 pentamers and 150 hexamers, but also 320 triplexes at quasi 3-fold axis. Furthermore, the capsomeres of semliki forest virus [13] at 2-fold axis are not connected closely, they separate from each other, 120 quadrangular holes at 2-fold axis and 80 triangular holes at quasi 3-fold axis have been formed. It means that Goldberg polyhedra failed to encode the locations of these triplexes and holes, so the new models of viral capsids [14, 15] should be developed.

A three-dimensional spherical space is the simplest compact 3-manifold [16], a polyhedron can be deformed into a topological rubber sphere, and it would preserve single connectivity through twisting, bending, stretching and pulling. According to this idea, we propose two topological approaches of ‘spherical rotating’ and ‘spherical stretching’. These methods applied to Goldberg polyhedra generate two infinite series of Extended Goldberg polyhedra of icosahedral symmetry. These Extended Goldberg polyhedra with Γ symmetry group having a-gonal and b-gonal faces added are defined as Γ (a, b)–Goldberg polyhedra. Particularly, they are used to explain some viral capsids whose capsomeres are rotated and separated from each other.

2. Rotate-Extended Goldberg polyhedra

Topologically, Goldberg polyhedra are homeomorphic to spheres, for this reason, a Rotate-Extended Goldberg polyhedron can be obtained by the spherical rotating in the following processes:

(i) Project points of a polyhedron *P* upon its circumscribed sphere S form the center of *S*.

As a result, all projection of faces of P will pack on a sphere surface without overlapping. It appears that F faces, E edges and V vertices are transformed into F spherical polygons, E arcs and V vertices.

(ii) Gradually increase the radius of the circumscribed ball, but keep the centers of spherical polygons and arc length unchanged, in this way, there are gaps gradually increased between original polygons. Let polygons rotate around the own centers in the same direction (clockwise or anticlockwise). Obviously, at a certain moment of expansion, every vertex would be connected to vertices of other polygons. Then we stop expansion and there are spherical triangles occurred among vertices, in this step the change of curvature of spherical polygons is allowed.

(iii) Project points of the expanded spherical surface S' back to its inscribed polyhedron P', it is said that the topological sphere has been assigned a geometric configuration of Rotate-Extended Goldberg polyhedron added with 3-gons.

For instance, Figure 1 describes the topological deformation processes of spherical rotating, the obtained Rotate-Extended 12-hedron defined as $I_h(3, 0)$-32-hedron corresponds to the icosidodecahedron belonging to Archimedean solids [17].

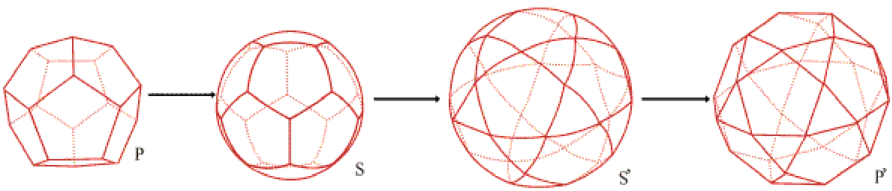

Figure 1. Processes of the spherical rotating for the Rotate-Extended 12-hedron

Here, we construct two classes of Rotate-Extended Goldberg polyhedra named as $\Gamma(3, 0)$ -Goldberg polyhedra. The type I Rotate-Extended Goldberg polyhedra is based on 42-hedron, 92-hedron, 162-hedron, ⋯ , the total number of faces F_n can be calculated by the following formula:

$$F_n = f_5 + f_6 + f_3 = 12 + 10(n^2+2n) + 20(n+1)^2$$

Where f_5, f_6, f_3 denote the number of 5-gons, 6-gons, and 3-gons, n=1, 2, 3, ⋯.

For n=1, as shown in Figure 2a, $f_5=12$, $f_6=10(1^2+2\times1)=30$, $f_3=20\times(1+1)^2=80$, $F_1=f_5+f_6+f_3=12+30+80=122$, the point group is I_h.

For n=2 (Figure 2b), $f_5=12$, $f_6=10(2^2+2\times2)=80$, $f_3=20\times(2+1)^2=180$, $F_2=f_5+f_6+f_3=12+80+180=272$, the point group is I_h.

For n=3 (Figure 2c), $f_5=12$, $f_6=10(3^2+2\times3)=150$, $f_3=20\times(3+1)^2=320$, $F_2=f_5+f_6+f_3=12+150+320=482$, the point group is I_h. It can be simulated the structure of herpes virus, and the added triangles may be used to simulate triplexes that on the surfaces of capsids.

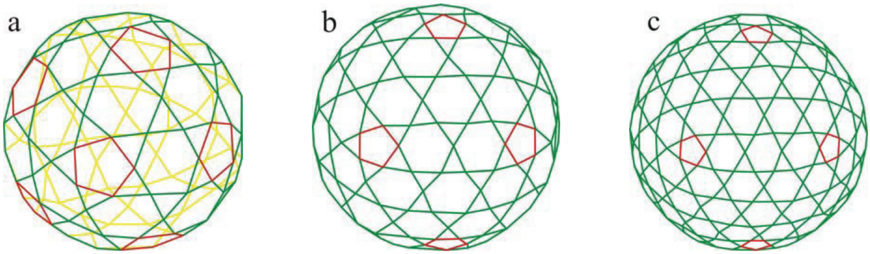

Figure 2. The type I Rotate-Extended Goldberg polyhedra
a. I_h (3, 0)-122-hedron; b. I_h (3, 0)-272-hedron; c. I_h (3, 0)-482-hedron

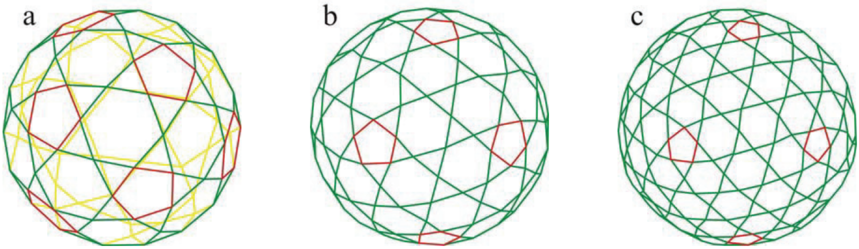

Figure 3. The type II Rotate-Extended Goldberg polyhedra
a. I_h (3, 0)-92-hedron; b. I (3, 0)-212-hedron; c. I (3, 0)-392-hedron

The type II Rotate-Extended Goldberg polyhedra is based on 32-hedron, 72-hedron, 132-hedron,⋯, the total number of faces F_n can be calculated by the following formula:

$$F_n=f_5+f_6+f_3=12+10(n^2+n)+20(n^2+n+1)$$

For n=1, 2, 3 (Figure 3), f_5 is only 12, f_6 is 20, 60, 120 and f_3 is 60, 140, 260, respectively, the total number faces F_1 =92, F_2=212, F_3=392. If n=1, the point group is I_h, when n=2 and n=3, the point group is I.

In particular, Rotate-Extended Goldberg polyhedra can be used to describe the surfaces of icosahedral capsids which capsomeres are rotated with each other. We use a pair of positive integer (h, k) to characterize these polyhedra: the number of vertices $V=30(h^2 + h k + k^2)$; the number of faces $F=30(h^2 + h k + k^2) + 2$; $0<h \geq k \geq 0$, $T= h^2 + h k + k^2$, T indicates the triangulation number [10].

3. Stretch-Extended Goldberg polyhedra

In contrast with a Rotate-Extended Goldberg polyhedron, beginning with a Goldberg polyhedron, a Stretch-Extended Goldberg polyhedron can be obtained by the spherical stretching in the following processes:

(i) As the same as the spherical rotating, project the points of a polyhedron P upon its circumscribed sphere S centrally.

(ii) Expand the spherical surface, but keep the positions of spherical polygons and arc length unchanged, allowing the change of bend degree of polygons to adapt the change of the curvature, so they can cover the sphere closely. Thus, the expanding of sphere stretches spaces between arcs and among vertices of original polygons. When the distances between arcs are stretched equal to the arc length, we stop expanding and there are spherical quadrangles occurred between arcs and spherical triangles formed among vertices.

(iii) Finally, project the points of the expanded spherical surface S' back to its inscribed polyhedron P', it is said that the topological sphere has been assigned a geometric configuration of Stretch-Extended Goldberg polyhedron added with 3-gons and 4-gons.

Take the dodecahedron, for example, Figure 4 depicts the topological deformation processes of spherical stretching, the obtained Stretch-Extended 12-hedron defined as I_h (3, 4)-62-hedron corresponds to the Rhombicosidodecahedron belonging to Archimedean solids [17].

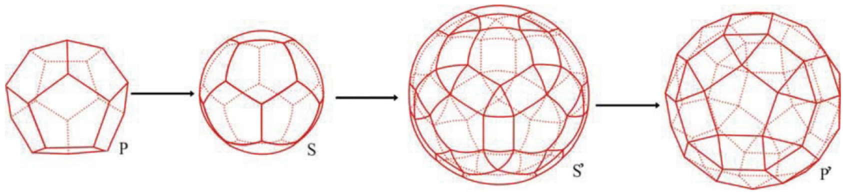

Figure 4. Processes of the spherical stretching for the Stretch-Extended 12-hedron

We construct two classes of Stretch-Extended Goldberg polyhedra named as Γ (3, 4) - Goldberg polyhedra. The type I Stretch-Extended Goldberg polyhedra is based on 42-hedron, 92-hedron, 162-hedron,⋯, the total number of faces F_n can be calculated by the following formula:

$$F_n = f_5 + f_6 + f_3 + f_4 = 12 + 10(n^2+2n) + 20(n+1)^2 + 30(n+1)^2$$

Where f_5, f_6, f_3, f_4 denote the number of 5-gons, 6-gons, 3-gons, and 4-gons, n=1, 2, 3, ⋯.

For n=1, as show in Figure 5a, $f_5=12$, $f_6=10(1^2+2\times1)=30$, $f_3=20\times(1+1)^2=80$, $f_4=30(1+1)^2=120$, $F_1= f_5+f_6+f_3=12+30+80+120=242$, the point group is I_h. The structure is similar to the capsid of semliki forest virus, whose edges between added triangles and quadrangles may be used to simulate linking protein strands.

For n=2 (Figure 5b), $f_5=12$, $f_6=10(2^2+2\times2)=80$, $f_3=20\times(2+1)^2=180$, $f_4=30(2+1)^2=270$, $F_2= f_5+f_6+f_3=12+80+180+270=542$, the point group is I_h.

For n=3 (Figure 5c), $f_5=12$, $f_6=10(3^2+2\times3)=150$, $f_3=20\times(3+1)^2=320$, $f_4=30(3+1)^2=480$, $F_2= f_5+f_6+f_3=12+150+320+480=962$, the point group is I_h.

The type II Stretch-Extended Goldberg polyhedra is based on 32-hedron, 72-hedron, 132-hedron,⋯, the total number of faces F_n can be calculated by the following formula:

$$F_n = f_5 + f_6 + f_3 + f_4 = 12 + 10(n^2+n) + 20(n^2+n+1) + 30(n^2+n+1)$$

For n=1, 2, 3 (Figure 6), f_5 is only 12, f_6 is 20, 60, 120, f_3 is 60, 140, 260 and f_4 is 90, 210, 390, respectively, the total number faces $F_1=182$, $F_2=422$, $F_3=782$. If n=1, the point group is I_h, when n=2 and n=3, the point group is I.

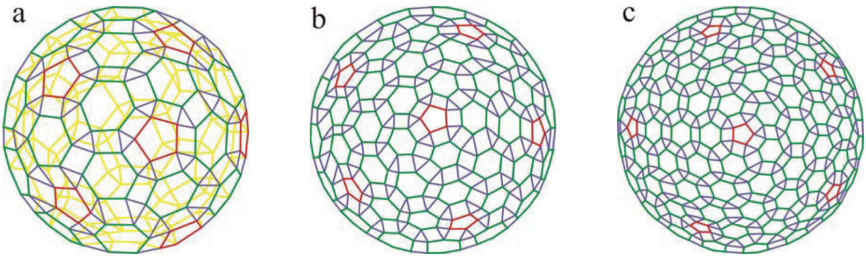

Figure 5. The type I Stretch-Extended Goldberg polyhedra
a. I_h (3, 4)-242-hedron; b. I_h (3, 4)-542-hedron; c. I_h (3, 4)-962-hedron

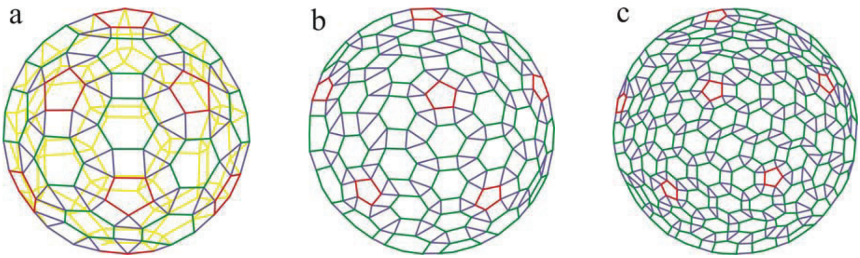

Figure 6. The type II Stretch-Extended Goldberg polyhedra
a. I_h (3, 4)-182-hedron; b. I (3, 4)-422–hedron; c. I (3, 4)-782-hedron

Particularly, Stretch-Extended Goldberg polyhedra can be used to describe the surfaces of icosahedral capsids whose capsomeres are separated. Use a pair of positive integer (h, k) to characterize these polyhedra: the number of vertices V=60(h^2 + h k + k^2); the number of faces F=60(h^2 + h k + k^2) + 2; $0<h \geq k \geq 0$, T= h^2 + h k + k^2.

4. Stability and symmetry

In graph theory, a polyhedron in three-dimensional space can be deformed into a plane graph known as Schlgel graph [18], if this graph has prefect matchings, the more perfect matchings the graph has, the more stable of the polyhedron is supposed to be. Schlgel graphs of Goldberg polyhedra are 3-regular and 3-connected, Zhang [19] got a lower bound 3(p+2)/4 of the number of perfect matchings of a fullerene graph with p vertices by finding its

2-extendability. Now, graphs of Extended Goldberg polyhedra are 4-regular and 4-connected, two of them visible in Figure 7, we find they are 1-extendable because every edge of them appears in some perfect matchings, and then, every 1-extendable graph with p vertices and q edges contains at least $(q-p)/2+2$ prefect matchings [20]. By calculation, for a Rotate-Extended Goldberg polyhedron graph, it contains at least $15T+2$ prefect matchings, for a Stretch-Extended Goldberg polyhedron graph, it contains at least $30T+2$ prefect matchings.

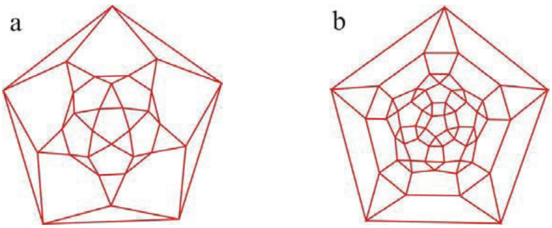

Figure 7.The schlgel graph of a. I_h (3, 0)-32-hedron; b. I_h (3, 4)-62-hedron

Goldberg polyhedra possess icosahedral symmetry (I or I_h) [21], they have 5, 3, 2-fold rotational axes. The symmetry of a polyhedron is decided by its mirror plane, *e.g.*, 72-hedron has no mirror plane, it is geometrically chiral with point symmetry group I; 92-hedron has planes of symmetry, which is geometrically achiral with point symmetry group I_h. For Rotate-Extended Goldberg polyhedra, whose pentagons and hexagons rotate by the same angle and preserve C_5 and C_6 rotational symmetry. Furthermore, the added 3-gons have C_3 rotational symmetry, so the symmetry of Goldberg polyhedra is maintained. Similarly, the added 4-gons and the added 3-gons in Stretch-Extended Goldberg polyhedra have C_4 and C_3 rotational symmetry, so the symmetry of Goldberg polyhedra is maintained too. Just like Goldberg polyhedra, the type I Extended Goldberg polyhedra have I_h symmetry, the type II Extended Goldberg polyhedra have I_h symmetry when n=1 and I symmetry when $n \geq 2$.

5. Conclusions

Geometrically, a new polyhedron can be obtained by operations such as truncating, snubbing, duality [19]. The paper develops two topological methods of the 'spherical rotating' and the 'spherical stretching' based on Goldberg polyhedra, just as doing rotating, stretching, bending these topological deformations on a sphere, construct two kinds of Extended Goldberg polyhedra which possess only tetrahedral vertices. These polyhedra preserve icosahedral symmetry and satisfy the Euler's polyhedral formula $f + v = e + 2$[20], so these two Extended polyhedra are both fully closed and stabilized in structure. From the biological point of view, our models are similar to some viral capsids which abide by CK theory [10], but are not corresponding to Goldberg polyhedra, which not only encode the locations of the proteins but also inter-subunit bonds that connect capsomeres.

Extended Goldberg polyhedra, the new isosahedral architectures, are of fundamental importance in understanding the molecular design of polyhedral links [3]. We shall discuss this idea in detail elsewhere.

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Referrences

[1] M. Goldberg, A class of Multi-Symmetric Polyhedra, *Tohoku Math. J.* **43** (1937) 104-108.

[2] H. S. M. Coxeter, Virus macromolecules and geodesic domes, *In A spectrum of mathematics (ed. J.C. Butcher)*, Oxford University Press/Auckland University Press, 1972, pp. 98-107.

[3] W.-Y. Qiu, X.-D. Zhai, Molecular design of Goldberg polyhedral links, *J. Mol. Struct. (THEOCHEM)* **756** (2005)163-166.

[4] H. W. Kroto, J. R. Health, S. C. O'Brien, R. F. Curl , R. E. Smalley, C_{60}-Buckminsterfullerene, *Nature* **318** (1985) 163–165.

[5] O. Delgado Friedrichs, M. Deza, in: Discrete Mathematical Chemistry, eds. P. Hausen, P. Fowler, M. Zheng, *DIMACS Series in Discrete Mathematics and Theoretical Computer Science*, Vol. 51 (2000) 97–115.

[6] A. W. M. Dress, G. Brinkmann, Phantasmagorical fulleroids, *MATCH Commun. Math. Comput. Chem.* **33** (1996) 87-100.

[7] S. Jendrol', M. Trenkler, More icosahedral fulleroids, *J. Math. Chem.* **29** (2001) 235-243.

[8] F. Kardos, Tetrahedral fulleroids, *J .math. chem*. **41** (2007) 101-111.

[9] F. Kardos, Fulleroids with Dihedral Symmetry, *Electronic Notes in Discrete Mathematics* **28** (2007) 287-292.

[10] D. L. D. Casper, A. Klug, Physical principles in the construction of regular viruses, *Cold Spring Harbor Symp. Quant, Biol*. **17** (1962) 1-24.

[11] A. Klug, Molecular structure: Architectural design of spherical viruses, *Nature* **303** (1983) 378-379.

[12] Z. H. Zhou, M. Dougherty, *et al.*, Seeing the Herpesvirus Capsid at 8.5Angstrom, *Science* **288** (2000) 877-880.

[13] E. J. Mancini, M. Clarke, *et al*., Cryo-electron microscopy reveals the functional organization of an enveloped virus, Semliki Forest virus, *Mol. Cell*. **5** (2000) 255-266.

[14] F. Kovács, T. Tarnai, P. W. Fowler, S. D. Guest, Double-link expandohedra: a mechanical model for expansion of a virus, *Pro. R. Soc. A*. **460** (2004) 3191-3202.

[15] R. Twarock, Mathematical Virology: A Novel approach to the Structure and Assembly of Viruses, *Philos. Trans. R. Soc. A*. **364** (2006) 3357–3373.

[16] Graham P. Collins, The Shapes of Space, *Sci. Amer*. July (2004) 94-103.

[17] H. M. Cundy, A. P. Rollet, *Mathematical Models,* Clarendon Press, Oxford, 1954.

[18] H. S. M. Coxeter, *convex Polytopes, 3rd ed*. Dover, New York, 1973.

[19] H.-P. Zhang, F.-J. Zhang, New lower bound on the number of perfect matchings in fullerene graphs in fullerene graphs, *J. Math. Chem.* **30** (2001) 343-347.

[20] T. Došlić, On lower bounds of number of perfect matchings in fullerene graphs, *J. Math. Chem.* **24** (1998) 359–364.

[21] F. A. Cotton, *Chemical Applications of Group Theory*, Wiley, New York, 1964.