Description of a highly symmetric polytope observed in Thomson's problem of charges on a hypersphere

J. Roth*

Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Pfaffenwaldring 57, D-70550 Stuttgart, Germany

(Received 23 July 2007; published 24 October 2007)

In a recent paper, Altschuler and Pérez-Garrido [Phys. Rev. E **76**, 016705 (2007)] have presented a four-dimensional polytope with 80 vertices. We demonstrate how this polytope can be derived from the regular four-dimensional 600-cell with 120 vertices if two orthogonal positive disclinations are created. Some related polytopes are also described.

DOI: 10.1103/PhysRevE.76.047702 PACS number(s): 02.70.−c, 02.40.−k

In 1904 Thomson [1] presented his "plum pudding" model of the atom, where pointlike electrons are embedded in a positively charged background. Since electrons repel each other, they have to find the lowest energy configuration on the surface of the sphere. Although Thomson's model has been outdated for a long time by quantum mechanics, his problem of placing charges on a sphere is still noteworthy. The results for a circular disk are trivial, namely regular polygons. The problem on the ordinary sphere is well studied (see, for example, Altschuler and Pérez-Garrido [2] for recent references). The problem on a four-dimensional hypersphere has not been treated in depth up to now. For arbitrary dimensions there are mathematical proofs that certain special configurations [3] are optimal for small numbers of charges.

Quite recently Altschuler and Pérez-Garrido [2] studied Thomson's problem on the hypersphere and discovered an unknown, highly symmetrical four-dimensional polytope with 80 vertices, but they failed to describe the polytope in detail. Since we believe that the polytope could be a prototype for other charge configurations on the hypersphere, we will describe it in detail trying to bring it down to three dimensions as far as possible. We show how the polytope can be derived from the regular 600-cell in four dimensions and that it is the member of a family of four-dimensional polytopes.

As an example, let us start with an icosahedron in three dimensions. We place one vertex at the north pole and the opposite one at the south pole (Fig. 1). Five other vertices lie on the northern hemisphere and five on the southern hemisphere. If we cut out a wedge with an angle of 72° between the poles as indicated in Fig. 1 and glue together the open lips, we get a square antiprism with two pyramids placed on the square faces, a polytope also called a gyroelongated square antiprism (gesa). The polyhedron belongs to the famous Bernal hole polyhedra where it is called Z10 [4]. The icosahedron has 12 vertices, 30 edges, and 20 faces. We remove a vertex on the northern hemisphere, glue together two vertices on the southern hemisphere and remove two triangles and four half triangles, furthermore, five edges, and glue together another edge. In total this leads to the gesa with 10 vertices, 24 edges, and 16 faces. Compared to the icosahedron, the gesa possesses a positive disclination characterized as a line through the poles and its center. If the surface is considered only, then the disclination is characterized by the angular deficiency at the poles.

Instead of cutting out a piece we could also squeeze in a wedge into the icosahedron thus forming a negative disclination. The resulting polyhedron is a gyro-elongated hexagonal antiprism with 14 vertices, 36 edges, and 24 faces. It is known as the Frank-Kasper polyhedron Z14 [5]. Repeated additions and removal of wedges are also possible and lead to multiple disclinations. The polytopes, however, become more and more distorted. By similar repeated surgeries one can derive all the deltahedra in three dimensions from the icosahedron, including the octahedron and the tetrahedron.

Now let us turn to four dimensions. The same surgeries are also possible for the 600-cell. Usually this polytope is described by its shells around a vertex [6]: starting from a vertex as the north pole, an icosahedra, a dodecahedron, and a second icosahedron follow. A subsequent icosadodecahedron forms the equatorial polyhedron. On the southern hemisphere the sequence repeats in the opposite order. The four-dimensional equivalent of the wedge would be a slice with a spindlelike three-dimensional surface.

This construction, however, does not lead to the desired 80-vertex polytope. To obtain it, we have to introduce another kind of shelling, namely the toroidal one. We select a chain of ten vertices connected by edges and situated in a two-dimensional plane. We can project the four-dimensional polytope into three dimensions such that the chain lies in the x-y plane, for example (see Fig. 2). Then there are 50 vertices which are connected to the chain by edges and form a torus around the chain. Additional 50 vertices are connected

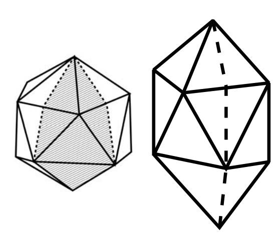

FIG. 1. Transformation of a icosahedron (left) into a gyroelongated square antiprism (gesa, right). The shaded wedge is cut out and the left and right lips are glued together at the dashed line in the gesa.

*johannes@itap.physik.uni-stuttgart.de; URL: www.itap.physik.uni-stuttgart.de\~johannes

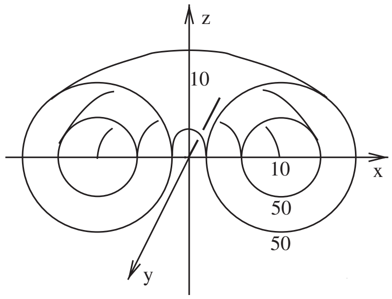

FIG. 2. Cut through the 600-cell in toroidal orientation. The numbers indicated the number of vertices on the chains and tori.

by edges to the first torus and lie on a second torus. The remaining vertices form a second chain in a plane perpendicular to the x-y plane. In Fig. 2 these vertices are placed on the z axis. The upper and lower end of the second chain are connected in four dimensions, but this is not possible in the projection due to topological restrictions of the visualization in three dimensions. The correctness of the shelling can be checked easily using the coordinates given in Ref. [6], for example.

Now we have the prerequisites to construct the 80-vertex polytope. There are two equivalent ways. The first one is to introduce a positive disclination in the x-y plane. The surface of the three-dimensional wedge becomes a lens with the x-y chain as its circumference. To remove the material we shorten the z chain by two vertices. The outer torus loses a pentagonal antiprismatic ring centered around the z axis with ten vertices. The inner torus is shrunk in diameter around the x-y chain from pentagonal to square antiprismatic also losing 10 vertices. Up to now all neighbor polytopes stay icosahedra. The x-y chain will be unaltered in length but its neighbor polytopes are changed from icosahedra to gesa since the vertices of the chain lie on the disclination line. The other possibility to construct the same polytope is to start with the x-y chain and shorten it by two vertices, thus taking the z chain as the disclination line. Now the torus around the x-y chain is shortened by an antiprismatic ring and the other torus is changed from pentagonal to square antiprismatic. The z chain remains unaltered, but the neighbor polyhedra of its vertices are gesa now.

The 600-cell has 120 vertices, 720 edges, 1200 faces, and 600 cells. The new polytope with one positive disclination possesses 88 vertices with icosahedral neighbor shells and ten vertices with gesa neighbor shells. This leads to $(12\times 88+10\times 10)/2=578$ edges, since each edge connects two vertices. Similarly we have $(30\times 88+24\times 10)/3=960$ triangular faces and $(20\times 88+16\times 10)/4=480$ tetrahedral cells.

The 80-vertex polytope is now simply generated if both disclinations are built in: both chains are shrunk by two vertices each and both tori lose ten vertices in the first and eight vertices in the second step. The result can be compared to Ref. [2], Fig. 1, especially to the part with the red edges: the vertices with the red dots lie on the disclination lines. As given by Altschuler and Pérez-Garrido, the polytope possesses 64 vertices with icosahedral neighborhood and 16 with gesa neighborhood. This leads to $(12\times 64+10\times 16)/2=464$ edges as can be checked also from Fig. 1 in Ref. [2]. Similarly we have $(30\times 64+24\times 16)/3=768$ triangular faces and $(20\times 64+16\times 16)/4=384$ tetrahedral cells.

If we denote a positive disclination along the $x-y$ plane as d_1 and a negative as $-d_1$ and similarly disclinations along the z axis with d_2 and $-d_2$, then a (d_1,d_2) polytope contains $10-2d_1+2(5-d_1)(5-d_2)+2(5-d_2)(5-d_1)+10-2d_2=120-22(d_1+d_2)+2d_1d_2$ vertices, since it consists of a $(10-2d_1)$ and a $(10-2d_2)$ polygon, a $(5-d_1)$-antiprismatic torus with $2(5-d_2)$ segments, and a $(5-d_2)$-antiprismatic torus with $2(5-d_1)$ segments. The number of edges, vertices, and cells can be found by evaluating the neighbor polyhedra as given in the first section. Since all cells are tetrahedra it follows that the number of faces has to be twice the number of cells. All the counts can be checked by the four-dimensional Euler formula: the number of vertices plus the number of faces has to be equal to the number of edges plus the number of cells.

The symmetry group of the (d_1,d_2) polytopes can also be given: The symmetry of a n-fold symmetric polygon is the dihedral group D_n of order $2n$. But since the tori are formed of antiprismatic rings, the symmetry reduces to $D_{(n/2)}$. By the way, this is the reason why we have to remove or add at least two vertices perpendicular to the disclination line (changing lengths by an odd number of vertices may also be possible, but lead to helically twisted polytopes). The symmetry group of the (d_1,d_2) polytopes is at least the direct product $D_{(5-d_1)}\times D_{(5-d_2)}$. If $d_1=d_2$, then there is an additional involution which maps the two chains onto one another. And for $d_1=d_2=0$ we obtain the famous 600-cell with a much larger symmetry group. Knowing the symmetry group is very helpful for the derivation of coordinates for the (d_1,d_2) polytopes.

There are a lot more possibilities to construct the four-dimensional analogs of the deltahedra in three dimensions. Most of them, like the 98- and the 80-vertex polytopes presented here cannot be realized by regular tetrahedra but by distorted ones only. Thus they are not included in the complete list of four-dimensional deltatopes made of regular tetrahedra as given in Refs. [7,8].

In conclusion, we have analyzed a highly symmetrical polytope discovered as a solution of Thomson's problem on the hypersphere. It would be interesting to test if other polytopes out of the family of polytopes which we described are also solutions of the problem. In general we do not expect this to be the case, since the disclinations and antidisclinations lead to a strong deviation of the shape of the polytope from a perfect hypersphere if nearest neighbor distances are equal. If the charges are forced to stay on the hypersphere this will cause a strongly stressed state.

In three dimensions it is well known that the hexagonal lattice, which is the solution of the problem in the two-dimensional plane, is adapted to the curved sphere through the introduction of defects, in this case disclinations, dislocation clusters, and grain boundaries [9]. We expect that the polytope discovered by Altschuler and Pérez-Garrido and described in this paper is a prototype of a similar adaption of the unique regular 600-cell to different numbers of charges. Here we have limited our analysis to the case of polytopes with two closed loop disclinations. But intersections of disclinations are also possible and lead to the well-known Frank-Kasper [5] phases as a result of squeezing the 600-cell into three dimensions. If we combine all those types of defects we can produce a huge amount of interesting polytopes. The next step will be to test these predictions by optimization of charge configurations on the four-dimensional hypersphere.

[1] J. J. Thomson, Philos. Mag. **7**, 237 (1904).
[2] E. L. Altschuler and A. Pérez-Garrido, Phys. Rev. E **76**, 016705 (2007).
[3] H. Cohn and A. Kumar, J. Am. Math. Soc. **20**, 99 (2006).
[4] J. D. Bernal, Proc. R. Soc. London, Ser. A **280**, 299 (1964).
[5] F. C. Frank and J. S. Kasper, Acta Crystallogr. **11**, 184 (1958); **12**, 483 (1959).
[6] H. S. M. Coxeter, *Regular Polytopes* (Dover, New York, 1973).
[7] G. Blind and R. Blind, Monatshefte für Mathematik **89**, 87 (1980).
[8] J. M. Sullivan (unpublished).
[9] M. J. Bowick, A. Cacciuto, D. R. Nelson, and A. Travesset, Phys. Rev. B **73**, 024115 (2006).