A Realistic Upper Bound for the Number of Facets of 3-dimensional Dirichlet Stereohedra

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Introduction

The goal of this work is to find a realistic upper bound for the maximal number of facets of 3-dimensional Dirichlet ~~stereohedra~~. We reduce the [redacted] upper bound of Delaunay (390) to 198 ~~number of facets for 3-dimensional Dirichlet streohedra~~.

A *stereohedral tiling* of the Euclidean space $\mathbb{R}^d$ is a decomposition of $\mathbb{R}^d$ into convex congruent polytopes (*tiles*) which intersect properly and whose symmetry group acts transitively on the tiles. A *stereohedron* is a convex polytope which is the tile of a stereohedral tiling.

The following is a particular way to obtain stereohedral tilings. Given a crystallographic group G and a point P with trivial stabilizer by the action of G, the Voronoi diagram of the orbit GP of P is a stereohedral tiling and, in particular, the Voronoi region $Vor_{GP}(P)$ is a stereohedron. Such stereohedra are called *Dirichlet stereohedra.*

The number of *aspects* of a crystallographic group G is the order of the quotient group G/G_T, where G_T is the subgroup of translations of G. The fundamental theorem of the theory of stereohedra, due to Delaunay ([Delaunay'61], see [Štogrin'75] for a proof in English) states that a *stereohedron* in d-space whose associated crystallographic group has *a aspects* is bounded above by $2^d(a+1)-2$. For $d=3$, the maximal number of aspects that a crystallographic group can have is 48, which produces a bound of 390 for the number of facets.

On the other hand, the stereohedron with the maximum number of facets known is a Dirichlet one corresponding to a cubic group and it has 38 facets ([Engel'86]).

There seems to be an agreement that the maximum number of facets has to be closer to 38 than to 390 ([Gru-She'80, page 960]; [Engel'86, page 214]). It is not known whether all stereohedra are combinatorially equivalent to Dirichlet stereohedra, but the absence of any method to study stereohedra in general leads to consider the special case of Dirichlet stereohedra ([Gru-She'80], page 965).

The results obtained so far are summerized in the following table :

Groups with reflexions			
Reflexions	Aspects	Groups	Facets
3	≤ 48	22	≤ 11
2	≤ 48	44	≤ 20
1	≤ 24	34	≤ 24
Groups without reflexions			
Cryst. system	Aspects	Groups	Facets
non-cubic	≤ 16	107	≤ 102
cubic	≤ 24	20	≤ 198
cubic	48	3	≤ 162

1 Groups with reflexions

We classify the groups which contain reflexions according to whether the set of normal vectors to the reflexion planes span a 1-dimensional, 2-dimensional or the whole 3-dimensional space. We say that the group " has reflexions in 1, 2 or 3 independent directions", respectively.

Let G be a crystallographic group which contains reflexions and G_r the subgroup of G generated by reflexions. We define the *reflexion cells* of G to be the minimal regions of the space with all facets supported by reflexion planes. The reflexion cells are all congruent to one another and tile the space, since they are Dirichlet domains of G_r.

Proposition 1 *Let R be a reflexion cell and $P \in R$. Let $S = GP \cap R$ be the subset of GP inside R. Then,*

$$Vor_{GP}(P) = R \cap Vor_S(P).$$

The neighbours of P outside R will be at most one for each facet of R. We call *external neighbours* of P those outside R and *internal neighbours* those inside R.

Groups with reflexions in 3 independent directions

Let G be a group with reflexions in 3 independent directions. Reflexion cells for these groups are bounded regions (3-polytopes) with at most 6 facets. Therefore the number of external neighbours is at most 6. The points $GP \cap R$ lie on a sphere , then using Euler formula for the sphere one can prove easily that the maximum number of internal neighbours of P is at most 5. From the above observations we have that *$Vor_{GP}(P)$ has at most 11 facets.*

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Groups with reflexions in 2 independent directions

Let G be a group with reflexions in 2 independent directions. In this case, the reflexion cell R is an infinite prism having as "base" one of the 5 possible bounded reflexion cells in 2 dimensions.

The number of external neighbours is at most 4. Concerning the internal neighbours, it happens that the points inside the prism R lie on a small number of parallel lines on the direction of the prism. The number of these lines is at most the number of symmetries of the planar reflexion cell. If $P \in R$ and $l \subset R$ is one of the parallel lines which contains points of the orbit, then P has at most 2 neighbours on l. Since the maximum number of parallel lines is 8, we have that: $Vor_{GP}(P)$ *has at most 20 facets.*

Groups with reflexions in 1 direction

Let G be a group with reflexions in 1 direction. For these groups the reflexion cell is an infinite band, thus P has at most 2 external neighbours. We can assume the family of the reflexion planes to be the horizontal planes at odd integer heights and R to be the band between $z = 1$ and $z = -1$. Let h be the horizontal plane which contains the point P. All the points of the orbit of P inside the band R lie on the planes h or $-h$.

Let $G_0 = \{g \in G | g(\alpha) = \alpha, \forall \text{ horizontal plane } \alpha\}$.

On the plane h, P has at most 6 neighbours, since $GP \cap h = G_0P$, and G_0 is a planar crystallographic group.

G_0 either is $p6$ or it has at most 4 aspects.

Using similar arguments to those that Delaunay uses for proving the fundamental theorem of stereohedra, we prove that P has at most 4 neighbours for each aspect of the 2-dimensional crystallographic group G_0 in the plane $-h$. We have then at most 16 internal neighbours in $-h$, except perhaps for $p6$. Nevertheless, when $G_0 = p6$, it can be proved easily that P has at most 6 neighbours in $-h$. Thus $Vor_{GP}(P)$ *has at most 24 facets.*

2 Groups without reflexions

Any crystallographic group with more than 4 aspects contains a translation perpendicular to ~~the~~ other two (we assume this to be the vertical direction).

All neighbours of P are inside the horizontal infinite band centered at P of width 2.

Let α and β be two horizontal planes, then $GP \cap \alpha$ and $GP \cap \beta$ are orbits of the *same* 2-dimensional crystallographic group (namely G_0) on the planes α and β, respectively.

In these conditions, if Q is a neighbour of P, then $Vor_{G_0Q}(Q) \cap Vor_{G_0P}(P) \neq \emptyset$. Since $Vor_{G_0Q}(Q)$ and $Vor_{G_0P}(P)$ are vertical infinite prisms, we have to study how the Dirichlet domains of two different orbits in a planar crystallographic group intersect.

Let G_0 be a planar crystallographic group and D a fundamental domain for G_0.

Without loss of generality, we assume P to lie in a fixed *fundamental subdomain* D_s for G_0: the quotient of D by its symmetries.

Given D_s a fundamental subdomain for G_0, we define:

- the *extended Voronoi region corresponding to* D_s the union $Ext_{G_0}D_s$ of all Voronoi regions $Vor_{G_0P}(P)$ when P moves inside D_s.

- *influence region of* D_s the union $Infl(D_s)$ of all fundamental subdomains D' of G_0 such that $Ext_{G_0}D_s \cap Ext_{G_0}D_s' \neq \emptyset$.

If P and Q are in fundamental subdomains D_s and D_s',respectively, then the number of regions of $Vor_{G_0}Q$ which intersect $Vor_{G_0P}(P)$ is at most the number of fundamental subdomains equivalent to D_s' contained in $Infl(D_s)$.

Non-cubic systems

Using the above property, we study each of the 4 groups with 16 aspects and we obtain~~ed~~ an upper bound of 94.

Each of the rest of groups has no more than 12 aspects, therefore $Vor_{GP}(P)$ *has at most 102 facets.*

The cubic system

Note that in the cubic system each translational vector is perpendicular to the others. Therefore we can apply the planar approach explained above 3 times, for each of the translational direction.

We study each of the 3 groups with 48 aspects from the cubic system and we obtain~~ed~~ a maximal number of 162 facets for $Vor_{GP}(P)$.

Any other group has no more than 24 aspects, thus $Vor_{GP}(P)$ *has at most 198 facets.*

References

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