Towards 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 current upper bound of 390 facets [Delaunay'61] to 198 in general and to 102 for all but 18 particular crystallographic groups in the cubic system.

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 (in particular, the symmetry group is a crystallographic group). 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 whose symmetry group is G 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 the number of facets of 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 3-dimensional 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]). Our results indicate that this is true at least for Dirichlet stereohedra. It is not known whether all stereohedra are combinatorially equivalent to Dirichlet stereohedra, but the absence of any good method to study stereohedra in general leads us to consider the special case of Dirichlet stereohedra (as in [Gru-She'80], page 965).

Our results are summarized in the following table. They are very good for groups which contain reflexion planes. For the groups without reflexions our strategy (explained in Section 2) has to be applied to each group individually. We have done this for all the non-cubic groups with 16 aspects and the cubic ones with 48 aspects, obtaining bounds of 94 and 162, respectively. In the rest of cases we keep Delaunay's bounds of 102 and 198, respectively.

Five among the 23 cubic groups without reflexions have 12 aspects and the bound of 102 is valid for them. We are studying the other 18 and our results so far indicate that the strategy we use will give a bound of about 100 facets for at least half of them.

Groups with reflexions		
Reflexions	Groups	Facets
3 directions		≤ 11
2 directions	99	≤ 20
1 direction		≤ 24

Groups without reflexions			
Cryst. system	Aspects	Groups	Facets
non-cubic	16 or ≤ 12	108	≤ 102
cubic	48 or ≤ 24	23	≤ 198

1 Groups with reflexions

Let G be a crystallographic group which contains reflexions and G_r the subgroup of G generated by reflexions. We will say that G "has reflexions in 1, 2 or 3 independent directions", 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 call *reflexion cells* of G the minimal regions of the space with all facets supported by reflexion planes. The reflexion cells are all congruent and tile the space, since they are Dirichlet domains of G_r.

Let P be a point in the reflexion cell R. We call *internal facets* of $Vor_{GP}(P)$ those which intersect the interior of R and *external facets* those which do not. We call external and internal neighbours of P the points which produce those facets. The following proposition implies that P has at most one external neighbour per facet of R and that all the internal neighbours of P are inside R.

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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,*

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

One can prove that:

• If G has **reflexions in 3 independent directions**, the reflexion cells 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 and by Euler's formula for the sphere the number of internal neighbours of P is at most 5. Thus, $Vor_{GP}(P)$ **has at most 11 facets**.

• If G has **reflexions in 2 independent directions**, the reflexion cells are infinite prisms having as "base" one of the possible bounded reflexion cells in 2 dimensions (which are all triangles or quadrilaterals). The number of external neighbours is at most 4.

Concerning the internal neighbours, the points inside the prism R lie on a certain number of parallel lines on the direction of the prism, all equivalent to one another by transformations from the group. The maximal number of these lines is 8 (the number of symmetries of a square) and we prove that P has at most 2 neighbours on each line, so that the number of internal neighbours is at most 16. Thus, $Vor_{GP}(P)$ **has at most** $8 \times 2 + 4 =$**20 facets**.

• If G has **reflexions in only 1 direction**, we can assume the reflexion planes to be the horizontal planes at odd integer heights and R to be the band between $z = 1$ and $z = -1$. Then, P has at most two external neighbours.

Let h be the horizontal plane which contains the point P. All the points of the orbit of P inside the band R (in particular, all the internal neighbours of P) lie on the planes h or $-h$. P can only have at most six neighbours at height h, since the points at height h form a two dimensional crystallographic orbit. Considering the different possibilities for the subgroup G_0 of G consisting of transformations which preserve height, we prove that P cannot have more than 16 neighbours at height $-h$. Thus, $Vor_{GP}(P)$ **has at most** 16+6+2=**24 facets**.

2 Groups without reflexions

Any crystallographic group with more than 4 aspects contains 3 independent translations t_1, t_2 and t_3 with t_1 perpendicular to t_2 and t_3. We assume t_1 to be the vertical translation of length 1. (Observe that t_1, t_2 and t_3 might not generate the subgroup of translations).

All neighbours of P are inside the horizontal infinite band centered at P of width 2 and lie on a finite (and "small") number of horizontal planes. On each horizontal plane, the subset of the orbit GP is an orbit of one and the same planar crystallographic group, namely the subgroup of G_0 consisting of transformations which preserve the vertical coordinate.

In these conditions, if Q is a neighbour of P then $Vor_{G_0Q}(Q) \cap Vor_{G_0P}(P) \neq \emptyset$. In particular, we can bound the number of neighbours of P as follows: for each horizontal plane between -1 and 1 containing a point Q of GP we bound the number of regions of Vor_{G_0Q} which can intersect $Vor_{G_0P}(P)$. Since $Vor_{G_0Q}(Q)$ and $Vor_{G_0P}(P)$ are vertical infinite prisms, P and Q can not be neighbours unless the planar Dirichlet regions of P and Q with respect to the group G_0 intersect.

In other words, we are led to study how two planar Voronoi diagrams produced by different orbits of the same crystallographic group G_0 intersect to one another. We formalize this as follows: Let D be a fundamental domain for G_0 and let us divide it into a number of *fundamental subdomains*, congruent to one another (we typically take as fundamental subdomains the quotient of D by its symmetry group). Then we define:

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

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

With this notation, a necessary condition for P and Q being neighbours is that the fundamental subdomain of Q lies in the influence region of P. Then:

In the **non-cubic systems** there are some hexagonal groups with 16 aspects, for which the above method gives a bound of 94 for the maximal number of facets. The rest of groups have at most 12 aspects, for which Delaunay bound gives 102.

In the **cubic system**, since there are three translations orthogonal to one another we can apply the above method three times and reduce further the number of neighbors. For the three cubic groups without reflexions and with 48 aspects this gives a bound of 162 facets. The rest of groups have 24 aspects, for which Delaunay's bound is 198.

References

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