On the Number of Facets of Three-Dimensional Dirichlet Stereohedra III: Cubic Group

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Abstract

We prove that Dirichlet stereohedra for cubic crystallographic groups cannot have more than 105 facets. This improves a previous bound of 162 [3].

1 Introduction

A *stereohedron* is any bounded convex polyhedron which tiles the space by the action of a crystallographic group. A particular case is the Voronoi region of a point P in the Voronoi diagram of its orbit GP under the action of a crystallographic group. These stereohedra are called *Dirichlet stereohedra* and are the object of study in this paper.

The study of the possible combinatorial types of stereohedra and, in particular, of their maximum number of facets, is related to Hilbert's 18th problem [9]. The two main previous results are:

- The *fundamental theorem of stereohedra* (Delone, 1961 [5]) asserts that a stereohedron of dimension d for a crystallographic group G with a aspects cannot have more than $2^d(a+1)-2$ facets, where the number of *aspects* of G is the number of translational lattices in which a generic orbit of G decomposes. 3D crystallographic groups can have a maximum of 48 aspects, so 3D stereohedra cannot have more than 390 facets.

- P. Engel (see [6] and [7, p. 964]), using a computer search, found in 1980 a 3-dimensional Dirichlet stereohedron with 38 facets, for a cubic group with 24 aspects. This is the stereohedron with the maximum number of facets known.

In previous papers, the second author together with D. Bochiş has initiated an exhaustive study of the number of facets of Dirichlet stereohedra for the different 3D crystallographic groups. They divided the 219 affine conjugacy clases of 3-dimensional crystallographic groups in three blocks, and gave upper bounds for the number of facets of Dirichlet stereohedra in them:

- Within the 100 crystallographic groups which contain reflection planes, the exact maximum number of facets is 18 [1].

- Within the 97 non-cubic crystallographic groups without reflection planes, there are Dirichlet stereohedra with 32 facets and no Dirichlet stereohedron can have more than 80 [2].

For cubic groups without reflection planes (there are 22 of them), Bochiş and Santos were only able to prove an upper bound of 162 facets [3]. Here we improve this bound, and hence the general upper bound for the number of facets of 3D Dirichlet stereohedra, to 105. More precisely, our bound goes "group by group" and it lies below 38 except in the eight so-called "quarter groups" [4]. Our bounds for these eight groups are respectively 42, 43, 53, 66, 73, 74, 73 and 105. Curiously enough, the last (and biggest) one is precisely for the crystallographic group that produces Engel's Dirichlet stereohedron with 38 facets.

2 Outline of the method

The sketch of the method is as follows:

1. We choose a tessellation of the 3-dimensional Euclidean space "adapted" to the group G under study. We call the tiles *fundamental subdomains*. By "adapted" we mean that the tiles are in a finite (and small) number of classes modulo the normalizer of G. We choose one fundamental subdomain of each class, and call them *basic fundamental subdomains*. If two points lie in the same orbit of the normalizer of G then the Dirichlet stereohedra based on them are affinely equivalent. Hence, every Dirichlet stereohedra for G is affinely equivalent to one with basis point in a basic fundamental subdomain.

2. For each basic fundamental subdomain, say D_0, we compute an *extended Voronoi region*, i.e., a region that is guaranteed to contain the union of the Dirichlet stereohedra generated by all the points in D_0. We do this cutting out parts of space that are guaranteed not to belong to any Voronoi region with basis in D_0 because of the presence of certain rotations or translations in G. The precise method is the same used in 2D in [2], except here we do it on the computer because of the extra complexity of the problem.

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Of course, the extended Voronoi region is not uniquely defined, and the smaller the one we get is, the better the final bound will result.

3. The extended Voronoi region of a non-basic fundamental subdomain D is now trivial to compute: Find the basic fundamental subdomain D_0 related to $D = \rho D_0$ by a motion ρ in the normalizer of G, and apply ρ to the extended Voronoi region of D_0. We call *influence region* of a basic subdomain D_0 the union of all the subdomains whose extended Voronoi regions intersect the extended Voronoi region of D_0.

Theorem 1 *For every $p \in D_0$, the neighbors of p in the Voronoi diagram of the orbit of p are contained in the influence region of D_0.*

Corollary 2 *The number of facets of Dirichlet stereohedra with base point in D_0 is bounded above by the number of fundamental subdomains in the influence region of D_0 "counted with multiplicity" (i.e., each one counted as many times as the number, perhaps zero, of transformations in G that send it to D_0. In particular only those in the same class of D_0 modulo the action of G are counted).*

All of the above actually follows the [Bochiş-Santos]'s approach, but with two new ingredients:

- [Bochiş-Santos] compute 2-dimensional influence regions for certain planar subgroups of G, and take as 3D influence region the intersection of the rectangular prisms over the 2D influence regions. We bound directly in dimension 3, with the aid of a computer program,resulting in a smaller region.
- Our understanding of cubic groups is greatly simplified by a new classification of 3D crystallographic groups given by Thurston et al. [4].

Let us briefly describe this classification. Thurston et al. first divide crystallographic groups into reducible and irreducible, were *irreducible groups* are those that do not have any invariant direction. They coincide with the cubic groups.

For an irreducible subgroup G, they define its *odd subgroup* as the one generated by the rotations of order three, and they observe that there are only two possible odd subgroups, that they denote T_1 and T_2. The odd subgroup T of a group G is normal, and so G lies between T and its normalizer $N(T)$. This is a powerful property, because it reduces the enumeration of irreducible space groups to the enumeration, up to conjugacy, of subgroups of two finite groups $N(T_1)/T_1$ and $N(T_2)/T_2$.

Hence, we study the cubic groups in two blocks. The 27 groups with odd subgroup T_1 are called "full groups" in [4], and they include all the cubic groups with reflections. The 8 groups with odd subgroup T_2 are called "quarter groups".

3 The 27 "full groups"

These are the groups between T_1 and $N(T_1)$. $N(T_1)$ is the automorphism group $I\frac{4}{m}\overline{3}\frac{2}{m}$ of the body centered cubic lattice (here and elsewhere we use the International Crystallographic Notation for crystallographic groups, see [8]). T_1 is the crystallographic group $F23$, generated by the triad rotations whose axes are the diagonals of the unit cube and by the translations of length 2 in the three edge directions of the cube. T_1 coincides the crystallographic group $F23$.

We take as fundamental subdomains of any group between T_1 and $N(T_1)$ the Delaunay tetrahedra of a body centered cubic lattice. They have two opposite perpendicular edges with length 1/2 (in relation to the fundamental translations of T_1) and four edges parallel to the four diagonals of the cube, with length $\frac{\sqrt{3}}{4}$. $N(T_1)$ has diad rotations over the first type of edges, and triad rotations over the second type of edges. The extended Voronoi region consists of five fundamental subdomains: a central one and its four neighbors. The influence region is made up of these tetrahedra plus their 10 neighbors. These 15 tetrahedra fall into two classes modulo T_1, with 11 and 4 elements.

Now let G be one of the full groups. Let s be the number of elements of G that preserve a fundamental subdomain. Then, the bound for G derived from the influence region we have calculated is $15s - 1$ or $11s - 1$ depending on whether G contains elements that exchange the two classes of subdomains or not. Since the order of $N(T_1)/T_1$ is 16, the values of s for groups other than $N(T_1)$ (which has reflections) are 1, 2, 4 and 8. This, in principle, gives a bound of 119 facets for these groups.

But we can do better. The worse this bound is the more motions we have in G, not present in T_1, that can be used to cut the extended Voronoi region further and produce better influence regions. Doing this, we get the upper bounds of the following table for the 14 full crystallographic groups without reflections.

Group	Our bound	Previous bound
$F23$	10	102
$F432$	5	21
$F\overline{4}3c$	14	44
$F\frac{2}{d}\overline{3}$	14	69
$P23$	21	102
$F4_132$	21	72
$P432$	12	15
$I23$	29	102
$P\frac{2}{n}\overline{3}$	24	79
$F\frac{4_1}{d}\overline{3}\frac{2}{n}$	29	89
$P\overline{4}3n$	29	72
$P4_232$	33	79
$P\frac{4}{n}\overline{3}\frac{2}{n}$	26	30
$I432$	26	33

4 The 8 "quarter groups"

The normalizer $N(T_2)$ of the second odd group consists of the automorphisms of the following arrangement of lines: the lines $x = y = z$, $1 + y = z = -x$, $1+z = x = -y$, and $1+x = y = -z$, together with all their translates by vectors with integer even coordinates. The odd subgroup T_2 itself is generated by the triad rotations on all these lines. The index of T_2 in its normalizer is eight. In crystallographic notation, $N(T_2)$ is $I\frac{4_1}{g}\bar{3}\frac{2}{d}$ and $T2$ is $P2_13$. There are 8 groups between (and including $N(T_2)$ and T_2. We can see their graphic representations [8] in Figures 1 to 8.

For quarter groups we choose a more complicated tesselation of space into fundamental subdomains. They are of two types, with different volumes. In type A the basic subdomain is the convex hull of the following five points: $(0, 0, 0)$, $(1/4, 0, 0)$, $(1/4, 1/4, 1/4)$, $(1/4, 1/8, 0)$ and $(1/4, 0, 1/8)$. For type B we use the convex hull of $(0, 0, 0)$, $(1/4, 1/4, -1/4)$, $(1/4, 0, 0)$, $(1/4, 0, -1/4)$, $(1/4, 1/4, 0)$, $(1/8, 0, -1/4)$ and $(1/8, 1/4, 0)$. Replicating these two bodies by the motions in $N(T_2)$ (Figure 1), tesselates space.

To calculate the extended Voronoi region we cut using the translations $(1/2, 0, 0)$, $(-1/2, 0, 0)$, $(0, 1/2, 0)$, $(0, -1/2, 0)$, $(0, 0, 1/2)$ and $(0, 0, -1/2)$, and the following list of triad rotations, which belong to T_2, hence to all the groups. The two entries in each row of the list are a point and the direction of the rotation axis:

Triad rotations

Point	Vector
$(0, 0, 0)$	$(1, 1, 1)$
$(0, 1/2, 0)$	$(-1, 1, 1)$
$(-1/2, 0, 0)$	$(-1, -1, 1)$
$(-1/2, 1/2, 0)$	$(1, -1, 1)$
$(1/2, 0, 0)$	$(-1, -1, 1)$
$(1/2, 1/2, 0)$	$(1, -1, 1)$
$(1/2, -1/2, 0)$	$(1, -1, 1)$
$(1/2, 1, 0)$	$(-1, -1, 1)$
$(0, -1/2, 0)$	$(-1, 1, 1)$
$(-1, 3/2, 0)$	$(-1, 1, 1)$
$(1, 1, 0)$	$(1, 1, 1)$
$(-3/2, -1, 0)$	$(-1, -1, 1)$
$(-1/2, -1, 0)$	$(-1, -1, 1)$
$(3/2, -1/2, 0)$	$(1, -1, 1)$
$(-1, -1, 0)$	$(1, 1, 1)$
$(-1, 0, 0)$	$(1, 1, 1)$
$(0, -1, 0)$	$(1, 1, 1)$
$(0, 1, 0)$	$(1, 1, 1)$
$(1, 0, 0)$	$(1, 1, 1)$
$(1, -1/2, 0)$	$(-1, 1, 1)$
$(1, 1/2, 0)$	$(-1, 1, 1)$
$(-1, 1/2, 0)$	$(-1, 1, 1)$

The resulting bounds with these extended Voronoi regions are in the first column of Table 1. They are not very good, the biggest being above 500. But, as in the case of full groups, the worse bounds are in groups where additional motions can be used to cut the extended Voronoi region. In particular, some of the groups have diad rotations parallel to the coordinate axes or to the diagonals of the faces of the unit cube, which we use too where we can. The list of rotations is the following, and the resulting bounds are in columns 2 and 3 of Table 1:

Diad rotations parallel to the coordinate axes

Point	Vector
$(1/2, 0, 1/4)$	$(0, 1, 0)$
$(0, 1/4, 0)$	$(1, 0, 0)$
$(1/4, 1/2, 0)$	$(0, 0, 1)$
$(0, 0, 1/4)$	$(0, 1, 0)$
$(-1/4, 1/2, 0)$	$(0, 0, 1)$
$(0, -1/4, 0)$	$(1, 0, 0)$
$(1/4, 0, 0)$	$(0, 0, 1)$
$(1/2, 0, -1/4)$	$(0, 1, 0)$
$(0, 1/4, -1/2)$	$(1, 0, 0)$
$(-1/4, 0, 0)$	$(0, 0, 1)$
$(0, 0, -1/4)$	$(0, 1, 0)$
$(0, -1/4, -1/2)$	$(1, 0, 0)$
$(0, 1/4, 1/2)$	$(1, 0, 0)$
$(0, -1/4, 1/2)$	$(1, 0, 0)$
$(0, 3/4, 0)$	$(1, 0, 0)$
$(0, 3/4, 1/2)$	$(1, 0, 0)$
$(0, 3/4, -1/2)$	$(1, 0, 0)$
$(-1/2, 0, 1/4)$	$(0, 1, 0)$
$(-1/2, 0, -1/4)$	$(0, 1, 0)$
$(-1/2, 0, -3/4)$	$(0, 1, 0)$
$(1/2, 0, -3/4)$	$(0, 1, 0)$
$(0, 0, -3/4)$	$(0, 1, 0)$
$(-1/4, -1/2, 0)$	$(0, 0, 1)$
$(1/4, -1/2, 0)$	$(0, 0, 1)$
$(3/4, 1/2, 0)$	$(0, 0, 1)$
$(3/4, 0, 0)$	$(0, 0, 1)$
$(3/4, -1/2, 0)$	$(0, 0, 1)$
$(-1/2, 0, 3/4)$	$(0, 1, 0)$
$(0, 0, 3/4)$	$(0, 1, 0)$
$(1/2, 0, 3/4)$	$(0, 1, 0)$

Point	Vector
$(3/4, 0, 3/8)$	$(-1, 1, 0)$
$(1/4, 0, 1/8)$	$(1, 1, 0)$
$(1/4, 0, 5/8)$	$(1, 1, 0)$
$(-3/4, 0, 1/8)$	$(1, 1, 0)$
$(-3/4, 0, 5/8)$	$(1, 1, 0)$
$(7/4, 0, 3/8)$	$(-1, 1, 0)$
$(3/8, 3/4, 0)$	$(0, -1, 1)$
$(1/8, 1/4, 0)$	$(0, 1, 1)$
$(5/8, 1/4, 0)$	$(0, 1, 1)$
$(1/8, -3/4, 0)$	$(0, 1, 1)$
$(5/8, -3/4, 0)$	$(0, 1, 1)$
$(3/8, 7/4, 0)$	$(0, -1, 1)$
$(0, 3/8, 3/4)$	$(1, 0, -1)$
$(0, 1/8, 1/4)$	$(1, 0, 1)$
$(0, 5/8, 1/4)$	$(1, 0, 1)$
$(0, 1/8, -3/4)$	$(1, 0, 1)$
$(0, 5/8, -3/4)$	$(1, 0, 1)$
$(0, 3/8, 7/4)$	$(1, 0, -1)$

Finally, in order to get better bounds in some of the groups, we intersect the final influence region

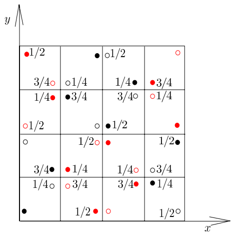

Figure 1: $I\frac{4_1}{g}\overline{3}\frac{2}{d}$

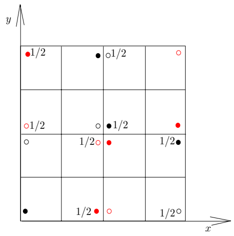

Figure 2: $I\frac{2}{g}\overline{3}$

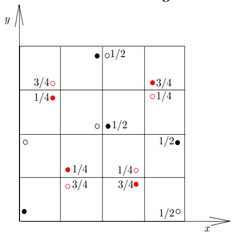

Figure 3: $I\overline{4}3d$

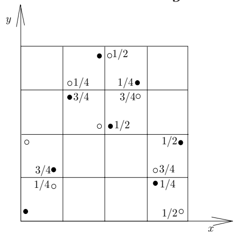

Figure 4: $I4_132$

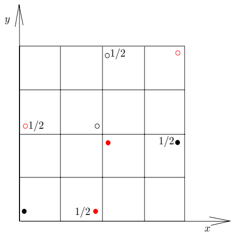

Figure 5: $P\frac{2_1}{a}\overline{3}$

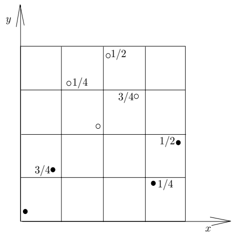

Figure 6: $P4_132 \approx P4_332$

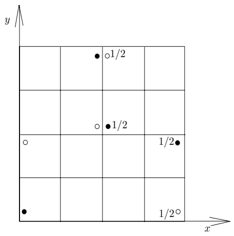

Figure 7: $I2'3$

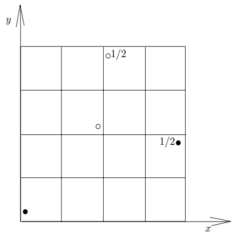

Figure 8: $P2_13$

that we obtain with the one obtained in [3] with the method of intersecting prisms over 2-dimensional regions. Our final bounds are in column four, compared tothe bounds in [3] in the last column.

Group	Our bounds				Bound from [3]
	(1)	(2)	(3)	(4)	
$I\frac{4_1}{g}\overline{3}\frac{2}{d}$	530	166	138	73	161
$I4_132$	246	94	70	53	162
$I\overline{4}3d$	276	87		74	135
$I\frac{2}{g}\overline{3}$	268	81		43	103
$P4_132$	129		105	105	89
$I2'3$	130	47		42	102
$P\frac{2_1}{a}\overline{3}$	137			73	94
$P2_13$	66			66	102

(1) Bounds after applying the triad rotations.
(2) Bounds after applying the diad rotations with axes parallel to the coordinate axes.
(3) Bounds after applying the diad rotations with axes parallel to the diagonals of the faces of the cube.
(4) Bounds after intersecting with planar projections in [3].

Table 1: Results for quarter groups.

References

[1] D. Bochiş and F. Santos. On the number of facets of 3-dimensional Dirichlet stereohedra I: groups with reflections. *Discrete Comput. Geom.* ***25:3*** (2001), 419–444.

[2] D. Bochiş and F. Santos. On the number of facets of 3-dimensional Dirichlet stereohedra II: non-cubic groups. *Preprint December 2000, revised April 2002, 27 pages.* http://arxiv.org/abs/math.CO/0204231

[3] D. Bochiş. Estereoedros de Dirichlet en 2 y 3 dimensiones. *Ph. D. Thesis, Universidad de Cantabria*, 1999.

[4] J. H. Conway, O. Delgado Friedrichs, D.H. Huson and W.P. Thurston. On Three-Dimensional Space Groups. *Contributions to Algebra and Geometry. Vol 42. No 2* (2001), 475–507.

[5] B. N. Delone (or Delaunay). A proof of the fundamental theorem of the theory of stereohedra. In *Dokl. Akad. Nauk. SSSR* ***138*** (1961), 1270–1272. (In Russian)

[6] P. Engel, *Über Wirkungsbereichsteilungen von kubischer Symmetrie*, *Z. Krist.* **154** (1981), no. 3-4, 199–215.

[7] B. Grünbaum and G. C. Shephard, Tilings with congruent tiles, *Bul. Amer. Math. Soc.* **3** (1980), 951–973.

[8] E. H. Lockwood and R. H. Macmillan. Geometric Symmetry. *Cambridge University Press*, Cambridge, 1978.

[9] J. Milnor. Hilbert's 18 problem: on crystallographic groups, fundamental domains, and on sphere packing. In *Proceedings of Symposium in Pure Mathematics of American Mathematical Society*, pages 491–507. Northern Illinois University, Dekalb, Illinois, 1974.