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

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Abstract We are interested in the maximum possible number of facets that Dirichlet stereohedra for three-dimensional crystallographic groups can have. In two previous papers, D. Bochiş and the second author studied the problem for noncubic groups. This paper deals with “full” cubic groups, while “quarter” cubic groups are left for a subsequent paper. Here, “full” and “quarter” refers to the recent classification of three-dimensional crystallographic groups by Conway, Delgado-Friedrichs, Huson and Thurston.

This paper’s main result is that Dirichlet stereohedra for any of the 27 full groups cannot have more than 25 facets. We also find stereohedra with 17 facets for one of these groups.

Keywords Stereohedra · Plesiohedra · Dirichlet domain · Crystallographic group · Cubic group

1 Introduction

Tiling problems are among the most classical problems in discrete geometry, yet they include many basic questions that are still open. See [4, Chap. 4] for a recent survey. A fundamental question, explicitly asked in [4, p. 177], [14, p. 959], and [20], and related to Hilbert’s 18th problem [18] is:

What is the maximum number of facets of a convex polytope P such that $\mathbb{R}^3$ can be tiled by congruent copies of P ?

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The fact is that there is no known upper bound for the number of facets of such a polytope. Only in the special case—where the symmetry group of the tiling acts transitively over the tiles—is a global upper bound known. In this case, the tiling is called *stereohedral* and the tile is a *stereohedron*.

Theorem 1.1 (Delone [6]) *A stereohedron in Euclidean d -space with respect to a symmetry group G cannot have more than $2^d(a+1)-2$ facets, where a is the number of aspects of G .*

The group $G \subset \text{Isom}(\mathbb{R}^d)$ that acts transitively on a stereohedral tiling is necessarily a *crystallographic group*. That is, it contains a full-dimensional discrete lattice $T \cong \mathbb{Z}^d$ as a subgroup of finite index. The quotient group G/T is usually called the *point group* of G , and its cardinality is the number of *aspects* of G . Equivalently, the number of aspects of G equals the number of translational lattices in which a generic orbit of G decomposes. In dimension three, crystallographic groups can have up to 48 aspects. Hence, the above “fundamental theorem of the theory of stereohedra” implies that three-dimensional stereohedra cannot have more than 390 facets.

On the other hand, the stereohedron with the maximum number of facets known so far has “only” 38 of them. It was found by P. Engel in 1980 (see [8] and [14, p. 964]), using a computer search, and it tiles space under the action of the cubic group $I4_132$, with 24 aspects.

It is also interesting to observe that “unbounded stereohedra”, that is, unbounded polyhedra that tile $\mathbb{R}^d$ by congruent copies under the action of a discrete transformation group, can have arbitrarily many facets, even in dimension 3. See [11], or Lemma 4.2 in [3].

A special case of stereohedral tiling is the Voronoi diagram of an orbit of points in a crystallographic group. The stereohedra obtained are called *Dirichlet stereohedra* or *plesiohedra*. The fact that Engel’s 38 face stereohedron is actually a Dirichlet stereohedron seems to indicate that Dirichlet stereohedra can have as many facets as general stereohedra (although there is no proof of this). Since Dirichlet stereohedra are much easier to analyze, the second author together with D. Bochiş (in previous papers) initiated an exhaustive study of the number of facets of Dirichlet stereohedra for the different three-dimensional crystallographic groups. They proved:

- Within the 100 crystallographic groups that contain reflection planes, the exact maximum number of facets of Dirichlet stereohedra is 18. Within *cubic* groups containing reflection planes the maximum number of facets is eight [2].
- Within the 97 noncubic crystallographic groups without reflection planes, no Dirichlet stereohedron can have more than 80 facets [3]. The same paper shows an explicit construction of Dirichlet stereohedra with 32 facets for a tetragonal group.

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 [1]. Here and in [19] we improve this bound, and hence the general upper bound for the number of facets of three-dimensional Dirichlet stereohedra. For technical reasons, we do this separately for “full groups” (this paper) and “quarter groups” (paper [19]). Among other things,

the proof we present here for full groups is “computer-free”, while the proof for quarter groups is not.

Our work takes great advantage of the new classification of crystallographic groups developed by Conway et al. in [5]. To enumerate cubic groups, they used the fact that every cubic group contains rotations of order three in the four diagonal directions of the orthonormal lattice $\mathbb{Z}^3$. They called the subgroup generated by all these rotations the *odd subgroup* of a cubic crystallographic group G . They showed that:

Theorem 1.2 (Conway et al. [5]) *For every cubic crystallographic group G :*

- (1) *Its odd subgroup is one of two possible groups R_1 or R_2 .*
- (2) *R_1 and R_2 are normal in $\text{Isom}(\mathbb{R}^3)$, hence G lies between R_i and its normalizer $\mathcal{N}(R_i)$, for the appropriate i .*

In particular, the classification of cubic groups is equal to the classification of (conjugacy classes of) subgroups of the finite groups $\mathcal{N}(R_1)/R_1$ and $\mathcal{N}(R_2)/R_2$, which are of orders 16 and 8. (The latter is isomorphic to the dihedral group D_8 ; the former contains D_8 as an index two subgroup.) The odd subgroups R_1 and R_2 differ in that R_1 contains rotation axes of order three that intersect one another while all rotation axes of order three in R_2 are mutually disjoint. Conway et al. called a cubic group *full* or *quarter* depending on whether its odd subgroup equals R_1 or R_2 . (The reason is that R_2 is a subgroup of R_1 of index four. That is, quarter groups contain only one quarter of the possible rotation axes.) There are 27 full groups (14 of them without reflection planes) and eight quarter groups (none with reflection planes, since $\mathcal{N}(R_2)$ does not contain reflections).

The main result in this paper is:

Theorem 1.3 *Dirichlet stereohedra for full cubic groups cannot have more than 25 facets.*

More precisely, for each of the 14 full groups without reflections we obtain the upper bound shown in Table 1. Here and in the rest of the paper we use the International Crystallographic Notation for crystallographic groups, see [17]. Let us remind the reader that for cubic groups with reflections, Theorem 2.4 in [2] gives a bound of eight facets.

Although, as far as we know, our work represents the first significant improvement to Delone’s global upper bound on the number of facets of general Dirichlet stereohedra, there are at least the following previous classifications of special Dirichlet stereohedra:

- Engel [9] completely classified Dirichlet stereohedra for the *symmorphic cubic groups*. G is called symmorphic if it is the semidirect product of its translation subgroup and its point group. Equivalently, if there is an orbit of G on which the translational subgroup acts transitively.

Symmorphic cubic groups are obviously all full. There are nine of them with reflections, six without reflections. Engel found that their Dirichlet stereohedra have up to 17 facets.

Table 1 Our bound for the number of facets of Dirichlet stereohedra of full cubic groups without reflections. The six groups marked with an asterisk are *symmorphic*. Their Dirichlet stereohedra were completely described by Engel (1981), and have at most 17 facets

$ G : R_1 $	Group G	Our bound	Proved by
1	$R_1 = F23^*$	10	Corollary 3.5
2	$F432^*$	14	Corollary 3.5
	$F\bar{4}3c$	14	Corollary 3.5
	$F\frac{2}{d}\bar{3}$	14	Corollary 3.5
	$P23^*$	15	Section 5
	$F4_132$	17	Corollary 3.5
4	$P432^*$	11	Corollary 4.3
	$I23^*$	21	Section 5
	$P\frac{2}{n}\bar{3}$	23	Section 5
	$F\frac{4}{d}\bar{3}\frac{2}{n}$	25	Corollary 3.5
	$P\bar{4}3n$	23	Section 5
	$P4_232$	25	Section 6
8	$P\frac{4}{n}\bar{3}\frac{2}{n}$	23	Corollary 4.3
	$I432^*$	22	Corollary 4.3

- Koch [15] (see also [16]) completely classified Dirichlet stereohedra for cubic orbits with less than three degrees of freedom. She found 117 types of stereohedra, with up to 23 facets.
- Dress et al. [7] completely classified the stereohedral tilings whose symmetry group acts transitively on the two-dimensional faces. There are 88 types of tilings, and seven types of tiles.

Remark 1.4 In the previous papers in this series we always assumed that the base point p for the orbit has trivial stabilizer for the crystallographic group G under study. We believed this was not a loss of generality in the sense that every crystallographic orbit with nontrivial stabilizer for a group G is also an orbit with smaller stabilizer for another group G' . That is actually not true, but we prove in [Appendix](#) that there are only four groups G in which it fails, all of them cubic and without reflections. These cases were previously found by Fischer [12, 13] by an exhaustive study of cubic orbits with less than three degrees of freedom.

We also show in [Appendix](#) that in the full case these special orbits produce stereohedra with at most 12 facets. In the quarter case we refer to the classification of Koch mentioned earlier, which gives a bound of 23 facets.

2 The Structure of Full Cubic Groups

The odd group R_1 of full cubic groups is a crystallographic group of type $F23$ (in International Crystallographic Notation). It is generated by rotations of order three in all the lines with directions $(\pm 1, \pm 1, \pm 1)$ and passing through integer points. In

Fig. 1 The body-centered cubic lattice I . The Delaunay tetrahedra fall into two classes, according to the orientation induced on them by the labeling. A representative of each class is shown

particular, the points where two or more axes meet form a body-centered lattice

$$I = \left\{ (0, 0, 0), \left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right) \right\} r + \mathbb{Z}.$$

To understand full groups, the Delaunay tessellation of this lattice is particularly helpful. Each Delaunay tetrahedron has two opposite dihedral angles equal to $\pi/2$, and the other four dihedral angles equal to $\pi/3$. The latter lie along rotation axes of order three and the former on rotation axes of order two, parallel to coordinate axes. Since every edge has an even number of incident Delaunay tetrahedra, the Delaunay tessellation is 2-colorable. The group R_1 acts transitively and with trivial stabilizer on the Delaunay tetrahedra of a given color.

Another way to define the coloring is as follows. The action of R_1 divides the lattice I into four orbits, namely:

$$F_i := \left\{ (a, b, c) \in I : a + b + c - \frac{i}{2} \in 2\mathbb{Z} \right\}, \quad i = 1, 2, 3, 4.$$

Each orbit is a face-centered cubic lattice. F_2 and F_4 together form a primitive lattice, and F_1 and F_3 form another.

Each Delaunay tetrahedron has a vertex in one of each of the F_i 's, and two Delaunay tetrahedra have the same color if and only if the isometry that sends one to the other and keeps the labels of vertices is orientation-preserving. In Fig. 1, lattice points are labeled according to their four orbits, and two Delaunay tetrahedra, which belong to different “colors”, have been shaded.

We fix, for the rest of the paper, the following “base Delaunay tetrahedron” T :

$$T := \text{conv}\left(\left\{ (1/2, -1/2, 1/2), (1, 0, 0), (1/2, 1/2, 1/2), (0, 0, 0) \right\}\right).$$

T is one of the two shaded tetrahedra in Fig. 1. We call its four vertices v_1 , v_2 , v_3 and v_4 , in the order we have given them, so that $v_i \in F_i$. We also introduce the following notation:

- Let T_i , $i = 1, \dots, 4$ be the tetrahedron adjacent to T and sharing with it the triangle opposite to v_i . Let v'_i be the vertex of T_i not in T .
- Similarly, let T_{ij} , with $i \neq j$, denote the neighbor of T_i and sharing with it the triangle opposite to v_j . Its vertices of T_{ij} are v_k , v_l , v'_i and a certain vertex v''_{ij} , where $\{i, j, k, l\} = \{1, 2, 3, 4\}$.

Observe that:

- If $i - j$ is odd, then T , T_{ij} and T_{ji} are related by the rotation of order three on the axis passing through v_k and v_l .
- If $i - j$ is even, then $v''_{ij} = v'_j$. That is, $T_{13} = T_{31}$ and $T_{42} = T_{24}$. Moreover, T_{ij} is related to T by an order two rotation on the axis passing through v_k and v_l . The rotation of order four on this same axis relates the two of them with T_i and T_j .

The normalizer $\mathcal{N}(R_1)$ of R_1 is the symmetry group of the lattice I . It acts transitively over all the Delaunay tetrahedra and with a stabilizer of order eight, isomorphic to the dihedral group D_8 (this stabilizer is the symmetry group of the Delaunay tetrahedron itself). Hence, the index of R_1 in $\mathcal{N}(R_1)$, that is, the order of the quotient group $\mathcal{N}(R_1)/R_1$, is 16.

Knowing $\mathcal{N}(R_1)$ and R_1 we can give the whole list of all full groups. They are shown in Table 2. We classify them with two parameters: the order s of the stabilizer of T , and a number $m = 0$ or $m = 1$ depending on whether the group acts on the Delaunay tessellation of the lattice I with one or two orbits of tetrahedra.

A group G with $m = 0$ is completely characterized by the stabilizer of the base tetrahedron T . Indeed, G is generated by R_1 together with this stabilizer. Hence, such groups are in bijection to the eight (conjugacy classes of) subgroups of D_8 , the symmetry group of T . The lattice of those groups is shown in Fig. 2. For each group we have drawn a projection of T in the vertical direction and, inside it, the orbit of a generic point. The dots representing an orbit are drawn—some black and some white—depending on whether the corresponding point lies above or below the horizontal plane at height $1/4$, which bisects T . The corresponding full cubic groups are listed in the first column of Table 2, with the same picture. The three groups that contain reflection planes are shaded.

For a group G with $m = 1$, we first look at the transformations in G that send Delaunay tetrahedra to Delaunay tetrahedra of the same R_1 -orbit. They form a subgroup H of index two in G , and H is one of the eight groups of the previous paragraph. Then, G is generated by H together with any single transformation $\rho \in G$ that sends T to one of its neighbors, say T_4 . Let H_T denote the stabilizer of T in H , and let ρ_T be ρ composed with the mirror reflection on the plane through v_1 , v_2 and v_3 (that is, the unique transformation that sends T_4 to T , keeping the labels of vertices). Let G_T be the group generated by H_T and ρ_T . Then, G is completely characterized by H_T and G_T and the conditions on H_T and G_T are that $H_T \leq G_T \leq D_8$ and $|G_T : H_T|$ equals 1 or 2.

To visualize these groups, Table 2 shows the image in T_4 of the orbit of H pictured in T . The rule of thumb is that the two orbits, when superimposed by composing one with the mirror symmetry on the plane containing v_1 , v_2 and v_3 should together form another orbit of a subgroup of D_8 . This happens automatically when $s = 8$ or $s = 4$. For $s = 1$, it is equivalent to the transformation between the two orbits being an

Table 2 The 27 full cubic groups

	m=0	m=1				
s=1	F_{23}	F_{43m}	F_{432}	$F_{\frac{2}{d}3}$	F_{43c}	
s=2	P_{23}	P_{43m}	P_{432}	I_{23}	$P_{\frac{2}{n}3}$
	$F_{41}32$	$F_{\frac{4}{m}3\frac{2}{n}}$	$F_{\frac{4}{d}3\frac{2}{n}}$
	$F_{\frac{2}{m}3}$	$F_{\frac{4}{m}3\frac{2}{m}}$	$F_{\frac{4}{d}3\frac{2}{m}}$			
s=4	$P_{42}32$	$P_{\frac{4}{n}3\frac{2}{m}}$	I_{432}
	P_{43n}	I_{43m}	$P_{\frac{4}{n}3\frac{2}{n}}$
	$P_{\frac{2}{n}3}$	$P_{\frac{4}{m}3\frac{2}{m}}$	$I_{\frac{2}{m}3}$			
s=8	$P_{\frac{4}{m}3\frac{2}{n}}$	$I_{\frac{4}{m}3\frac{2}{m}}$				

Fig. 2 The subgroups of symmetries of the base tetrahedron T

involution of T . For $s = 2$, it is necessary but not sufficient that the transformation be an involution.

Depending on the particular H , there may be one or more possibilities for G . There is always at least one, in which ρ is the mirror symmetry itself (and the involution is the identity). That is the first group shown after H in each row of Table 2, and it is shaded since it obviously contains reflections. The other ones contain reflections if and only if H contains reflections.

3 A First Upper Bound

Now let G be one of the 27 full groups, let T be a Delaunay tetrahedron of the lattice I , and p a point in T , whose Dirichlet stereohedron we want to study. We assume that p has trivial stabilizer for the action of G on Gp . That is to say, that the only motion in G that fixes p is the identity. In [Appendix](#) we treat the case of nontrivial stabilizers and correct statements made about this in the previous papers [\[2, 3\]](#). The main reason for this assumption is the following lemma.

Lemma 3.1 *If p has trivial stabilizer, then a small perturbation of it cannot decrease the number of facets of the Dirichlet stereohedron $\text{Vor}_{Gp}(p)$. That is, the maximum number of facets for a Dirichlet stereohedron with trivial stabilizer is achieved when p is generic.*

As a consequence, from now on we assume that p is generic, in particular that it lies in the interior of T .

Proof Let $p_1 \in Gp$ be a neighbor of p in the Voronoi diagram. We claim that when p is perturbed to a position p' sufficiently close to p the point $p'_1 \in Gp'$ corresponding to p_1 will be a neighbor of p' .

For this, let $x \in \mathbb{R}^3$ be a point whose distance to p and p_1 is equal, and smaller than the distance to any other point in Gp . By continuity, a small perturbation of p will make p' and p'_1 still be the two orbit points closest to x , except perhaps not equidistant to it. Assume, without loss of generality, that after the perturbation we have $d(x, p') > d(x, p'_1)$. Then, moving x in a straight line towards p' makes $d(x, p')$ decrease faster than the distance to any other point in Gp' . Hence, when x reaches a position equidistant to p' and p'_1 , the distance to all other orbit points will be bigger, which proves that p' and p'_1 are neighbors in $\text{Vor}_{Gp'}$. $\square$

Lemma 3.2 *The Dirichlet stereohedron $\text{Vor}_{Gp}(p)$ is fully contained in the (nonconvex) polyhedron obtained as the union of T and its four neighbors T_1, T_2, T_3 and T_4 . Moreover, no facet of $\text{Vor}_{Gp}(p)$ lies in the boundary of this polyhedron.*

Proof We start with the following simple observation: if a group G contains a rotation ρ of angle α and axis on the line l , then $\text{Vor}_{Gp}(p)$ is fully contained on the dihedral sector of angle α with edge l and centered around p . Indeed, this dihedral sector equals $\text{Vor}_S(p)$ where $S \subseteq Gp$ is the orbit of p under the cyclic group generated by ρ .

In our case, since the six edges of T are rotation axes for every full group, $\text{Vor}_{Gp}(p)$ will be contained in the intersection of the six corresponding dihedral sectors. For each rotation of order three on edges of T , say the one on the edge v_1v_2 , the sector of angle $2\pi/3$ in question is in turn contained in the half-space delimited by the plane containing the vertices v_1, v_2, v'_3 and v'_4 . The intersection of the four half-spaces is an infinite square prism circumscribed to T . Similarly, the rotations of order two on the axes v_1v_3 and v_2v_4 , cut this infinite square prism by two sectors of $3\pi/2$ with dihedral angle at the edges v_1v_3 and v_2v_4 . The nonconvex polyhedron obtained in this way coincides with the union of T and its four neighbors T_1, T_2, T_3 and T_4 .

For the “moreover” observe that p being interior to T implies that the half-spaces and dihedral sectors can be taken open, except for the corresponding axes. $\square$

Lemma 3.3 *Let $q \in Gp$ be a point whose Dirichlet stereohedron $\text{Vor}_{Gp}(q)$ shares a facet with $\text{Vor}_{Gp}(p)$. Then, q lies in the interior of one of the following 15 Delaunay tetrahedra of I : T , its four neighbors T_i , or the ten additional neighbors of the latter T_{ij} .*

Proof By definition, p and q are neighbors if and only if $\text{Vor}_{Gp}(p)$ and $\text{Vor}_{Gp}(q)$ share a facet. Lemma 3.2 implies that this facet (except perhaps some of its edges) is contained in the interior of the union of T and its neighbors. The same lemma applied to q , implies that q lies either in T , or in a neighbor of T , or in a neighbor of a neighbor of T . $\square$

Since each Delaunay tetrahedron contains at most eight points of Gp (because $Gp \subseteq \mathcal{N}(R_1)(p)$, which has exactly eight points in each tetrahedron), this lemma already gives a global upper bound of $8 \times 15 - 1 = 119$ facets for Dirichlet stereohedra of full cubic groups. Even more, full groups that contain eight points per tetrahedron necessarily have reflection planes. So, every full group without reflection planes has

at most four orbit points in each tetrahedron, which gives a bound of $4 \times 15 - 1 = 59$. But a more refined bound can be given using the following ideas:

- First, we will give bounds for each group G separately, using as parameters the numbers $s(G)$ and $m(G)$ introduced in the previous section. We do this to identify which groups are worth closer study. For example, in case $m(G) = 0$, then the list of 15 tetrahedra given in Lemma 3.3 goes down to only 11: T and the ten “neighbors of neighbors” T_{ij} of T .
- Second, the following lemma allows us to proceed almost as if the number of “neighbors of neighbors” of T was only six and not ten.

Lemma 3.4 *Let $G \in \text{Isom}(\mathbb{R}^3)$ be a crystallographic group and $\rho \in G$ a rotation. Let $p \in \mathbb{R}^3$ and let q a point of the orbit of p , Gp . Let S be the orbit of q by the rotation ρ . Then, at most two points of S are neighbors of p in the Voronoi diagram of Gp , namely, those which make the smallest dihedral angle with p , in both directions, when seen from the axis of ρ .*

Proof Let $S = S_q$ be the orbit of q by the rotation ρ , and let S_p denote the orbit of p . Clearly, $(S_p \cup S_q) \subseteq Gp$ implies $\text{Vor}_{Gp}(p) \subseteq \text{Vor}_{S_p \cup S_q}(p)$ and, in particular, points of S_q that are neighbors of p in Vor_{Gp} must also be neighbors in $\text{Vor}_{S_p \cup S_q}$.

We now claim that if a point $q' \in S_q$ is a neighbor of p in $\text{Vor}_{S_p \cup S_q}$, then the relative interiors of the regions $\text{Vor}_{S_p}(p)$ and $\text{Vor}_{S_q}(q')$ intersect (this is actually a variation of Lemma 1.2 in [3] and can be stated more generally). The reason is that if a point x lies in the common facet of the Voronoi regions of p and q' in $\text{Vor}_{S_p \cup S_q}$, then p and q' are the unique closest points to x in S_p and S_q , respectively.

With this claim the proof is easy to finish. The Voronoi diagrams of both S_p and S_q consist of dihedra with an edge in the axis of ρ and with angle 2π divided by the order of ρ . The dihedron $\text{Vor}_{S_p}(p)$ can only overlap with (at most) two such dihedra of the diagram Vor_{S_q} .

Perhaps the special case where p and q lie in the same orbit modulo $\langle \rho \rangle$ needs an extra word. In this case, $S = S_p = S_q$ and the Voronoi diagram $\text{Vor}_{S_p \cup S_q}(p)$ equals the cycle of dihedra around the axis of ρ mentioned earlier. It is then clear that in it every cell (in particular, the one of p) has exactly two neighbors. $\square$

In the following statement, we say that a full cubic group G “mixes colors” if it contains transformations that send black tetrahedra to white tetrahedra, and vice versa, in the 2-coloring of the Delaunay tessellation of the lattice I described in Sect. 2.

Corollary 3.5 *Let G be a full group. Let $s(G)$ be the order of the stabilizer of T in G , and let $m(G)$ be equal to 1 if G mixes colors of Delaunay tetrahedra and 0 if it does not. Then, the number of facets of any Dirichlet stereohedron for the group G is bounded above by*

$$(7 + 4m(G))s(G) + 3.$$

Proof The neighbors of p in the Voronoi diagram of Gp fall into one of the three following cases:

Table 3 The upper bound derived from Corollary 3.5

$s(G)$	$m(G)$	Bound	Groups
1	0	10	F23
	1	14	$F432, F\frac{2}{d}\bar{3}, F\bar{4}3c, (F\bar{4}3m)$
2	0	17	$F4_132, P23, (F\frac{2}{m}\bar{3})$
	1	25	$F\frac{4}{d}\bar{3}\frac{2}{n}, I23, P432, P\frac{2}{n}\bar{3},$ $(F\frac{4}{d}\bar{3}\frac{2}{m}), (F\frac{4}{m}\bar{3}\frac{2}{n}), (P\bar{4}3m), (F\frac{4}{m}\bar{3}\frac{2}{m})$
4	0	31	$P4_232, P\bar{4}3n, (P\frac{2}{m}\bar{3})$
	1	47	$I432, P\frac{4}{n}\bar{3}\frac{2}{n},$ $(P\frac{4}{m}\bar{3}\frac{2}{m}), (I\frac{2}{m}\bar{3}), (P\frac{4}{n}\bar{3}\frac{2}{m}), (I\bar{4}3m)$
8	0	59	$(P\frac{4}{m}\bar{3}\frac{2}{n})$
	1	91	$(I\frac{4}{m}\bar{3}\frac{2}{m})$

- Those in T , which are at most $s(G) - 1$.
- Those in one of the four neighbor tetrahedra, which are at most $4s(G)$, but are present only if $m(G) = 1$. That is, they are $4s(G)m(G)$.
- Those in one of the ten “neighbors of neighbors” of T . In principle the bound would be $10s(G)$, but it gets reduced to $6s(G) + 4$ using Lemma 3.4. Indeed, let $S = \{p_1, \dots, p_{s(G)}\}$ be the set of points of Gp inside the base tetrahedron T , with $p = p_1$. Similarly, let S_{ij} be the set of points of Gp inside the tetrahedron T_{ij} . Then, S_{ij} is obtained from S by the rotation of order two or three that sends T to T_{ij} . In particular, Lemma 3.4 says that for (i, j) equal to one of $(1, 2)$, $(1, 4)$, $(3, 2)$ and $(3, 4)$, S_{ij} and S_{ji} contain, in total, at most $s(G) + 1$ neighbors of p in the Dirichlet tessellation of Gp : the two obtained from p_1 by the rotation of order three, and only one of the two obtained from each of the other points in S . That is, the total number of neighbors in the ten T_{ij} ’s is bounded above by $2s(G) + 4(s(G) + 1) = 6s(G) + 4$.

Adding up, the number of neighbors is at most

$$s(G) - 1 + 4s(G)m(G) + 6s(G) + 4 = 4s(G)m(G) + 7s(G) + 3. \quad \square$$

Table 3 shows the bound given in this statement for each of the 27 full groups. Those that contain reflections appear in parentheses. As a conclusion, the global upper bound derived from this statement is 47.

4 Groups that Contain Rotations of Order Four

Corollary 3.5 is ultimately based on the fact that every full group contains the rotations of order three or two on all the edges of the Delaunay tetrahedra (see the proof of Lemma 3.2). But, of course, the groups for which the bound obtained is worse are

precisely those that have more transformations. Here and in the next section we take advantage of this fact by using additional rotations present in some of the full groups.

In this section we look at the groups which contain the rotations of order four in the two edges of T with dihedral angle of $\pi/2$. We call ρ_{13} and ρ_{24} these two rotations (ρ_{ij} is meant to have axis on the edge $v_i v_j$). Certainly, every group containing them has $m = 1$, since both rotations send T to one of its neighbors. Moreover, to locate them in Table 2 we just need to observe that ρ_{13} and ρ_{24} act on the four labels 1, 2, 3 and 4 of points in the lattice I as the transpositions $2 \leftrightarrow 4$ and $1 \leftrightarrow 3$, respectively. So, a group from Table 2 contains these two rotations if and only if the corresponding pictures contain two specific dots, namely those in the picture for the group $P432$ (said differently, $P432$ is the group generated by R_1 and the rotations ρ_{13} and ρ_{24}).

That is, the groups we are interested in are

$$P432, \quad I432, \quad P \frac{4-2}{3 \quad n} \quad \left(P \frac{4-2}{m \quad m} \right) \quad \text{and} \quad \left(I \frac{4-2}{m \quad m} \right).$$

As usual, those with reflection planes are in parentheses.

Our goal is to prove the analogues of Lemmas 3.2 and 3.3 in this case. That is to say, we want to specify a region guaranteed to contain $\text{Vor}_{Gp}(p)$ and derive from it a region guaranteed to contain all neighbors of p . To do this we introduce the following setting, which will be used again in the next section: (1) We divide the base tetrahedron T in eight smaller tetrahedra $T^A, T^B, T^C, T^D, T^E, T^F, T^G$, and T^H , via the two mirror reflection planes of T and their two bisectors. These eight tetrahedra are congruent to one another. The labels A to H are given cyclically, as shown in Fig. 3. That is, T^A is incident to vertex v_1 and edge $v_1 v_2$, T^B is incident to vertex v_2 and edge $v_1 v_2$, and so on. The same decomposition will be assumed in all the other Delaunay tetrahedra, with similar notation. For example, T_{12}^C denotes the image of T^C by the unique transformation that sends T to T_{12} preserving the labels of vertices or, equivalently, the subtetrahedron in T_{12} incident to its vertex v''_{12} and to the edge $v''_{12} v_3$. Figure 3 not only shows the decomposition of T , but also those of its neighbors T_1, T_2, T_3 and T_4 . The T_i are drawn smaller and using the same projection we used for T . Observe that this projection makes the vertices v'_i and v_{i+2} coincide (indices assumed modulo four).

We call the eight tetrahedra in which each Delaunay tetrahedron is divided *fundamental subdomain*. This is justified by the fact that they are fundamental domains of the normalizer $\mathcal{N}(R_1)$. In particular, they are permuted transitively by the normalizer $\mathcal{N}(G)$ of any full group.

(2) Using the same arguments as in Lemma 3.2, we will construct a region $\text{VorExt}(T^A)$ with the following properties: it is a union of several fundamental subdomains and, for every p in the interior of T^A , $\text{Vor}_{Gp}(p)$ is contained in $\text{VorExt}(T^A)$; no facet of $\text{Vor}_{Gp}(p)$ is in the boundary of $\text{VorExt}(T^A)$.

We call this region an *extended Voronoi region* of T^A . Lemma 3.2 says that the union of T and its four neighbors (which is the union of 40 fundamental subdomains) would be a valid $\text{VorExt}(T^A)$. But, of course, we want to find one as small as possible, since this will produce better bounds.

Lemma 4.1 *Let G be a full cubic group. Let S be a fundamental subdomain, obtained from T^A by a certain transformation $g \in \mathcal{N}(R_1)$. Then, for every q in the*

Fig. 3 The decomposition of a Delaunay tetrahedron into eight “fundamental subdomains”

interior of S we have

$$\text{Vor}_{Gq}(q) \subseteq g(\text{VorExt}(T^A)).$$

Proof Since $g \in \mathcal{N}(R_1) \subset \mathcal{N}(G)$, we have that $\text{Vor}_{Gq}(q) = g(\text{Vor}_{Gp}(p))$, where $p = g^{-1}(q)$. This, together with $\text{Vor}_{Gp}(p) \subseteq \text{VorExt}(T^A)$, finishes the proof. $\square$

In the conditions of this lemma, we call $g(\text{VorExt}(T^A))$ the extended Voronoi region of the subdomain S , and denote it $\text{VorExt}(S)$.

(3) We call *influence region* of T^A the union of all the fundamental subdomains S such that $\text{VorExt}(S)$ and $\text{VorExt}(T^A)$ overlap. We denote it $\text{Infl}(T^A)$. We have that:

Corollary 4.2 *Let p be a point in the interior of T^A and let $q \in Gp$ be a point whose Dirichlet stereohedron $\text{Vor}_{Gp}(q)$ shares a facet with $\text{Vor}_{Gp}(p)$. Then, q lies in $\text{Infl}(T^A)$.*

Proof Same as the proof of Lemma 3.3. $\square$

In particular, Lemma 3.3 implies that $\text{Infl}(T^A)$ will be contained in the union of T , its four neighbors, and the ten neighbors of the latter.

Let us mention that this method of using fundamental subdomains, extended Voronoi regions, and influence regions was already used in [2] and [3], with the same names, although applied to planar crystallographic groups.

Fig. 4 The extended Voronoi region for groups that contain rotations of order four

Figure 4 shows the extended Voronoi region obtained for the groups that contain the two rotations of order four. Our method to compute it is to start with the union of T and its four neighbors and cut some fundamental subdomains from it via the additional rotations present in these groups. For example, the rotation ρ_{13} allows us to exclude the whole of T_2 and half of T_4 and the rotation ρ_{24} allows us to exclude the whole of T_1 and half of T_3 . Finally, the order two rotation ρ_0 in the axis perpendicular to both $v_1 v_3$ and $v_2 v_4$, which is an element in all these groups, allows us to exclude the fundamental subdomains T^D , T^E and T^F . So, the extended Voronoi region consists of the following 11 fundamental subdomains:

$$\text{VorExt}(T^A) = \{T^A, T^B, T^C, T^G, T^H, T_3^A, T_3^B, T_3^G, T_3^H, T_4^A, T_4^B, T_4^C, T_4^D\}.$$

The influence region is shown in Fig. 5. Its computation is a bit more complicated. In principle, one should compute the 120 extended Voronoi regions for the fundamental subdomains contained in the 15 tetrahedra of Lemma 3.3 and check which ones overlap $\text{VorExt}(T^A)$. But things can be slightly simplified. On the one hand, we have observed (a posteriori) that the influence region does not increase when adding T^D , T^E , and T^F to $\text{VorExt}(T^A)$. That is, we can act as if the extended Voronoi region of any given fundamental subdomain S consisted of the whole Delaunay tetrahedron containing S plus half of two of its neighbors, namely those closest to S . With this

Fig. 5 The influence region for groups that contain rotations of order four

simplification, the reader should be able to check quickly that the influence region consists of the 48 fundamental subdomains of Fig. 5, which are three full Delaunay tetrahedra plus six halves of them.

Corollary 4.3 *Dirichlet sterohedra for groups of types $P432$, $I432$ and $P\frac{4}{n}\bar{3}\frac{2}{n}$ cannot have more than 11, 22 and 23 facets, respectively.*

Proof We start with the case of $G = P432$. If p is a point in T^A , then Gp contains exactly one pair of antipodal points in T , and in every Delaunay tetrahedron T_i or T_{ij} . Since $\text{Infl}(T^A)$ is made of 12 “half-tetrahedra”, it contains exactly 12 points of Gp , that is, 11 plus p itself.

Similarly, since $I432$ and $P\frac{4}{n}\bar{3}\frac{2}{n}$ contain two pairs of opposite points in each of T , T_i or T_{ij} , $\text{Infl}(T^A)$ contains exactly 24 points of Gp , that is, 23 plus p . In $I432$ we subtract one, because in this case we have counted points in both T_{34}^B and T_{43}^B , of which only one can be a neighbor of p by Lemma 3.4. $\square$

5 Groups that Contain the Transversal Rotation of Order Two

We call “transversal rotation of order two” the symmetry ρ_0 of T that exchanges $v_1 \leftrightarrow v_3$ and $v_2 \leftrightarrow v_4$. That is, the rotation of order two on the axis perpendicular to the edges v_1v_3 and v_2v_4 , and crossing both of them. (It is one of the transformations used in the previous section to cut out the extended Voronoi region.)

Equivalently, in this section we are interested in the full groups that contain $P23$ as a subgroup. The list of them, excluding the ones already considered in the previous section and the ones that contain reflections, is

$$P23, I23, P\frac{2}{n}\bar{3}, P4_232, P\bar{4}3n.$$

Figure 6 shows the extended Voronoi region. The rotations used to cut it from the union of T and its four neighbors T_i are:

- The transversal rotation ρ_0 itself, which excludes the following fundamental sub-domains:

from T : T^D, T^E, T^F ,

from T_1 : $T_1^A, T_1^D, T_1^E, T_1^F, T_1^G, T_1^H$,

Fig. 6 The extended Voronoi region for groups that contain the transversal rotation of order two

from T_2 : $T_2^C, T_2^D, T_2^E, T_2^F$.

- The rotation of order two on the axis v_1v_3 , which excludes the following fundamental subdomains from T_2 :

$$T_2^A, T_2^B, T_2^C, T_2^D.$$

- The rotation of order two on the axis v_2v_4 , which excludes the following fundamental subdomains from T_1 :

$$T_1^A, T_1^B, T_1^G, T_1^H.$$

- The rotation of order two on the axis perpendicular to v_1v_3 and $v_2v'_4$; that is, the conjugate of ρ_0 with axis crossing T_4 and T_2 . It excludes the following fundamental subdomains from T_4 :

$$T_4^E, T_4^F.$$

- The rotation of order two on the axis perpendicular to $v_1v'_3$ and v_2v_4 ; that is, the conjugate of ρ_0 with axis crossing T_1 and T_3 . It excludes the following fundamental subdomains from T_3 :

$$T_3^D, T_3^E, T_3^F.$$

We leave it to the reader to verify the above assertions. There are 19 fundamental subdomains not excluded by any of the above, namely those not shadowed in Fig. 6.

We also leave out the details of the computation of the influence region. The interested reader should verify that sending $\text{VorExt}(T^A)$ to be based at each of the 31 shadowed fundamental subdomains of Fig. 7 produces a region $\text{VorExt}(S)$ that does not intersect $\text{VorExt}(T^A)$ itself. Hence, the influence region of T^A consists of the 89 fundamental subdomains that are not shadowed.

These 89 subdomains are divided as follows, according to the action of the group R_1 . Representatives for the 16 orbits of fundamental subdomains via this action are, for example, the eight subdomains contained in T and the eight contained in any specific neighbor T_i . The numbers of them are given in Table 4.

In the case of the subdomains in T , the table contains two numbers. The first number is the number of fundamental subdomains of that orbit contained in $\text{Infl}(T^A)$. That is, a mere counting of the “white triangles” of each type in Fig. 7. The second number is the amount by which the subdomains of a given type contribute to the upper bound on the number of facets. It is obtained from the first number by subtracting 1 to T^A because of the base subdomain p , plus one to the corresponding class by the presence of the following pairs of subdomains in $\text{Infl}(T^A)$. Of each pair, only one

Fig. 7 The influence region for groups that contain the transversal rotation of order two

Table 4 Subdomains in the influence region for the groups in Sect. 5

Orbit	Subdomains in $\text{Infl}(T^A)$	Bound on nbr. of facets	Orbit	Subdomains in $\text{Infl}(T^A)$
T^A	9	8	T_i^A	4
T^B	9	6	T_i^B	4
T^C	6	4	T_i^C	3
T^D	6	4	T_i^D	3
T^E	11	7	T_i^E	4
T^F	8	7	T_i^F	4
T^G	6	4	T_i^G	3
T^H	6	4	T_i^H	3
Total	61	44	Total	28

Table 5 Final bounds for Sect. 5

Group G	Subdomains containing points of Gp	Bound on the number of facets
$P23$	T^A, T^E	$8 + 7 = 15$
$I23$	T^A, T^E, T_i^C, T_i^G	$8 + 7 + 3 + 3 = 21$
$P\frac{2}{n}\bar{3}$	T^A, T^E, T_i^B, T_i^F	$8 + 7 + 4 + 4 = 23$
$P4_232$	T^A, T^E, T^B, T^F	$8 + 7 + 6 + 7 = 28$
$P\bar{4}3n$	T^A, T^E, T^C, T^G	$8 + 7 + 4 + 4 = 23$

subdomain may produce a facet, by Lemma 3.4:

$$\begin{array}{cccc}
 (T_{23}^B, T_{32}^B) & (T_{34}^B, T_{43}^B) & (T_{14}^B, T_{41}^B) & \\
 & (T_{34}^C, T_{43}^C) & (T_{14}^C, T_{41}^C) & \\
 & (T_{34}^D, T_{43}^D) & (T_{14}^D, T_{41}^D) & \\
 (T_{12}^E, T_{21}^E) & (T_{23}^E, T_{32}^E) & (T_{34}^E, T_{43}^E) & (T_{14}^E, T_{41}^E) \\
 & & & (T_{23}^F, T_{32}^F) \\
 & (T_{23}^G, T_{32}^G) & (T_{34}^G, T_{43}^G) & \\
 & (T_{23}^H, T_{32}^H) & (T_{34}^H, T_{43}^H) & .
 \end{array}$$

In order to obtain the specific bound for each of the five groups we are interested in, we just need to add, for each of them, the bounds corresponding to the fundamental subdomains that contain a point of Gp , for each specific G . The result is in Table 5.

6 The Group $P4_232$

In this section we analyze in a bit more detail the group on which the methods so far give the worst upper bound, namely $P4_232$. Summing up, what we have said in the previous sections is that for every choice of a base point p in the fundamental subdomain T_0^A :

- Only the 37 orbit points lying in the following fundamental subdomains can possibly be neighbors of p in the Voronoi diagram of the orbit Gp :

$$\begin{array}{cccccccccccc}
 T_0^B, & T_0^E, & T_0^F, & T_{13}^A, & T_{13}^B, & T_{13}^E, & T_{13}^F, & T_{24}^A, & T_{24}^B, & T_{24}^E, & T_{24}^F, \\
 & & & & & T_{12}^E, & & & & T_{21}^E, & T_{21}^F, \\
 T_{14}^A, & T_{14}^B, & T_{14}^E, & T_{14}^F, & T_{41}^A, & T_{41}^B, & T_{41}^E, & T_{41}^F, & & & \\
 T_{23}^A, & T_{23}^B, & T_{23}^E, & T_{23}^F, & T_{32}^A, & T_{32}^B, & T_{32}^E, & T_{32}^F, & & & \\
 T_{34}^A, & T_{34}^B, & T_{34}^E, & & T_{43}^A, & T_{43}^B, & T_{43}^E, & T_{43}^F. & & &
 \end{array}$$

- The count gets down to 28 because the two orbit points in T_{ij}^x and T_{ji}^x , with $x \in \{B, E, F\}$ and $|i - j| \neq 2$, cannot be neighbors for the same choice of p (Lemma 3.4).

In what follows we investigate in further detail which fundamental subdomains produce a neighbor for all choices of p or for none. We also examine which further dependencies exist between fundamental subdomains that prevent them from producing neighbors simultaneously. Our main goal is to lower the upper bound a bit for this particular group, but this analysis also gives an idea of how far our bound is from being tight.

We start with the following relatively easy observations:

Lemma 6.1 *For any base point p in general position in the region T_0^A :*

- (1) *The orbit points in $T_0^A, T_{34}^A, T_{43}^A, T_0^B, T_{34}^B$, and T_{43}^B form a Delaunay cell, with the combinatorial type of an octahedron in which the opposite point to T_0^A is either T_{34}^B or T_{43}^B .*
- (2) *Similarly, the orbit points in $T_0^A, T_{23}^A, T_{32}^A, T_0^F, T_{23}^F$, and T_{32}^F form a Delaunay cell, with the combinatorial type of an octahedron in which the opposite point to T_0^A is either T_{23}^F or T_{32}^F .*
- (3) *The four orbit points T_0^A, T_0^B, T_0^E and T_0^F also form a Delaunay tetrahedron.*
- (4) *Let π be the plane that bisects T_0 along the mid-points of the four edges $v_i v_{i+1}$. Let π^+ and π^- be the half-spaces containing v_1 (and v_3) and v_2 (and v_4), respectively. If p is in π^+ , then T_0^A, T_0^E, T_{13}^A and T_{13}^E form a Delaunay tetrahedron. Otherwise, T_0^A, T_0^E, T_{24}^A and T_{24}^E form one. That is, for every base point either both T_{13}^A and T_{13}^E or both T_{24}^A and T_{24}^E are neighbors. This is not exclusive, in principle the four of them could be neighbors simultaneously.*

Proof In part one, the six points in question are equidistant to the mid-point of the segment $v_1 v_2$, and closer to this mid-point than any other orbit point. Actually, the points in $T_0^A, T_{34}^A, T_{43}^A$ form an equilateral triangle on the side of v_1 and those in T_0^B, T_{34}^B and T_{43}^B form another, on the side of v_2 . Depending on the direction of the plane $v_1 v_2 p$, the points of the second triangle closer to p will be T_0^B and T_{34}^B or T_0^B and T_{43}^B .

The same arguments, on the edge $v_1 v_4$, prove part 2.

Part 3 holds since these four points are equidistant and closest to the centroid of T . For part 4, the four points in question are equidistant and closest to the midpoint of $v_1 v_3$ or to the midpoint of $v_2 v_4$, depending on whether p lies in the half-space π^+ or π^- . $\square$

Corollary 6.2 *For every base point in general position, the Dirichlet stereohedron formed by the crystallographic group $P4_232$ has at least 11 facets. More precisely:*

- $T_{34}^A, T_{43}^A, T_0^B, T_{23}^A, T_{32}^A, T_0^F$ and T_0^E are always neighbors of T_0^A .
- Exactly one of T_{34}^B or T_{43}^B and one of T_{23}^F or T_{32}^F is a neighbor of T_0^A .
- Either both of T_{13}^A and T_{13}^E or both of T_{24}^A and T_{24}^E are neighbors of T_0^A .

We have done experiments with 150 base points in general position in T_0^A and the result is that the number of facets has always been between 14 and 17. This shows that the lower bound of the corollary is fairly good, while the upper bound of 28 can perhaps be lowered. In what follows we actually lower it to 25.

Fig. 8 Experiments with the group $P4_232$. The base point is arbitrary

Our experimental results are shown graphically in Figs. 8, 9 and 10. Each figure shows the 37 fundamental subdomains that can possibly produce neighbors. Subdomains are colored white, gray or black according to whether the observed behavior is that they *always*, *sometimes* or *never* produce a neighbor. We do this for an arbitrary base point (Fig. 8) and also separately for base points chosen in the lower and upper halfspaces π^- and π^+ of part 4 of Lemma 6.1.

The first observation is that the statement in Corollary 6.2 is tight in the sense that all the subdomains that are white in the pictures are mentioned in that statement. In fact, the only white subdomains in any of the three figures that do not follow from the considerations of Lemma 6.1 are T_{34}^B and T_{32}^F in Fig. 9. Apparently, when p is in the lower half-space, T_{43}^B and T_{23}^F are always opposite to T_0^A in the octahedra of parts 1 and 2 of the lemma.

More important for our purposes, however, is to understand the black subdomains in Figs. 8, 9 and 10. What we experimentally observe is:

- (1) In both the upper and lower cases, only five of the eight possible subdomains in the tetrahedra T_{13} and T_{24} produce neighbors. More precisely, if p is in the lower

Fig. 9 Experiments with the group $P4_232$. The base point is in the lower half-space

half-space, then T_{24}^E , T_{24}^F and T_{13}^F are never neighbors, while if p is in the upper half-space, then T_{13}^A , T_{13}^B and T_{24}^B are never neighbors.

- (2) The following six subdomains never produce a neighbor: T_{34}^E , T_{43}^E , T_{12}^E , T_{21}^E , T_{14}^E and T_{23}^E .
- (3) There are another four and three, respectively, subdomains that never produce a neighbor for a base point in the lower and upper half-spaces.

In our next and last result we prove part 1 of the above list, which decreases our upper bound for the group $P4_232$ from 28 to 25. Proving part 2 would decrease it to 23 (subtract one for each pair $T_{34}^E - T_{43}^E$, $T_{12}^E - T_{21}^E$) and proving part 3 would further decrease it to 21.

To lower the bound we consider the subgroup of motions of G that send the vertical axis of T_0 (the line passing through the midpoints of v_1v_3 and v_2v_4) to itself. This subgroup can be generated, for example, by the three rotations of order two that stabilize T_0 plus those on the edges v_1v_3 and v_2v_4 of T_0 (two of these five rotations are redundant, but not any two).

Fig. 10 Experiments with the group $P4_232$. The base point is in the upper half-space

Let G' denote this subgroup, and let $G'p$ denote the orbit of an arbitrarily chosen point in the fundamental subdomain T_0^A .

In order to simplify our arguments, we slightly translate the system of coordinates that we have been using so far to one in which the vertical axis of T_0 is actually a coordinate axis with the origin in the centroid of T_0 . More precisely, we take as coordinate system the one in which

$$\begin{aligned} v_1 &= (0, -1/2, 1/4), & v_2 &= (1/2, 0, -1/4), \\ v_3 &= (0, 1/2, 1/4), & v_4 &= (-1/2, 0, -1/4). \end{aligned}$$

The generating rotations of G' then are on the following axes:

- The vertical coordinate axis $\{x = y = 0\}$.
- The diagonal horizontal axes at height zero $\{z = 0, x + y = 0\}$ and $\{z = 0, x - y = 0\}$.
- The horizontal axes in the coordinate directions at height $1/4$ and/or height $-1/4$.

More generally, G' contains rotations of order four in the “diagonal horizontal” lines at height every integer or half-integer, and the “coordinate horizontal” axes at every height $n/4$ for an odd integer n . It also contains the two screw rotations of order four with axis $\{x = y = 0\}$ and translation vector $(0, 0, \pm 1/2)$.

We can also relax our conditions on the base point p a bit, so that for the purposes of the following theorem we can consider T_0 to be the whole strip delimited by the planes $z = \pm 1/4$, and divide it into eight sectors such as the following one that we call T_0^A :

$$T_0^A := \{(x, y, z) \in \mathbb{R}^3 : -1/4 < z < 1/4, x > 0, x + y < 0\}.$$

We also use the rest of labels T_0^x or T_{ij}^x in this extended sense.

One nice feature of this subgroup G' , highlighted by our choice of coordinates, is that the reflection that interchanges the two half-spaces π^+ and π^- (now the reflection on the plane $z = 0$) is in its normalizer. In particular, the choices of base point in the “upper” and “lower” part of T_0^A produce equivalent Dirichlet tessellations. In what follows we assume that the base point is chosen in the upper part of T_0^A . What we say is true for the lower part too, except that there is the following involution that has to be applied to the names of subdomains when passing from an upper to a lower base point (or vice-versa). Those in T_0 remain the same, while those in T_{13} and T_{24} are exchanged as follows:

$$T_{13}^A \leftrightarrow T_{24}^E, \quad T_{13}^B \leftrightarrow T_{24}^F, \quad T_{13}^E \leftrightarrow T_{24}^A, \quad T_{13}^F \leftrightarrow T_{24}^B.$$

Of course, only the subdomains of types A , B , E or F will contain orbit points when the base point is in T_0^A . Figure 11 schematically shows a vertical projection of these subdomains together with (part of) an orbit for this group. The figure is designed to aid in the proof of the following result.

Theorem 6.3 *All Voronoi diagrams for a generic orbit of the group G' are equivalent, and their Voronoi cells have nine facets. More precisely, the neighbors of a generic base point in the upper half of T_0^A are the orbit points in the following eleven fundamental subdomains:*

$$T_{13}^E, T_{13}^F, T_0^B, T_0^E, T_0^F, T_{24}^A, T_{24}^E, T_{24}^F, T_+^A, T_-^A, \text{ and } T_+^F,$$

where $T_+^A = T_0^A + (0, 0, 1)$, $T_-^A = T_0^A - (0, 0, 1)$ and $T_+^F = T_0^F + (0, 0, 1)$ denote the translates of T_0^A and T_0^F one unit up or down.

Observe that we have three “extra” neighbors, such as T_+^A , in this statement which do not appear anywhere else in this paper. The reason is that this is a neighbor in the Dirichlet tessellation of the group G' (not a crystallographic one) that is never a neighbor in a crystallographic full cubic group. Observe also that the notation T_+^A is a bit misleading, since this fundamental subdomain should be considered “of type E ” rather than A . Indeed, the screw rotation of order two with translation vector $(0, 0, 1)$ is an element in the odd subgroup, and gives T_+^A as the transformed of T_0^E , while the translation $(0, 0, 1)$ itself is not in the odd subgroup.

Fig. 11 Part of an orbit of the subgroup G' of the group $G = P4_232$

Proof Let $p = p_0 = (\alpha, -\beta, h)$ be our base point, with $0 < h < 1/4$, $0 < \alpha < \beta$. We introduce the following names for the other relevant points in the orbit. The following list also shows the fundamental subdomain they lie in. As in the statement, the subdomain $T_{\pm}^x$ denotes the subdomain T_0^x translated one unit up or down:

$$\begin{array}{ll}
 p_{-4} = (-\alpha, \beta, h-1) \in T_{-}^E, & q_{-4} = (\alpha, -\beta, h-1) \in T_{-}^A, \\
 p_{-3} = (\alpha, \beta, -h-1/2) \in T_{13}^A, & q_{-3} = (-\alpha, -\beta, -h-1/2) \in T_{13}^E, \\
 p_{-2} = (\beta, \alpha, h-1/2) \in T_{13}^B, & q_{-2} = (-\beta, -\alpha, h-1/2) \in T_{13}^F, \\
 p_{-1} = (\beta, -\alpha, -h) \in T_0^B, & q_{-1} = (-\beta, \alpha, -h) \in T_0^F, \\
 p_0 = (\alpha, -\beta, h) \in T_0^A, & q_0 = (-\alpha, \beta, h) \in T_0^E, \\
 p_1 = (-\alpha, -\beta, -h+1/2) \in T_{24}^A, & q_1 = (\alpha, \beta, -h+1/2) \in T_{24}^E, \\
 p_2 = (-\beta, -\alpha, h+1/2) \in T_{24}^B, & q_2 = (\beta, \alpha, h+1/2) \in T_{24}^F, \\
 p_3 = (-\beta, \alpha, -h+1) \in T_{+}^F, & q_3 = (\beta, -\alpha, -h+1) \in T_{+}^F, \\
 p_4 = (-\alpha, \beta, h+1) \in T_{+}^E, & q_4 = (\alpha, -\beta, h+1) \in T_{+}^A.
 \end{array}$$

That the neighbors of p_0 must be contained in this list follows from the fact that the translations $(0, 0, \pm 1)$ lie in G' .

The structure of the orbit is a double helix: The points p_i are cyclically ordered on the edges of an infinite prism over a (nonregular) octagon, and each point q_i is “opposite” and at the same height as the corresponding p_i . The pairs of points have their heights ordered by i , since $0 < h < 1/4$. Figure 11 shows (the projection of) the spiral of points p_i , with p_4 superimposed over p_{-4} , indicating for each point the subdomain in which it lies.

From this double helix structure we can derive some properties of the Dirichlet tessellation or, rather, its dual Delaunay triangulation:

Fig. 12 Two consecutive layers (three tetrahedra each) in $\text{Vor}_{G'p_0}$. In between the two layers lie the four tetrahedra $q_{-2}q_{-1}p_1p_2$, $q_{-1}q_0p_0p_1$, $p_{-1}p_0q_0q_1$, and $p_{-2}p_{-1}q_1q_2$

- For every i , the tetrahedron $\{p_{i-1}, q_{i-1}, p_i, q_i\}$ is a Delaunay tetrahedron. Indeed, its four points are equidistant and closest to the point $(0, 0, i/4)$.
- For every i , the tetrahedron $\{q_{i-2}, q_{i-1}, p_i, p_{i+1}\}$ is a Delaunay tetrahedron. Here we work out the details for $i = 0$, the other cases being symmetric to it.

Consider the empty sphere with center at the point $o = (-c, -c, 0)$, for a positive c . The orbit points closest to it for c sufficiently large are clearly p_1 and q_{-2} . On the other hand, when c approaches zero, the closest points to o are those with minimum (in absolute value) height and lying in the half-space $x + y < 0$; that is, p_0 and q_{-1} . Moreover, it is easy to show that at any intermediate c the closest points to o must be one of these two pairs. Hence, there must be a c where these four points are equidistant and closest to o , hence they form a Delaunay tetrahedron.

- Similarly, for every i , the tetrahedron $\{p_{i-2}, p_{i-1}, q_i, q_{i+1}\}$ is a Delaunay tetrahedron.

These three classes of tetrahedra do not cover completely the convex hull of the orbit (which is an infinite prism over an octagon) but almost: indeed, for each i these three tetrahedra form a “layer” separate the prism into two parts, so that every other Delaunay tetrahedron must lie in between two layers. See Fig. 12, where (the vertical projection of) the layers with $i = 0$ and $i = 1$ are drawn.

Moreover, the $i - 1$ th and the i th layers have three edges in common, so that the space between them consists of four nonoverlapping and triangle-disjoint tetrahedra. These four tetrahedra must then also be Delaunay (and add no Delaunay edges except for $p_iq_{i\pm 4}$), which finishes the description of the Delaunay tessellation.

Hence, the list of neighbors of p_0 in the Delaunay tessellation is

$$q_{-4}, q_{-3}, q_{-2}, q_{-1}, q_0, q_1, q_2, q_3, q_4, p_{-1}, p_1,$$

as claimed. $\square$

We remark that a “single helix” analogue of this last statement was proved as Lemma 4.2 in [3, Lemma 2.8] and, independently, in [10, Lemma 2.1].

Appendix and Erratum: Orbits with Nontrivial Stabilizer

In this and the previous papers in this series we have always assumed that the base point p for the crystallographic orbit Gp under consideration has trivial stabilizer in G . That is, there is no nontrivial element $g \in G$ with $gp = p$. We believed this was no loss of generality “since otherwise Gp is also an orbit of a proper subgroup of G ” (cf. [3, p. 92]). This sentence is actually false. In this appendix we show that:

- The sentence only fails in tetragonal and cubic groups, and only for orbits with stabilizer of order two.
- In the tetragonal case, the sentence is almost true: every tetragonal crystallographic orbit Gp is also an orbit with trivial stabilizer for a different group G' , except G' may not be a subgroup of G .
- In the cubic case, there are exactly four (one-parameter families of) cubic orbits that are not orbits with trivial stabilizer for any crystallographic group. Two arise in full groups and produce stereohedra with at most 12 facets, and two in quarter groups. For the latter, results of Koch [15] give a bound of 23 facets.

A.1. Nontrivial Stabilizers Have at Most Order Two Let D be a stereohedron for a crystallographic group G (not necessarily a Dirichlet one). Suppose that the stabilizer of D in G is a nontrivial subgroup $H_0 \leq G$, but that D is still not a stereohedron for any proper subgroup of G . That is, there is no proper subgroup F such that $\{fD : f \in F\} = \{gD : g \in G\}$.

Observe that H_0 can naturally be considered a subgroup of the point group G_0 of G : every element of H_0 fixes the centroid of D , which we take as the origin.

Lemma A.1 *There is no proper subgroup $F_0 \leq G_0$ such that $F_0H_0 = G_0$.*

Here $F_0H_0 = \{hf : h \in H_0, f \in F_0\}$ is not necessarily a subgroup of G_0 . It is a union of right cosets of F_0 and also a union of left cosets of H_0 . It is guaranteed to be a subgroup only if one (or both) of F_0 and H_0 are normal.

Proof Let H and F denote the preimages of H_0 and F_0 under the canonical quotient map $G \rightarrow G_0$. Suppose that $F_0H_0 = G_0$ and let gD be a copy of D obtained by some element $g \in G$. We want to show that $gD = fD$ for some $f \in F$.

Let $g_0 \in G_0$ be the point transformation corresponding to g . Since $F_0H_0 = G_0$, there are elements $h_0 \in H_0$ and $f_0 \in F_0$ such that $f_0h_0 = g_0$. Since $H_0 \leq G$, we can consider h_0 as an element of G , not only a point transformation. Let $f \in F$ be any element that projects to f_0 . Then, $fh_0D = fD$ is a translated copy of gD . That is, $gD = tfD$ for some translation t . But $f \in F$ implies $tf \in F$, which finishes the proof. $\square$

Corollary A.2 *H_0 is contained in all the subgroups of G_0 of index two.*

Proof If $F_0 \leq G_0$ has index two and H_0 is not contained in F_0 , then $F_0H_0 = G_0$. $\square$

Theorem A.3 *If H_0 is not trivial, then it has order two. More precisely, either*

- (1) G is tetragonal, and H_0 is generated by a vertical rotation of order two; or
- (2) G is cubic, and H_0 is generated by a rotation of order two in one of the coordinate directions.

Proof (1) Let P_{2i} , with $i \in \{1, 2, 3\}$ denote the point group $\frac{2i}{m} \frac{2}{m} \frac{2}{m}$. Put differently, P_6 , P_4 and P_2 are the symmetry groups of a hexagonal prism, square prism, and parallelepiped, respectively. The last one is contained in the other two.

Every noncubic point group is contained in one of these three groups. More precisely: triclinic, monoclinic and orthorhombic point groups are contained in P_2 ; tetragonal point groups are those contained in P_4 but not on P_2 ; and trigonal and hexagonal are those contained in P_6 but not on P_2 . So, let i be such that $G_0 \leq P_{2i}$.

For each index two subgroup N of P_{2i} , $N \cap G_0$ is either G_0 or an index two subgroup of G_0 . Hence, by the previous corollary, H_0 is contained in the intersection of the following three subgroups of P_{2i} , of index two: The group of orientation-preserving symmetries, the group of transformations sending the positive vertical direction to itself, and the group P_i of “symmetries of the i -gonal prism” (P_1 is the order four group generated by the mirror reflections with respect to a vertical and the horizontal plane).

In the three cases this intersection is the group of order i generated by a rotation around the vertical axis. (Of course, the “rotation of order one” is the identity.) If $i = 1$, then the intersection is trivial, and the case $i = 2$ is the one allowed in the statement. In the case $i = 3$, if H_0 is not trivial (hence equal to the C_3 generated by a vertical rotation of order three) we can apply Lemma A.1 to the index three subgroup $F_0 := P_2 \cap G_0$ of G_0 . The three elements of C_3 belong to the three different cosets of P_2 in P_6 , hence to the three of F_0 in G_0 .

(2) If G is cubic, then G_0 is contained in the symmetry group of the regular cube. By the corollary, H_0 must be contained in the subgroups of orientation preserving transformations and of symmetries of the inscribed regular tetrahedron. The intersection of them is the group 23 of order 12 consisting of the identity, the three rotations of order two in coordinate directions, and the eight rotations of order three in the four diagonal directions. But H_0 cannot contain a rotation ρ of order 3. If it did, let F_0 be the subgroup of G_0 consisting of transformations that send the z axis to itself. Since 1 , ρ and ρ^2 lie in the three cosets of F_0 in G_0 , we have that $F_0 H_0 = G_0$.

So, H_0 must be contained in the group 222 of order four generated by the rotations of order two in the three coordinate directions. It cannot equal that group either, or otherwise we could take F_0 the subgroup of G_0 that sends the diagonal axis $\{x = y = z\}$ to itself. Since the four diagonal axes are permuted transitively by the group 222, $F_0 H_0$ would equal G_0 . $\square$

A.2. Nontrivial Stabilizers Exist only in Cubic Groups Here we assume that p is a base point with stabilizer generated by a rotation of order two in the vertical direction of a tetragonal group G . We prove that Gp is also an orbit with trivial stabilizer for another group G' .

Since G is tetragonal and Gp lies in order two rotation axes, the horizontal projection of Gp is a square lattice. For the sake of concreteness, let us introduce coordinates in which this lattice is the integer two-dimensional lattice $\mathbb{Z}^2$.

Let G_h be the subgroup of G generated by the vertical rotations of order two on axes that contain orbit points. Let $T_h \leq G_h$ be the subgroup of translations in G_h . T_h is the group of horizontal translations by vectors with even coordinates. Put differently, T_h splits the rotation axes in G_h into four orbits, with representatives in the vertical lines $l_{(0,0)}$, $l_{(1,0)}$, $l_{(1,1)}$ and $l_{(0,1)}$. ($l_{(x,y)}$ denotes the vertical line through $(x, y, 0)$.)

Also, let T_v be the minimal vertical translation under which the orbit Gp is invariant, and let c be its length. On each vertical axis, Gp splits into either one or two orbits of T_v and it thus is an orbit of T_v together with perhaps a reflection. We choose the vertical coordinate so that the orbit along the line $l_{(0,0)}$ is symmetric under the change of sign in this coordinate.

Only three possibilities are compatible with G being a tetragonal group:

- On all the $l_{(x,y)}$'s, the orbit points lie at the same height. Then, we let G' be generated by the translations with integer horizontal coordinates and vertical coordinates multiple of c , together with a mirror reflection in the horizontal plane at height zero, if needed.
- On all the $l_{(x,y)}$'s the orbit points lie at different heights. This can happen only if G contains a screw rotation ρ of type 4_1 (or 4_3) on the vertical axis through the point $(1/2, 1/2, 0)$. The translation part of ρ is of length $c/4$. We let G' be generated by T_h , T_v , ρ and a rotation of order two on the horizontal axis passing through $(0, 0, 0)$ and $(1, 1, 0)$. By our choice of the third coordinate this rotation keeps the orbit Gp invariant. Hence Gp is still an orbit of G' and it has trivial stabilizer in it.
- On $l_{(0,0)}$ and $l_{(1,1)}$ the orbit points are at the same height, but different from that of $l_{(1,0)}$ and $l_{(0,1)}$ (and the latter are equal to one another). If this happens, then along each vertical axis there is only one translational orbit, or there are two but then the orbit on the axes $l_{(0,0)}$ and $l_{(1,1)}$ is displaced a vertical length of exactly $c/2$ with respect of the orbit on $l_{(1,0)}$ and $l_{(0,1)}$ (if none of this happens, then there is no transformation of 3-space that sends Gp to Gp and switches the two translational orbits along the axis $l_{(0,0)}$). In the first case we let G' be generated by T_h , T_v , the translation with vector $(0, 1, 1)$, and a rotation of order two in a horizontal axis through the points $(0, 1/2, \alpha)$ and $(1, 1/2, \alpha)$. Here, α is half the vertical displacement between the orbits in $l_{(0,0)}$ and $l_{(1,0)}$. In the second case, we let G' be generated by T_h , T_v , and the translations with vectors $(1, 1, 0)$ and $(0, 1, c/2)$.

A.3. Dirichlet Stereohedra with Nontrivial Stabilizer, for Cubic Groups Fischer [12] completely classified the cubic orbits with less than three degrees of freedom. This includes the case of all cubic orbits with nontrivial stabilizer. His findings in this respect are as follows (see also [13]):

Proposition A.4 (Fischer) *There exist exactly five cubic groups with orbits that are not orbits with trivial stabilizer for noncubic groups: the quarter groups $I\bar{4}3d$ and $I\frac{4}{g}\bar{3}\frac{2}{d}$, and the full groups $F\frac{2}{d}\bar{3}$, $F4_132$ and $F\frac{4}{m}\bar{3}\frac{2}{n}$.*

Here we recover this result and show that, in the full case, Dirichlet stereohedra produced by these orbits have at most 12 facets. The group $F\frac{4}{m}\bar{3}\frac{2}{n}$ is superfluous for us, since the “bad” orbits in it are also orbits of its proper subgroup $F4_132$.

Theorem A.5 *Let p be a base point with nontrivial stabilizer in a full cubic group G , and suppose Gp is not an orbit with smaller stabilizer for any other crystallographic group. Then G is one of the groups $F4_132$ or $F\frac{2}{d}\bar{3}$ and the Dirichlet stereohedra of this orbit have at most 12 facets.*

Proof By Theorem A.3, p lies in an order-two coordinate-parallel rotation axis. There are two types of coordinate-parallel rotations of order two in full cubic groups. Those on the long sides of the fundamental subdomains and those in the common perpendicular line to the two long sides of one fundamental subdomain.

If p lies in a rotation axis of the second type, then Gp is an orbit for some proper subgroup of G . If there is one orbit point in each fundamental subdomain, then Gp is an orbit with trivial stabilizer for either $F23$, $F432$ or $F\frac{2}{d}\bar{3}$. If there are two (symmetrically placed) orbit points in each fundamental subdomain, then Gp is an orbit for either $F4_132$, or $F\frac{4}{d}\bar{3}\frac{2}{n}$. See Table 2.

If p lies in a long side of the fundamental subdomain, suppose that it lies on the edge v_1v_3 of T and closer to v_1 than to v_3 . We say that p lies “near v_1 ”. The whole orbit Gp decomposes into at most four orbits of $F23$, one “near v_i ” for each $i = 1, 2, 3, 4$. There are four cases, depending on the action of G on the four symbols 1, 2, 3 and 4 of the lattice points. That is, on how G mixes the four sublattices of type F that make the I lattice whose Delone tetrahedra we call fundamental subdomains:

- If G does not mix the sublattices, then the orbit consists of six points near each center of the lattice F , lying in the two directions of the three coordinate axes from that center. This is also an orbit for the semidirect product of the translational lattice F and the order six point group $\bar{3}$ generated by the inversion and a diagonal rotation of order three.
- If G mixes the four sublattices, then the same is true except now for the lattice I .
- If G mixes 1 only with 3 and 2 only with 4, then the same holds for the lattice P .
- So, the only problematic case is when G mixes the sublattice 1 with the sublattices of 2 and 4 and the sublattice 3 with the other. Looking at Table 2, we see that the only full groups that do this are $F\frac{2}{d}\bar{3}$, $F4_132$ and $F\frac{4}{m}\bar{3}\frac{2}{n}$. The latter is discarded since then the stabilizer of p contains not only the rotation on the axis v_1v_3 , but also a mirror reflection.

In this case we consider Gp as the union of two orbits of the index two subgroup $F23$. The Dirichlet stereohedra for each $F23$ -orbit are the octahedra obtained gluing the four fundamental subdomain that share a long edge, the edge being v_1v_3 for one orbit and v_2v_4 for the other. Then, p has at most eight neighbors in its own $F23$ -orbit (corresponding to the eight facets of the octahedron), and at most four in the other $F23$ -orbit (because each octahedron from one orbit intersects four from the other). $\square$

For quarter groups, a quick look at the list of them (Fig. 2 in [19]) easily implies:

Lemma A.6 *If p has nontrivial stabilizer in a quarter group G and Gp is not an orbit for a proper subgroup of G , then G is either $I\bar{4}3d$ or $I\frac{4}{g}\bar{3}\frac{2}{d}$.*

Proof Of the other six quarter groups, three do not have rotations of order two and the other three contain the first three as subgroups of index two. $\square$

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