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DENSEST BALL PACKINGS BY ORBITS OF THE 10 FIXED POINT FREE EUCLIDEAN SPACE GROUPS

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0. Introduction

Let G be a fixed point free Euclidean space group, i.e. any group from among the crystallographic groups

1. P1; 2. P2_1; 7. Pb; 9. Bb; 19. P$2_12_12_1$; 29. Pca2_1; 33. Pna2_1; 76. P4_1; 144. P3_1; 169. P6_1 (see [3], [7]).

Take a point X in the Euclidean space E^3, and consider the G-orbit of X

$$X^G := \{X^g \in E^3 : g \in G\}. \tag{0.1}$$

The radius $r(X^G)$ of the ball packing with centres by the orbit X^G is defined as follows:

$$r(X^G) = (1/2)\inf\{\varrho(X, X^g) : g \in G \setminus \{1\}\} \tag{0.2}$$

where ϱ is the distance function in E^3. We are interested in the optimal ball packing of the group G whose radius is

$$r(G) = \sup\{r(X^G) : X \in E^3\}. \tag{0.3}$$

The optimal density of the ball packing by G is

$$\delta(G) = \frac{\operatorname{Vol} B(r(G))}{\operatorname{Vol} F(G)} \tag{0.4}$$

where the volume of the optimal ball is related to the volume of the fundamental domain of G. This density $\delta(G)$ depends on the free parameters of G. Finally, we optimize $\delta(G)$ also by the free parameters of G. Thus the optimal density $\delta(G)$ will be determined by the isomorphy class of G as it is natural to expect.

This program generalizes the problem of finding the densest lattice-like ball packing in the Euclidean space E^3, where the group $G = \mathrm{P1}$ generated

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by 3 independent translations. The result, due to Gauss is well-known [1]. The optimal packing provides the face centred cubic lattice, spanned by the vectors $\mathbf{f}_1, \mathbf{f}_2, \mathbf{f}_3$ with Gramian matrix

$$(0.5) \qquad (f_{ik}) = (\langle \mathbf{f}_i, \mathbf{f}_k \rangle) = \begin{bmatrix} 1 & 1/2 & 1/2 \\ 1/2 & 1 & 1/2 \\ 1/2 & 1/2 & 1 \end{bmatrix}, \qquad \det(f_{ik}) = 1/2,$$

$$(0.6) \qquad r(\mathrm{P1}) = 1/2; \ \operatorname{Vol} F(\mathrm{P1}) = (1/2)^{1/2}; \ \delta(\mathrm{P1}) = \pi(18)^{-1/2} \approx 0.7405.$$

It is clear that congruent orbits of G provide ball packings of the same density. Therefore, those isometries of E^3, which preserve the G-orbits, play important role. These isometries constitute the metric normalizer of the space group G as a supergroup

$$(0.7) \qquad M_G = \{\mu \in \operatorname{Iso} E^3 \mid \mu^{-1} G \mu = G\}.$$

A fundamental set of M_G, denoted by $F(M_G)$ has the basic property

$$(0.8) \qquad r(G) = \sup\{r(X^G) \mid X \in F(M_G)\}$$

because $F(M_G)$ consists of points providing all noncongruent G-orbits. Since we know the metric normalizer for each group G considered [2], it is reasonable to assign a suitable $F(M_G)$ as a parameter domain for determining the optimal radius $r(G)$. It will turn out that each above group G provides the optimal ball packing of the same density by (6). For the first 9 groups one extremal arrangement is the same as the lattice-like one. The groups $\mathrm{P2_12_12_1}$; $\mathrm{P2_1}$; Bb; $\mathrm{Pna2_1}$ and $\mathrm{Pca2_1}$ has two different extremal arrangements, one of them is lattice-like. The other optimal ball packing of these five groups coincides with the unique one of $\mathrm{P6_1}$. This non-lattice arrangement is also well-known.

1. The method of the proof, the case $\mathrm{P2_12_12_1}$

In the International Tables [3], for each Euclidean space group G there is given its lattice L_G, related to a primitive Bravais lattice with the corresponding centering. The coordinate presentation of the so-called point-group G_0 is expressed in the basis of L_G. Moreover, a so-called vector-system, associated with the point group G_0 is given which describes the images of the origin O under G.

For instance let the group $\mathrm{P2_12_12_1}$ be fixed as G. The primitive orthorombic lattice L_G is spanned by the orthogonal basis $\{\mathbf{e}_i\}$ with Gramian

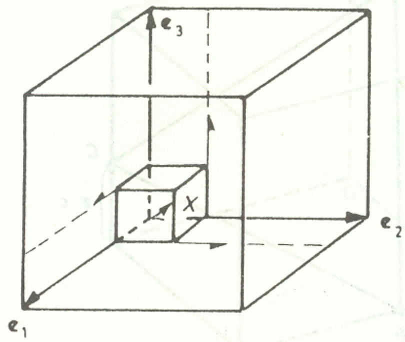
$$(1.1) \qquad (e_{ij}) = (\langle \mathbf{e}_i, \mathbf{e}_j \rangle) = \begin{bmatrix} a^2 & 0 & 0 \\ 0 & b^2 & 0 \\ 0 & 0 & c^2 \end{bmatrix}, \quad 0 < a \leqq b \leqq c, \ abc = 1.$$

The parameters a, b, c are characteristic for G, but we may normalize $abc = 1$.

The point positions are:

$$X(x,y,z), X^{S1}(x+1/2, -y, -z+1/2), X^{S2}(-x+1/2, y+1/2, -z), \quad (1.2)$$
$$X^{S3}(-x, -y+1/2, z+1/2).$$

S_1, S_2, S_3 mean screw motions indicated in the Figure 1.



$X(x,y,z) \in F(M_G)$.

Fig. 1

The vectors XX^g, $g \in G$, are of the form

$$\mathrm{t}_0, XX^{S1} + \mathrm{t}_1, XX^{S2} + \mathrm{t}_2, XX^{S3} + \mathrm{t}_3 \quad \text{with} \quad \mathrm{t}_0, \mathrm{t}_1, \mathrm{t}_2, \mathrm{t}_3 \in L_G.$$

These are in coordinates:

(1.3) $\quad (0,0,0),\ (1/2, -2y, -2z+1/2),\ (-2x+1/2, 1/2, -2z),$

plus an integer tripel to any of them, describing a lattice vector from L_G. Here $X(x,y,z)$ runs over a fundamental set of the metric normalizer M_G. Now $M_G = \mathrm{Pmmm}$ is generated by plane reflections in the walls of the brick with edge measures $a/4, b/4, c/4$. The lattice L_{Pmmm} is generated by $(1/2)\mathrm{e}_1$, $(1/2)\mathrm{e}_2$, $(1/2)\mathrm{e}_3$ (see [2]). Hence a fundamental set of M_G is defined by

(1.4) $\quad F(M_G) = \{X(x,y,z) \in E^3,\ 0 \leqq x \leqq 1/4,\ 0 \leqq y \leqq 1/4,\ 0 \leqq z \leqq 1/4\}.$

From (1.3) we see that the infimum by the formula (0.2) comes from the length minimum of 4 vectors as follows

$$l = \min\Big\{ a, [a^2/4 + 4y^2b^2 + (1/2-2z)^2c^2]^{1/2}, \quad (1.5)$$
$$[(1/2-2x)^2a^2 + b^2/4 + 4z^2c^2]^{1/2},\ [4x^2a^2 + (1/2-2y)^2b^2 + c^2/4]^{1/2}\Big\}.$$

By (0.3) and (0.4) we look for

(1.6) $\quad \delta(G) = (2\pi/3)\max\{l^3 \mid 0 \leqq x, y, z \leqq 1/4,\ 0 < a \leqq b \leqq c; abc = 1\}$

since now Vol $F(G) = 1/4$, Vol $B(l/2) = (1/6)l^3\pi$. To prove $\delta(G) \leqq \pi/(18)^{1/2}$, we shall show that $l \leqq 2^{-1/2}$ in (1.5). So we may assume that

(1.7) $\quad 2^{-1/2} \leqq a \leqq b \leqq c, \quad \text{moreover} \quad 0 \leqq x, y, z \leqq 1/4$

hold in (1.5) and (1.6). We sketchily prove the following

LEMMA. *If a brick has a unit volume, its side lengths are not less than $2^{-1/2}$ and the vertices of a triangle lie on the skew edges of this brick, then there is a side of the triangle whose length is not greater than $2^{1/2}$* (see Figure 2).

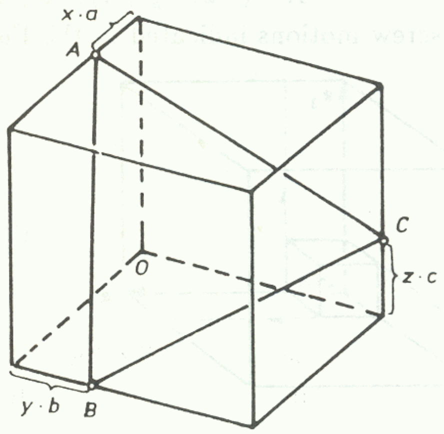


Fig. 2

We may assume that the triangle is regular and prove that the optimal triangle have two common vertices with the brick containing it. Consider the orthogonal projection of the triangle onto any face P of the brick. So we obtain a triangle which has a common vertex A' with the rectangle P and the other vertices B', C' lie on those sides of P which are opposite to A'. A short calculation shows that the indirect assumption, i.e. P has neither B' nor C' as its vertex, may allow choosing a bigger triangle ABC on the skew edges of the brick. So two vertices of the optimal regular triangle are vertices of the brick. From this we derive three optimal cases with the parameters:

1. $a^2 = 1/2, \quad b^2 = 1, \quad c^2 = 2;$
2. $a^2 = 1/2, \quad b^2 = 4/3, \quad c^2 = 3/2;$
3. $a^2 = 1, \quad b^2 = 1, \quad c^2 = 1$

(see Figure 3).

For more details see [4].

Replace x, y, z of Fig. 2 by $1-4x$, $1-4y$, $1-4z$, respectively. Then, e.g., the length $|AB|$ is equal to $2[4x^2a^2 + (1/2-2y)^2b^2 + c^2/4]^{1/2}$ and so on, as (1.5) and (1.6) imply. Finally, by the lemma we have obtained three optimal ball systems with the density in (0.6). These are:

1. $a^2 = 1/2,\ b^2 = 1,\ \ c^2 = 2,\ \ x = 0,\ \ y = 1/4,\ z = 1/8;$
2. $a^2 = 1/2,\ b^2 = 4/3,\ c^2 = 3/2,\ x = 1/4,\ y = 1/4,\ z = 1/12;$
3. $a^2 = 1,\ \ b^2 = 1,\ \ c^2 = 1,\ \ x = 1/4,\ y = 1/4,\ z = 1/4.$

The first and third arrangements are lattice-like, the second is not.

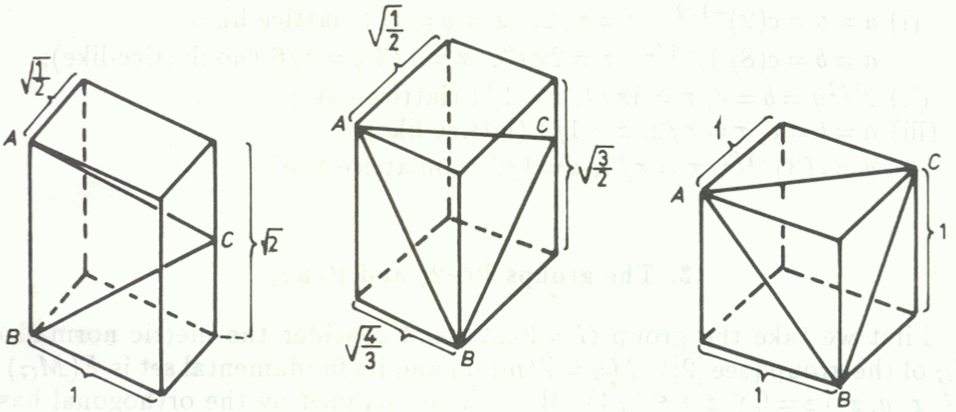


Fig. 3

2. The cases of the groups $P2_1$, Pb, Bb

These three space-groups G generates double lattice-like ball packings, respectively. The optimal ball systems give the density by (0.6) (see [5], [6], [8]). We can prove this in a direct way, too. Namely we regard the metric normalizers M_G and their fundamental sets $F(M_G)$ (see [2]). We have to solve the following problems, respectively:

(i) $$\delta(\mathrm{P}2_1) = \max\left\{ \frac{(l^3\pi)/6}{(abc\sin\tau)/2} \;\middle|\; z = 0 \leqq x, y;\ x + y = 1/2;\ \pi/2 \leqq \tau < 2\pi/3;\ 0 < a, b, c \right\},$$

where

$$l = \min\{a, c, (4x^2a^2 + 2ab\cos\tau(2x)(2y) + 4y^2b^2 + c^2/4)^{1/2}\};$$

(ii) $$\delta(\mathrm{Pb}) = \max\left\{ \frac{(l^3\pi)/6}{(abc\sin\tau)/2} \;\middle|\; x = y = 0 \leqq z \leqq 1/4;\ \pi/2 \leqq \tau < \pi;\ 0 < a \leqq b;\ 0 < c \right\},$$

where

$$l = \min\{a, c, (b^2/4 + 4z^2c^2)^{1/2}\};$$

(iii) $$\delta(\mathrm{Bb}) = \max\left\{ \frac{(l^3\pi)/6}{(abc\sin\tau)/4} \;\middle|\; x = y = 0 \leqq z \leqq 1/4;\ \pi/2 \leqq \tau < \pi;\ 0 < a, b, c \right\},$$

where

$$l = \min\left\{a, b, c, (a^2+c^2)^{1/2}/2, [(a^2+c^2)/4 + ab\cos\tau + b^2]^{1/2}, (b^2/4 + 4z^2c^2)^{1/2}\right\}.$$

Since these results are treated in [5], [6] as particular cases, we omit here the lengthy calculations which are similar to those at the other groups. The parameters of the optimal ball packings are as follows:

(i) $a=b=c(2)^{-1/2},\quad \tau=\pi/2,\quad x=y=1/4$ (lattice-like)
$a=b=c(8/3)^{-1/2},\quad \tau=2\pi/3,\quad x=1/3\ y=1/6$ (nonlattice-like);
(ii) $2^{1/2}a=b=c$, $\tau=3\pi/4$, $z=1/4$ (lattice-like);
(iii) $a=b=c$, $\tau=\pi/2$, $z=1/4$ (lattice-like)
$a=c(3)^{-1/2}$, $\tau=\pi/2$, $z=1/6$ (nonlattice-like).

3. The groups $\mathrm{Pca2_1}$ and $\mathrm{Pna2_1}$

First we take the group $G=\mathrm{Pca2_1}$ and consider the metric normalizer M_G of the group (see [2]). $M_G=\mathrm{Z^1mmm}$ and its fundamental set is $F(M_G)= =\{(x,y,z)\,|\,z=0\leqq x,y\leqq 1/4\}$. Here L_G is spanned by the orthogonal basis $\{\mathbf{e}_i\}$ where $|\mathbf{e}_1|=a$, $|\mathbf{e}_2|=b$, $|\mathbf{e}_3|=c$. The point positions are:

$$X(x,y,z), X^{2_1}(-x,-y,z+1/2), X^c(-x+1/2,y,z+1/2), X^a(x+1/2,-y,z)$$

and the vectors XX^g, $g\in G$ are of the form:

$$(0,0,0),\ (-2x,-2y,1/2),\ (1/2-2x,0,1/2),\ (1/2,-2y,0) \tag{3.1}$$

plus an integer triple from L_G. Since $0\leqq x,\ y\leqq 1/4$ we see from (3.1) that the infimum in (0.2) is nothing but

$$l=\min\Big\{a,b,c,(4x^2a^2+4y^2b^2+c^2/4)^{1/2},\\ [(1/2-2x)^2a^2+c^2/4]^{1/2},(a^2/4+4y^2b^2)^{1/2}\Big\} \tag{3.2}$$

and we look for

$$\delta(G)=(2\pi/3)\max\{l^3\,|\,z=0\leqq x,y\leqq 1/4,\ 0<a,b,c,\ abc=1\}. \tag{3.3}$$

Since by (3.2) l is increasing in y, we may suppose that y is equal to 1/4. Then we see that in the case $x=0$, $y=1/4$, $z=0$ the ball packing is lattice-like since XX^G, $g\in G$ are of the form

$$(0,0,0),\ (0,-1/2,1/2),\ (1/2,0,1/2),\ (1/2,-1/2,0) \tag{3.4}$$

plus any triple of integers from L_G. We obtain the optimal face centered cubic lattice iff $a=b=c=1$, then $l=2^{-1/2}$ and $\delta=\pi/(18)^{1/2}$.

To prove $l\leqq 2^{-1/2}$ we may assume $x>0$, moreover,

$$1/2\leqq a^2,b^2,c^2=(ab)^{-2},(a^2+b^2)/4\ \text{ and}\\ d^2=4x^2a^2+(b^2+c^2)/4=(1/2-2x)^2a^2+c^2/4. \tag{3.5}$$

From (3.5) we have

$$0<x=\frac{a^2-b^2}{8a^2}<1/4 \text{ and } d^2=(1/2-2x)^2a^2+c^2/4=\frac{(a^2+b^2)^2}{16a^2}+\frac{c^2}{4}. \tag{3.6}$$

First we assume that $3b^2 = a^2$, hence $l^2 = \min\{1/3b^4, b^2, b^2/3 + 1/12b^4\} = 1/2$ by easy calculations, we get the optimal non-lattice arrangement with the parameters $b^2 = 1/2$, $a^2 = 3/2$, $c^2 = 4/3$, $x = 1/12$, $y = 1/4$, $z = 0$. The vectors XX^G, $g \in G$ will be

(3.4*) $$(0,0,0),\ (-1/16; -1/2; 1/2),\ (1/3; 0; 1/2),\ (1/2; -1/2; 0)$$

plus any integer triple from the lattice L_G. We shall prove that $l^2 \leqq 1/2$ holds also in the other cases. We introduce a new variable u by

(3.7) $$u^2 = a^2/b^2 > 1.$$

1) Assume that

(3.8) $$1/2 \leqq c^2 \leqq (a^2 + b^2)/4 < b^2 < a^2, \text{ i.e. by substitution, } 1 < u^2 < 3$$

and $1/2 \leqq c^2 \leqq 2^{-4/3}u^{-2/3}(u^2+1)^{2/3}$ for any fixed u. Then $d^2 = \frac{1}{16c}\frac{(u^2+1)^2}{u^3} + \frac{c^2}{4}$ stands by (3.6) and

(3.9) $$d^2 \leqq \max\{2^{-7/2}u^{-3}(u^2+1)^2 + 2^{-4}; 2^{-10/3}u^{-8/3}(2u^2+1)(u^2+1)^{2/3}\}$$

holds for any fixed $u \in (1, 3^{1/2})$. Since both the above functions of u would take their maxima either at 1 or at $3^{1/2}$, hence

(3.10) $$d^2 < \max\{2^{-3/2} + 2^{-4}; 2^{1/2}3^{-3/2} + 2^{-4}; 3(2^{-8/3}); 7(2^{-2})3^{-4/3}\} < 1/2.$$

2) Assume that $1 < u^2 < 3$ and $1/2 \leqq (a^2 + b^2)/4 \leqq c^2$. Introducing $e^2 = (a^2 + b^2)/4$, we express all the variables by e and u. Then we have our assumptions:

(3.11) $$1 < u^2 < 3 \text{ and } 1/2 \leqq e^2 \leqq 2^{-4/3}u^{-2/3}(u^2+1)^{2/3}$$

for any fixed u. By (3.6) we have

(3.12) $$d^2 = \frac{e^2}{4}\frac{(u^2+1)}{u^2} + \frac{1}{64e^4}\frac{(u^2+1)^2}{u^2}$$

and, again by substitution

(3.13) $$d^2 \leqq \max\{2^{-4}u^{-2}(u^2+1)(u^2+3); 2^{-10/3}u^{-8/3}(2u^2+1)(u^2+1)^{2/3}\}$$

holds for any fixed $u \in (1, 3^{1/2})$. Again, taking $u^2 = 1$ and 3 in (3.13) we obtain

(3.14) $$d^2 < \max\{1/2; 1/2; 3(2)^{-8/3}; 7(2)^{-2}(3)^{-4/3}\} = 1/2.$$

3) Assume $1/2 \leqq c^2 \leqq b^2 < (a^2+b^2)/4$. We express all the variables by c and u. Then

$$(3.15) \qquad 3 < u^2 \text{ and } 1/2 \leqq c^2 \leqq u^{-2/3} \text{ means also } u^2 \leqq 8.$$

Again $d^2 = \frac{1}{16c}\frac{(u^2+1)^2}{u^3} + \frac{c^2}{4}$ and

$$(3.16) \qquad d^2 \leqq \max\{2^{-7/2}u^{-3}(u^2+1)^2 + 2^{-4}; 2^{-4}; 2^{-4}u^{-8/3}(u^4+6u^2+1)\}$$

holds for any fixed $u^2 \in (3,8]$. Hence

$$(3.17) \qquad d^2 \leqq \max\{2^{1/2}3^{-3/2} + 2^{-4}; 5^2 2^{-8}; 7(2^{-2})3^{-4/3}; 2^{-8}113\} < 1/2.$$

4) Finally, assume $3 < u^2$ and $1/2 \leqq b^2 \leqq c^2$. Then

$$(3.18) \qquad 1/2 \leqq b^2 \leqq u^{-2/3} \quad \text{and} \quad 3 < u^2 \leqq 8$$

hold. Now

$$(3.19) \qquad d^2 = \frac{b^2}{16}\frac{(u^2+1)^2}{u^2} + \frac{1}{4u^2b^4}$$

stands and

$$(3.20) \qquad d^2 \leqq \max\{2^{-5}u^{-2}(u^2+1)^2 + u^{-2}; 2^{-4}u^{-8/3}(u^4+6u^2+1)\}$$

holds for any fixed $u^2 \in (3,8]$. Hence

$$(3.21) \qquad d^2 < \max\{1/2; 2^{-8}113; 7(2)^{-2}3^{-4/3}; 2^{-8}113\} = 1/2.$$

So, we have two optimal ball systems for $G = \mathrm{Pca}2_1$

$$(3.22) \qquad \begin{array}{l} 1.\ a=b=c=1, \quad x=0, \quad y=1/4, \quad z=0 \quad (3.4) \\ 2.\ a^2=3/2,\ b^2=1/2,\ c^2=4/3,\ x=1/12,\ y=1/4,\ z=0 \quad (3.4^*). \end{array}$$

Secondly, we take the group $G = \mathrm{Pna}2_1$. In this case the lattice L_G is also spanned by the orthogonal basis $\{\mathbf{e}_i\}$ where the lengths of these vectors are a, b, c, respectively. The point positions are:

$$(3.23) \qquad \begin{array}{c} X(x,y,z),\ X^{2_1}(-x,-y,z+1/2),\ X^n(1/2-x,1/2+y,1/2+z) \\ \text{and } X^a(1/2+x,1/2-y,z) \end{array}$$

and the vectors XX^g, $g \in G$ are of the form:

$$(3.24) \qquad (0,0,0),\ (-2x,-2y,1/2),\ (1/2-2x,1/2,1/2),\ (1/2,1/2-2y,0)$$

plus an integer triple from L_G.

Since the metric normalizer is $M_G = \mathrm{Z}^1\mathrm{mmm}$ and its fundamental set is $F(M_G) = \{(x,y,z) \mid z = 0 \leqq x, y \leqq 1/4\}$ we get the following:

$$l = \min\Big\{a, b, c, (4x^2a^2 + 4y^2b^2 + c^2/4)^{1/2}, \tag{3.25}$$
$$[(1/2-2x)^2a^2 + (b^2+c^2)/4]^{1/2},\ [a^2/4 + (1/2-2y)^2b^2]^{1/2}\Big\}$$

and

$$\delta(G) = (2\pi/3)\max\{l^3 \mid 0 \leqq x, y \leqq 1/4,\ 0 < a, b, c, \text{ and } abc = 1\}, \tag{3.26}$$

for this reason we have to prove the inequality $l^2 \leqq 1/2$, too. Certainly we may assume that $a^2, b^2, c^2 \geqq 1/2$ (3.27) and prove

$$\max\Big\{\min\{(4x^2a^2 + 4y^2b^2 + c^2/4), [(1/2-2x)^2a^2 + (b^2+c^2)/4],$$
$$[a^2/4 + (1/2-2y)^2b^2]\} \mid 0 \leqq x, y \leqq 1/4,\ 1/2 < a^2, b^2, c^2 = (ab)^{-2}\Big\} = 1/2.$$

We have the same geometric statement as in the Lemma at the group $\mathrm{P}2_12_12_1$ (see Figure 4).

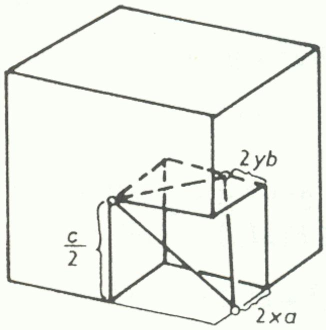


Fig. 4

The optimal arrangements in this case are as follows:

1. $a^2 = 2,\quad b^2 = 1/2,\quad c^2 = 1,\quad x = 1/8,\quad y = 1/4,\quad z = 0;$
2. $a^2 = 3/2,\quad b^2 = 1/2,\quad c^2 = 4/3,\quad x = 1/6,\quad y = z = 0;$
3. $a = b = c = 1,\quad x = 1/4,\quad y = z = 0.$

4. The groups $\mathrm{P}4_1$, $\mathrm{P}3_1$, and $\mathrm{P}6_1$

First we take the group $G = \mathrm{P}4_1$. The translation lattice L_G is spanned by the orthogonal basis $\{\mathbf{e}_i\}$ with the lengths a, a, c, respectively. The point positions are:

$$X(x,y,z),\ X^s(-y,x,z+1/4),\ X^{s^2}(-x,-y,z+1/2)$$
$$X^{s^3}(y,-x,z+3/4) \tag{4.1}$$

and the vectors XX^g, $g \in G$ are:

$$(4.2)\quad (0,0,0),\ (-y-x, x-y, 1/4),\ (-2x, -2y, 1/2),\ (y-x, -x-y, 3/4)$$

plus an integer triple from L_G. The metric normalizer M_G is the group Z^1422 and its fundamental domain is

$$(4.3)\qquad F(M_G) = \{(x,y,z) \mid z=0,\ x \geqq 0,\ y-x \geqq 0,\ 1/2-x-y \geqq 0\}.$$

Let l be the $\inf\{\varrho(XX^g) \mid g \in G\}$. It is easy to see that

$$(4.4)\quad l = \min\{a, c, [2(x^2+y^2)a^2 + c^2/16]^{1/2}, [(4x^2+(1-2y)^2)a^2 + c^2/4]^{1/2}\}$$

and

$$(4.5)\qquad \delta(G) = (2\pi/3)\max\{l^3/a^2c \mid x, y \in F(M_G),\ a, c > 0\}.$$

Suppose that $a^2c = 1$ and $a, c \geqq 2^{-1/2}$. This means that we have to prove the following inequality:

$$(4.6)\qquad \max\Big\{\min\{2(x^2+y^2)a^2 + c^2/16, (4x^2+(1-2y)^2)a^2 + c^2/4\} \mid \\ \mid 1/2 \leqq a^2 = 1/c, c^2; x, y \in F(M_G)\Big\} \leqq 1/2.$$

First we assume that $2^{-1/2} \leqq c \leqq (8/3)^{1/3}$. Fixing the value c we look for those points $(x,y,0) \in F(M_G)$ where

$$(4.7)\qquad 2(x^2+y^2)a^2 + c^2/16 = [4x^2 + (1-2y)^2]a^2 + c^2/4 =: d^2.$$

It is easy to see that from this we get

$$(4.8)\qquad c^3 = (32/3)[-x^2 - (y-1)^2 + 1/2] \leqq 8/3$$

and so

$$x^2 = 1/2 - (y-1)^2 - 3c^3/32.$$

That means

$$(4.9)\qquad d^2 = 2(x^2+y^2)a^2 + c^2/16 = (-1+4y)/c - c^2/8.$$

Since by (4.3) the inequalities $0 \leqq x \leqq 1/2 - y$ hold, from (4.8) we get

$$(4.10)\quad 1/2 - 3c^3/32 = (y-1)^2 + x^2 \leqq (y-1)^2 + (1/2-y)^2 = 2y^2 - 3y + 5/4$$

and so

$$(4.11)\qquad y \leqq 3/4 - (12-3c^3)^{1/2}/8.$$

By (4.9) we have

$$d^2 \leqq 2/c - c^2/8 - (3/c^2 - 3c/4)^{1/2} =: g(c). \tag{4.12}$$

A difficult computation shows that $g(c) \leqq 1/2$ on the closed interval $[2^{-1/2}, (8/3)^{1/3}]$.

Consider now $5^{1/2} - 1 \leqq c \leqq 2$. Since the points $(x, y, 0)$ are elements of $F(M_G)$, it is easy to see that $0 \leqq x^2 + y^2 \leqq 1/4$ and so

$$2(x^2 + y^2)a^2 + c^2/16 \leqq 1/2c + c^2/16 \leqq 1/2. \tag{4.13}$$

By (4.6) we have considered each occurring c, and the optimal packing is the following: 1, $a^2 = 1/2$, $c = 2$, $x = z = 0$, $y = 1/2$.

Secondly, we take the group $G = \mathrm{P}3_1$. Now the translation lattice L_G is spanned by the basis $\{\mathbf{e}_i\}$ with Gramian matrix

$$(\langle \mathbf{e}_i, \mathbf{e}_j \rangle) = \begin{bmatrix} a^2 & -a^2/2 & 0 \\ -a^2/2 & a^2 & 0 \\ 0 & 0 & c^2 \end{bmatrix}. \tag{4.15}$$

The point positions are

$$X(x, y, z),\ X^s(-y, x - y, z + 1/3),\ X^{s^2}(y - x, -x, z + 2/3) \tag{4.16}$$

and the vectors XX^g, $g \in G$ are

$$(0, 0, 0),\ (-y - x, x - 2y, 1/3),\ (y - 2x, -x - y, 2/3) \tag{4.17}$$

plus a vector from L_G. The metric normalizer M_G is the group $\mathrm{Z}^1 622$ and its fundamental domain is

$$F(M_G) = \{(x, y, z) \mid z = 0,\ 0 \leqq y,\ 0 \leqq 1/3 - x,\ 0 \leqq x/2 - y\}. \tag{4.18}$$

Let l be the infimum by (0.2) then

$$\delta(G) = \frac{\pi l^3}{a^2 c 3^{1/2}}. \tag{4.19}$$

If $l^3 = a^2 c/6^{1/2}$ then $\delta(G) = \pi/18^{1/2}$. Suppose $a^2 c = 1$ then we have to prove that the maximum l^2 is not greater than $6^{-1/3}$ if the number c is on the closed interval $[6^{-1/6}, 6^{1/3}]$. But

$$\begin{aligned} l^2 &\leqq (y + x)^2 a^2 + (x - 2y)^2 a^2 - (x + y)(2y - x)a^2 + c^2/9 = \\ &= (3/4)[3x^2 + (x - 2y)^2]a^2 + c^2/9 \leqq a^2/3 + c^2/9 =: d^2, \end{aligned} \tag{4.20}$$

where the equality stands iff $x=1/3$, $y=0$. Taking into consideration $a^2 = c^{-1}$, the function $d^2 := (a^2/3 + c^2/9)^{1/2}$ is not greater than $6^{-1/6}$ on the interval $[6^{-1/6}, 6^{1/3}]$. If $c = 6^{1/3}$ then $d^2 = 6^{-1/6}$. Thus

$$\delta(G) = \pi/18^{1/2} \tag{4.21}$$

holds, too. The optimal arrangement is the following:

$$a^2 = 6^{-1/3}, \quad c = 6^{1/3}, \quad x = 1/3, \quad y = z = 0, \tag{4.22}$$

and the packing is the densest lattice-like one. This is the well-known double lattice-like packing with the density $\pi/18^{1/2}$.

We take now the space group $G = \mathrm{P}6_1$. The lattice L_G is the same as in the previous case of $\mathrm{P}3_1$. Figure 5 shows the projection onto the plane $(0; \mathbf{e}_1, \mathbf{e}_2)$.

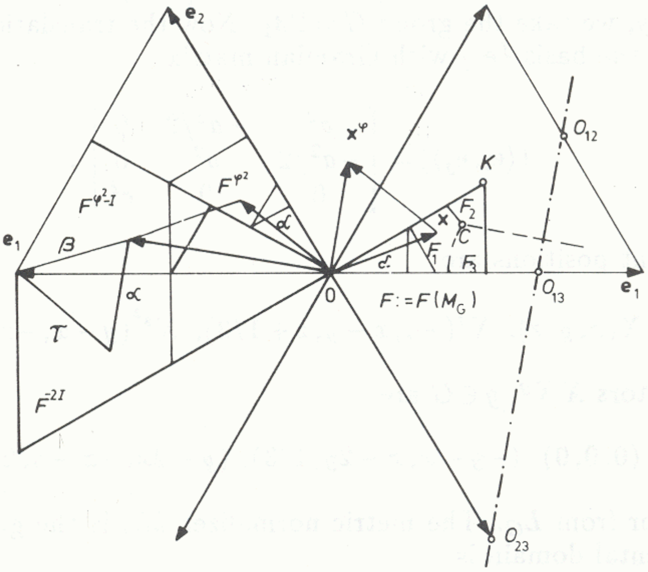


Fig. 5

Denote $X(x,y,z)$ a general point. The vectors XX^g, $g \in G$ are

$$\begin{gathered}(0,0,0),\ (-y, x-y, 1/6),\ (-y-x, x-2y, 1/3),\ (-2x, -2y, 1/2),\\ (y-2x, x-y, 2/3),\ (y-x, -x, 5/6)\end{gathered} \tag{4.23}$$

plus an integer triple from L_G.

The metric normalizer M_G is the group $\mathrm{Z}^1 622$ with the fundamental domain

$$F := F(M_G) = \{X(x,y,z) \mid z = 0,\ 0 \leqq y,\ 0 \leqq y - 2x + 1,\ 0 \leqq x - 2y\}. \tag{4.24}$$

In Figure 5 we see F with the projection vector $\mathbf{x}(x,y)$ of OX. Let $\varphi\colon \mathbf{x} \longmapsto \mathbf{x}^\varphi$ denote the 6-rotation through $\pi/3$. Then the vectors in (4.23) have components in the $(\mathbf{e}_1, \mathbf{e}_2)$-plane:

$$\mathbf{x} - \mathbf{x} = 0,\ \mathbf{x}^\varphi - \mathbf{x} = \mathbf{x}^{\varphi^2},\ \mathbf{x}^{\varphi^2} - \mathbf{x},\ \mathbf{x}^{\varphi^3} - \mathbf{x} = -2\mathbf{x}, \dots,$$

which determine also the corresponding images of F denoted by

(4.25) $$F^{\varphi^2}, F^{\varphi^2-I}, F^{-2I}, \quad \text{respectively.}$$

We look for the maximal density

$$\delta(G) = \frac{2\pi l^3}{a^2 c(3)^{1/2}}$$

where l is the infimum by (0.2). We may assume $a^2c = 1$ and conclude that

$$l^2 = \min\{d_1^2, d_2^2, d_3^2, c^2, a^2 = 1/c\} \quad \text{with}$$

$$d_1^2 = [(-y)^2 + (x-y)^2 + y(x-y)]/c + c^2/36 = (x^2+y^2-xy)/c + c^2/36 =:$$
$$=: \alpha^2/c + c^2/36,$$

(4.26) $$d_2^2 = [(-1+y+x)^2 + (-x+2y)^2 - (-1+y+x)(-x+2y)]/c + c^2/9 =$$
$$= (3\alpha^2 - 3x + 1)/c + c^2/9 =: \beta^2/c + c^2/9,$$
$$d_3^2 = [(-1+2x)^2 + (2y)^2 - (-1+2x)(2y)]/c + c^2/4 =$$
$$= (4\alpha^2 - 4x + 2y + 1)/c + c^2/4 =: \tau^2/c + c^2/4.$$

To show $\delta(G) \leqq \pi(18)^{-1/2}$, we shall prove that

(4.27) $$\min\{d_1^2, d_2^2, d_3^2\} \leqq (24)^{-1/3} \quad \text{if } c \in [(24)^{-1/6}, (24)^{1/3}].$$

We draw three curves $c_{ij} := \{(x,y) \in F \mid d_i^2 = d_j^2\}$ $i \neq j = 1,2,3$. These are circle arcs with centres $O_{12}(1, 1/2)$, $O_{13}(2/3, 0)$, $O_{23}(0, -1)$ as follows:

(4.28) $$c_{12} : (x-1)^2 + (y-1/2)^2 - (x-1)(y-1/2) = 1/4 - c^3/24, \quad c^3 \leqq 6;$$

(4.29) $$c_{13} : (x-2/3)^2 + y^2 - (x-2/3)y = 1/9 - 2c^3/27, \quad c^3 \leqq 3/2;$$

(4.30) $$c_{23} : x^2 + (y+1)^2 - x(y+1) = 1 - 5c^3/36, \quad c^3 \leqq 36/5.$$

Thus we determine the domain F_i in F, where d_i^2 is the minimum in (4.27). The pencil of circles c_{ij} may have a common point C where the minimum d_i^2 is maximal. This fact depends on the parameter c of the group $G = \mathrm{P}6_1$. A straightforward but awful computation yields the coordinates of the extremal point C. First, C lies on the power line of the circle pencil $\{c_{ij}\}$:

(4.31) $$x + 4y = 1 - 7c^3/36.$$

Then we substitute, say, into (4.28) and solve the equation of second degree. We obtain $C(x_c, y_c)$

(4.32)
$$x_c = \frac{5}{7} - \frac{c^3}{36} - \frac{1}{2(3)^3 7}[2^4 3^6 - 2^3 3^3 5(7)c^3 - 3(7)^2 c^6]^{1/2},$$
$$y_c = \frac{1}{14} - \frac{c^3}{24} + \frac{1}{2^3 3^3 7}[2^4 3^6 - 2^3 3^3 5(7)c^3 - 3(7)^2 c^6]^{1/2},$$

whenever $c^3 \leqq (2^2 3^2/7)(2(7)^{1/2} - 5) = 1.4992$, i.e. $c \leqq 1.1445$.

C just lies on F if (x_c, y_c) satisfies (4.24) besides

$$0.5888 = (24)^{-1/6} \leqq c \leqq (24)^{1/3} = 2.8845.$$

We obtain for $C \in F$ the interval

(4.33) $$0.5888 = (24)^{-1/6} \leqq c \leqq 7^{-2/3}(162(57)^{1/2} - 1170)^{1/3} = 1.0270,$$

(4.34) $$d_1^2(C) = \frac{2^2}{7c} - \frac{c^2}{18} - \frac{1}{2^2 3^2 7c}[2^4 3^6 - 2^3 3^3 5(7)c^3 - 3(7)^2 c^6]^{1/2}.$$

A careful computation shows that $d_1^2(C) \leqq (24)^{-1/3}$ holds on the interval (4.33). If C lies out of F, then the intersection of c_{12} and the segment on $y = 2x - 1$, i.e.

(4.35) $$H(3/4 - (9 - 2c^3)^{1/2}/12; 1/2 - (9 - 2c^3)^{1/2}/6)$$

provides the minimum by (4.27), and we obtain

(4.36) $$d_1^2(H) = 5/(8c) - c^2/72 - (9 - 2c^3)^{1/2}/(8c) \text{ for } 1.027 \leqq c \leqq 4^{1/3}.$$

We need again a careful computation to show that $d_1^2(H) \leqq (24)^{-1/3} = 0.34668$ holds on the interval (4.36). If $c^3 = 4$ then we arrive into the vertex $K(2/3, 1/3)$ of F. In the interval

(4.37) $$4 \leqq c^3 \leqq 24, \text{ i.e. } 1.5874 \leqq c \leqq 2.8845$$

the point $K(2/3, 1/3)$ provides the minimum in (4.27) and

(4.38) $$d_1^2(K) = 1/(3c) + c^2/36$$

is a convex function in (4.37), taking its maximum at $c = (24)^{1/3}$. Then $d_1^2 = (24)^{-1/3}$ as we stated at (4.27). We have got the optimal ball arrangement parametrized by

(4.39) $$c = (24)^{1/3} \quad a = (24)^{-1/6} \quad x = 2/3 \quad y = 1/3.$$

This arrangement is not lattice-like.

We remark that the last observation at (4.38) would give the estimate $l^2 \leqq (24)^{-1/3}$ in the interval

$$1.0558 = 3^{5/6} - 3^{1/3} \leqq c \leqq (24)^{-1/3} = 2.8845,$$

but this does not give more and we need such awful computations as we did.

Now the result formulated at the end of the introduction is completely proved.

REFERENCES

[1] HILBERT, D. and COHN-VOSSEN, S., *Anschauliche Geometrie*, Die Grundlehren der mathematischen Wissenschaften in Einzeldarstellungen, Bd. 37, Springer-Verlag, Berlin, 1932. *Jb. Fortschritte Math.* **58**, 597

[2] KOCH, E. and FISCHER, W., Euclidean and affine normalizers of space groups and their use in crystallography, *International tables for X-ray crystallography*, Vol. A, Ed. by Theo Hahn, Reidel, 1983.

[3] *International tables for X-ray crystallography*, Vol. A, Ed. by Theo Hahn, Reidel, 1983.

[4] HORVÁTH, Á. G., Egy nehezen kezelhető geometriai szélsőérték problémáról, *Mat. Lapok* (to appear).

[5] HOLLAI, M., Doppelgitterförmige Lagerungen inkongruenter Kreise und Kugeln, *Ann. Univ. Sci. Budapest. Eötvös Sect. Math.* **18** (1975), 75–86. *MR* **54** #5978a

[6] HORVÁTH, Á. G., On double lattice-like sphere packing, *Ann. Univ. Sci. Budapest. Eötvös Sect. Math.* **33** (1990), 53–60.

[7] MOLNÁR, E., Minimal presentation of the 10 compact Euclidean space forms by fundamental domains, *Studia Sci. Math. Hungar.* **22** (1987), 19–51. *MR* **88j**: 51029

[8] HORVÁTH, Á. G., Correction to my paper "On double lattice-like sphere packing", *Ann. Univ. Sci. Budapest. Eötvös Sect. Math.* (to appear).

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