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ON FINITE SPHERE-PACKINGS

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Abstract: Given k unit balls in Euclidean d-space E^d, what is the minimal volume of their convex hull? In E^2 hexagonal circle-packings, possibly degenerate, are best possible ([6], [8]). In E^d, $d \geq 5$ the linear arrangement of the k balls is conjectured to be optimal. L. Fejes Tóth's sausage conjecture [3], and several partial results (cf. [1],[4]) support this conjecture. In E^3 and E^4 no such general results can be expected, because the situation is more complicated. We consider $d = 3$: In the sausage-catastrophe (cf [9]) it is conjectured that for all $k < 56$ the linear arrangement is optimal, whereas for all but finitely many $k \geq 56$ clusters of spheres are best possible. Although this is supported by computer-aided calculation, a proof seems to be very hard. However, we can prove: For no $k \geq 56$ but 57,58,63 and 64 the sausage is optimal.

1. Introduction

Dense packings of finitely many spheres are good models for atom clusters. So in recent years there were several investigations about various aspects on finite circle- or sphere-packings (cf. e.g. [1], [3] – [6], [8], [9]). In this paper we define the density of finite sphere-packings via the minimal volume of the convex hull of the spheres. For simplicity we only consider unit spheres, i.e. $B^3 = \{x \in E^3 | \, ||x|| \le 1\}$. Further $\mathcal{L}$ denotes the lattice of the densest lattice packing of unit spheres. Given k unit spheres $B_i^3 = B^3 + c_i$, $i = 1, \dots, k$ in E^3 with mutual disjoint interiors, the volume of their convex hull is given by the Steiner formula (cf. e.g. [7])

$$V(C_k + B^3) = V(C_k) + F(C_k) + M(C_k) + \frac{4}{3}\pi,$$

where $C_k = \text{conv}(c_1, \dots, c_k)$ and V, F, M denote the volume, surface area and integral of mean curvature.

The problem is to minimize $V(C_k + B^3)$ for a given fixed k and all possible C_k i.e. with mutual distance ≥ 2 of any of the c_i.

The "icefern"-theorem ([1], Th. 2) says that if one restricts oneself to planar C_k, then the linear arrangement, i.e. $C_k = S_k$, where S_k is a segment of length $2(k-1)$, is minimal, i.e.

$$V(S_k + B^3) \le V(C_k + B^3).$$

In other words, the sausage is better than any other planar arrangement of k unit balls. It is conjectured that for all $k < 56$ this inequality even holds for arbitrary C_k. Although computer-aided calculations support this conjecture, called sausage-catastrophe, an exact proof is still open for all $k \ge 4$. On the other hand simple considerations show that for all sufficiently large k there are lattice points $c_i \in \mathcal{L}$, $i = 1, \dots, k$ such that for the lattice-polyhedron $C_k = \text{conv}(c_1, \dots, c_k)$ holds

$$(*) \qquad V(C_k + B^3) < V(S_k + B^3).$$

Obviously for sufficiently large k there are also C_k with $(*)$, which are no lattice-polyhedra. For k not too large, say $k < 100$, the difference in $(*)$ is so small that no general proof for $(*)$ and all possible k can be expected. However, the following result solves the problem for all but four $k \ge 56$.

Theorem. *For each $k \ge 56$, $k \ne 57, 58, 63, 64$ there is a C_k with $(*)$.*

Remarks. 1) For $k = 61, 67, 71, 77, 81, 83$ the C_k with $(*)$ are no lattice polyhedra. It remains open if for these k there are lattice polyhedra C_k with $(*)$.

2) We conjecture that for $k = 57, 58, 63$ and 64 the sausage is optimal. For the proof we need 11 lemmas. The theorem follows from Lemmas 5,6,7,8,9 and 11.

2. Definitions. The lattice polyhedra

Definition 1. Let T_1^n be the basic regular tetrahedron of $\mathcal{L}$ with edge-length 2, i.e. the convex hull of 4 lattice-points of $\mathcal{L}$. For $n \in \mathbb{N}$ let $T_n = nT_1$.

Definition 2. Let $P_{1,1,1}$ be the lattice parallelohedron of $\mathcal{L}$ with edges of length 2 parallel to those of T_1, i.e. the convex hull of 8 lattice-points of $\mathcal{L}$. For $0 \leq a \leq b \leq c$, $a, b, c \in \mathbb{N} \cup \{0\}$ let $P_{a,b,c}$ denote the lattice parallelohedron with edge-lengths $2a \leq 2b \leq 2c$, generated from $P_{1,1,1}$.

Remark. For $a = b = 0$, $c = k-1$ we get $P_{0,0,k-1} = S_k$ and $P_{0,0,k-1} + +B^3$ is the sausage with k balls. Besides this case we will only consider $2 \leq a \leq b \leq c$.

The T_n and $P_{a,b,c}$ are the basic lattice polyhedra and we obtain our general lattice polyhedra C_k for the theorem by omitting suitable lattice-points, or, in other words, by suitable truncations of the T_n and $P_{a,b,c}$. We will have two types of truncations: 1) by regular simplices, 2) by nonregular simplices. We start with the easier case:

1) From a vertex of T_n we cut off a copy of T_p, $p < n$. After compactifying the truncated or snub tetrahedron again we denote it by T_n^p. If we do so with each vertex of T_n we obtain

$$T_n^{p,q,r,s},\ 0 \leq p \leq q \leq r \leq s,$$

where 0 means no truncation; in particular $T_n^{0,0,0,0} = T_n$. Further we only consider n, p, q, r, s such that $T_n^{p,q,r,s} \neq \emptyset$. We can do the same truncation with $P_{a,b,c}$:

Each $P_{a,b,c}$ with $a \geq 1$ has exactly 2 acute vertices of the same type as T_n. So from these 2 vertices we cut off a copy of T_p and T_q with $0 \leq p \leq q \leq a$. After compactifying we obtain the truncated lattice parallelohedron $P_{a,b,c}^{p,q}$. For $P_{a,b,c}$ we write $P_{a,b,c}^{0,0}$.

2) The second type of truncation we describe via $T_2^{1,0,0,0}$ which has 3 vertices c_1, c_2, c_3 of the same type as a regular tetrahedron and 3 vertices v_1, v_2, v_3 of same type, which we call obtuse vertices. So

$T_2^{1,0,0,0} = \text{conv}(c_3, v_1, v_2, v_3)$ with $||c_i - v_i|| = 2$ $(i = 1, 2, 3)$, $||v_i - v_j|| = 2$ and $||c_i - c_j|| = 4$ $(i \neq j)$. Now let $T = \text{conv}(c_1, c_2, c_3, v_1, v_2, v_3)$ and $T^* = \text{conv}(c_1, c_2, c_3, v_2, v_3)$. Then $T \cup T^* = T_2^{1,0,0,0}$ and $T \cap T^* = \text{conv}(c_1, v_2, v_3) = T'$. Simple considerations show $||c_1 - v_2|| = ||c_1 - v_3|| = 2\sqrt{3}$. So T' is a triangle with two edges of length $2\sqrt{3}$ and one edge length 2. Further T is a tetrahedron with two edges of length $2\sqrt{3}$ and four edges of length 2.

The truncations of second type will be truncations of congruent copies of T. For this we consider $P_{a,b,c}^{p,q}$ with $a \geq 2$ and $0 < p \leq q < a$. Then easy considerations show that $P_{a,b,c}^{p,q}$ has at least two obtuse vertices as the vertices v_1, v_2, v_3 of $T_2^{1,0,0,0}$. At one or both of these vertices we cut off one or two copies of T and compactify. The new truncated polyhedron we denote by $P_{a,b,c}^{p,q,t}$ with $t \in \{1, 2\}$ and $0 < p \leq q < a$.

If we write $P_{a,b,c}^{p,q,o} = P_{a,b,c}^{p,q}$, we obtain the general truncated parallelohedron

$$P_{a,b,c}^{p,q,t} \; 0 \leq p \leq q \leq a \leq b \leq c, \quad t \in \{0, 1, 2\}, \tag{4}$$

which will solve $(*)$ for all but 14 values of k in the theorem.
This second type of truncation is only needed once for $T_n^{a,b,c,d}$ (namely for $k = 84$), so we do not introduce an extra notation for this special case.

3. Basic lemmas on lattice polyhedra

In this section we calculate V, F and M for the simplest polyhedra in our proof.

Lemma 1. $k(P_{a,b,c}) = (a+1)(b+1)(c+1)$, $V(P_{a,b,c}) = 4\sqrt{2}abc$, $F(P_{a,b,c}) = 4\sqrt{3}(ab + ac + bc)$, $M(P_{a,b,c}) = 2\pi(a + b + c)$.

Proof. Elementary calculation shows
$V(P_{1,1,1}) = 4\sqrt{2}$, $F(P_{1,1,1}) = 4\sqrt{3}(1+1+1)$, $M(P_{1,1,1}) = 2\pi(1+1+1)$. From this one obtains the general case if one observes that $P_{a,b,c}$ can be dissected into abc copies of $P_{1,1,1}$. The calculation of $k(P_{a,b,c})$ is simple. $\diamondsuit$

Lemma 2. $k(T_n) = \binom{n+3}{3}$, $V(T_n) = \frac{2}{3}\sqrt{2}n^3$, $F(T_n) = 4\sqrt{3}n^2$,

$M(T_n) = 11,4638\ldots n$ $k(T'_n) = \binom{n+2}{2}$, $F(T'_n) = 2\sqrt{3}n^2$, $M(T'_n) = 3\pi n$, *where* T'_n *is a facet of* T_n.

Proof. For $k(T_n)$ see [7], for $M(T_1)$ and hence for $M(T_n)$ see [2] or [7]. The other results are simple. ♢

In the following lemma we calculate V, F and M for the non-regular tetrahedron T (described in Sect. 2) and for its largest facet T'.

Lemma 3. $V(T) = V(T_1) = \frac{2}{3}\sqrt{2}$, $F(T) = 3\sqrt{3} + \sqrt{11}$, $M(T) = 14,3441\ldots$, $F(T') = 2\sqrt{11}$, $M(T') = 14,0244\ldots$.

Proof. For the calculation of $M(T)$ we introduce coordinates (only in this lemma). Again $T = \mathrm{conv}(v_1, v_2, v_3, c_3)$.

Let $v_1 = \sqrt{2}(1,0,0)$, $v_2 = \sqrt{2}(0,1,0)$, $v_3 = \sqrt{2}(0,0,1)$, $c_3 = \sqrt{2}(-1,-1,1)$. Then $||v_1 - v_2|| = ||v_1 - v_3|| = ||v_2 - v_3|| = ||v_3 - c_3|| = 2$ and $||v_1 - c_3|| = ||v_2 - c_3|| = 2\sqrt{3}$ as required.

Elementary calculation shows $V(T) = V(T_1) = \frac{2}{3}\sqrt{2}$, $F(T) = 3\sqrt{3} + \sqrt{11}$ and $F(T') = 2\sqrt{11}$. (The surface area of T' is twice its 2-dimensional volume). Further $M(T')$ is the sum of the length of its three edges multiplied with $\frac{\pi}{2}$, hence $M(T') = \frac{\pi}{2}(2 + 2\sqrt{3}) = 14,0244\ldots$.

It remains to calculate $M(T)$. For this we determine the affine hulls of the 4 facets of T:

$$E_1 = \mathrm{aff}(v_1, v_2, v_3) = \{(x,y,z) | x + y + z = \sqrt{2}\}$$
$$E_2 = \mathrm{aff}(v_1, v_3, c_3) = \{(x,y,z) | x - y + z = \sqrt{2}\}$$
$$E_3 = \mathrm{aff}(v_2, v_3, c_3) = \{(x,y,z) | -x + y + z = \sqrt{2}\}$$
$$E_4 = \mathrm{aff}(v_1, v_2, c_3) = \{(x,y,z) | -x - y - 3z = \sqrt{2}\}.$$

From this one gets the angles of the outer normals of the E_i:

$$\cos(E_1, E_2) = \cos(E_1, E_3) = \tfrac{1}{3} = \cos\alpha$$
$$\cos(E_2, E_3) = -\tfrac{1}{3} = \cos\beta$$
$$\cos(E_1, E_4) = -5/\sqrt{33} = \cos\gamma$$
$$\cos(E_2, E_4) = \cos(E_3, E_4) = -3/\sqrt{33} = \cos\delta$$

and hence (normalized to 2π):$\alpha = 0,5148\ldots$,$\beta = 1,0213\ldots$,$\gamma = 1,9106\ldots$, $\delta = 1,2310\ldots$. Now for M holds $M(T) = \sum_i \alpha_i l_i$ (cf. e.g. [7]), where the sum is taken over the 6 edges of T; l_i is the length of the i-th edge and α_i is the measure of the corresponding outer normals, normalized to π such that $\alpha_1 = \alpha_2 = \frac{1}{2}\alpha$, $\alpha_3 = \beta$, $\alpha_4 = \gamma$, $\alpha_5 = \alpha_6 = \frac{1}{2}\delta$. Then with $l_{1,2,3,4} = 2$, $l_5 = l_6 = 2\sqrt{3}$ one obtains $M(T) = 2\alpha + \beta + \gamma + 2\sqrt{3}\delta = 14,3441\ldots$. ♢

4. The general case. Parallelohedra

Lemma 4. $k\left(P^{p,q,t}_{a,b,c}\right) = (a+1)(b+1)(c+1) - \binom{p+2}{3} - \binom{q+2}{3} - t.$

Proof. From the construction of $P^{p,q,t}_{a,b,c}$ and the additivity of the lattice point number follows with the Lemmas 1 and 2:

$$k\left(P^{p,q,t}_{a,b,c}\right) = (a+1)(b+1)(c+1) - \binom{p+3}{3} + \binom{p+2}{2} - \binom{q+3}{3} + \binom{q+2}{2} - t$$
$$= (a+1)(b+1)(c+1) - \binom{p+2}{3} + \binom{q+2}{3} - t.$$

Lemma 5. *Let* $k = (a+1)(b+1)(c+1) - \binom{p+2}{3} - \binom{q+2}{3}$ $(p, q \in \{0,1,2\})$ *and*

(a) $a \geq 2$, $b \geq 3$, $c \geq 8$ *or*
(b) $a \geq 2$, $b \geq 4$, $c \geq 5$ *or*
(c) $a \geq 3$, $b \geq 3$, $c \geq 4$.

Then $(*)$ *holds with* $C_k = P^{p,q}_{a,b,c}$.

Proof. Let k be given as above. Then by Lemma 4 we can choose $C_k = P^{p,q}_{a,b,c}$.

Further $V(S_k + B^3) = 2\pi(k - 1 + \frac{4}{3}\pi = 2\pi((a+1)(b+1)(c+1) - 1) - 2\pi\left(\binom{p+2}{3} + \binom{q+2}{3}\right) + \frac{4}{3}\pi$. From Lemmas 1 and 2 we have $V(C_k + B^3) = \{V(P_{a,b,c}) - V(T_p) - V(T_q)\} + \{F(P_{a,b,c}) - F(T_p) + F(T'_p) - F(T_q) + F(T'_q)\} + \{M(P_{a,b,c}) - M(T_p) + M(T'_p) - M(T_q) + M(T'_q)\} + \frac{4}{3}\pi = \{4\sqrt{2}abc - \frac{2}{3}\sqrt{2}(p^3 + q^3)\} + \{4\sqrt{3}(ab + ac + bc) - 2\sqrt{3}(p^2 + q^2)\} + \{2\pi(a+b+c) - (11{,}4638\ldots - 3\pi)(p+1)\} + \frac{4}{3}\pi$. So we get $V(C_k + B^3) - V(S_k + B^3) = abc(4\sqrt{2} - 2\pi) + (ab + ac + bc)(4\sqrt{3} - 2\pi) - \frac{1}{3}(2\sqrt{2} - \pi)(p^3 + q^3) - (2\sqrt{3} - \pi)(p^2 + q^2) + \delta(p+q) = \beta abc(a^{-1} + b^{-1} + c^{-1} - \gamma) + \{\frac{1}{6}\beta\gamma(p^3 + q^3) - \frac{1}{2}\beta(p^2 + q^2) + \delta(p+q)\} = A + B$, where $\beta = 2(2\sqrt{3} - \pi) = 0{,}64502\ldots$, $\gamma = (\pi - 2\sqrt{2}) : (2\sqrt{3} - \pi) = 0{,}9710\ldots$ and $\delta = 3\pi + \frac{2}{3}\pi - 11{,}4638\ldots = 0{,}0553\ldots$.

We show that $A + B < 0$. In all cases (a), (b), (c) we have

$$a^{-1} + b^{-1} + c^{-1} \leq \tfrac{23}{24} < \gamma,$$

hence $A < 0$. To show $B \leq 0$ it suffices to consider only p: $B_p = \frac{1}{6}\beta\gamma p^3 - \frac{1}{2}\beta p^2 + \delta p$. Now $B_0 = 0$, $B_1 = \frac{1}{2}\beta(\frac{1}{3}\gamma - 1) + \delta < 0$, $B_2 = \beta(\frac{4}{3}\gamma - 2) + 2\delta < 0$. So $B \leq 0$, i.e. $A + B < 0$ and $V(C_k + B^3) - V(S_k + B^3) < 0$.

Lemma 6. *Let* $k = 16(c+1) - \binom{p+2}{3} - \binom{q+2}{3} - t$, *and*
(a) $c \geq 4,\ t = 0,\ p, q \in \{0,1,2,3\}$ *or*
(b) $c \geq 5,\ t = 1,\ p, q \in \{1,2,\}$ *or*
(c) $c \geq 6,\ t = 1,\ p \in \{1,2\},\ q = 3$ *or*
(d) $c \geq 7,\ t = 2,\ q \in \{2,3\}$.
Then $(*)$ *holds with* $C_k = P^{p,q,t}_{3,3,c}$.

Proof. Let k be given as above. Then by Lemma 4 we can choose $C_k = P^{p,q,t}_{3,3,c}$. As in the proof of Lemma 5 we get (now with $a = b = 3$) and with Lemma 3 for $(*)$:

$V(C_k + B^3) - V(S_k + B^3) = A + B - t\{V(T) + F(T) - F(T') +$
$+ M(T) - M(T') - 2\pi\} = A + B - t(\frac{2}{3}\sqrt{2} + 3\sqrt{3} - \sqrt{11} + 0{,}3197\ldots - 2\pi) =$

$$= A + B - Ct = \Delta, \text{where} \tag{4.1}$$

$$A = 9\beta c(\tfrac{2}{3} + c^{-1} - \gamma) = 3\beta(2c + 3 - 3c\gamma)$$

$$B = \tfrac{1}{6}\beta\gamma(p^3 + q^3) - \tfrac{1}{2}\beta(p^2 + q^2) + \delta(p + q) = B_p + B_q,$$

$$C = 3{,}14\ldots.$$

It remains to prove $\Delta < 0$ in all cases. From the proof of Lemma 5 we have $B_0 = 0$, $B_1 = -0{,}162\ldots$, $B_2 = -0{,}344\ldots$, $B_3 = \frac{9}{2}\beta(\gamma - 1) + 3\delta = 0{,}082\ldots$, hence $B_2 < B_1 < B_0 = 0 < B_3$. To prove $\Delta < 0$ it suffices to prove $(*)$ for the worst cases in (a), (b), (c), (d):

(a) $c = 4,\ t = 0,\ p = q = 3$.
Then $\Delta = 3\beta(11 - 12\gamma) + 2B_3 < 0$.
(b) $c = 5,\ t = 1,\ p = q = 1$.
Then $\Delta = 3\beta(13 - 15\gamma) + 2B_1 + C < 0$.
(c) $c = 6,\ t = 1,\ p = 1,\ q = 3$.
Then $\Delta = 3\beta(15 - 18\gamma) + B_1 + B_3 + C < 0$.
(d) $c = 7,\ t = 2,\ p = 1,\ q = 3$.
Then $\Delta = 3\beta(17 - 21\gamma) + B_1 + B_3 + 2C < 0$.

These inequalities prove Lemma 6. ◊

Lemma 7. *The* k *in Lemmas 5 and 6 cover all* k *of the theorem except the fifteen cases* $k \in \{56, 59, 61, 62, 65, 67, 68, 71, 73, 74, 77, 81, 83, 84\}$.

Proof. We start with Lemma 6 which covers nearly all of these k. We write $k = 16c + 16 - R$, $R = \binom{p+2}{3} + \binom{q+2}{3} + t$ and calculate R for (a), (b), (c), (d):

(a) $t = 0,\ p, q \in \{0,1,2,3\}$ yield $R = 0, 1, 2, 4, 5, 8, 10, 11, 14$ and 20.
(b) $t = 1,\ p, q \in \{1,2\}$ yield $R = 3, 6, 9$.

(c) $t = 1,\ p \in \{1, 2\},\ q = 3$ yield $R = 12, 15$.
(d) $t = 2,\ p = 1,\ q \in \{2, 3\}$ yield $R = 7, 13$.
The special case $p = q = 3$, i.e. $R = 20$, is only needed for $c = 4$ and yields $k = 60$.
The other cases in (a),(b),(c),(d) cover all residue classes modulo 16, and from Lemma 6 follows with $c \geq 7$ that all $k \geq 112$ are covered.
For $c = 6$ the only missing k are $k = 112 - R$, $R = 7$ and 13, hence $k = 105$ and 99.
For $c = 5$ the only missing k are $k = 96 - R$, $R = 7, 12, 13, 15$, hence $k = 81, 83, 84, 89$.
For $c = 4$ the only missing k are $k = 80 - R$, $R = 3, 6, 7, 9, 12, 13, 15$, hence $k = 65, 67, 68, 71, 73, 74, 77$.
Three of these k are covered by Lemma 5, namely $k = 3 \cdot 5 \cdot 7 = 105$, $k = 4 \cdot 4 \cdot 5 - 1 = 99$, and $k = 3 \cdot 5 \cdot 6 - 1 = 89$.
This proves Lemma 7.

5. Truncated tetrahedra

In the preceeding section the theorem was proved for all but 14 k. In this section we prove it for eight of these k; seven in Lemma 8, one in Lemma 9.

Lemma 8. *Let $k \in \{56, 59, 62, 65, 68, 73, 74\}$. Then there are positive integers n, p, q, r, s with $p \leq q \leq r \leq s$, $r + s \leq n$ such that $(*)$ holds with $C_k = T_n^{p,q,r,s}$.*

Proof. From Lemma 2 and $r + s \leq n$ follows, if one observes that V is simply additive and that F, M and k are additive:

$$V(T_n^{p,q,r,s}) = \tfrac{2}{3}\sqrt{2}(n^3 - p^3 - q^3 - r^3 - s^3)$$

$$F(T_n^{p,q,r,s}) = 2\sqrt{3}(2n^2 - p^2 - q^2 - r^2 - s^2)$$

$$M(T_n^{p,q,r,s}) = 11,4638\ldots(n - p - q - r - s) + 3\pi(p + q + r + s)$$

$$(5.1) \qquad k(T_n^{p,q,r,s}) = \binom{n+3}{3} - \binom{p+2}{3} - \binom{q+2}{3} - \binom{r+2}{3} - \binom{s+2}{3}.$$

So $k = \frac{1}{6}(n^3 - p^3 - q^3 - r^3 - s^3) + \frac{1}{2}(2n^2 - p^2 - q^2 - r^2 - s^2) + \frac{1}{3}(\frac{11}{2}n -$

$-p-q-r-s)+1$ and

$$V(C_k+B^3)-V(S_k+B^3)=$$

$$=\tfrac{1}{3}(2\sqrt{2}-\pi)(n^3-p^3-q^3-r^3-s^3)+(2\sqrt{3}-\pi)(2n^2-p^2-q^2-r^2-s^2)-$$

$$-(\tfrac{11}{3}\pi-11,4638\ldots)(n-p-q-r-s)=$$

$$=-0,10438\ldots(n^3-p^3-q^3-r^3-s^3)+0,3225\ldots(2n^2-p^2-q^2-r^2-s^2)$$

$$(5.2)\qquad -0,055\ldots(n-p-q-r-s)=\Delta.$$

We now consider the 7 cases separately by calculating k from (5.1) and Δ from (5.2). We omit the easy calculations for Δ.

(1) $k(T_6^{2,2,3,3})=56;\ \Delta=-0,183\ldots<0$

(2) $k(T_6^{1,2,3,3})=59;\ \Delta=-0,002\ldots<0$

(3) $k(T_6^{2,2,2,3})=62;\ \Delta=-0,610\ldots<0$

(4) $k(T_6^{1,2,2,3})=65;\ \Delta=-0,428\ldots<0$

(5) $k(T_6^{2,2,2,2})=68;\ \Delta=-1,036\ldots<0$

(6) $k(T_6^{1,1,2,2})=74;\ \Delta=-0,673\ldots<0$

(7) $k(T_7^{2,2,2,5})=73;\ \Delta=-0,356\ldots<0$

These seven inequalities prove Lemma 8. ◊

Lemma 9. *For* $k=84$ *holds* $(*)$.

Proof. From (5.1) we get $k(T_7^{1,2,3,4})=85$.

With $C_{85}=T_7^{1,2,3,4}$ we get from (5.2) with some calculation $V(C_{85}+$ $+B^3)-V(S_{85}+B^3)=-3,27\ldots<0$.

Now $T_7^{1,2,3,4}$ obviously has at least one (in fact six) obtuse vertex as defined in Section 2. We cut off the irregular tetrahedron associated to this vertex as described for $P_{a,b,c}^{p,q,t}$, $t=1$ and obtain a truncated tetrahedron $\bar{T}_7^{1,2,3,4}$. Obviously $k(\bar{T}_7^{1,2,3,4})=84$, so we write $C_{84}=$ $=\bar{T}_7^{1,2,3,4}$. As in (4.1) we now get $C=3,14\ldots$: $V(C_{84}+B^3)-V(S_{84}-$ $-B^3)=V(C_{85}+B^3)-V(S_{85}+B^3)+C=$ $=-3,27\ldots+3,14\ldots<0$ which proves the lemma. ◊

6. Double tetrahedra

In this section we consider non-lattice packings for the last six k. If we fit two copies of T_n together at one facet, one obtains in an obvious way a double-tetrahedron (or bipyramide) D_n, endowed with the sphere-centres c_i of the two copies of T_n. D_n has exactly two acute vertices of same type as T_n. Hence we can truncate D_n by copies of T_p, T_q $(p, q < n)$ in the same way as we did to obtain $P^{p,q}_{a,b,c}$ and $T^{p,q,r,s}_n$. We denote this truncated and compactified D_n by $D^{p,q}_n$.

Lemma 10. *For $p \leq q < n$ we have*
$V(D^{p,q}_n) = \frac{2}{3}\sqrt{2}(2n^3 - p^3 - q^3)$
$F(D^{p,q}_n) = 2\sqrt{3}(3n^2 - p^2 - q^2)$
$M(D^{p,q}_n) = (2M(T_1) - 3\pi)n - (M(T_1) - 3\pi)(p + q)$
$k(D^{p,q}_n) = \binom{n+3}{3} + \binom{n+2}{3} - \binom{p+2}{3} - \binom{q+2}{3}$.

Proof. The results follow from Lemma 2, from the definition of $D^{p,q}_n$, and from the fact that V is simply additive and that F, M and k are additive. ♢

Lemma 11. *Let $k \in \{61, 67, 71, 77, 81, 83\}$. Then there are positive integers $p \leq q < n$, such that $(*)$ holds with $C_k = D^{p,q}_n$.*

Proof. From Lemma 10 we have

$$(6.1) \quad k(D^{p,q}_n) = \binom{n+3}{3} + \binom{n+2}{3} - \binom{p+2}{3} - \binom{q+2}{3} =$$
$$= \tfrac{1}{6}(2n^3 - p^3 - q^3) + \tfrac{1}{2}(3n^2 - p^2 - q^2) + \tfrac{13}{6}n - \tfrac{1}{3}(p+1) + 1.$$

So we get as in Lemma 8

$$V(C_k + B^3) - V(S_k + B^3) = V(D^{p,q}_n) + F(D^{p,q}_n) + M(D^{p,q}_n) - 2\pi(k-1) =$$
$$= \tfrac{1}{3}(2\sqrt{2} - \pi)(2n^3 - p^3 - q^3) + (2\sqrt{3} - \pi)(3n^2 - p^2 - q^2) + (2M(T_1) -$$
$$-3\pi - \tfrac{13}{3}\pi)n - (M(T_1) - 3\pi - \tfrac{2}{3}\pi)(p + q) = -0,104\ldots(2n^3 - p^3 - q^3) +$$
$$+0,3225\ldots(3n^2 - p^2 - q^2) - 0,11\ldots n - 0,055\ldots(p+q) = \Delta$$

We now consider the six cases separately by calculating k from (6.1) and Δ from the last equality. We omit the easy calculations for Δ.

(1) $k(D^{3,4}_5) = 61, \ \Delta = -1,40\ldots < 0$

(2) $k(D^{2,4}_5) = 67, \ \Delta = -1,72\ldots < 0$

(3) $k(D^{3,3}_5) = 71, \ \Delta = -2,95\ldots < 0$

(4) $k(D^{2,3}_5) = 77, \ \Delta = -3,27\ldots < 0$

(5) $k(D^{0,3}_5) = 81, \ \Delta = -2,70\ldots < 0$

(6) $k(D^{2,2}_5) = 83, \ \Delta = -3,58\ldots < 0$

These six inequalities prove Lemma 12. ◇

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References

[1] BETKE, U.; GRITZMANN, P; WILLS, J.M.: Slices of L. Fejes Tóth's sausage conjecture; *Mathematika* **29** (1982), 194-201.

[2] COXETER, H.S.M : Regular polytopes, 3rd ed., Dover, New York, 1973.

[3] FEJES TÓTH, L.: Research problem 13; *Period. Math. Hungar.* **6** (1975), 197-199.

[4] FEJES TÓTH, G.; GRITZMANN, P; WILLS, J.M.: Finite sphere packing and sphere covering; *Disc. Comp. Geom.* **4** (1889), 19-40.

[5] GRAHAM, R.L.; SLOANE, N.J.A.: Penny-packing and two-dimensional codes; *Disc. Comp. Geom.* **5** (1990), 1-11.

[6] GROEMER, H.: Über die Einlagerung von Kreisen in einen konvexen Bereich; *Math. Z.* **73** (1960), 285-294.

[7] HADWIGER, H. : Altes und Neues über konvexe Körper; Birkhäuser, Basel, 1955.

[8] WEGNER, G.: Über endliche Kreispackungen in der Ebene; *Studia Sci. Math. Hungar.* **21** (1986), 1-28.

[9] WILLS, J.M.: On the density of finite packings; *Acta Math. Hungar.* **46** (1985), 205-210.