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Contact Numbers for Congruent Sphere Packings in Euclidean 3-Space

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Abstract The contact graph of an arbitrary finite packing of unit balls in Euclidean 3-space is the (simple) graph whose vertices correspond to the packing elements and whose two vertices are connected by an edge if the corresponding two packing elements touch each other. One of the most basic questions on contact graphs is to find the maximum number of edges that a contact graph of a packing of n unit balls can have. Our method for finding lower and upper estimates for the largest contact numbers is a combination of analytic and combinatorial ideas and it is also based on some recent results on sphere packings. In particular, we prove that if $C(n)$ denotes the largest number of touching pairs in a packing of $n>1$ congruent balls in Euclidean 3-space, then $0.695 < \frac{6n-C(n)}{n^{\frac{2}{3}}} < \sqrt[3]{486} = 7.862\ldots$ for all $n = \frac{k(2k^2+1)}{3}$ with $k \geq 2$.

Keywords Congruent sphere packing · Contact number · Density · (truncated) Voronoi cell · Union of balls · Isoperimetric inequality · Spherical cap packing

1 Introduction

Let $\mathbb{E}^d$ denote the d-dimensional Euclidean space. Then the *contact graph* of an arbitrary finite packing of unit balls (i.e., of an arbitrary finite family of non-overlapping balls having unit radii) in $\mathbb{E}^d$ is the (simple) graph whose vertices correspond to the

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packing elements and whose two vertices are connected by an edge if and only if the corresponding two packing elements touch each other. One of the most basic questions on contact graphs is to find the maximum number of edges that a contact graph of a packing of n unit balls can have in $\mathbb{E}^d$. In 1974 Harborth [6] proved the following optimal result in $\mathbb{E}^2$: the maximum number $c(n)$ of touching pairs in a packing of n congruent circular disks in $\mathbb{E}^2$ is precisely $\lfloor 3n-\sqrt{12n-3}\rfloor$ implying that

$$\lim_{n\to+\infty}\frac{3n-c(n)}{\sqrt{n}}=\sqrt{12}=3.464\ldots.$$

Some years later the author [2] has proved the following estimates in higher dimensions. The number of touching pairs in an arbitrary packing of $n>1$ unit balls in $\mathbb{E}^d$, $d\geq 3$ is less than

$$\frac{1}{2}\tau_d\, n-\frac{1}{2^d}\delta_d^{-\frac{d-1}{d}}n^{\frac{d-1}{d}},$$

where τ_d stands for the kissing number of a unit ball in $\mathbb{E}^d$ (i.e., it denotes the maximum number of non-overlapping unit balls of $\mathbb{E}^d$ that can touch a given unit ball in $\mathbb{E}^d$) and δ_d denotes the largest possible density for (infinite) packings of unit balls in $\mathbb{E}^d$. Now, recall that on the one hand, according to the well-known theorem of Kabatiansky and Levenshtein [7] $\tau_d\leq 2^{0.401d(1+o(1))}$ and $\delta_d\leq 2^{-0.599d(1+o(1))}$ as $d\to+\infty$ on the other hand, $\tau_3=12$ (for the first complete proof see [12]) moreover, according to the recent breakthrough result of Hales [5] $\delta_3=\frac{\pi}{\sqrt{18}}$. Thus, by combining the above results together we find that the number of touching pairs in an arbitrary packing of $n>1$ unit balls in $\mathbb{E}^d$ is less than

$$\frac{1}{2}2^{0.401d(1+o(1))}n-\frac{1}{2}2^{-0.401(d-1)(1-o(1))}n^{\frac{d-1}{d}}$$

as $d\to+\infty$ and in particular, it is less than

$$6n-\frac{1}{8}\left(\frac{\pi}{\sqrt{18}}\right)^{-\frac{2}{3}}n^{\frac{2}{3}}=6n-0.152\ldots n^{\frac{2}{3}}$$

for $d=3$. The main purpose of this note is to improve further the latter result. In order, to state our theorem in a proper form we need to introduce a bit of additional terminology. If $\mathcal{P}$ is a packing of n unit balls in $\mathbb{E}^3$, then let $C(\mathcal{P})$ stand for the number of touching pairs in $\mathcal{P}$, that is, let $C(\mathcal{P})$ denote the number of edges of the contact graph of $\mathcal{P}$ and call it the *contact number* of $\mathcal{P}$. Moreover, let $C(n)$ be the largest $C(\mathcal{P})$ for packings $\mathcal{P}$ of n unit balls in $\mathbb{E}^3$. Finally, let us imagine that we generate packings of n unit balls in $\mathbb{E}^3$ in such a special way that each and every center of the n unit balls chosen, is a lattice point of the face-centered cubic lattice Λ_{fcc} with shortest non-zero lattice vector of length 2. Then let $C_{fcc}(n)$ denote the largest possible contact number of all packings of n unit balls obtained in this way. Before stating our main theorem we make the following comments. First, recall that according to [5] the lattice unit sphere packing generated by Λ_{fcc} gives the largest possible density for unit ball packings in $\mathbb{E}^3$, namely $\frac{\pi}{\sqrt{18}}$ with each ball touched by 12 others such that their centers form the vertices of a cuboctahedron. Second, it is easy to see that $C_{fcc}(2)=C(2)=1$, $C_{fcc}(3)=C(3)=3$, $C_{fcc}(4)=C(4)=6$. Third, it is natural to conjecture that $C_{fcc}(9) = C(9) = 21$. If this were true, then based on the trivial inequalities $C(n+1) \geq C(n)+3$, $C_{fcc}(n+1) \geq C_{fcc}(n)+3$ valid for all $n \geq 2$, it would follow that $C_{fcc}(5) = C(5) = 9$, $C_{fcc}(6) = C(6) = 12$, $C_{fcc}(7) = C(7) = 15$, and $C_{fcc}(8) = C(8) = 18$. Furthermore, we note that $C(10) \geq 25$, $C(11) \geq 29$, and $C(12) \geq 33$. In order to see that, one should take the union $\mathbf{U}$ of two regular octahedra of edge length 2 in $\mathbb{E}^3$ such that they share a regular triangle face T in common and lie on opposite sides of it. If we take the unit balls centered at the nine vertices of $\mathbf{U}$, then there are exactly 21 touching pairs among them. Also, we note that along each side of T the dihedral angle of $\mathbf{U}$ is concave and in fact, it can be completed to 2π by adding twice the dihedral angle of a regular tetrahedron in $\mathbb{E}^3$. This means that along each side of T two triangular faces of $\mathbf{U}$ meet such that for their four vertices there exists precisely one point in $\mathbb{E}^3$ lying outside $\mathbf{U}$ and at distance 2 from each of the four vertices. Finally, if we take the twelve vertices of a cuboctahedron of edge length 2 in $\mathbb{E}^3$ along with its center of symmetry, then the thirteen unit balls centered about them have 36 contacts implying that $C(13) \geq 36$. Whether in any of the inequalities $C(10) \geq 25$, $C(11) \geq 29$, $C(12) \geq 33$, and $C(13) \geq 36$ we have equality is a challenging open question. In the rest of this note we give a proof of the following theorem.

Theorem 1.1

(i) $C(n) < 6n - 0.695n^{\frac{2}{3}}$ *for all* $n \geq 2$.
(ii) $C_{fcc}(n) < 6n - \frac{3\sqrt[3]{18\pi}}{\pi}n^{\frac{2}{3}} = 6n - 3.665\ldots n^{\frac{2}{3}}$ *for all* $n \geq 2$.
(iii) $6n - \sqrt[3]{486}n^{\frac{2}{3}} < C_{fcc}(n) \leq C(n)$ *for all* $n = \frac{k(2k^2+1)}{3}$ *with* $k \geq 2$.

As an immediate result we get

Corollary 1.2

$$0.695 < \frac{6n - C(n)}{n^{\frac{2}{3}}} < \sqrt[3]{486} = 7.862\ldots$$

for all $n = \frac{k(2k^2+1)}{3}$ *with* $k \geq 2$.

The following was noted in [2]. Due to the Minkowski difference body method (see for example, Chap. 6 in [11]) the family $\mathcal{P}_{\mathbf{K}} := \{\mathbf{t}_1 + \mathbf{K}, \mathbf{t}_2 + \mathbf{K}, \ldots, \mathbf{t}_n + \mathbf{K}\}$ of n translates of the convex body $\mathbf{K}$ in $\mathbb{E}^d$ is a packing if and only if the family $\mathcal{P}_{\mathbf{K_o}} := \{\mathbf{t}_1 + \mathbf{K_o}, \mathbf{t}_2 + \mathbf{K_o}, \ldots, \mathbf{t}_n + \mathbf{K_o}\}$ of n translates of the symmetric difference body $\mathbf{K_o} := \frac{1}{2}(\mathbf{K} + (-\mathbf{K}))$ of $\mathbf{K}$ is a packing in $\mathbb{E}^d$. Moreover, the number of touching pairs in the packing $\mathcal{P}_{\mathbf{K}}$ is equal to the number of touching pairs in the packing $\mathcal{P}_{\mathbf{K_o}}$. Thus, for this reason and for the reason that if $\mathbf{K}$ is a convex body of constant width in $\mathbb{E}^d$, then $\mathbf{K_o}$ is a ball of $\mathbb{E}^d$, Theorem 1.1 extends in a straightforward way to translative packings of convex bodies of constant width in $\mathbb{E}^3$.

For the sake of completeness we mention that the nature of contact numbers changes dramatically for non-congruent sphere packings in $\mathbb{E}^3$. For more details on that we refer the interested reader to the elegant paper [8] of Kuperberg and Schramm.

Last but not least, it would be interesting to improve further the estimates of Theorem 1.1. In the last section of this paper we mention a particular packing conjecture that could lead to a significant improvement on the estimate (i) in Theorem 1.1.

2 Proof of Theorem 1.1

2.1 Proof of (i)

Let $\mathbf{B}$ denote the (closed) unit ball centered at the origin $\mathbf{o}$ of $\mathbb{E}^3$ and let $\mathcal{P} := \{\mathbf{c}_1 + \mathbf{B}, \mathbf{c}_2 + \mathbf{B}, \dots, \mathbf{c}_n + \mathbf{B}\}$ denote the packing of n unit balls with centers $\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_n$ in $\mathbb{E}^3$ having the largest number $C(n)$ of touching pairs among all packings of n unit balls in $\mathbb{E}^3$. ($\mathcal{P}$ might not be uniquely determined up to congruence in which case $\mathcal{P}$ stands for any of those extremal packings.) Now, let $\hat{r} := 1.81383$. The following statement shows the main property of $\hat{r}$ that is needed for our proof of Theorem 1.1.

Lemma 2.1 *Let $\mathbf{B}_1, \mathbf{B}_2, \dots, \mathbf{B}_{13}$ be 13 different members of a packing of unit balls in $\mathbb{E}^3$. Assume that each ball of the family $\mathbf{B}_2, \mathbf{B}_3, \dots, \mathbf{B}_{13}$ touches $\mathbf{B}_1$. Let $\hat{\mathbf{B}}_i$ be the closed ball concentric with $\mathbf{B}_i$ having radius $\hat{r}$, $1 \le i \le 13$. Then the boundary $\mathrm{bd}(\hat{\mathbf{B}}_1)$ of $\hat{\mathbf{B}}_1$ is covered by the balls $\hat{\mathbf{B}}_2, \hat{\mathbf{B}}_3, \dots, \hat{\mathbf{B}}_{13}$, that is,*

$$\mathrm{bd}(\hat{\mathbf{B}}_1) \subset \bigcup_{j=2}^{13} \hat{\mathbf{B}}_j.$$

Proof Let $\mathbf{o}_i$ be the center of the unit ball $\mathbf{B}_i$, $1 \le i \le 13$ and assume that $\mathbf{B}_1$ is tangent to the unit balls $\mathbf{B}_2, \mathbf{B}_3, \dots, \mathbf{B}_{13}$ at the points $\mathbf{t}_j \in \mathrm{bd}(\mathbf{B}_j) \cap \mathrm{bd}(\mathbf{B}_1)$, $2 \le j \le 13$.

Let α denote the measure of the angles opposite to the equal sides of the isosceles triangle $\Delta\mathbf{o}_1\mathbf{p}\mathbf{q}$ with $\mathrm{dist}(\mathbf{o}_1, \mathbf{p}) = 2$ and $\mathrm{dist}(\mathbf{p}, \mathbf{q}) = \mathrm{dist}(\mathbf{o}_1, \mathbf{q}) = \hat{r}$, where $\mathrm{dist}(\cdot, \cdot)$ denotes the Euclidean distance between the corresponding two points. Clearly, $\cos\alpha = \frac{1}{\hat{r}}$ with $\alpha < \frac{\pi}{3}$.

Proposition 2.2 *Let $\mathbf{T}$ be the convex hull of the points $\mathbf{t}_2, \mathbf{t}_3, \dots, \mathbf{t}_{13}$. Then the radius of the circumscribed circle of each face of the convex polyhedron $\mathbf{T}$ is less than $\sin\alpha$.*

Proof Let F be an arbitrary face of $\mathbf{T}$ with vertices $\mathbf{t}_j$, $j \in I_F \subset \{2, 3, \dots, 13\}$ and let $\mathbf{c}_F$ denote the center of the circumscribed circle of F. Clearly, the triangle $\Delta\mathbf{o}_1\mathbf{c}_F\mathbf{t}_j$ is a right triangle with a right angle at $\mathbf{c}_F$ and with an acute angle of measure β_F at $\mathbf{o}_1$ for all $j \in I_F$. We have to show that $\beta_F < \alpha$. We prove this by contradiction. Namely, assume that $\alpha \le \beta_F$. Then either $\frac{\pi}{3} < \beta_F$ or $\alpha \le \beta_F \le \frac{\pi}{3}$. First, let us take a closer look of the case $\frac{\pi}{3} < \beta_F$. Reflect the point $\mathbf{o}_1$ about the plane of F and label the point obtained by $\mathbf{o}_1'$. Clearly, the triangle $\Delta\mathbf{o}_1\mathbf{o}_1'\mathbf{o}_j$ is a right triangle with a right angle at $\mathbf{o}_1'$ and with an acute angle of measure β_F at $\mathbf{o}_1$ for all $j \in I_F$. Then reflect the point $\mathbf{o}_1$ about $\mathbf{o}_1'$ and label the point obtained by $\mathbf{o}_1''$ furthermore, let $\mathbf{B}_1''$ denote the unit ball centered at $\mathbf{o}_1''$. As $\frac{\pi}{3} < \beta_F$ therefore $\mathrm{dist}(\mathbf{o}_1, \mathbf{o}_1'') < 2$, and so one can simply translate $\mathbf{B}_1''$ along the line $\mathbf{o}_1\mathbf{o}_1''$ away from $\mathbf{o}_1$ to a new position say, $\mathbf{B}_1'''$ such that it is tangent to $\mathbf{B}_1$. However, this would mean that $\mathbf{B}_1$ is tangent to 13 non-overlapping unit balls namely, to $\mathbf{B}_1''', \mathbf{B}_2, \mathbf{B}_3, \dots, \mathbf{B}_{13}$, clearly contradicting to the well-known fact [12] that this number cannot be larger than 12. Thus, we are left with the case when $\alpha \le \beta_F \le \frac{\pi}{3}$. By repeating the definitions of $\mathbf{o}_1'$, $\mathbf{o}_1''$, and $\mathbf{B}_1''$, the inequality $\beta_F \le \frac{\pi}{3}$ implies in a straightforward way that the 14 unit balls $\mathbf{B}_1, \mathbf{B}_1'', \mathbf{B}_2, \mathbf{B}_3, \dots, \mathbf{B}_{13}$ form a packing in $\mathbb{E}^3$. Moreover, the inequality $\alpha \le \beta_F$ yields that $\operatorname{dist}(\mathbf{o}_1, \mathbf{o}_1'') \le 4\cos\alpha = \frac{4}{\hat{r}} = 2.205278333691\ldots < 2.205279217705$. Finally, notice that the latter inequality contradicts to the following recent result of Böröczky and Szabó [3].

Lemma 2.3 *Let* $\mathbf{B}_1, \mathbf{B}_2, \dots, \mathbf{B}_{14}$ *be* 14 *different members of a packing of unit balls in* $\mathbb{E}^3$. *Assume that each ball of the family* $\mathbf{B}_2, \mathbf{B}_3, \dots, \mathbf{B}_{13}$ *touches* $\mathbf{B}_1$. *Then the distance between the centers of* $\mathbf{B}_1$ *and* $\mathbf{B}_{14}$ *is at least*

$$2.205279217705.$$

This completes the proof of Proposition 2.2. □

Now, we are ready to prove Lemma 2.1. First, we note that by projecting the faces F of $\mathbf{T}$ from the center point $\mathbf{o}_1$ onto the sphere $\operatorname{bd}(\hat{\mathbf{B}}_1)$ we get a tiling of $\operatorname{bd}(\hat{\mathbf{B}}_1)$ into spherically convex polygons $\hat{F}$. Thus, it is sufficient to show that if F is an arbitrary face of $\mathbf{T}$ with vertices $\mathbf{t}_j$, $j \in I_F \subset \{2, 3, \dots, 13\}$, then its central projection $\hat{F} \subset \operatorname{bd}(\hat{\mathbf{B}}_1)$ is covered by the closed balls $\hat{\mathbf{B}}_j$, $j \in I_F \subset \{2, 3, \dots, 13\}$. Second, in order to achieve this it is sufficient to prove that the projection $\hat{\mathbf{c}}_F$ of the center $\mathbf{c}_F$ of the circumscribed circle of F from the center point $\mathbf{o}_1$ onto the sphere $\operatorname{bd}(\hat{\mathbf{B}}_1)$ is covered by each of the closed balls $\hat{\mathbf{B}}_j$, $j \in I_F \subset \{2, 3, \dots, 13\}$. Indeed, if in the triangle $\Delta\mathbf{o}_1\mathbf{o}_j\hat{\mathbf{c}}_F$ the measure of the angle at $\mathbf{o}_1$ is denoted by β_F, then Proposition 2.2 implies in a straightforward way that $\beta_F < \alpha$. Hence, based on $\operatorname{dist}(\mathbf{o}_1, \mathbf{o}_j) = 2$ and $\operatorname{dist}(\mathbf{o}_1, \hat{\mathbf{c}}_F) = \hat{r}$, a simple comparison of the triangle $\Delta\mathbf{o}_1\mathbf{o}_j\hat{\mathbf{c}}_F$ with the triangle $\Delta\mathbf{o}_1\mathbf{p}\mathbf{q}$ yields that $\operatorname{dist}(\mathbf{o}_j, \hat{\mathbf{c}}_F) < \hat{r}$ holds for all $j \in I_F \subset \{2, 3, \dots, 13\}$, finishing the proof of Lemma 2.1. □

Next, let us take the union $\bigcup_{i=1}^n (\mathbf{c}_i + \hat{r}\mathbf{B})$ of the closed balls $\mathbf{c}_1 + \hat{r}\mathbf{B}, \mathbf{c}_2 + \hat{r}\mathbf{B}, \dots, \mathbf{c}_n + \hat{r}\mathbf{B}$ of radii $\hat{r}$ centered at the points $\mathbf{c}_1, \mathbf{c}_2, \dots, \mathbf{c}_n$ in $\mathbb{E}^3$.

Lemma 2.4

$$\frac{n\operatorname{vol}_3(\mathbf{B})}{\operatorname{vol}_3(\bigcup_{i=1}^n (\mathbf{c}_i + \hat{r}\mathbf{B}))} < 0.7785,$$

where $\operatorname{vol}_3(\cdot)$ *refers to the* 3*-dimensional volume of the corresponding set.*

Proof First, partition $\bigcup_{i=1}^n (\mathbf{c}_i + \hat{r}\mathbf{B})$ into truncated Voronoi cells as follows. Let $\mathbf{P}_i$ denote the Voronoi cell of the packing $\mathcal{P}$ assigned to $\mathbf{c}_i + \mathbf{B}$, $1 \le i \le n$, that is, let $\mathbf{P}_i$ stand for the set of points of $\mathbb{E}^3$ that are not farther away from $\mathbf{c}_i$ than from any other $\mathbf{c}_j$ with $j \ne i, 1 \le j \le n$. Then, recall the well-known fact (see for example, [11]) that the Voronoi cells $\mathbf{P}_i$, $1 \le i \le n$ just introduced form a tiling of $\mathbb{E}^3$. Based on this it is easy to see that the truncated Voronoi cells $\mathbf{P}_i \cap (\mathbf{c}_i + \hat{r}\mathbf{B})$, $1 \le i \le n$ generate a tiling of the non-convex container $\bigcup_{i=1}^n (\mathbf{c}_i + \hat{r}\mathbf{B})$ for the packing $\mathcal{P}$. Second, as

$\sqrt{\frac{3}{2}} = 1.2247\ldots < \hat{r} = 1.81383$ therefore the following recent result (Corollary 3 in [1]) of the author applied to the truncated Voronoi cells $\mathbf{P}_i \cap (\mathbf{c}_i + \hat{r}\mathbf{B})$, $1 \le i \le n$ implies the inequality of Lemma 2.4 in a straightforward way.

Lemma 2.5 *Let $\mathcal{F}$ be an arbitrary (finite or infinite) family of non-overlapping unit balls in $\mathbb{E}^3$ with the unit ball $\mathbf{B}$ centered at the origin $\mathbf{o}$ of $\mathbb{E}^3$ belonging to $\mathcal{F}$. Let $\mathbf{P}$ stand for the Voronoi cell of the packing $\mathcal{F}$ assigned to $\mathbf{B}$. Moreover, let $r := \sqrt{\frac{3}{2}} = 1.2247\ldots$ and let $r\mathbf{B}$ denote the (closed) ball of radius r centered at the origin $\mathbf{o}$ of $\mathbb{E}^3$. Then*

$$\frac{\mathrm{vol}_3(\mathbf{B})}{\mathrm{vol}_3(\mathbf{P})} \le \frac{\mathrm{vol}_3(\mathbf{B})}{\mathrm{vol}_3(\mathbf{P} \cap r\mathbf{B})}$$
$$\le \frac{20\sqrt{6}\arctan(\frac{\sqrt{2}}{2}) - 2(2\sqrt{6}-1)\pi}{5\sqrt{2} + 3\pi - 15\arctan(\frac{\sqrt{2}}{2})} = 0.77842\ldots < 0.7785.$$

This finishes the proof of Lemma 2.4. □

The well-known isoperimetric inequality [10] applied to $\bigcup_{i=1}^{n}(\mathbf{c}_i + \hat{r}\mathbf{B})$ yields

Lemma 2.6

$$36\pi \,\mathrm{vol}_3^2\left(\bigcup_{i=1}^{n}(\mathbf{c}_i + \hat{r}\mathbf{B})\right) \le \mathrm{svol}_2^3\left(\mathrm{bd}\left(\bigcup_{i=1}^{n}(\mathbf{c}_i + \hat{r}\mathbf{B})\right)\right),$$

where $\mathrm{svol}_2(\cdot)$ *refers to the* 2*-dimensional surface volume of the corresponding set.*

Thus, Lemmas 2.4 and 2.6 generate the following inequality.

Corollary 2.7

$$14.849236n^{\frac{2}{3}} < 14.84923634\ldots n^{\frac{2}{3}} = \frac{4\pi}{(0.7785)^{\frac{2}{3}}}n^{\frac{2}{3}}$$
$$< \mathrm{svol}_2\left(\mathrm{bd}\left(\bigcup_{i=1}^{n}(\mathbf{c}_i + \hat{r}\mathbf{B})\right)\right).$$

Now, assume that $\mathbf{c}_i + \mathbf{B} \in \mathcal{P}$ is tangent to $\mathbf{c}_j + \mathbf{B} \in \mathcal{P}$ for all $j \in T_i$, where $T_i \subset \{1, 2, \ldots, n\}$ stands for the family of indices $1 \le j \le n$ for which $\mathrm{dist}(\mathbf{c}_i, \mathbf{c}_j) = 2$. Then let $\hat{S}_i := \mathrm{bd}(\mathbf{c}_i + \hat{r}\mathbf{B})$ and let $\hat{\mathbf{c}}_{ij}$ be the intersection of the line segment $\mathbf{c}_i\mathbf{c}_j$ with $\hat{S}_i$ for all $j \in T_i$. Moreover, let $C_{\hat{S}_i}(\hat{\mathbf{c}}_{ij}, \frac{\pi}{6})$ (resp., $C_{\hat{S}_i}(\hat{\mathbf{c}}_{ij}, \alpha)$) denote the open spherical cap of $\hat{S}_i$ centered at $\hat{\mathbf{c}}_{ij} \in \hat{S}_i$ having angular radius $\frac{\pi}{6}$ (resp., α with $0 < \alpha < \frac{\pi}{2}$ and $\cos\alpha = \frac{1}{\hat{r}}$). Clearly, the family $\{C_{\hat{S}_i}(\hat{\mathbf{c}}_{ij}, \frac{\pi}{6}),\ j \in T_i\}$ consists of pairwise disjoint open spherical caps of $\hat{S}_i$; moreover,

$$\frac{\sum_{j\in T_i} \mathrm{svol}_2(C_{\hat{S}_i}(\hat{\mathbf{c}}_{ij}, \frac{\pi}{6}))}{\mathrm{svol}_2(\bigcup_{j\in T_i} C_{\hat{S}_i}(\hat{\mathbf{c}}_{ij}, \alpha))} = \frac{\sum_{j\in T_i} \mathrm{svol}_2(C(\mathbf{u}_{ij}, \frac{\pi}{6}))}{\mathrm{svol}_2(\bigcup_{j\in T_i} C(\mathbf{u}_{ij}, \alpha))}, \tag{1}$$

where $\mathbf{u}_{ij} := \frac{1}{2}(\mathbf{c}_j - \mathbf{c}_i) \in \mathbb{S}^2 := \mathrm{bd}(\mathbf{B})$ and $C(\mathbf{u}_{ij}, \frac{\pi}{6}) \subset \mathbb{S}^2$ (resp., $C(\mathbf{u}_{ij}, \alpha) \subset \mathbb{S}^2$) denotes the open spherical cap of $\mathbb{S}^2$ centered at $\mathbf{u}_{ij}$ having angular radius $\frac{\pi}{6}$ (resp., α). Now, Molnár's density bound (Satz I in [9]) implies that

$$\frac{\sum_{j \in T_i} \mathrm{svol}_2(C(\mathbf{u}_{ij}, \frac{\pi}{6}))}{\mathrm{svol}_2(\bigcup_{j \in T_i} C(\mathbf{u}_{ij}, \alpha))} < 0.89332. \tag{2}$$

In order to estimate $\mathrm{svol}_2(\mathrm{bd}(\bigcup_{i=1}^n (\mathbf{c}_i + \hat{r}\mathbf{B})))$ from above let us assume that m members of $\mathcal{P}$ have 12 touching neighbors in $\mathcal{P}$ and k members of $\mathcal{P}$ have at most nine touching neighbors in $\mathcal{P}$. Thus, $n - m - k$ members of $\mathcal{P}$ have either 10 or 11 touching neighbors in $\mathcal{P}$. (Here we have used the well-known fact that $\tau_3 = 12$, that is, no member of $\mathcal{P}$ can have more than 12 touching neighbors.) Without loss of generality we may assume that $4 \le k \le n - m$.

First, we note that $\mathrm{svol}_2(C(\mathbf{u}_{ij}, \frac{\pi}{6})) = 2\pi(1 - \cos\frac{\pi}{6}) = 2\pi(1 - \frac{\sqrt{3}}{2})$ and $\mathrm{svol}_2(C_{\hat{S}_i}(\hat{\mathbf{c}}_{ij}, \frac{\pi}{6})) = 2\pi(1 - \frac{\sqrt{3}}{2})\hat{r}^2$. Second, recall Lemma 2.1 according to which if a member of $\mathcal{P}$ say, $\mathbf{c}_i + \mathbf{B}$ has exactly 12 touching neighbors in $\mathcal{P}$, then $\hat{S}_i \subset \bigcup_{j \in T_i} (\mathbf{c}_j + \hat{r}\mathbf{B})$, i.e., $\mathrm{svol}_2(\mathrm{bd}(\bigcup_{i=1}^n (\mathbf{c}_i + \hat{r}\mathbf{B})))$ has zero contribution coming from $\hat{S}_i$. These facts together with (1) and (2) imply the following estimate.

Corollary 2.8

$$\mathrm{svol}_2\left(\mathrm{bd}\left(\bigcup_{i=1}^n (\mathbf{c}_i + \hat{r}\mathbf{B})\right)\right) < \frac{32.04253}{3}(n - m - k) + 32.04253k.$$

Proof

$$\begin{aligned}
&\mathrm{svol}_2\left(\mathrm{bd}\left(\bigcup_{i=1}^n (\mathbf{c}_i + \hat{r}\mathbf{B})\right)\right) \\
&\quad < \left(4\pi\hat{r}^2 - \frac{10 \cdot 2\pi(1 - \frac{\sqrt{3}}{2})\hat{r}^2}{0.89332}\right)(n - m - k) + \left(4\pi\hat{r}^2 - \frac{3 \cdot 2\pi(1 - \frac{\sqrt{3}}{2})\hat{r}^2}{0.89332}\right)k \\
&\quad < 10.34119(n - m - k) + 32.04253k < \frac{32.04253}{3}(n - m - k) + 32.04253k. \qquad \square
\end{aligned}$$

Hence, Corollary 2.7 and Corollary 2.8 yield in a straightforward way that

$$1.39026n^{\frac{2}{3}} - 3k < n - m - k. \tag{3}$$

Finally, as the number $C(n)$ of touching pairs in $\mathcal{P}$ is obviously at most

$$\frac{1}{2}\big(12n - (n - m - k) - 3k\big),$$

therefore (3) implies that

$$C(n) \le \frac{1}{2}\big(12n - (n - m - k) - 3k\big) < 6n - 0.69513n^{\frac{2}{3}} < 6n - 0.695n^{\frac{2}{3}},$$

finishing the proof of (i) in Theorem 1.1.

2.2 Proof of (ii)

Although the idea of the proof of (ii) is similar to that of (i) they differ in the combinatorial counting part (see (9)) as well as in the density estimate for packings of spherical caps of angular radii $\frac{\pi}{6}$ (see (8)). Moreover, the proof of (ii) is based on the new parameter value $\bar{r} := \sqrt{2}$ (replacing $\hat{r} = 1.81383$). The details are as follows.

First, recall that if Λ_{fcc} denotes the face-centered cubic lattice with shortest non-zero lattice vector of length 2 in $\mathbb{E}^3$ and we place unit balls centered at each lattice point of Λ_{fcc}, then we get the fcc lattice packing of unit balls, labeled by $\mathcal{P}_{fcc}$, in which each unit ball is touched by 12 others such that their centers form the vertices of a cuboctahedron. (Recall that a cuboctahedron is a convex polyhedron with 8 triangular faces and 6 square faces having 12 identical vertices, with 2 triangles and 2 squares meeting at each, and 24 identical edges, each separating a triangle from a square. As such it is a quasiregular polyhedron, i.e. an Archimedean solid, being vertex-transitive and edge-transitive.) Second, it is well known (see [4] for more details) that the Voronoi cell of each unit ball in $\mathcal{P}_{fcc}$ is a rhombic dodecahedron (the dual of a cuboctahedron) of volume $\sqrt{32}$ (and of circumradius $\sqrt{2}$). Thus, the density of $\mathcal{P}_{fcc}$ is $\frac{\frac{4\pi}{3}}{\sqrt{32}} = \frac{\pi}{\sqrt{18}}$.

Now, let $\mathbf{B}$ denote the unit ball centered at the origin $\mathbf{o} \in \Lambda_{fcc}$ of $\mathbb{E}^3$ and let $\mathcal{P} := \{\mathbf{c}_1 + \mathbf{B}, \mathbf{c}_2 + \mathbf{B}, \ldots, \mathbf{c}_n + \mathbf{B}\}$ denote the packing of n unit balls with centers $\{\mathbf{c}_1, \mathbf{c}_2, \ldots, \mathbf{c}_n\} \subset \Lambda_{fcc}$ in $\mathbb{E}^3$ having the largest number $C_{fcc}(n)$ of touching pairs among all packings of n unit balls being a sub-packing of $\mathcal{P}_{fcc}$. ($\mathcal{P}$ might not be uniquely determined up to congruence in which case $\mathcal{P}$ stands for any of those extremal packings.) As the Voronoi cell of each unit ball in $\mathcal{P}_{fcc}$ is contained in a ball of radius $\bar{r} = \sqrt{2}$ therefore, based on the corresponding decomposition of $\bigcup_{i=1}^n (\mathbf{c}_i + \bar{r}\mathbf{B})$ into truncated Voronoi cells, we get

$$\frac{n \operatorname{vol}_3(\mathbf{B})}{\operatorname{vol}_3(\bigcup_{i=1}^n (\mathbf{c}_i + \bar{r}\mathbf{B}))} < \frac{\pi}{\sqrt{18}} = 0.7404\ldots. \tag{4}$$

As a next step we apply the isoperimetric inequality [10]:

$$36\pi \operatorname{vol}_3^2\left(\bigcup_{i=1}^n (\mathbf{c}_i + \bar{r}\mathbf{B})\right) \le \operatorname{svol}_2^3\left(\operatorname{bd}\left(\bigcup_{i=1}^n (\mathbf{c}_i + \bar{r}\mathbf{B})\right)\right). \tag{5}$$

Thus, (4) and (5) in a straightforward way yield

$$15.3532\ldots n^{\frac{2}{3}} = 4\sqrt[3]{18\pi} n^{\frac{2}{3}} < \operatorname{svol}_2\left(\operatorname{bd}\left(\bigcup_{i=1}^n (\mathbf{c}_i + \bar{r}\mathbf{B})\right)\right). \tag{6}$$

Now, assume that $\mathbf{c}_i + \mathbf{B} \in \mathcal{P}$ is tangent to $\mathbf{c}_j + \mathbf{B} \in \mathcal{P}$ for all $j \in T_i$, where $T_i \subset \{1, 2, \ldots, n\}$ stands for the family of indices $1 \le j \le n$ for which $\operatorname{dist}(\mathbf{c}_i, \mathbf{c}_j) = 2$. Then let $\bar{S}_i := \operatorname{bd}(\mathbf{c}_i + \bar{r}\mathbf{B})$ and let $\bar{\mathbf{c}}_{ij}$ be the intersection of the line segment $\mathbf{c}_i\mathbf{c}_j$ with $\bar{S}_i$ for all $j \in T_i$. Moreover, let $C_{\bar{S}_i}(\bar{\mathbf{c}}_{ij}, \frac{\pi}{6})$ (resp., $C_{\bar{S}_i}(\bar{\mathbf{c}}_{ij}, \frac{\pi}{4})$) denote the open spherical cap of $\bar{S}_i$ centered at $\bar{\mathbf{c}}_{ij} \in \bar{S}_i$ having angular radius $\frac{\pi}{6}$ (resp., $\frac{\pi}{4}$). Clearly, the family $\{C_{\bar{S}_i}(\bar{\mathbf{c}}_{ij}, \frac{\pi}{6}), j \in T_i\}$ consists of pairwise disjoint open spherical caps of $\bar{S}_i$; moreover,

$$\frac{\sum_{j\in T_i} \mathrm{svol}_2(C_{\bar{S}_i}(\bar{\mathbf{c}}_{ij}, \frac{\pi}{6}))}{\mathrm{svol}_2(\bigcup_{j\in T_i} C_{\bar{S}_i}(\bar{\mathbf{c}}_{ij}, \frac{\pi}{4}))} = \frac{\sum_{j\in T_i} \mathrm{svol}_2(C(\mathbf{u}_{ij}, \frac{\pi}{6}))}{\mathrm{svol}_2(\bigcup_{j\in T_i} C(\mathbf{u}_{ij}, \frac{\pi}{4}))}, \tag{7}$$

where $\mathbf{u}_{ij} = \frac{1}{2}(\mathbf{c}_j - \mathbf{c}_i) \in \mathbb{S}^2$ and $C(\mathbf{u}_{ij}, \frac{\pi}{6}) \subset \mathbb{S}^2$ (resp., $C(\mathbf{u}_{ij}, \frac{\pi}{4}) \subset \mathbb{S}^2$) denotes the open spherical cap of $\mathbb{S}^2$ centered at $\mathbf{u}_{ij}$ having angular radius $\frac{\pi}{6}$ (resp., $\frac{\pi}{4}$). Now, the geometry of the cuboctahedron representing the 12 touching neighbors of an arbitrary unit ball in $\mathcal{P}_{fcc}$ implies in a straightforward way that

$$\frac{\sum_{j\in T_i} \mathrm{svol}_2(C(\mathbf{u}_{ij}, \frac{\pi}{6}))}{\mathrm{svol}_2(\bigcup_{j\in T_i} C(\mathbf{u}_{ij}, \frac{\pi}{4}))} \leq 6\left(1 - \frac{\sqrt{3}}{2}\right) = 0.8038\ldots \tag{8}$$

with equality when 12 spherical caps of angular radius $\frac{\pi}{6}$ are packed on $\mathbb{S}^2$.

Finally, as $\mathrm{svol}_2(C(\mathbf{u}_{ij}, \frac{\pi}{6})) = 2\pi(1 - \cos\frac{\pi}{6})$ and $\mathrm{svol}_2(C_{\bar{S}_i}(\bar{\mathbf{c}}_{ij}, \frac{\pi}{6})) = 2\pi \times (1 - \frac{\sqrt{3}}{2})\bar{r}^2$ therefore (7) and (8) yield that

$$\begin{aligned} \mathrm{svol}_2\left(\mathrm{bd}\left(\bigcup_{i=1}^{n} \mathbf{c}_i + \bar{r}\mathbf{B}\right)\right) &\leq 4\pi\bar{r}^2 n - \frac{1}{6(1-\frac{\sqrt{3}}{2})} 2\left(2\pi\left(1 - \frac{\sqrt{3}}{2}\right)\bar{r}^2\right) C_{fcc}(n) \\ &= 8\pi n - \frac{4\pi}{3} C_{fcc}(n). \end{aligned} \tag{9}$$

Thus, (6) and (9) imply that

$$4\sqrt[3]{18\pi}\, n^{\frac{2}{3}} < 8\pi n - \frac{4\pi}{3} C_{fcc}(n). \tag{10}$$

From (10) the inequality $C_{fcc}(n) < 6n - \frac{3\sqrt[3]{18\pi}}{\pi} n^{\frac{2}{3}} = 6n - 3.665\ldots n^{\frac{2}{3}}$ follows in a straightforward way for all $n \geq 2$. This completes the proof of (ii) in Theorem 1.1.

2.3 Proof of (iii)

It is rather easy to show that for any positive integer $k \geq 2$ there are $n(k) := \frac{2k^3+k}{3} = \frac{k(2k^2+1)}{3}$ lattice points of the face-centered cubic lattice Λ_{fcc} such that their convex hull is a regular octahedron $\mathbf{K} \subset \mathbb{E}^3$ of edge length $2(k-1)$ having exactly k lattice points along each of its edges. Now, draw a unit ball around each lattice point of $\Lambda_{fcc} \cap \mathbf{K}$ and label the packing of the $n(k)$ unit balls obtained in this way by $\mathcal{P}_{fcc}(k)$. It is easy to check that if the center of a unit ball of $\mathcal{P}_{fcc}(k)$ is a relative interior point of an edge (resp., of a face) of $\mathbf{K}$, then the unit ball in question has seven (resp., nine) touching neighbors in $\mathcal{P}_{fcc}(k)$. Last but not least, any unit ball of $\mathcal{P}_{fcc}(k)$ whose center is an interior point of $\mathbf{K}$ has 12 touching neighbors in $\mathcal{P}_{fcc}(k)$. Next we note that the number of lattice points of Λ_{fcc} lying in the relative interior of the edges (resp., faces) of $\mathbf{K}$ is $12(k-2) = 12k - 24$ (resp., $8(\frac{1}{2}(k-3)^2 + \frac{1}{2}(k-3)) = 4(k-3)^2 + 4(k-3)$). Furthermore the number of lattice points of Λ_{fcc} in the interior of $\mathbf{K}$ is equal to $\frac{2}{3}(k-2)^3 + \frac{1}{3}(k-2)$. Thus, the contact number $C(\mathcal{P}_{fcc}(k))$ of the packing $\mathcal{P}_{fcc}(k)$ is equal to

$$\frac{12}{2}\left(\frac{2}{3}(k-2)^3+\frac{1}{3}(k-2)\right)+\frac{9}{2}\big(4(k-3)^2+4(k-3)\big)+\frac{7}{2}(12k-24)+\frac{24}{2}$$
$$=4k^3-6k^2+2k.$$

As a result we get

$$C\big(\mathcal{P}_{fcc}(k)\big)=6n(k)-6k^2. \tag{11}$$

Finally, as $\frac{2k^3}{3}<n(k)$ therefore $6k^2<\sqrt[3]{486}n^{\frac{2}{3}}(k)$, and so (11) implies (iii) of Theorem 1.1 in a straightforward way.

3 On Improving (i) in Theorem 1.1

Let $\delta(\mathbf{K})$ denote the largest density of packings of translates of the convex body $\mathbf{K}$ in $\mathbb{E}^d$, $d\geq 3$. The following result has been proved by the author in [2].

Lemma 3.1 *Let $\mathbf{K_o}$ be a convex body in $\mathbb{E}^d$, $d\geq 2$ symmetric about the origin $\mathbf{o}$ of $\mathbb{E}^d$ and let $\{\mathbf{c}_1+\mathbf{K_o},\mathbf{c}_2+\mathbf{K_o},\dots,\mathbf{c}_n+\mathbf{K_o}\}$ be an arbitrary packing of $n\geq 1$ translates of $\mathbf{K_o}$ in $\mathbb{E}^d$. Then*

$$\frac{n\,\mathrm{vol}_d(\mathbf{K_o})}{\mathrm{vol}_d(\bigcup_{i=1}^n(\mathbf{c}_i+2\mathbf{K_o}))}<\delta(\mathbf{K_o}).$$

Let $\mathbf{B}$ denote the unit ball centered at the origin $\mathbf{o}$ of $\mathbb{E}^3$ and let $\mathcal{P}:=\{\mathbf{c}_1+\mathbf{B},\mathbf{c}_2+\mathbf{B},\dots,\mathbf{c}_n+\mathbf{B}\}$ denote the packing of n unit balls with centers $\mathbf{c}_1,\mathbf{c}_2,\dots,\mathbf{c}_n$ having the largest number $C(n)$ of touching pairs among all packings of n unit balls in $\mathbb{E}^3$. ($\mathcal{P}$ might not be uniquely determined up to congruence in which case $\mathcal{P}$ stands for any of those extremal packings.) The well-known result of Hales [5] according to which $\delta_3=\frac{\pi}{\sqrt{18}}$ and Lemma 3.1 imply in a straightforward way

Lemma 3.2

$$\frac{n\,\mathrm{vol}_3(\mathbf{B})}{\mathrm{vol}_3(\bigcup_{i=1}^n(\mathbf{c}_i+2\mathbf{B}))}<\delta(\mathbf{B})=\frac{\pi}{\sqrt{18}}.$$

The isoperimetric inequality [10] yields

Lemma 3.3

$$36\pi\,\mathrm{vol}_3^2\left(\bigcup_{i=1}^n(\mathbf{c}_i+2\mathbf{B})\right)\leq \mathrm{svol}_2^3\left(\mathrm{bd}\left(\bigcup_{i=1}^n(\mathbf{c}_i+2\mathbf{B})\right)\right).$$

Thus, Lemmas 3.2 and 3.3 generate the following inequality.

Corollary 3.4

$$4\sqrt[3]{18\pi}\,n^{\frac{2}{3}}<\mathrm{svol}_2\left(\mathrm{bd}\left(\bigcup_{i=1}^n(\mathbf{c}_i+2\mathbf{B})\right)\right).$$

Now, assume that $\mathbf{c}_i+\mathbf{B}\in\mathcal{P}$ is tangent to $\mathbf{c}_j+\mathbf{B}\in\mathcal{P}$ for all $j\in T_i$, where $T_i\subset\{1,2,\dots,n\}$ stands for the family of indices $1\le j\le n$ for which $\|\mathbf{c}_i-\mathbf{c}_j\|=2$. Then let $S_i:=\mathrm{bd}(\mathbf{c}_i+2\mathbf{B})$ and let $C_{S_i}(\mathbf{c}_j,\frac{\pi}{6})$ denote the open spherical cap of S_i centered at $\mathbf{c}_j\in S_i$ having angular radius $\frac{\pi}{6}$. Clearly, the family $\{C_{S_i}(\mathbf{c}_j,\frac{\pi}{6}),\ j\in T_i\}$ consists of pairwise disjoint open spherical caps of S_i; moreover,

$$\frac{\sum_{j\in T_i}\mathrm{svol}_2(C_{S_i}(\mathbf{c}_j,\frac{\pi}{6}))}{\mathrm{svol}_2(\bigcup_{j\in T_i}C_{S_i}(\mathbf{c}_j,\frac{\pi}{3}))}=\frac{\sum_{j\in T_i}\mathrm{svol}_2(C(\mathbf{u}_{ij},\frac{\pi}{6}))}{\mathrm{svol}_2(\bigcup_{j\in T_i}C(\mathbf{u}_{ij},\frac{\pi}{3}))},$$

where $\mathbf{u}_{ij}:=\frac{1}{2}(\mathbf{c}_j-\mathbf{c}_i)\in\mathbb{S}^2$ and $C(\mathbf{u}_{ij},\frac{\pi}{6})\subset\mathbb{S}^2$ (resp., $C(\mathbf{u}_{ij},\frac{\pi}{3})\subset\mathbb{S}^2$) denotes the open spherical cap of $\mathbb{S}^2$ centered at $\mathbf{u}_{ij}$ having angular radius $\frac{\pi}{6}$ (resp., $\frac{\pi}{3}$). Now, we are ready to state the main conjecture of this section.

Conjecture 3.5 *Let $\{C(\mathbf{u}_m,\frac{\pi}{6}),\ 1\le m\le M\}$ be a family of M pairwise disjoint open spherical caps of angular radii $\frac{\pi}{6}$ in $\mathbb{S}^2$. Then*

$$\frac{\sum_{1\le m\le M}\mathrm{svol}_2(C(\mathbf{u}_m,\frac{\pi}{6}))}{\mathrm{svol}_2(\bigcup_{1\le m\le M}C(\mathbf{u}_m,\frac{\pi}{3}))}\le 6\left(1-\frac{\sqrt{3}}{2}\right)=0.8038\dots$$

with equality when $M=12$ spherical caps of angular radii $\frac{\pi}{6}$ are packed on $\mathbb{S}^2$.

Clearly, $M\le\tau_3=12$. Moreover, if true, then Conjecture 3.5 can be used to improve the upper bound for $C(n)$ in (i) of Theorem 1.1 as follows. First, Conjecture 3.5 implies in a straightforward way that

$$\mathrm{svol}_2\left(\mathrm{bd}\left(\bigcup_{i=1}^{n}(\mathbf{c}_i+2\mathbf{B})\right)\right)\le 16\pi n-\frac{1}{6(1-\frac{\sqrt{3}}{2})}16\pi\left(1-\frac{\sqrt{3}}{2}\right)C(n)=16\pi n-\frac{8\pi}{3}C(n).$$

Second, the above inequality combined with Corollary 3.4 yields

$$4(18\pi)^{\frac{1}{3}}n^{\frac{2}{3}}<16\pi n-\frac{8\pi}{3}C(n),$$

from which the inequality

$$C(n)<6n-\frac{3\sqrt[3]{18\pi}}{2\pi}n^{\frac{2}{3}}=6n-1.8326\dots n^{\frac{2}{3}}$$

follows. Clearly, this would be a significant improvement on (i) in Theorem 1.1.

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