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On Mixed Sphere Packings

Salvatore Vassallo and **Jörg M. Wills***

Università Cattolica del Sacro Cuore, Istituto de Matematica
Largo A. Gemelli, 1, I - 20123 Milano

Fachbereich Mathematik, Universität Siegen
Hölderlinstraße 3, D-57068 Siegen

Abstract. Balls of two different radii $r_1 < r_2$ can trivially be packed in E^3 with density better than the classical packing density $\delta_L^3 = 0.74048\ldots$, if $r_1/r_2 \leq 0.41$... We show that this even holds for $r_1/r_2 = 0.623\ldots$ Further we show, under strong restrictions, that r_1/r_2 close to 1 does not yield a density $> \delta_L^3$. These results correspond to similar results on circle packings in the plane by G. Blind, L. Fejes Tóth and A. Florian.

1. Introduction and Definitions

Let $B^d \subset E^d, d \geq 2$ denote the unit d-ball in euclidian d-space and $B_i^d = c_i + r_i B^d$, $i = 1, 2, \ldots$ If for each r_i either $r_i = r$ with $r \in [0, 1]$ or $r_i = 1$, then

$$P_r^d = \{B_i^d \subset E^d \mid i = 1, 2 \ldots \text{ with } \operatorname{int}(B_i^d \cap B_j^d) = \emptyset \text{ for } i \neq j\}$$

is called an infinite packing of balls of two radii or briefly a two-radii packing. For its density function $\delta(P_r^d)$ let as usual V denote the volume, in particular $V(B^d) = \kappa_d$ and $V(RB^d) = \kappa_d R^d$. Then

$$\delta(P_r^d) = \limsup_{R \to \infty} \{(\kappa_d R^d)^{-1} \sum_{B_i^d \subset RB^d} V(B_i^d) \mid B_i^d \in P_r^d\}.$$

The set of all two-radii-packings is denoted by $\mathcal{P}_r^d$. Then let

$$\delta^d(r) = \sup\{\delta(P_r^d) \mid P_r^d \in \mathcal{P}_r^d\}.$$

Clearly $\delta^d(1) = \delta^d$ is the classical packing density of E^d by translates of B^d. We further define $\delta^d(0) = \limsup_{r \to 0} \delta^d(r)$. Then

$$0 < \delta^d(r) < 1 \text{ for } 0 \leq r \leq 1. \tag{1}$$

* The paper was initiated while the second author was as a visiting professor at the University of Torino.

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It is a natural question to compare $\delta^d(r)$ with δ^d and with the classical lattice packing density δ^d_L. Obviously for all sufficently small r one has $\delta^d(r) > \delta^d \geq \delta^d_L$. So the most interesting partial problems are to find

$$r_d = \sup\{r \mid \delta^d(r) > \delta^d\}$$

and

$$r^L_d = \sup\{r \mid \delta^d(r) > \delta^d_L\}.$$

2. Known results

For $d = 2$ one has $\delta^2 = \delta^2_L = \pi/\sqrt{12}$, hence $r_2 = r^L_2$. G. Blind [1] proved

$$r_2 \leq 0.74299. \tag{2}$$

Weaker upper bounds were given in [4] and [7], cf. also [3] and [5].

L. Fejes Tóth ([4] p.78) gave the lower bound

$$r_2 \geq 0.6 \tag{3}$$

and proved further ([4] p.71 ff.)

$$\delta^2(0) = \delta^2(2 - \delta^2). \tag{4}$$

The simple proof of (4) works for all d, hence

$$\delta^d(0) = \delta^d(2 - \delta^d). \tag{5}$$

This implies $\delta^d(r) > \delta^d$ for all sufficiently small r, i.e. $r_d > 0$, but (as far as we know) no nontrivial lower bound for r_d, $d \geq 3$ is known. Moreover, for no $d \geq 3$ it is known if $r_d < 1$, although it seems to be plausible.

Slightly more can be said for r^L_d, because δ^L_d is known for $d \leq 8$: If ρ_d denotes the covering radius (cf. [2] p.6,33) of a densest packing lattice, then the deep holes (cf. [2] p.6,33) can be filled by balls of radius $\rho_d - 1$ so

$$\begin{gathered} r^L_d \geq \rho_d - 1\ ,\ d \leq 8 \\ \text{with} \qquad \rho_2 = 2/\sqrt{3},\ \rho_3 = \rho_4 = \rho_8 = \sqrt{2},\ \rho_5 = \sqrt{5/2},\ \rho_6 = \sqrt{8/3},\ \rho_7 = \sqrt{3}. \end{gathered} \tag{6}$$

For $d = 2$ (6) yields $r^L_2 = r_2 \geq 0.1547\cdots$, which is much smaller than the bound in (3).

Although one can slightly improve on (6) by varying the radii r and 1 with $r + 1 = \rho_d$ and renormalization, no essential improvement on (6) for $d \geq 3$ is known. For $d = 3$ (6) yields

$$r^L_3 \geq 0.414\cdots \tag{7}$$

It is the first goal of this note to improve this bound (Theorem 1). For $d = 3$ the problem has connections to crystallography, hence there are some more partial results (cf. [8], [9] p.492) and in particular by Few [6].

Few investigated particular 2-radii-packings in E^3 by superposing a lattice packing $\Lambda + B^3$ and with suitable $x \in E^3$ and $r > 0$ a grid packing or "displaced" lattice packing $x + \Lambda + rB^3$. He called this superposed packing a "mixed lattice packing". If for a given $r \in (0, 1]$ $\delta^3_\star(r)$ denotes the density of the densest mixed lattice packing, then the following holds with a slight reformulation (Few used R with $R - 1 = r$):

Theorem (Few, 1960).

$$\begin{aligned}
\delta^3_\star(r) &= \frac{\pi}{3\sqrt{2}}(1 + r^3) && 0 \le r \le \sqrt{2} - 1 \\
\delta^3_\star(r) &= \frac{\pi}{3}\frac{1 + r^3}{2r + r^2}(3 - 2r - r^2)^{-1/2} && \sqrt{2} - 1 \le r \le \sqrt{3} - 1 \\
\delta^3_\star(r) &= \frac{\pi}{6}(1 + r^3)(r^2 + 2r - 1)^{-1/2} && \sqrt{3} - 1 \le r \le 1
\end{aligned}$$

By definition one has $\delta^3_\star(r) \le \delta^3(r)$. Further $\delta^3_\star(1) = \delta^3_L$. Elementary but tedious calculation shows $\delta^3_\star(r) < \delta^3_L$ for $1/2 \le r < 1$. So Few's result supports the general opinion that $\delta^3(r) < \delta^3_L$, if $1 - r = \varepsilon$ is small. Our second result (Theorem 2), which is related to L. Few's theorem, also supports this conjecture. But still it seems to be hard to find a 3-dimensional analogue of Blind's result.

3. Results

The first result improves (7):

Theorem 1.

$$r_3^L \ge 0.623\ldots$$

Remarks. a) Theorem 1 improves (7), but note that it does not imply $\delta(P^3_r) > \delta^3_L$ for all $r \le r^L_3$. In fact there remains a gap $0.44\ldots \le r \le 0.57\ldots$, for which it is open if $\delta(P^3_L) > \delta^3_L$ or not.

b) For Theorem 2 let Λ_c denote the face-centered cubic lattice (fcc), i.e. the critical lattice of B^3, which generates the densest sphere packing in E^3.

Theorem 2. *Let P^3_r be a 2-ball-packing with $\{c_i\} = \Lambda_c$ and $\delta(P^3_r) > \delta^3_L$. Then $r < 0.29\ldots$*

4. Proof of Theorem 1

Let $x_i = (2\cos(\pi i/3),\ 2\sin(\pi i/3),\ h)$, $i = 1, \ldots, 6$, and $x_i = (2\cos(\pi i/3), 2\sin(\pi i/3), -h)$, $i = 7, \ldots, 12$, where $h \ge 1$ will be determined later. Then $||x_i - x_j|| \ge 2$ for $i \ne j$ and $||x_i||^2 = 4 + h^2$.

Further $P = \operatorname{conv}\{x_1, \dots, x_{12}\}$ is an orthogonal prism with regular hexagon as basis, height $2h$ and volume $V(P) = 12\sqrt{3}h$.

Obviously P is a spacefiller and we denote by P_j, $j = 1, 2, \dots$ the congruent copies of P, such that $\bigcup_{j\in N} P_j = E^3$ is a lattice-tiling of E^3. We now construct the two-radii-packing: Let each vertex x_i of P be the center of a unit ball B_i, $i = 1, \dots, 12$. Further let O be the center of a ball B_{13} with radius ρ such that

$$(\rho+1)^2 = 2^2 + h^2, \quad \rho \le \sqrt{3} \quad \text{and} \quad \rho \le h. \tag{8}$$

(8) implies $\rho \ge \frac{3}{2}$ and $h = h(\rho) = ((\rho+1)^2 - 4)^{1/2} = (\rho^2 + 2\rho - 3)^{1/2} \le \sqrt{2}\sqrt[4]{3} = 1.86\dots$ Then the 13 B_i do not overlap each other and $B_{13} \subset P$.

If we proceed periodically for all P_j, we get a nonlattice 2-radii- packing of E^3 with the radii $r_1 = 1$ and $r_2 = \rho > 1$. With $r_1/r_2 = 1/\rho = r$ we have the density

$$\delta^3(r) = \delta^3\left(\frac{1}{\rho}\right) = (V(P))^{-1}\sum_{i=1}^{13} V(B_i \cap P) = (12\sqrt{3})^{-1}(\rho^2+2\rho-3)^{-1/2}\frac{4\pi}{3}(2+\rho^3) =$$
$$= \frac{\pi}{\rho\sqrt{3}}(2+\rho^3)(\rho^2+2\rho-3)^{-1/2}.$$

From $\delta^3(r) = \delta^3(\frac{1}{\rho}) > \delta^3_L = \pi/3\sqrt{2}$ follows $\sqrt{2}(2+\rho^3) > 3\sqrt{3}(\rho^2+2\rho-3)^{1/2}$ or $\rho^6+4\rho^3+4 > \frac{27}{2}(\rho^2+2\rho-3)$.

So we have to find a zero of

$$f(\rho) = \rho^6 + 4\rho^3 - \frac{27}{2}\rho^2 - 27\rho + \frac{89}{2}$$

for $3/2 \le \rho \le \sqrt{3}$. Simple calculation shows $f(\frac{3}{2}) < 0$, $f(\sqrt{3}) > 0$ and $f'(\rho) > 0$ for $\rho \ge \frac{3}{2}$. So there is exactly one $\rho' \in (\frac{3}{2}, \sqrt{3})$ with $f(\rho') = 0$. Again simple calculation shows $\rho' = 1.604\dots$, hence $r' = \frac{1}{\rho'} = 0.623\dots$ and $\delta^3(r) > \delta^3_L$ for $0.577 < r < 0.623$.

5. Proof of Theorem 2

If some balls are enlarged in the densest sphere packing $\Lambda + B^3$, then obviously some other balls have to shrink in order to obtain a two-radii-packing. We first determine the optimal relation of large and small balls. For this we consider a fixed ball B of Λ and its 12 neighbours. If B is enlarged, then all of its 12 neighbours have to shrink.

On the other hand, if B shrinks then at most 4 of its neighbours can be enlarged. For this let C be the convex hull of the centers of the 12 balls, i.e. the regular cuboctahedron. Its vertex graph is 3-colourable, so each of the 12 balls corresponds to one colour. No two balls of different colours can be enlarged, so at most 4 balls can. So the relation of large and small balls is at most 4:12 or 1:3, and in fact this relation can globally be attained in Λ as one can easily check.

Hence we get from $\delta^3(P^3_L) > \delta^3_L$: For $\varepsilon \in [0,1]$ with $(1-\varepsilon)/(1+\varepsilon) = r$ holds

$$\frac{4\pi}{3}\{(1+\varepsilon)^3 + 3(1-\varepsilon)^3\} > \frac{4\pi}{3}4$$

or

$$(1+\varepsilon)^3 + 3(1-\varepsilon)^3 > 4$$

or

$$-\varepsilon^3 + 6\varepsilon^2 - 3\varepsilon > 0. \tag{9}$$

The roots of $\varepsilon^3 - 6\varepsilon^2 + 3\varepsilon = 0$ are

$$\varepsilon_1 = 0, \ \varepsilon_2 = 3 - \sqrt{6} \ \text{and} \ \varepsilon_3 = 3 + \sqrt{6}.$$

Hence (9) holds in particular for $\varepsilon_2 < \varepsilon \leq 1$, but not for $0 \leq \varepsilon \leq \varepsilon_2$.

With $(1-\varepsilon_2)/(1+\varepsilon_2) = \frac{1}{5}(\sqrt{6}-1) = 0,289898\ldots$ Theorem 2 is proved.

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