THE DENSEST PACKING OF SIX SPHERES IN A CUBE

J. Schaer

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This packing problem is obviously equivalent to the problem of locating six points $P_i (1 \leq i \leq 6)$ in a closed unit cube C such that $\min_{i \neq j} d(P_i, P_j)$ is as large as possible, where $d(P_i, P_j)$ denotes the distance between P_i and P_j. We shall prove that this minimum distance cannot exceed $\frac{3\sqrt{2}}{4}$ (= m, say), and that it attains this value only if the points form a configuration which is congruent to the one of the points $R_i (1 \leq i \leq 6)$ shown in fig. 1. Note that $d(R_i, A_i) = \frac{1}{4} (1 \leq i \leq 6)$, and so the six points are the vertices of a regular octahedron.

1) For our proof we shall need the solution of the analogous problem for three points in a right square prism P of side 1 and height $\frac{1}{4}$: $0 \leq y_i \leq 1$ $(i=1, 2)$, $0 \leq y_3 \leq \frac{1}{4}$.

PROPOSITION 1. For any three points Q_1, Q_2, Q_3 of P, $\min_{i \neq j} d(Q_i, Q_j) \leq \frac{3\sqrt{2}}{4} = m$, and equality holds only for a configuration congruent to the set of the points $V_1(\frac{1}{4}, 1, \frac{1}{4})$, $V_2(1, \frac{1}{4}, \frac{1}{4})$, and $V_3(0, 0, 0)$. See fig. 2. Note that $d(V_i, V_j) = m \, (i \neq j)$.

Proof. Consider any best configuration[1] T of three points Q_1, Q_2, Q_3 in P. Of course

[1] i.e., a configuration for which $\min_{i \neq j} d(Q_i, Q_j)$ is maximum.

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(1) $$\min_{i \neq j} d(Q_i, Q_j) \geq m.$$

(A) Assume first that a point of T lies in a vertex of P, say $Q_3 = V_3$. Then by (1) no other point of T can lie in the convex hull H of the vertices V_3, $(0, 0, \frac{1}{4})$, $(1, 0, 0)$, $(1, 0, \frac{1}{4})$, $(0, 1, 0)$, $(0, 1, \frac{1}{4})$ of T, V_1, V_2, $U_1(\frac{\sqrt{2}}{4}, 1, 0)$, and $U_2(1, \frac{\sqrt{2}}{4}, 0)$, except possibly at V_1, V_2, U_1, or U_2. Note that $d(V_3, V_i) = d(V_3, U_i) = m$ $(i=1, 2)$. Therefore Q_1 and Q_2 must lie in the closure of P - H. But this polyhedron[2] assumes its diameter m only between the points V_1 and V_2. Therefore $\{Q_1, Q_2\} = \{V_1, V_2\}$.

(B) We are left to show that at least one point of T must lie in a vertex of P. If we assume the contrary, then Q_1, Q_2, and Q_3 must lie on mutually orthogonal non-intersecting edges of P. This follows from the basic lemma according to which on every face of P there must be at least one point of any best configuration [1]. Thus we may assume $Q_1 = (y_1, 1, \frac{1}{4})$, $Q_2 = (1, y_2, 0)$, and $Q_3 = (0, 0, y_3)$, with $0 < y_i < 1$ (i=1,2), and $0 < y_3 < \frac{1}{4}$. By (1) $d^2(Q_3, Q_i) > m^2$ (i=1, 2). This leads to

$$y_1 > \sqrt{\frac{1}{8} - (\frac{1}{4} - y_3)^2} \text{ and } y_2 > \sqrt{\frac{1}{8} - y_3^2}\ .$$

But then $d^2(Q_1, Q_2) = (1-y_1)^2 + (1-y_2)^2 + \frac{1}{16}$

$$< 2 + \frac{1}{2}y_3 - 2y_3^2 - 2\sqrt{\frac{1}{8} - (\frac{1}{4} - y_3)^2} - 2\sqrt{\frac{1}{8} - y_3^2}\ .$$

For $0 < y_3 < \frac{1}{4}$ this expression is less than $\frac{9}{8}$, in contradiction to (1), q.e.d.

This proves that if three points with mutual distances at least $m = \frac{3\sqrt{2}}{4}$ lie in a right square prism of side 1, then the height of the prism must be at least $\frac{1}{4}$.

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[2] The diameter of a closed polyhedron is obviously always assumed between two of its vertices.

2) Let S be any set of six points $P_i (1 \leq i \leq 6)$ of C such that

(2) $$d(P_i, P_j) \geq m \quad (1 \leq i < j \leq 6)$$

We shall prove that $\{R_i (1 \leq i \leq 6)\}$ of fig. 1 is, up to congruent ones, the only such set.

The unit cube C: $0 \leq x_j \leq 1$ $(1 \leq j \leq 3)$ is the union of eight closed cubes C_k of side $\frac{1}{2}$: $a_j \leq x_j \leq b_j$, where either $a_j = 0$ and $b_j = \frac{1}{2}$, or $a_j = \frac{1}{2}$ and $b_j = 1$. Let us enumerate them such that the vertices $A_k \epsilon C_k$ $(1 \leq k \leq 8)$ (see fig. 1). Since $\frac{\sqrt{3}}{2} < m$, by (2) in every C_k there can at most be one point of S. Therefore we may choose six cubes C_k containing one point of S each, and two "empty" cubes that do not contain any point of S except possibly on their intersection with a "containing" cube. This choice may be not unique, but all we need is the existence of (at least) two such "empty" cubes C_k .

PROPOSITION 2. If two "containing" cubes C_i, C_j are adjacent, then the points of S which they contain have at least a distance $\frac{1}{2} - a$ from their common face, $a \equiv 1 - \frac{\sqrt{10}}{4} < \frac{1}{4}$.

Indeed, consider the right square prism of side $\frac{1}{2}$ and diagonal m which contains all of C_i and as much of C_j as possible (see fig. 3). Excluding its base, which lies completely in C_j, it can, because of (2), contain at most one point of S. But it contains already the point of S in C_i. Therefore the point of S in C_j must lie in the indicated right square prism of side $\frac{1}{2}$ and height a, a being defined by $(1-a)^2 + 2(\frac{1}{2})^2 = m^2$. q.e.d.

COROLLARY. If a "containing" cube C_k is adjacent to two other "containing" cubes, then the point of S in C_k is confined in a right square prism of side a and height $\frac{1}{2}$ with one edge common with that edge of C_k which has no points in

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common with the two adjacent "containing" cubes.

3) PROPOSITION 3. The six points P_i must lie in right square prisms of side $a(<\frac{1}{4})$ and height $\frac{1}{2}$, namely (see fig. 4) P_i in $\frac{1}{2} \leq x_i \leq 1$, $0 \leq x_j \leq a$ $(j \neq i)$ $(i=1,2,3)$ resp. in $0 \leq x_{i-3} \leq \frac{1}{2}$, $1-a \leq x_j \leq 1$ $(j \neq i-3)$ $(i=4,5,6)$

Proof. The two "empty" cubes C_k are not adjacent, nor can they have a common edge. Otherwise their centers would have at least one equal coordinate, say $x_3 = \frac{3}{4}$, and the four cubes C_k: $0 \leq x_3 \leq \frac{1}{2}$ would all be "containing". By the corollary of Proposition 2 the points of S which they contain would be confined to $0 \leq x_j \leq a$ or $1-a \leq x_j \leq 1$ $(j=1,2)$. The four right square prisms of side 1 and height $\frac{1}{4}$: $0 \leq x_j \leq \frac{1}{4}$ or $\frac{3}{4} \leq x_j \leq 1$ $(j=1$ or $2)$, $0 \leq x_h \leq 1$ $(h \neq j)$, would therefore already contain at least 2 points of S each. Thus by Proposition 1 the two other points of S, i.e. those with $\frac{1}{2} \leq x_3 \leq 1$, would be restricted to $\frac{1}{4} \leq x_j \leq \frac{3}{4}$ $(j=1,2)$. But this is impossible, because this point set is a cube of side $\frac{1}{2}$ and diameter $\frac{\sqrt{3}}{2} < m$.

Thus the two "empty" cubes must lie opposite to the center of C, e.g. let them be C_7 and C_8. We may then assume $P_i \in C_i$ $(1 \leq i \leq 6)$. Proposition 3 follows now from the corollary of Proposition 2.

4) Using Proposition 3 and applying Proposition 1 to the six right square prisms in C of height $\frac{1}{4}$, which contain one face of C each, the location of the P_i can in addition be restricted to P_1, P_2, P_3 all in $0 \leq x_j \leq \frac{3}{4}$ $(1 \leq j \leq 3)$, P_4, P_5, P_6 all in $\frac{1}{4} \leq x_j \leq 1$ $(1 \leq j \leq 3)$.

5) According to the solution of the analogous problem of placing three points in a cube [1] the only way to locate three

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points with minimum distance $\frac{3\sqrt{2}}{4}$ in a cube of side $\frac{3}{4}$ consists in placing them in vertices with mutual distances $\frac{3\sqrt{2}}{4}$.

Applying this result to 4) and Proposition 3 we deduce $P_i = R_i$ $(1 \leq i \leq 6)$.

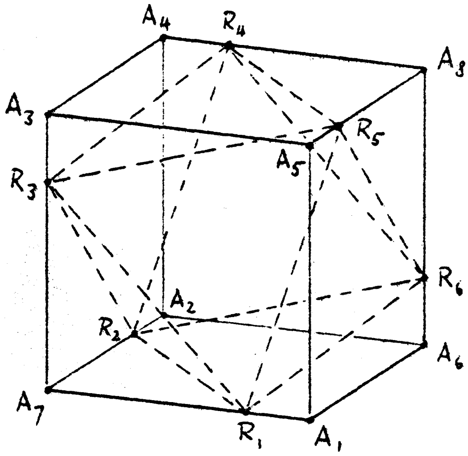

Figure 1

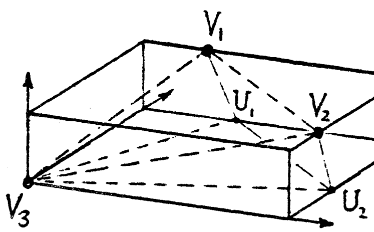

Figure 2

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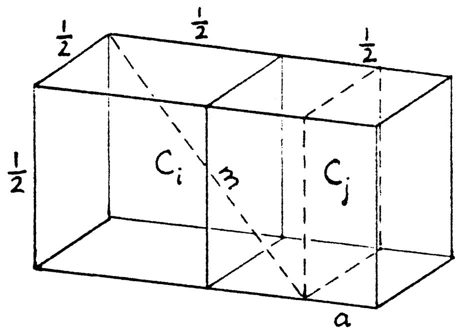

Figure 3

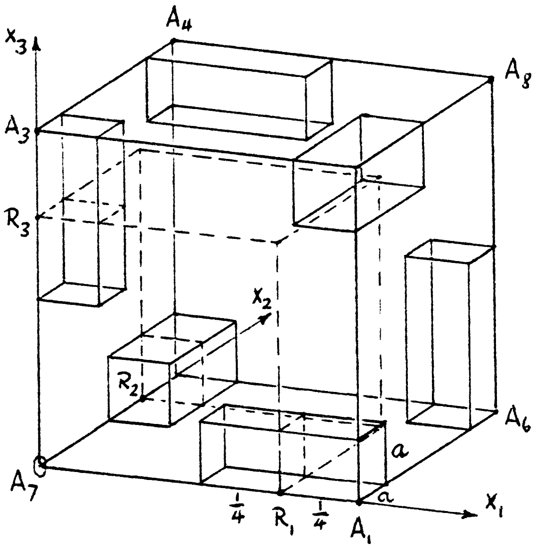

Figure 4

REFERENCES

1. J. Schaer, On the densest packing of spheres into a cube. Canad. Math. Bull. vol. 9, no. 3, 1966.

University of Alberta, Calgary

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