ON THE DENSEST PACKING OF SPHERES IN A CUBE

J. Schaer

(received February 22, 1965)

How many spheres of given diameter can be packed in a cube of given size? Or: What is the maximum diameter of k identical spheres if they can be packed in a cube of given size? These questions are obviously equivalent to the following problem:

Let $d(P_i, P_j)$ denote the distance between the points P_i and P_j, and Γ_k the set of all configurations of k points P_i $(1 \leq i \leq k)$ in a closed unit cube C. For which configuration $S \in \Gamma_k$ is $m_k(S) = \min\limits_{1 \leq i < j \leq k} d(P_i, P_j)$ as large as possible, and how large is $m_k = \max\limits_{S \in \Gamma_k} m_k(S)$? The maximum exists because of the compactness of Γ_k .

We shall call a <u>best configuration</u> any configuration for which the maximum is attained. In any dimension d we have the following Lemma:

BASIC LEMMA. Any best configuration contains at least one point on every face of C. The same is true not only for a cube, but also for any parallelotope.

Here we shall prove the lemma for right parallelotopes. For skew ones a simple modification of the proof would be needed.

In a suitably chosen Cartesian coordinate system a d-dimensional right parallelotope Π may be defined by $0 \leq x^i \leq a^i$ $(1 \leq i \leq d)$. If a configuration S of k points $P_j(x^1_j, \ldots, x^d_j)$ $(1 \leq j \leq k)$ contains no point of the face $x^1 = a^1$,

Canad. Math. Bull. vol. 9, no. 3, 1966

https://doi.org/10.4153/CMB-1966-033-0 Published online by Cambridge University Press

say, then it cannot be a best configuration. Numerate the points P_i according to non-decreasing first coordinate: $0 \leq x_1^1 \leq x_2^1 \leq \ldots \leq x_k^1 = a^1 - \epsilon$ $(\epsilon > 0)$. Then the k points $Q_j\left(x_j^1 + \frac{j-1}{k-1}\epsilon, x_j^2, \ldots, x_j^d\right)$ $(1 \leq j \leq k)$ are also all in Π, but $d(Q_i, Q_j) > d(P_i, P_j)$ $(1 \leq i < j \leq k)$, q.e.d.

For $k = 2$ clearly $m_2 = \sqrt{d}$, d denoting the dimension of the cube. The points of a best configuration lie in opposite vertices.

The determination of a general formula for m_k is a difficult problem. It seems that each value of k must be treated individually.

In $d = 2$ dimensions it has been solved [1] for $2 \leq k \leq 9$.

In this paper we shall give the solutions for $k = 2, 3, 4, 8$, and 9 in three dimensions. The cases $k = 5$ and $k = 6$ are treated in separate papers. Fig. 1 displays these known solutions.*

The case $\underline{k = 2}$ is trivial, $m_2 = \sqrt{3}$.

The cases $\underline{k = 3}$ and $\underline{k = 4}$ may be treated together, since we can assert $m_3 = m_4 = \sqrt{2}$. The configuration of four points is an inscribed regular tetrahedron, and for three points simply one of its four vertices is omitted.

For the proof let us consider any set S of three points $P_i (1 \leq i \leq 3)$ of C with

$$d(P_i, P_j) \geq \sqrt{2} = m_3 \quad (1 \leq i < j \leq 3). \tag{1.3}$$

We shall show that up to symmetric ones the only such set is the indicated one.

If no point of S would lie in a vertex of C, then according to the basic lemma the three points would have to lie on mutually orthogonal non-intersecting edges. With respect to suitably chosen coordinates we might therefore assume them to be $P_1(x_1, 0, 1)$, $P_2(1, x_2, 0)$, and $P_3(0, 1, x_3)$, with

* In the meantime the author has found the solution for $k=7$ as well.

(2) $$0 < x_i < 1 \quad (1 \leq i \leq 3) .$$

Now by (1.3)

$$d^2(P_1, P_2) = (1-x_1)^2 + x_2^2 + 1 \geq 2,$$

$$d^2(P_2, P_3) = 1 + (1-x_2)^2 + x_3^2 \geq 2 ,$$

and $$d^2(P_3, P_1) = x_1^2 + 1 + (1-x_3)^2 \geq 2 .$$

Adding these inequalities we would obtain

$$x_1^2 + x_2^2 + x_3^2 \geq x_1 + x_2 + x_3$$

in contradiction to (2).

Therefore at least one point of S lies in a vertex of C, say $P_1 = A_1$. (See fig. 2) Then by (1.3), P_2 and P_3 have to lie in the pyramid $A_3A_6A_7A_8$. This set assumes its diameter $m_3 = \sqrt{2}$ only between the vertices of the equilateral triangle $A_3A_6A_8$. Thus for $k = 3$ points without loss of generality $P_2 = A_3$, and $P_3 = A_6$. q.e.d.

A set of $k = 4$ points with

(1.4) $$d(P_i, P_j) \geq \sqrt{2} = m_4 \quad (1 \leq i < j \leq 4)$$

contains of course a subset of three points with (1.3). With the indicated solution for $k = 3$, the solution for $k = 4$ is therefore obvious: $P_4 = A_8$.

The case <u>$k = 8$</u>. It looks obvious, and is indeed readily proved, that the best configuration consists of the eight vertices of C. Consider any set S of eight points

(1.8) $P_i (1 \leq i \leq 8)$ of C with $$\min_{1 \leq i < j \leq 8} d(P_i, P_j) \geq 1 = m_8 .$$

We shall prove that there is just one such set; namely the conjectured one, for which in (1.8) equality holds. Consider C as the union of eight closed cubes C_i of side 1/2. Enumerate them such that the vertex $A_i \in C_i$ $(1 \leq i \leq 8)$. Their diameter is

https://doi.org/10.4153/CMB-1966-033-0 Published online by Cambridge University Press

$\sqrt{3/2} < 1$, such that in every cube C_i by (1.8) there can be at most one point of S. And since there are as many points P_i as cubes C_i, in every C_i there must lie exactly one point of S, say $P_i \in C_i$ $(1 \leq i \leq 8)$.

We shall now show how the location of every P_i may be restricted to a smaller cube $C_i^1 \subset C_i$. Iterating the process we find for every i a sequence of cubes $C_i \supset C_i^1 \supset C_i^2 \supset \ldots$, all containing A_i and P_i. Then we shall show that the sequence of the sides s_n of these cubes C_i^n approaches 0 as n tends to infinity, proving $P_i = A_i$. The process leading from C_i^n to C_i^{n+1} consists of the following: Consider the right square prism of side s_n and diagonal 1 which fully contains a closest neighbour cube C_j^n and as much as possible of C_i^n (see fig. 3). Excluding its face which lies entirely in C_i^n, by (1.8) it cannot contain more than one point of S. And because it contains already $P_j \in C_j^n$ its intersection with C_i^n is excluded as a possible location of P_i. Every C_i^n may be truncated in that manner by its three closest neighbours. What is left as a possible location of P_i is the cube C_i^{n+1} of side s_{n+1}.

Now $(1-s_{n+1})^2 = 1-2s_n^2$ and therefore

$$s_{n+1} = 1 - \sqrt{1-2s_n^2} = 2s_n^2 \left(1+\sqrt{1-2s_n^2}\right)^{-1} .$$

Thus for $s_n \leq s_o = 1/2$, $s_{n+1}(s_n)^{-1} = (1+\sqrt{1/2})^{-1} < 1$.

This proves $s_n \to 0$ $(n \to \infty)$ and hence $P_i = A_i$ $(1 \leq i \leq 8)$.

For the case <u>k = 9</u> the best configuration is also easily guessed: It contains the eight vertices A_i and the center M of C. We have to prove that this is the only configuration S of nine points P_i $(1 \leq i \leq 9)$ in C for which

(1.9) $$\min_{1 \leq i < j \leq 9} d(P_i, P_j) \geq \sqrt{3/2} = m_9 .$$

https://doi.org/10.4153/CMB-1966-033-0 Published online by Cambridge University Press

As in the case $k = 8$ we may write $C = \bigcup_{i=1}^{9} C_i$, where C_9 consists of M alone, and the $C_i (1 \leq i \leq 8)$ are cubes of side 1/2. But now we don't take them closed, but let each of their 26 vertices besides M belong to one C_i only in such a manner that no C_i $(1 \leq i \leq 8)$ contains a pair of opposite vertices. This may be achieved easily in many different ways. Then by (1.9) each $C_i (1 \leq i \leq 9)$ can contain at most one point of S, and because there are as many points in S as there are sets C_i, every $C_i (1 \leq i \leq 9)$ contains exactly one point of S, say $P_i \in C_i (1 \leq i \leq 9)$. Now $P_9 \in C_9$ means $P_9 = M$, and by (1.9) we deduce immediately $P_i = A_i$ $(1 \leq i \leq 8)$.

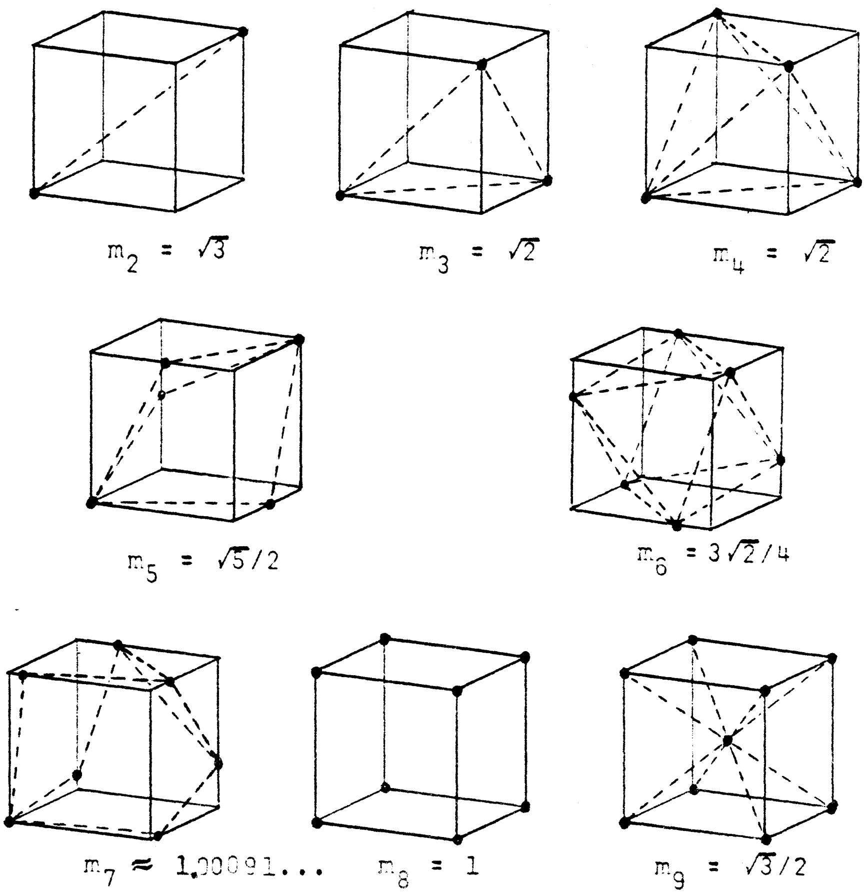

Figure 1.

https://doi.org/10.4153/CMB-1966-033-0 Published online by Cambridge University Press

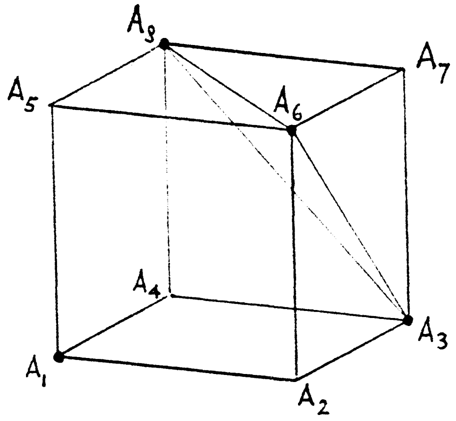

Figure 2.

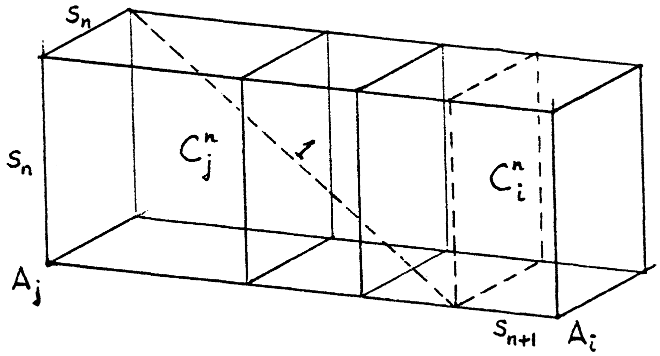

Figure 3.

REFERENCES

1. J. Schaer, The densest packing of nine circles in a square.

University of Alberta, Calgary