THE DENSEST PACKING OF FIVE SPHERES IN A CUBE

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(received February 22, 1965)

The purpose of this paper is to locate five points $P_i (1 \leq i \leq 5)$ 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 prove that this minimum distance cannot exceed $\frac{\sqrt{5}}{2}$ (=m, say), and if it is equal to m, then the corresponding configuration is congruent to the set of points shown in fig. 1, namely $P_1 = A_1(0, 0, 0)$, $P_2 = A_8(1, 1, 1)$, $P_3 = B_1(0, 1/2, 1)$, $P_4 = B_3(1/2, 1, 0)$ and $P_5 = B_5(1, 0, 1/2)$.

<u>Proof</u>. Let S be any set of 5 points $P_i (1 \leq i \leq 5)$ of C with mutual distances not less than m:

$$d(P_i, P_j) \geq m \quad (i \neq j). \tag{1}$$

We shall show that, up to symmetric ones, there is just one such set, namely the indicated one.

(A) If a point of S lies in a vertex of C, then S is the indicated set.

Indeed, assume for example $P_1 = A_1$ (see fig. 1). The plane through the center M and orthogonal to $A_1M: x_1 + x_2 + x_3 = 3/2$, intersects C in a regular hexagon $B_1B_2B_3B_4B_5B_6$ and divides C into two halves. Every point of the half $x_1 + x_2 + x_3 < 3/2$ has a distance less than m from $P_1 = A_1$ (this half being a polyhedron), for $d(B_iA_1) = m$ $(i = 1, 2, \ldots, 6)$ and for any X on the hexagon we have $d(X, A_1) < m$. By (1) the other four points of

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

S must therefore lie in the other half with $x_1 + x_2 + x_3 \geq 3/2$.

This other half may be divided into three parts by the three half planes through $A_8M : x_1 = x_2 \leq x_3$, $x_1 = x_3 \leq x_2$, and $x_2 = x_3 \leq x_1$, cutting the hexagon in MD_1, MD_2, and MD_3 respectively. These three parts, taken closed, are congruent. Since their union contains four points of S, one part must contain (at least) two points of S. But these parts have diameter m, which is assumed only between A_8 and the points B_i $(1 \leq i \leq 6)$. By (1) another point of S, say P_2, must therefore be located at A_8 and only the points B_i $(1 \leq i \leq 6)$ are left as possible locations of the last three points of S. It is easily seen that thus P_3, P_4, P_5 lie either at B_1, B_3, B_5 or at B_2, B_4, B_6. Both these configurations are congruent to the indicated solution, and so (A) is proved.

(B) We are left to show that there exists no set of five points P_i $(1 \leq i \leq 5)$ with (1), without at least one of the points P_i lying at a vertex of C.

Let us assume the contrary. Then around every vertex A_i there exists a largest open cube C_i $(1 \leq i \leq 8)$, with center A_i and edges parallel to those of C, which does not contain any point of S. With suitable numeration a smallest of them is C_1. Denote its side by $2a$ $(0 < a \leq 1/2)$. Let Q_i be the open cube with center A_i $(1 \leq i \leq 8)$, side $2a$, and edges parallel to those of C. Clearly $Q_i \subseteq C_i$, and therefore $S \subset C_Q$, where C_Q denotes the set of all points belonging to C but not to any Q_i. Since $Q_1 = C_1$, on its boundary there must lie (at least) one point of S, say P_1. Without loss of generality we may assume that P_1 lies on the square $\Sigma : 0 \leq x_i \leq a$ $(i = 1, 2)$, $x_3 = a$ (shaded in fig. 2).

By (1), the subset $S_1 \subset C_Q$ which is defined by the simultaneous conditions $x_1 + x_2 + x_3 \leq 3/2$ and $x_1 + x_2 \leq 3/2 - a$ (see fig. 2) cannot contain any point of S besides P_1, because all its points have a distance which is less than m from all the points of Σ. This latter statement is easily verified by showing that all the distances between any vertex of Σ and any vertex of S_1 are less than m.

The remaining part $C_Q - S_1$ of C_Q may now, by the same three half planes through A_8M as used in (A), be subdivided into three parts. But although that part which contains (1, 1, 1/2) is increased, in comparison with (A), by part of the half space $x_1 + x_2 \geq 3/2 - a$, because of the truncation of C by Q_i the diameters of all three parts are now less than m. (This is again proved by straight forward verification that the distance between any two vertices of such a part is less than m. For $a \leq 1/4$ the elimination of Q_8 would suffice; see fig. 2. For $a > 1/4$ also the elimination of Q_2 and Q_3 becomes important.) By (1) they can therefore lodge at most one point of S each, and S can contain at most four points, in contradiction to our assumption. This proves (B).

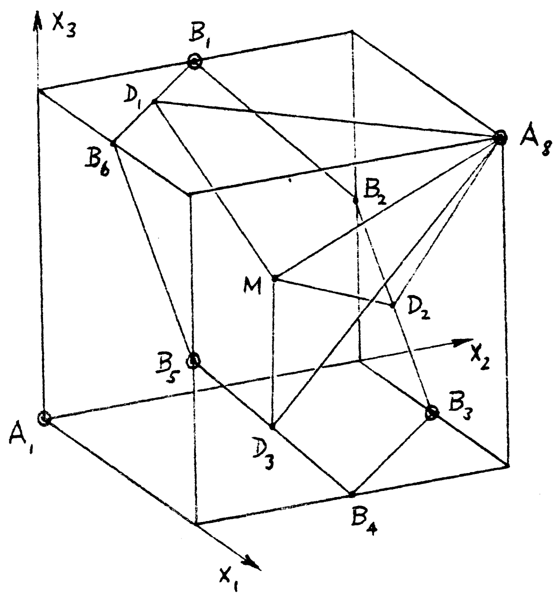

Fig. 1

https://doi.org/10.4153/CMB-1966-034-8 Published online by Cambridge University Press

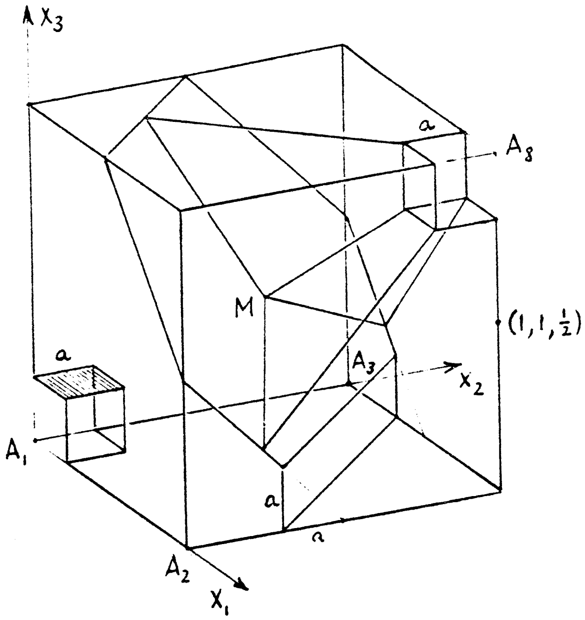

Fig. 2

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