

The densest and the least dense packings of equal spheres.

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The densest packings.—Of the results which have so far been achieved by study of the packing of equal spheres one of the most remarkable, both by reason of its simplicity and of its fundamental importance, was that announced by Barlow in 1883.¹ He called attention to the fact that equal spheres can be most densely packed in two ways, one possessing cubic symmetry and the other hexagonal (fig. 1).

Already in 1862 Tait² had investigated the piling of marbles of equal size and had noticed that ‘there are two obvious ways of constructing the layers, and two of applying layer to layer’: nevertheless his two densest arrangements are in fact identical. He saw that the cubic structure could be begun either upon a square base or a triangular base but failed to perceive the possibility of the hexagonal arrangement.

And even after Barlow announced his discovery, A. G. Greenhill³ dealing in 1889 with the piling of spherical shot concluded that ‘Whether we begin piling the shot in horizontal layers, in triangular order or in square order, the internal molecular arrangement of the spheres is the same’.

It was also in 1889 that Kelvin⁴ dealt with the densest packing of equal spheres in connexion with his development of Boscovich’s theory of the constitution of matter. While admitting that ‘Mr. Barlow, so far as I know, was the first to show a cubic part of the close-packed homogeneous assemblage of equal globes’, he declined to recognize the hexagonal structure as a homogeneous assemblage. But this came about through his adhering to a too-restricted definition of homogeneity.

In 1898 Barlow⁵ took up the subject of the densest packing of unequal spheres. ‘I may say’, he remarks, ‘that my general principle for getting closest-packing of the spheres is to produce a maximum number of

¹ W. Barlow, *Nature*, London, 1883, vol. 29, p. 186.

² P. G. Tait, *Proc. Roy. Soc. Edinburgh*, 1862, vol. 4, p. 535.

³ A. G. Greenhill, *Nature*, London, 1889, vol. 40, p. 10.

⁴ W. Thomson, *Proc. Roy. Soc. Edinburgh*, 1890, vol. 16, p. 693.

⁵ W. Barlow, *Proc. Roy. Dublin Soc.*, 1898, n. ser., vol. 8, p. 527 (preprints dated 1897).

contacts, so as to diminish, as far as possible, the amount of interstitial space.' In the case of equal spheres, it is taken as axiomatic that they are most densely packed when each is in contact with twelve others. He then goes on to remark that 'It is evident that twelve contacts for each sphere can be attained in a variety of different ways. There are two and two only, which give homogeneity of structure.'

However, by 1907 he had gained further light on the matter, and having once more described the arrangements shown in fig. 1, he adds:

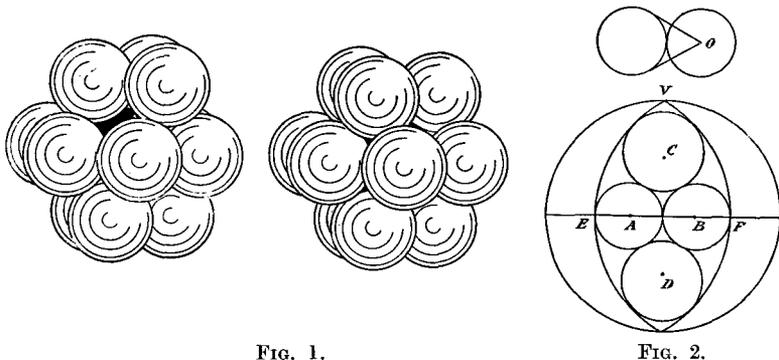


FIG. 1.

FIG. 2.

'The two assemblages above described are equally close packed and can, by combination or admixture, give rise to other equally close-packed homogeneous assemblages.'¹

The question as to how many such closest-packed homogeneous mixtures there might be was left by Barlow incompletely answered; but it has recently been found that there are four.² There are thus all together six homogeneous structures possessing 12-point contact and having therefore the same density³ of 0.74048. . .

It has lately been remarked as a curious fact that although it is obviously true that equal spheres are most densely packed when each is in contact with twelve, nobody has yet succeeded in proving it. Several persons have shown that it is true when the sphere-centres are at the corners of a parallelepiped, the earliest so far as I know being Kelvin in the paper already cited. But the problem still remains to be considered free from such restrictions.

¹ W. Barlow and W. J. Pope, Journ. Chem. Soc. London, 1907, vol. 91, p. 1158.

² S. Melmore, Nature, London, 1947, vol. 159, p. 817.

³ By *density* is meant the ratio of the total volume of the spheres in a lattice cell to the whole volume of the cell.

It might be thought that the property of dilatancy¹ is in itself a satisfactory proof: for if any distortion of normal piling with 12-point contact results in an increase in the overall volume, and therefore a diminution of density, it follows that 12-point contact is the condition for maximum density. But setting this aside, we may approach the matter in another way:

The upper part of fig. 2 represents two equal spheres (radius = 1) in contact: from O , the centre of one sphere, project the other on to it. The projection will be a small circle with an angular diameter of 60° : the area of the small circle is therefore 0.268π .

In place of the question: What is the greatest number of equal spheres that can be brought into contact with another of the same size?, we may now ask: What is the greatest number of non-intersecting small circles (diameter = 60°) that can be inscribed on a sphere?

In the stereographic projection, fig. 2, the four small circles are equal and have angular diameters of 60° : two, with their poles at A and B respectively, are in contact. A third, C , will be most closely packed when it is in contact with the first two; and again, a fourth, D , will be most closely packed in like circumstances. Through A and B draw a great circle intersecting the small circles A and B in E and F . Through E and F draw secondaries to this great circle. Then the angle of the lune $VEV'F$ is equal to the arc $EF = 120^\circ$. So the area of the lune is one-third the area of the whole sphere, that is to say, its area is $\frac{4}{3}\pi$.

The sum of the areas of the four small circles is $4 \times 0.268\pi = 1.072\pi$. The residual area is therefore $(1.333 - 1.072)\pi = 0.261\pi$, which is less than the area of one small circle. So not more than four circles can be accommodated within the lune, and therefore not more than twelve on the whole surface of the sphere. Hence not more than twelve equal spheres can be brought into contact with another of the same size.

Taking another view of the problem: It has been proved² that the closest packing of equal circles in a plane is that in which each circle is in contact with six, fig. 3. Let the middle circle rotate about a diameter so as to generate a sphere. We may then inquire: What is the greatest number of planes through the centre of this sphere upon which a like set of neighbouring circles can be inscribed, having regard to the symmetry?

¹ Osborne Reynolds, *Phil. Mag.*, 1885, ser. 5, vol. 20, p. 469. The sub-mechanics of the universe, Cambridge, 1903. Rede Lecture, Cambridge, 1902.

² B. Segre and K. Mahler, *Amer. Math. Monthly*, 1944, vol. 51, p. 261. But I have not seen this paper.

There is an axis of symmetry normal to the plane through the centre of the middle circle, which may be regarded as hexagonal or as trigonal. If hexagonal, then there can be only one plane: if trigonal, there may be four, but no more. These planes are parallel to the faces of the octahedron, and are represented by the great circles in the stereographic projection, fig. 4, where three of them are projected on the plane of the fourth.

The great circles may be thought of as passing through the centres of the six circles in their respective planes. It follows from considerations

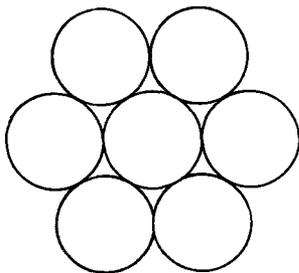


FIG. 3.

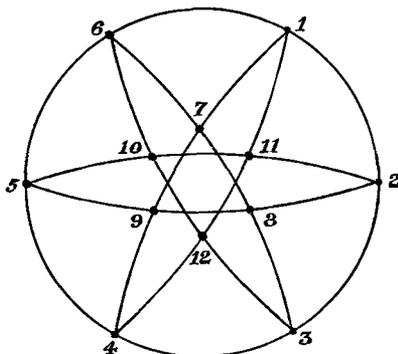


FIG. 4.

of symmetry that the centres of these latter circles lie at the intersections of the great circles (numbered in the figure); and since the great circles intersect in pairs, the total number of circles in contact with the central sphere is $\frac{4 \times 6}{2} = 12$.

It is easily seen that all the arc-segments joining the numbered points of intersection are arcs of 60° : therefore when all the twelve circles each rotate about a diameter they will generate spheres touching the central sphere and also touching their other neighbours.

The least dense packings.—Although the study of the most open packings of equal spheres is of comparatively recent date, some of the results have already found application in the elucidation of the structure of ionic minerals¹ and of the assemblages built up by ultra-microscopic dust particles.² The problem of the most open packing was first propounded by H. Heesch and F. Laves in 1933.³

¹ H. W. Fairbairn, *Bull. Geol. Soc. Amer.*, 1943, vol. 54, p. 1305. [M.A. 9-41.]

² H. Heywood, *Journ. Imp. Coll. Chem. Eng. Soc.*, 1946, vol. 2.

³ H. Heesch and F. Laves, *Zeits. Krist.* 1933, vol. 85, p. 443. [M.A. 5-342.]

The principal conditions they impose are that: (i) the structure is composed of congruent spheres, (ii) it is continuous, (iii) either sphere of a pair can be transformed into the other by symmetry operations, (iv) the lines joining the points of contact of successive spheres pass through the centres of the spheres, thus ensuring the stability of the structure. (It follows from this condition that when a sphere is in contact with no more than three others, the four sphere-centres must be coplanar.)

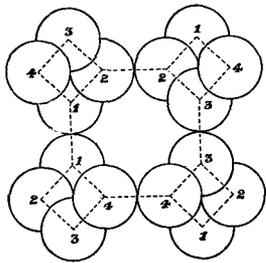


FIG. 5.

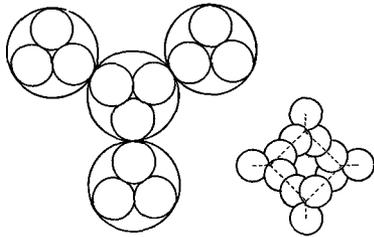


FIG. 6.

Condition (iii) is of some practical importance. It means that the whole structure can be developed by applying symmetry operations to a single sphere. If, on the other hand, we operate upon a group of spheres, structures can be developed which are even less dense than those found by Heesch and Laves.¹ However, in what follows, this condition is retained. Of the nine assemblages described by these authors, it is here necessary to consider only two; both possess cubic symmetry and are non-self-reflexible.

The nature of the first is indicated by the ground plan of the left-handed form, fig. 5. The spheres are arranged round tetragonal screw-axes having a pitch angle of 45° , and there are digonal axes of rotation between the screws. Each sphere makes contact with three others, and the lines of centres from any one sphere to its three neighbours make angles of 120° . This structure has a density of 0.185 . . .

From this assemblage Heesch and Laves derive another by applying an ingenious three-for-one substitution, the nature of which will be at once evident from the diagram in the left-hand half of fig. 6. When this is done, the tetragonal screws of fig. 5 become 2-point tetragonal screws with a connecting sphere between. One such element of the new structure is shown in the right-hand half of fig. 6.

¹ S. Melmore, *Nature*, London, 1942, vol. 149, p. 669. [M.A. 8-344, 9-139.]

The structure thus derived has a density of 0.056,¹ and is the most open described by Heesch and Laves. The opinion has been expressed² that this may perhaps be the most open structure possible (under condition (iii)), but till now no proof has been forthcoming.

The following considerations are based upon Barlow's conception of *singular points*.³ These are concisely defined in the Dublin paper (footnote to p. 627): 'Singular points in a homogeneous structure are points which occupy specially symmetrical situations, and so form point-

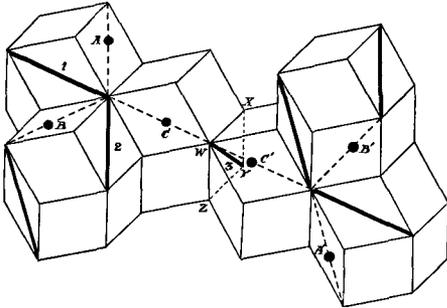


FIG. 7.

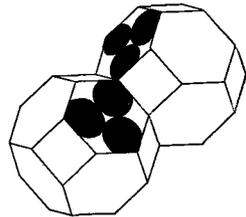


FIG. 8.

systems containing fewer points than ordinarily; they lie on axes of rotation or on planes of symmetry, or on both'; but the paper in the *Zeitschrift* must be consulted for the full exposition.

It is clear then, that if we are to fill a given space with a homogeneous arrangement of as few spheres as possible, the sphere-centres will be singular points. Following Barlow's train of thought (*Zeitschrift*, pp. 60-62) it is evident that if there are to be as few singular points as possible, then structures with a principal axis of rotation are ruled out, and we are left with the consideration of digonal axes only.

To visualize the position of all the possible digonal axes: Let space be partitioned into rhombic dodecahedral cells: then the digonal axes will be represented by the normals joining opposite faces.⁴ They lie in

¹ The value is thus given by Heesch and Laves. I have carried the calculation farther, using 7-figure logarithms, with the result 0.055515 . . .

² W. Nowacki, *Homogene Raumteilung und Kristallstruktur*. Zürich, 1935, p. 48.

³ W. Barlow, *Zeits. Kryst. Min.*, 1894, vol. 23, p. 1; *Proc. Roy. Dublin Soc.*, 1898, n. ser., vol. 8, p. 527.

⁴ The particular normals which are the digonal axes of the extended structure lie in the surface of the cells as indicated in fig. 7, which represents one of the models exhibited when the paper was read.

possible planes of reflection, and other symmetry elements are also potentially available. As will appear immediately, the question which and how few of all these potential elements are necessarily operative is automatically answered by the conditions of the problem.

In fig. 7, let A be a sphere-centre located on a digonal axis;¹ then the axis 1 will develop from it the point B . Axis 2 will carry B to C . We now have three sphere-centres A, B, C , defining a plane. Now by condition (iv) a fourth centre must lie in this plane and also on the diameter (produced) of one of the existing spheres. C' is therefore a possible position. To carry C to C' , two courses are open: either C may be reflected across the plane $WXYZ$, or the digonal axis no. 3 (i.e., WY) may be employed. But the first process leads merely to the development of a single sheet of spheres. On the other hand, by the operation of the digonal axis no. 3, C is carried to C' , A to A' , and B to B' , so that a 3-dimensional distribution of sphere-centres comes into being.

The structure developed by repetition of these rotations is identical with that of Heesch and Laves, having the density 0.056. (The points B, C, C', A' , for instance, are part of a 2-point tetragonal screw such as is shown in plan in fig. 6.) This structure, first discovered by Heesch and Laves, is then the most open possible under the given conditions.

It was necessary for the purposes of proof to employ digonal axes only; but now that this is done we see that of all the potential digonal axes those actually used are themselves distributed around threefold axes of rotation, and the sphere-centres are consequently similarly related.

As the normals to the faces of the octahedron are threefold axes of rotation, a conveniently compact model of this structure can be made by preparing several equal truncated octahedra, inscribing three circles (to represent spheres) on one hexagonal face of each octahedron, and fixing them together so that each is connected to four others at faces tetrahedrally related. Two such truncated octahedra are shown in fig. 8.

¹ In order that the spheres shall be in contact, A must bisect the long face diagonal in the ratio 0.758 : 0.875.