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Minimal-Energy Clusters of Hard Spheres

N. J. A. Sloane,[1] R. H. Hardin,[1] T. D. S. Duff,[1] and J. H. Conway[2]

[1]Mathematical Sciences Research Center, AT & T Bell Laboratories,
Murray Hill, NJ 07974, USA
njas@research.att.com; rhh@research.att.com; td@research.att.com

[2]Mathematics Department, Princeton University,
Princeton, NJ 08544, USA
conway@math.princeton.edu

Abstract. What is the tightest packing of N equal nonoverlapping spheres, in the sense of having minimal energy, i.e., smallest second moment about the centroid? The putatively optimal arrangements are described for $N \leq 32$. A number of new and interesting polyhedra arise.

1. Introduction

> **hardball**. 2. Informal. The use of any means, however ruthless, to attain an objective.
>
> *American Heritage Dictionary*, Third Edition, Houghton-Mifflin, New York, 1992

A number of papers have appeared in recent years in the mathematical literature dealing with questions of finding the best packings of N points (or equivalently congruent circles or spheres) in two and three dimensions from various points of view: see the surveys in [CFG] and [GW]. For example, [MP], [PWM], and [Me] study the problems of finding the densest packings of N equal circles in a square or equilateral triangle.

Statement of Problem

However, the problem considered in this paper, which is to find minimal-energy clusters of N equal and nonoverlapping spheres, seems to our surprise not to have been considered. Stated formally, we wish to determine points $P_1, \ldots, P_N$ in $\mathbb{R}^3$ so as to minimize the second moment

$$M = \sum_{i=1}^{N} |P_i - C|^2, \tag{1}$$

where $C = N^{-1}\sum_{i=1}^{N} P_i$ is the centroid, subject to the constraints $|P_i - P_j| \geq 2$ for $i \neq j$. Placing spheres of radius 1 at the P_i then gives a packing or cluster of hard spheres. Apart from a factor of N, M is the sum of the squared distances between all pair of points.

Such clusters are also of interest in the investigation of Kepler's problem of determining the densest sphere-packing in three dimensions, since the attacks on this problem involve (among other things) detailed analysis of small clusters of spheres [B], [Mu], [Hs], [Ha]. Although there is a standard way to define the density of a packing of infinitely many spheres, there is no single definition of the density of a finite cluster that is totally satisfactory. Our minimal-moment criterion offers another way to evaluate the "tightness" of a cluster.

The interpretation of $|P_i - C|^2$ as the energy in P_i is a standard one in communications, where $P_1, \ldots, P_N$ would represent a constellation of N signals with total energy M [CG], [FGW].

The analogous two-dimensional question of minimal-energy penny packings was studied in [GS] and [C].

Lennard–Jones Clusters

In the physics literature there have been a large number of papers that deal with the problem of finding arrangements of N points that minimize the Lennard–Jones potential

$$\sum_{1 \leq i < j \leq N} \left(\frac{1}{d_{ij}^{12}} - \frac{2}{d_{ij}^{6}} \right), \tag{2}$$

where $d_{ij} = |P_i - P_j|$—see [CSW1], [CSW2], [FFR], [HM1], [HM2], [HP1], [HP2], [MF], [N], [RFF], [S], and [Wi]. Reasonable candidates for minimal-potential arrangements have been found for up to several hundred points, although optimality has been rigorously established in only a few cases. However, in such arrangements the distances between pairs of neighboring points is not constant (for example, in the case $N = 5$ it varies between 0.996 and 1.002), so such clusters are packings of soft rather than hard spheres. Furthermore, even if we ignore this variation in minimal distance, the putatively optimal Lennard–Jones clusters are in general completely different from those found in this paper, so this is a strictly different problem. The Lennard–Jones problem also seems considerably easier than the minimal moment problem, essentially because (2) is differentiable but (1) is not. Using our techniques we were able to reproduce all the published optima for Leonard–Jones clusters of

Table 1. Conjectured minimal second moment M for any cluster of N unit spheres

N	M	N	M	N	M
1	0.	12	42.8163	23	131.7681
2	2.	13	47.7012	24	141.2778
3	4.	14	54.8783	25	151.6267
4	6.	15	62.1071	26	161.3333
5	9.3333	16	69.7926	27	172.8889
6	12.	17	78.1282	28	183.7619
7	16.6833	18	86.3012	29	193.4559
8	21.1567	19	95.1284	30	205.7136
9	25.8990	20	105.0434	31	217.3094
10	31.8279	21	114.2222	32	229.3750
11	37.8346	22	122.4848		

up to 75 spheres. To use a sporting metaphor which is also technically correct, their problem is softball, ours hardball.[1]

Other criteria for minimal clusters of spheres, also different from ours, and with different solutions, have been used in [We], [B], and [GW].

Summary

The main results of this paper are summarized in Table 1, which gives what we conjecture are the minimal second moments of arrangements of N spheres for $N \leq 32$. The arrangements themselves are illustrated in Fig. 1 and described in more detail in Section 2. We have in fact searched for optimal packings with up to 99 spheres, although since we are less confident of the optimality of the configurations with more than 32 spheres they will not be described here. Numerical coordinates for all these packings have been placed in the Netlib archive, and can be accessed via electronic mail, ftp, or Mosaic. The packings are in the directory att/math/sloane/cluster. Instructions for obtaining them can be obtained by sending the message send getting.stuff from att/math to netlib@research.att.com.

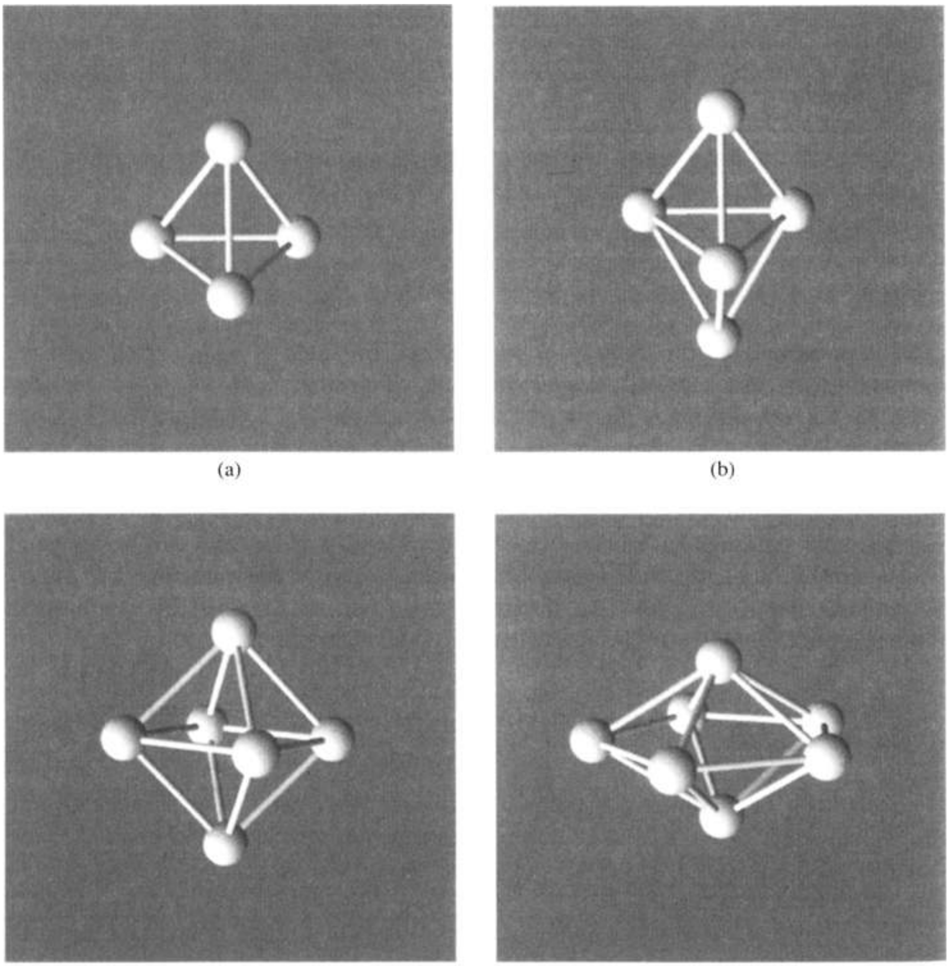
Discussion of Results

The character of the putatively optimal arrangements changes in an interesting way as N increases. For $4 \leq N \leq 10$ these arrangements (see Section 2) consist of the vertices of reasonably well-known polyhedra, the so-called *deltahedra*, whose faces are equilateral triangles [J].

For $N = 11$–13 the best arrangements consist of a central point together with $N - 1$ points at distance 2 from it. The 13-point answer is at first glance surprising, since it consists neither of the center and vertices of a regular icosahedron (which is

[1]As one reader of this paper has pointed out, softball is intrinsically underhanded.

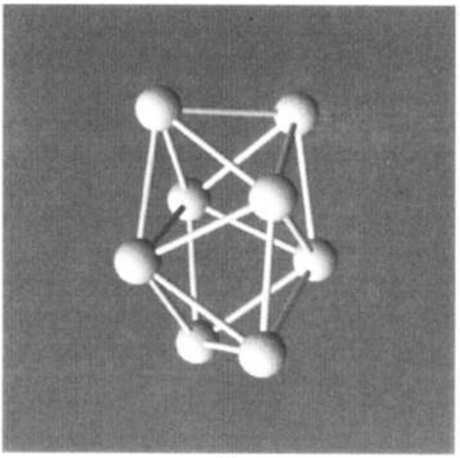
the 12-vertex deltahedron), nor the center and vertices of a cuboctahedron (the arrangement found in the face-centered cubic lattice). Instead, the answer is the center and vertices of the "weary icosahedron," obtained from a regular icosahedron by allowing the vertices to roll down the circumsphere toward the south pole until the *contact graph* of distance-2 neighbors is as shown in Fig. 3. This is understandable, however, when we recall that in a regular icosahedron the edge length is slightly greater than the circumradius, and therefore the second moment can be reduced by displacing the centroid away from the center, at the same time rolling the vertices in the direction of the centroid until their separation is equal to the circumradius. The equilibrium position is reached at the "weary icosahedron."



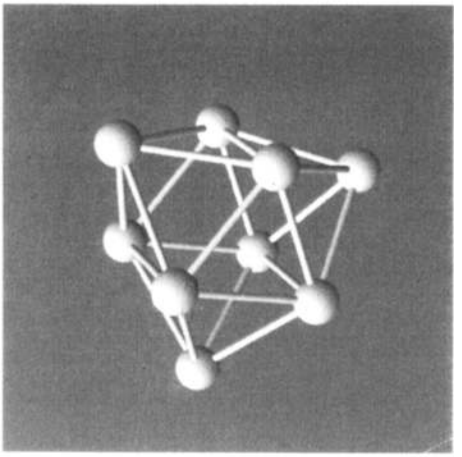
(a) (b)

(c) (d)

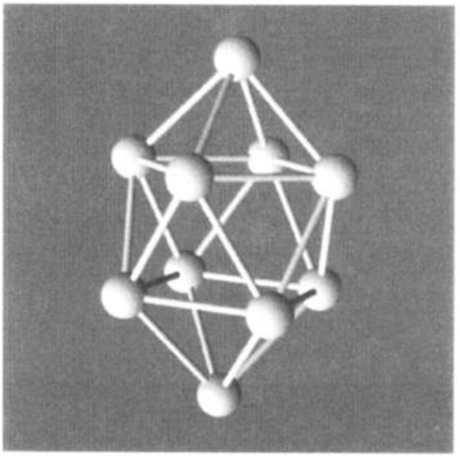
Fig. 1. Putatively optimal clusters of N spheres, for $N = 4$–10 (a)–(g) and 13–20 ((h)–(o)). For greater clarity the spheres have been reduced in size, contacts between adjacent spheres have been replaced by bonds, and for $N \geq 3$ the central sphere has been omitted.



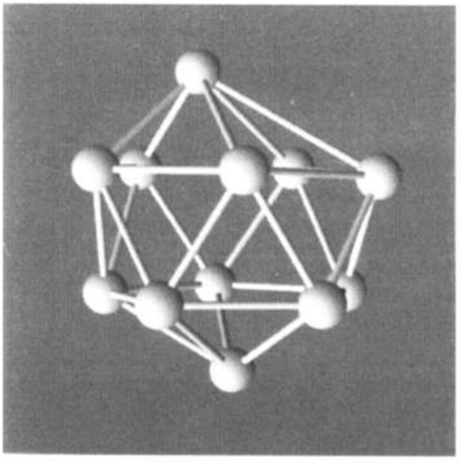
(e)



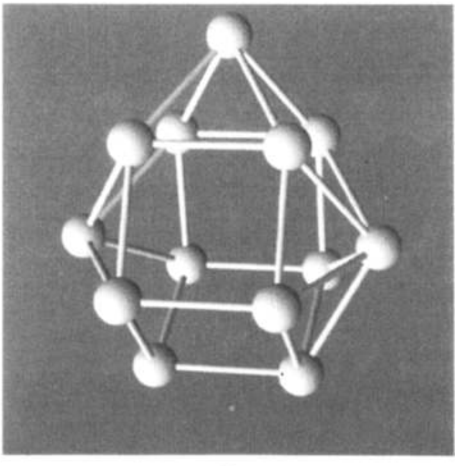
(f)



(g)



(h)



(i)

Fig. 1. Continued

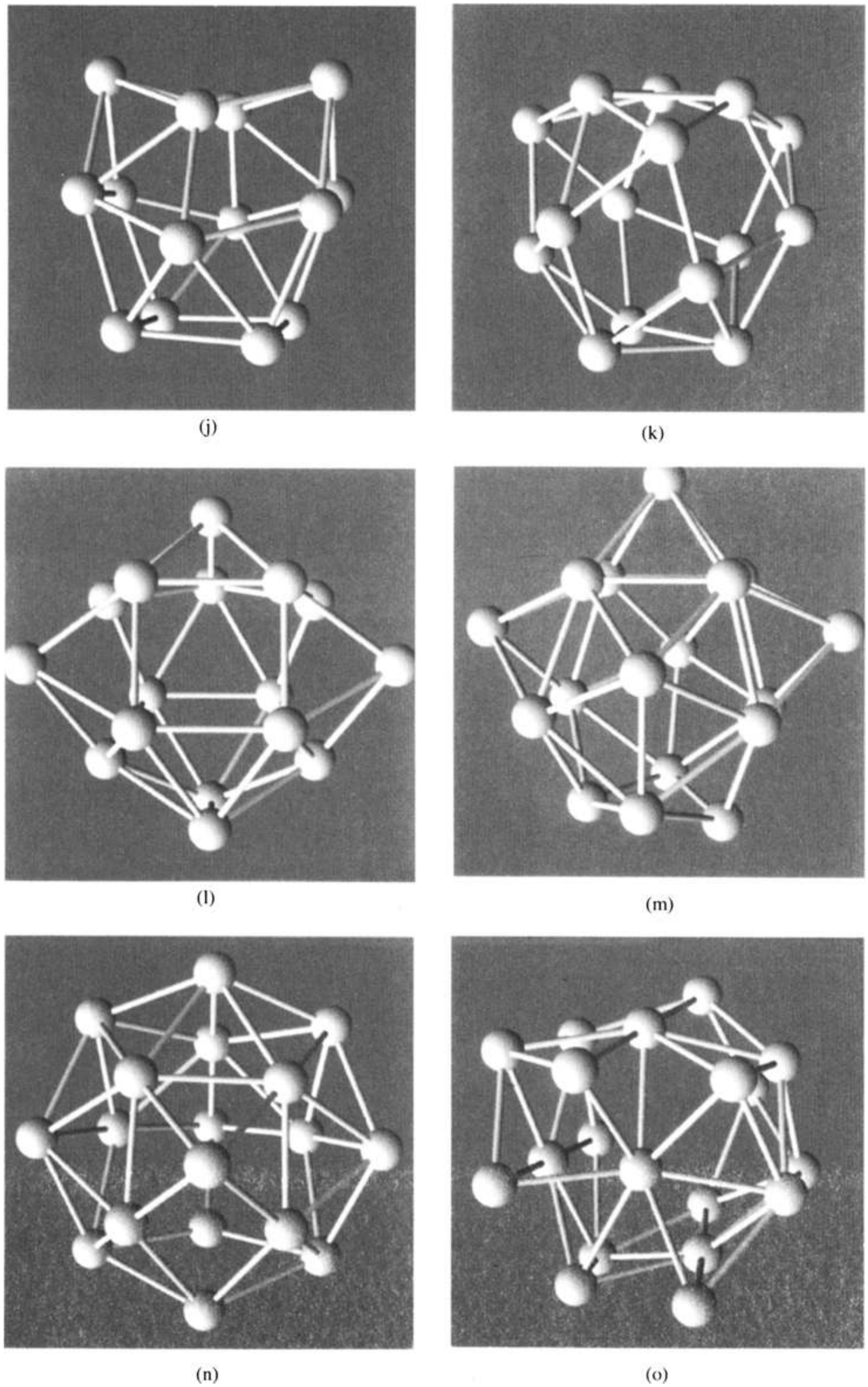


Fig. 1. Continued

The best arrangements for $N = 11$ and 12 are obtained by omitting points from the $N = 13$ solution.

For $N = 14$–20 the best arrangements we have found consist of a (roughly) central point together with the vertices of a convex polyhedron containing the central point. The central sphere often touches only a few of the other spheres (only seven when $N = 18$, for example). The polyhedra for $N = 14, 15, \ldots, 20$ are all quite different from each other. We believe that these polyhedra have not appeared in the literature before.

Our understanding of these polyhedra was greatly enhanced by making cardboard models of them, and the figures in Section 2 can be used as a guide for making such models.

For $N = 21$–32 the best arrangements can be built in a uniform manner (to be described in Section 2) from parallel one-dimensional strings (or "skewers") of spheres. All of $N = 21$–32 can be obtained as subsets or supersets of the clusters for $N = 26$ and 29.

Before beginning this investigation, we anticipated that many of the optimal arrangements for small N would consist of regular tetrahedra glued together. For $N \geq 6$, nothing could be further from the truth. The numbers of regular tetrahedra in the best arrangements for $N = 4$–20 are respectively 1, 2, 0, 0, 0, 3, 0, 8, 8, 8, 0, 8, 1, 0, 0, 0, 3.

The results are also in complete contrast to those obtained in [GS] for the analogous two-dimensional problem, in that

(a) the best arrangements are not those found in the densest lattice packing, and
(b) whereas in the two-dimensional case the greedy algorithm produces the best arrangements for $N \leq 21$, in three dimensions the greedy algorithm gives the best arrangements only for $N \leq 5$ and $N = 11, 12, 13$ (and, we conjecture, never again).

Finally, we give a brief comparison with the putatively optimal Lennard–Jones clusters given by Hoare and Pal [HP1]. For $N \leq 7$ these clusters are essentially the same as ours, except for having spheres of slightly different sizes. For $N \geq 8$ the clusters are quite different. For $N = 8, \ldots, 12$ the optimal Lennard–Jones clusters are essentially the vertices of a pentagonal bipyramid with $N - 7$ tetrahedra erected on consecutive faces of one of the two pentagonal pyramids, and for $N = 13$ the answer consists of the center and vertices of a regular icosahedron [HP1, p. 176].

How the Results were Obtained

Bearing in mind the epigraph to this paper, we tried a number of different techniques:

(i) The greedy algorithm, at each step adding a sphere in the optimal way. (The results from this method have already been mentioned.)
(ii) Extracting clusters of spheres from the face-centered cubic lattice, hexagonal close packing, etc., as in [GS] and [ST]. (This was successful—i.e.,

produced what we believe are the optimal configurations—only for $N \leq 5$ and $N = 26$.)

(iii) Simulated annealing applied to clusters from (i) and (ii). (Successful for $N = 21, 23\text{–}25, 27, 28$.)

(iv) Quadratic programming, to minimize (1) subject to the constraints $|P_i - P_j|^2 \geq 4$ $(i \neq j)$. (Successful for $N \leq 20$, not for larger N.) The programming language AMPL [FGK] made it particularly easy to apply quadratic programming to this problem. For each value of N we took several thousand random starting configurations and then optimized them (via AMPL) using both the MINOS [MS] and CONOPT [D] optimization programs.

(v) A modification of the "pattern search" used in [HS1], [HS2], and [HS3]. (Successful for all $N \leq 32$ except 29 and 30.) In this algorithm we approximated the minimal moment criterion of (1) by a sequence of potential functions

$$\Phi_k = \sum_{i=1}^{N} |P_i|^2 + \sum_{i<j} \frac{\beta_k}{|P_i - P_j| - \alpha_k}, \tag{3}$$

for $k = 0, 1, \ldots$, where α_k and β_k (respectively specifying the hardness and repulsion of the spheres) are given by $\alpha_0 = 0$, $\beta_0 = 1$, and

$$\alpha_k = \alpha_{k-1} + \tfrac{1}{2}\left\{\min_{i<j}|P_i - P_j| - \alpha_{k-1}\right\},$$

$$\beta_k = \tfrac{1}{2}\beta_{k-1}, \qquad k \geq 1. \tag{4}$$

A given starting configuration is minimized under Φ_0, the result then minimized under Φ_1, and so on, until no further improvement is obtained to the tolerance of the machine. At each stage the spheres get harder and less repellent.

This procedure has the drawback that since initially the spheres are soft and can squish by each other, only a small number of different final configurations were reached. To obtain further possibilities, even if only to reject them, we therefore removed a random sphere from the final cluster, placed it outside the cluster, softened the spheres slightly (by setting $\alpha_0 = 0.9 \min_{i<j} |P_i - P_j|$, and choosing a random β_0), and again minimizing under the sequence of potential functions. (The value 0.9 was determined by experimentation to produce good results.) After termination the cluster must be rescaled to have minimal separation 2.

The computer output from these algorithms was then "beautified" to produce the arrangements shown in Section 2. This process consisted in finding the contact graph, the full symmetry group, and coordinates for the points that reveal as much of the symmetry as possible. Some of the symmetry groups were found using MAGMA [CP].

(vi) Study of the beautified results from (v) for $N = 21\text{–}26$ revealed that these had a common construction, the "skewer" construction described in Section 2. A special search was therefore made for clusters of this type, which produced new records for $N = 29$ and 30.

(vii) After applying our pattern-search algorithm to the Lennard–Jones problem, we used the putatively optimal configurations for that problem as input to the program described in (v). This was successful only for $N \leq 9$.

(viii) Various iterative constructions, such as adding a random sphere to a good packing of $N - 1$ spheres and optimizing the result.

We are reasonably confident that the results in Table 1 are optimal, or at least very close to optimal. On the other hand we have no proofs of optimality for any N greater than 4. It would be possible, although laborious, to construct such proofs using the methods of [PWM], by considering all possible contact graphs with N nodes, and for each graph, using MAPLE or MACSYMA to determine the optimal arrangement of points with that contact graph.

We would be interested in hearing of any improvements to Table 1, or of optimality proofs. They should be sent to N. J. A. Sloane at the address at the beginning of the paper, or by electronic mail to njas@research.att.com.

Existence Questions

Once the contact graph is specified, the coordinates of the points are determined by the solution to a system of quadratic equations, and so are algebraic numbers. The computer output gives only an approximate solution to these equations, correct to about 10^{-12}. Formally, therefore, it is necessary to verify that there *is* a true solution to this system of equations in the neighborhood of the computer's approximate solution. For $N \leq 14$ we carried out this verification using MACSYMA, and in Section 2 give exact coordinates for the points. However, for $15 \leq N \leq 20$ we did not do this, since already at $N = 15$ the algebraic numbers involved are of quite large degree. Our experience (both in this problem and in related problems discussed in [HS1] and [HS3]) strongly suggests that for $N \leq 20$ the computer solutions are sufficiently precise and the equations are sufficiently well-behaved that there always is a true solution nearby. For $21 \leq N \leq 32$ the skewer construction directly leads to explicit coordinates.

If it were felt necessary to establish the formal existence of these arrangements for $15 \leq N \leq 20$, this could most easily be carried out by the interval arithmetic package INTBIS [KN].

Note that there is no question about the validity of the numbers in Table 1, only about the existence of the contact graphs. Even if some of the distances in the cluster are $2 + \varepsilon$ rather than 2, the values in Table 1 will not change.

One of the referees has kindly pointed out that it is easy to give existence proofs for the cases $N = 15$, 16, 17, and 19. With the editors' permission, we quote from the report. "Here is the argument for $N = 15$. If we delete the two edges $(12, 13)$ and $(11, 14)$ from the contact graph in Figure 5, so that these spheres overlap if necessary, a solution may be constructed by inserting one sphere after another. In fact, a continuous one-dimensional family of (symmetric) solutions exists and is parametrized by the distance t between the spheres 5 and 6. The distance $d(t)$ between spheres 12 and 13 is continuous in t. We find $d(2.76) = 1.99428$ and $d(2.77) = 2.0224$. Some intermediate value t_0 then gives $d(t_0) = 2$. By symmetry, the distance between spheres 11 and 14 must also be 2. The arguments for $N = 16$, 17, and 19 are similar. For $N = 18$, the existence argument involves a two-dimensional family of clusters."

Asymptotic Results

As the radius R of the clusters increases, N will grow like R^3, M like R^5, and the normalized second moment $M/N^{5/3}$ should approach

$$\frac{3}{5} \frac{1}{\Delta^{2/3}},$$

where Δ is the density of the packing. (This limiting expression is valid if the spheres form a roughly spherical subset of a lattice, as follows from Theorem 4 of [CS], and it is plausible that the same limit holds for arbitrary clusters.) Therefore, if Kepler's conjecture that no sphere packing can be denser than the face-centered cubic lattice is correct (see [Ha] and [Hs]), $M/N^{5/3}$ should approach

$$\left(\frac{2 \cdot 3^5}{5^3 \cdot \pi^2} \right)^{1/3} = 0.7331\ldots$$

as $N \to \infty$. Our results neither confirm nor contradict this: at $N = 99$, $M/N^{5/3}$ has very slowly risen to around 0.72. It certainly is true, as we have already discussed, that for $N \leq 99$ (with the exceptions $N \leq 5$, $N = 26$), extracting clusters of spheres from the face-centered cubic lattice of hexagonal close-packing does *not* yield minimal energy arrangements.

Notation

In Section 2 the N points are labeled $0, 1, \ldots, N - 1$, decimal expansions have been rounded to four places, the coordinates are labeled x, y, z, and G denotes the group order.

2. The Putatively Minimal-Energy Clusters

$N = $ **1–7.** The vertices of the following figures, in which all edges have length 2.

1: point
2: line segment
3: triangle
4: tetrahedron
5: triangular bipyramid
6: octahedron (= square bipyramid)
7: pentagonal bipyramid

$N = $ **8.** Vertices of dodecadeltahedron (a polyhedron with 12 triangular faces). Other names are Siamese dodecadeltahedron or snub disphenoid [FW], [J], [Wa, Fig. 2-A16 #5]. It is also the "3-into-2" mutated icosahedron, because it can be obtained from a regular icosahedron by converting a triad axis into a dyad one. Coordinates:

$$(\pm f, e, 0), (\pm 1, -g, 0), (0, -e, \pm f), (0, g, \pm 1),$$

where $e = 0.4111$ is the unique positive real root of $2X^6 + 11X^4 + 4X^2 - 1$, $g = \sqrt{(e^{-2} - 1)/2} = 1.5679$, $f = 2eg = 1.2892$. $C = (0,0,0)$, $M = (2 + 10e^2 - 4e^4)/e^2 = 21.1567$. $G = 8$: negate x; negate z; swap x, z and negate y.

$N = $ **9.** Vertices of tetrakis triangular prism. This is the deltahedron with 14 triangular faces (the tetrakaidecadeltahedron). Coordinates:

$$\left(0, \frac{2}{\sqrt{3}}, \pm 1\right), \left(\pm 1, -\frac{1}{\sqrt{3}}, \pm 1\right), \left(0, -\sqrt{2} - \frac{1}{\sqrt{3}}, 0\right), \left(\pm \frac{1+\sqrt{6}}{2}, \frac{1+\sqrt{6}}{2\sqrt{3}}, 0\right).$$

$C = (0,0,0)$, $M = 21 + 2\sqrt{6} = 25.8990$, $G = 12$.

$N = $ **10.** Vertices of tetrakis square antiprism. This is the deltahedron with 16 triangular faces (the hexakaidecadeltahedron). Coordinates: $(\pm 1, \pm 1, e)$, $(\pm \sqrt{2}, 0, -e)$, $(0, \pm \sqrt{2}, -e)$, $(0, 0, \pm f)$, where $e = 2^{-1/4}$, $f = e + \sqrt{2}$. $C = (0,0,0)$, $M = 20 + 5\sqrt{2} + 4.2^{1/4} = 31.8279$, $G = 16$.

$N = $ **11–13.** The 13-point cluster consists of the center (labeled 0) and 12 vertices (labeled 1–12) of a "weary icosahedron," defined as follows. Take a regular icosahedron whose circumsphere has radius 2, and so the edge lengths are $4/\sqrt{(\tau + 2)} = 2.1029$, where $\tau = (1 + \sqrt{5})/2$. Imagine the vertices are replaced by heavy particles, which then roll down the circumsphere toward the south pole (labeled 1) until the graph that shows adjacencies between points at distance $\sqrt{2}$ is as shown in Fig. 2. Coordinates: 0: $(0,0,0)$, 1: $(0,0,-2)$, 2: $(\sqrt{3}, 0, -1)$, 3, 4: $(1/\sqrt{3}, \pm\sqrt{\tfrac{8}{3}}, -1)$, 5, 6: $(-7/\sqrt{27}, \pm\sqrt{\tfrac{32}{27}}, -1)$, 7, 8: $(-8\sqrt{3}/27, \pm 20\sqrt{6}/27, \tfrac{2}{3})$, 9, 10: $(8/\sqrt{27}, \pm\sqrt{\tfrac{32}{27}}, \tfrac{2}{3})$, 11: $(-21\sqrt{3}/19, 0, \tfrac{11}{19})$, 12: $(5\sqrt{3}/19, 0, \tfrac{37}{19})$. $C = (233\sqrt{3}/6669, 0, 103/741)$, $M = 54398420/1140399 = 47.7012$, $G = 2$ (negate y).

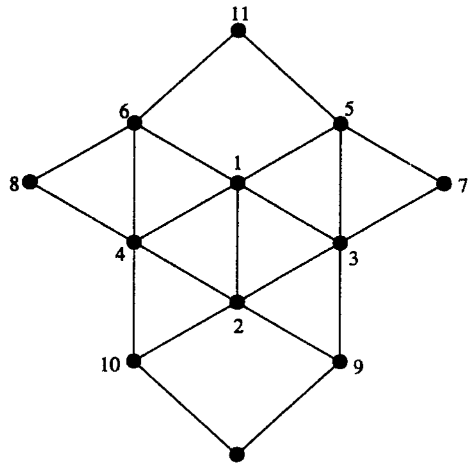


Fig. 2. $N = 13$. Contact graph for points 1–12. Point 0 (not shown) is joined to all twelve.

The convex hull of points 1–12 (which still lie on the circumscribing sphere) has the 1-skeleton shown in Fig. 3, so this is also an icosahedron. There are 30 edges, 21 of which (those shown in Fig. 2) now have length 2, the others being longer.

For $N = 12$, omit point 12; for $N = 11$, omit 11 and 12.

Incidentally the 13-sphere cluster described by Wefelmeier [We] as the "energetisch günstigsten Packung" appears to be simply the center and vertices of a regular icosahedron, rather than our arrangement.

$N = 14$. Construct the figure shown in Fig. 4 from cardboard, with all edges having length 2, and fold it so the points marked 1 all coincide, the points marked 2 coincide, and the points marked 13 coincide. Then adjoin a center point (0). Figure 4

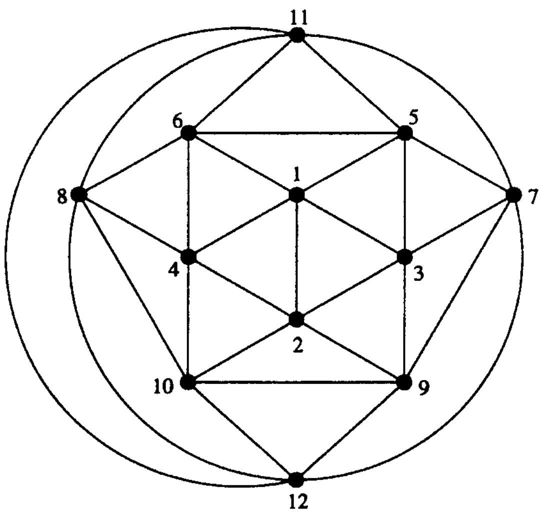


Fig. 3. $N = 13$. 1-skeleton of convex hull (the "weary icosahedron").

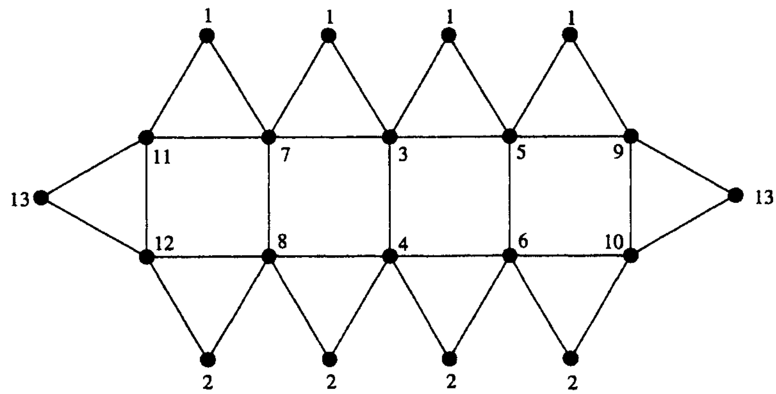


Fig. 4. Cardboard model for $N = 14$.

is also the contact graph of 1–13, the full contact graph being obtained by joining 0 to 1–12 (but not to 13).

Coordinates: 0: $(0,0,0)$, 1, 2: $(0,0,\pm 2)$, 3, 4: $(\sqrt{3},0,\pm 1)$, 5–8: $(1/\sqrt{3},\pm\sqrt{\frac{8}{3}},\pm 1)$, 9–12: $(-7/\sqrt{27},\pm\sqrt{\frac{32}{27}},\pm 1)$, 13: $(-14/\sqrt{27},0,0)$. $C=(-2/7\sqrt{3},0,0)$, $M = 10372/189 = 54.8783$, $G = 4$ (negate y; negate z).

The convex polyhedron formed by 1–13 is a pentakis prism, in which one of the square faces (9-10-12-11) has been opened slightly and point 13 placed above that face. The final polyhedron has ten equilateral triangular faces, four squares faces, and two faces (1-11-13-9 and 2-12-13-10) that are planar rhombi.

This 14-sphere cluster was discovered by Boerdijk [B], and appears as Figure 45/2 in [F].

$N = 15$. Whereas $N = 14$ was obtained by distorting a square face of a pentakis pentagonal prism, $N = 15$ is obtained by distorting two adjacent square faces of the same polyhedron. Point 0 is at the center, 1 and 2 are the apex vertices of the pentagonal pyramids, 3–12 are the vertices of the distorted pentagonal prism, and 13, 14 lie above the two adjacent faces. In the final figure, however, these two faces (7-11-10-12 and 8-12-11-9) have become nonplanar quadrilaterals. Also 1 and 2 are no longer antipodal, and it is best to take the north pole above the center (marked P in Fig. 5) of the rhombus 3-5-4-6. The contact graph for points 1–14 is shown in Fig. 5, and the full contact graph is obtained by joining 0 to 1–12. Coordinates:

0:	$(0.0000,\ 0.0000,\ 0.0000)$
1, 2:	$(0.0022, \pm 1.4459, \pm 1.3818)$
3, 4:	$(1.3825,\ 0.0000, \pm 1.4452)$
5, 6:	$(1.4466, \pm 1.3810, \pm 0.0000)$
7, 8:	$(-0.5235, \mp 0.4171, \pm 1.8847)$
9, 10:	$(-0.4166, \pm 1.8846, \mp 0.5240)$
11, 12:	$(-1.7301, \pm 0.6859, \mp 0.7324)$
13, 14:	$(-2.1985, \mp 1.2156, \pm 1.1384)$

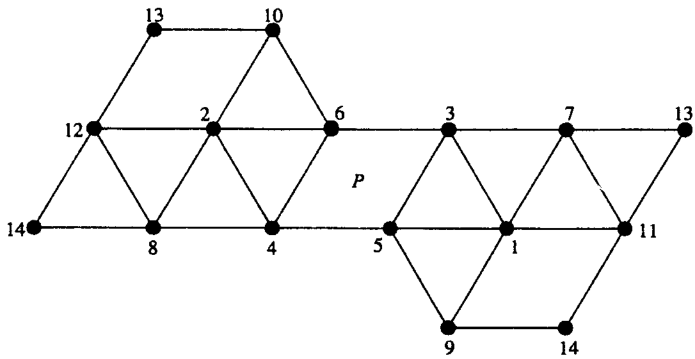


Fig. 5. $N = 15$. Contact graph for points 1–14. (Note that 13, 14 appear twice.) Point 0 (not shown) is joined to 1–12.

$C = (-0.2716, 0, 0)$, $M = 62.1071$, $G = 2$ (negate y, z). The north pole, P in Fig. 5, not one of the 15 points, is $(2, 0, 0)$.

This configuration exists in two enantiomorphic versions (the other being obtained by negation of the y coordinate).

$N = 16$. This cluster has a group of order 3, corresponding to cyclic shifts of the three coordinates. Point 0 is central, with points 1–15 arranged in rings of three about the north–south axis through 0 (the line P–Q in Fig. 6). A cardboard model for the polyhedron defined by 1–15 is shown in Fig. 6. As usual the edges have length 2, while the dotted edges have length 2.0572. All contacts among 1–15 are shown in the figure, while 0 (not shown) is jointed to 1–3, 7–12. Coordinates:

0:	(0.0000,	0.0000,	0.0000)
1, 2, 3:	(−1.4142,	−1.4142,	0.0000)
4, 5, 6:	(0.2739,	0.2739,	−2.4512)
7, 8, 9:	(−1.1076,	−0.3067,	1.6368)
10, 11, 12:	(−0.9967,	1.5547,	0.7678)
13, 14, 15:	(2.0207,	0.4263,	0.9180)

(The coordinates are shown for point 1, while 2, 3 are obtained by cycling the coordinates to the left, etc.). $C = (0.0114, 0.0114, 0.0114)$, $M = 69.7926$, $G = 3$. Again there are two enantiomorphic versions, the other being obtained by exchanging x and y.

$N = 17$. Point 0 is central, with 1–16 forming a polyhedron described in Fig. 7. Figure 7 shows all contacts among 1–16, while 0 (not shown) is joined to 5–8, 11–14. The convex hull of 1–16 is a polyhedron with 22 faces that are equilateral triangles (shown in Fig. 7), one square face (11-12-14-13), and four faces that are obtuse

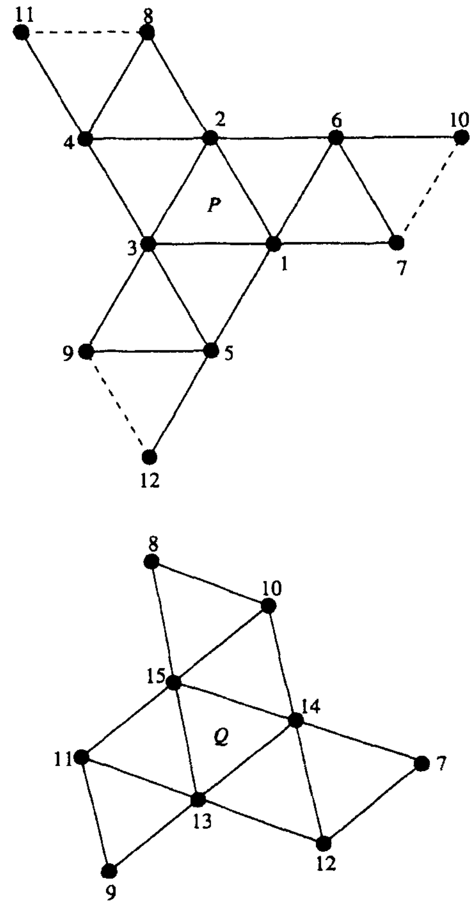


Fig. 6. Cardboard model for $N = 16$. Solid lines have length 2 and dashed lines have length 2.0572.

isosceles triangles (1-5-15, 1-7-15, 2-6-16, 2-8-16). Coordinates:

0:	$(0.0000, \quad 0.0000, \quad 0.0000)$
1, 2:	$(2.0248, \pm 1.0000, \quad 0.0000)$
3, 4:	$(1.6958, \quad 0.0000, \pm 1.7005)$
5, 6, 7, 8:	$(0.5062, \pm 1.5249, \pm 1.1910)$
9, 10:	$(-0.2247, \quad 0.0000, \pm 2.2590)$
11, 12, 13, 14:	$(-1.4142, \pm 1.0000, \pm 1.0000)$
15, 16:	$(-0.7052, \pm 2.5803, \quad 0.0000)$

$C = (0.1147, 0, 0)$, $M = 78.1282$, $G = 4$ (negate y; negate z).

$N = \mathbf{18}$. Point 0 is roughly central, and 1, 2, 3, 4, 5 form a square pyramid (with 1 at the apex) which we use to define the coordinate axes. All contacts among 1–17 are

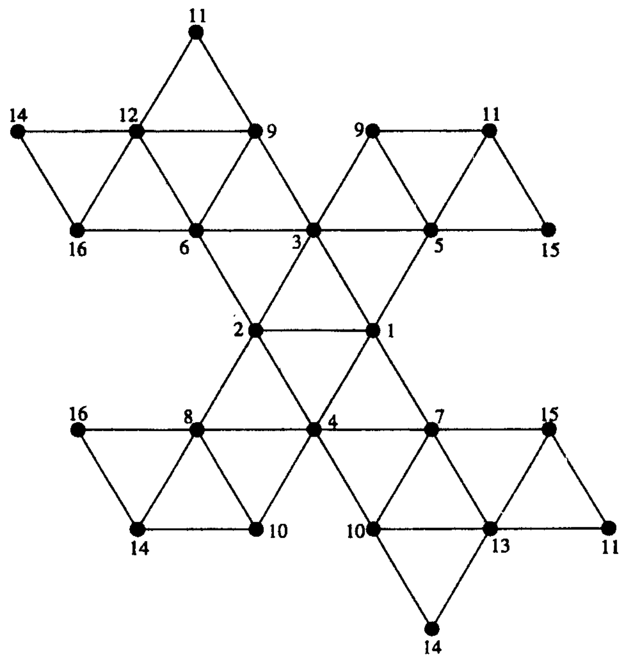


Fig. 7. Cardboard model for $N = 17$.

shown in Fig. 8, while 0 (not shown) should be joined to 2, 3, 10–13, 16. The convex hull of 1–17 is a polyhedron with 30 triangular faces. Twenty-six of the faces are equilateral and are shown in Fig. 8, the other four being the obtuse isosceles triangles 6-10-16, 6-11-16, 7-12-17, 7-13-17. Figure 8 thus serves as a cardboard model for this polyhedron. All the triangles should be made equilateral of side 2; in

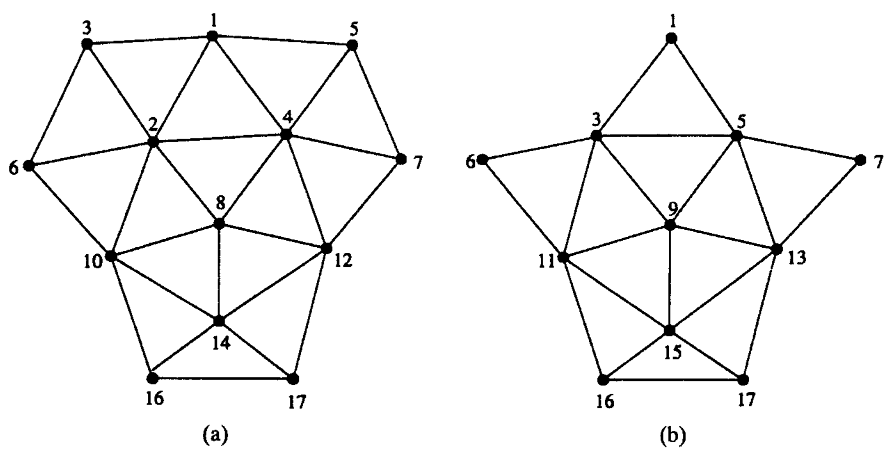


Fig. 8. Cardboard model (distorted) for $N = 18$.

Fig. 8(a), 8 should be pushed up out of the page and 3, 5, 16, 17 pushed down into the page; in Fig. 8(b), 9 should be pushed down and 16, 17 up; and corresponding nodes in Fig. 8(a), (b) should be identified. Joining 0 to 2, 3, 10–13, 16 then establishes the positions of all the points. Coordinates:

0:	$(0.1188,\ 0.1188,\ -1.5191)$
1:	$(0.0000,\ 0.0000,\ 1.4142)$
2, 3:	$(0.0000,\ 1.4142,\ 0.0000)$
4, 5:	$(-1.4142,\ 0.0000,\ 0.0000)$
6:	$(1.8215,\ 1.8215,\ -0.7186)$
7:	$(-1.8178,\ -1.8178,\ -0.7300)$
8, 9:	$(-1.6040,\ 1.6040,\ -1.1794)$
10, 11:	$(0.2093,\ 2.0852,\ -1.8724)$
12, 13:	$(-1.8030,\ -0.2316,\ -1.9481)$
14, 15:	$(-1.1445,\ 1.2676,\ -3.0966)$
16:	$(0.7885,\ 0.7885,\ -3.2806)$
17:	$(-0.6163,\ -0.6163,\ -3.5113)$

(The second point of each pair is obtained by interchanging the x and y coordinates.) $C = (0.0376, 0.0376, -1.3633)$, $M = 86.3012$, $G = 2$ (interchange x and y).

$N = \mathbf{19}$. The contact graph is shown in Fig. 9. Coordinates:

0:	$(0.0000,\ 0.0000,\ 0.0000)$
1:	$(0.0000,\ -2.1976,\ 0.7759)$
2:	$(0.0000,\ -1.3253,\ -2.4305)$
3:	$(0.0000,\ 1.9804,\ -1.6102)$
4:	$(0.0000,\ 1.9617,\ 0.3897)$
5:	$(0.0000,\ 1.4605,\ 2.3259)$
6:	$(0.0000,\ -0.5011,\ 1.9362)$
7, 8:	$(\pm 1.0806,\ -1.5030,\ -0.7570)$
9, 10:	$(\pm 1.6920,\ -1.1887,\ 1.1211)$
11, 12:	$(\pm 1.0000,\ 0.2514,\ -1.7137)$
13, 14:	$(\pm 2.4433,\ -0.0906,\ -0.3721)$
15, 16:	$(\pm 1.7189,\ 1.7581,\ -0.6123)$
17, 18:	$(\pm 1.4519,\ 0.7968,\ 1.1211)$

$C = (0, 0.0751, -0.0547)$, $M = 95.1284$, $G = 2$ (negate x).

$N = \mathbf{20}$. There is a central sphere that touches 11 others, but the cluster has no symmetry, and we do not give it here. In spite of its lack of symmetry, this cluster was found repeatedly by several different methods, and we believe that it (and indeed all the clusters described in this section) is (probably) optimal.

$N = \mathbf{21\text{–}32}$. For $N = 26$ the putatively optimal arrangement consists of a cluster of points from the hexagonal close packing, the center of the cluster being taken at the midpoint of a triangle lying between adjacent tetrahedra—see Fig. 10. (The theta

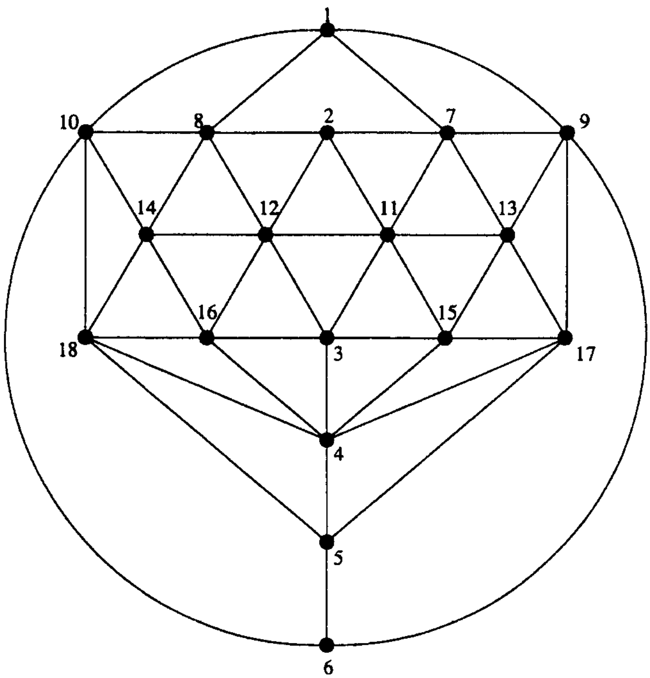


Fig. 9. $N = 19$. Contact graph for 1–18. Point 0 (not shown) is joined to 4, 6–8, 11, 12, 17, 18.

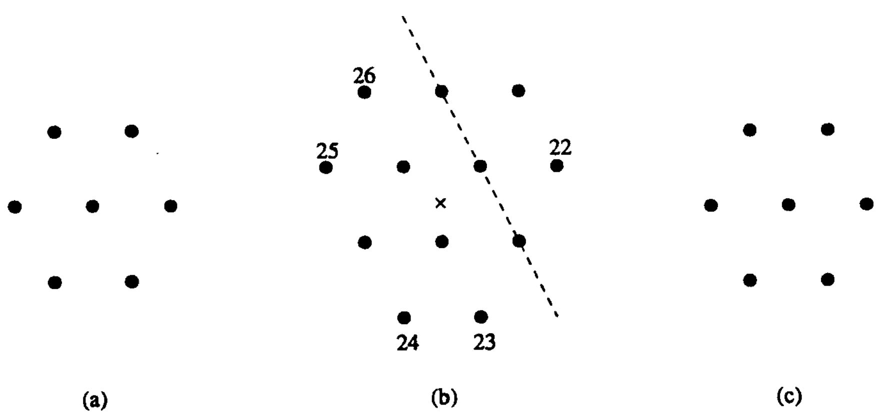


Fig. 10. Twenty-six-sphere cluster found inside hexagonal close packing. Points occur in three layers, and may be partitioned into ten parallel "skewers," one of which is indicated by the dashed line. The center of the cluster is indicated by $\times$.

series with respect to this point is given in Table 19 of [ST]) C is at the center of the layer shown in Fig. 10(b), $M = 484/3$, $G = 12$.

For $N = 25$–21, successively omit points 26–22 from Fig. 10.

There is an alternative way to describe this cluster, which leads to an interesting generalization. We may regard the spheres in Fig. 10 as arranged on ten parallel "skewers," one of which is indicated by the dashed line. Formally, we say that a cluster is a *skewer packing* if there is a coordinate system with the property that the z coordinates of all centers with the same x, y coordinates form a sequence of consecutive integers with the same parity. In this case we call the set of points with the same x, y coordinates a *skewer*. (The cluster could then be physically constructed using oranges impaled on skewers.)

After noticing that the best clusters we had found in the range $N \geq 21$ were skewer packings, we undertook a systematic search for such clusters. This produced new records for $N = 29, 30$, with the final result that in the range $4 \leq N \leq 32$ the best clusters are skewer packings for $N = 5$ and $21 \leq N \leq 32$.

In order to specify these clusters we use the notation $[l, m, n]$ (resp. $[l, m, n']$) to indicate a skewer with n spheres centered at points with

$$x = l\sqrt{\frac{2}{27}}, \qquad y = \frac{m}{\sqrt{27}},$$

and whose z coordinates are consecutive integers of the same parity centered at 0 (resp. at 1). The 26- and 29-sphere clusters are then described in Table 2. For $N = 27$, adjoin $[12, 12, 1]$ to $N = 26$; for $N = 28$, adjoin $[12, 12, 2]$ to $N = 26$; for $N = 30$, adjoin $[0, 0, 1']$ to $N = 29$; for $N = 31$, adjoin $[0, 0, 2]$ to $N = 29$; for $N = 32$, adjoin $[12, 12, 1']$ to $N = 31$.[2]

Table 2. Values of l, m, n for skewer clusters at $N = 26$ and 29

$N = 26$			$N = 29$		
0	0	2	0	9	3
0	9	3	0	18	4
0	18	4	0	32	2
0	27	3	± 4	25	3
± 6	6	2	± 6	6	2
± 6	15	3	± 6	15	3
± 6	24	2	± 10	22	2

The 26- and 29-sphere clusters are also shown in Figs. 11 and 12, in which the skewers are indicated by circles (the skewers are perpendicular to the page), and skewer $[l, m, n]$ is indicated by a circle of radius 1 centered at $x = l\sqrt{2/27}$, $y = m/\sqrt{27}$ with n written at the center. Because in some cases the spheres on adjacent

[2] To find these skewer packings, we established certain obvious rules that specify which combinations of skewers $[l, m, n]$ and $[l, m, n']$ are permissible, and then searched through all legal combinations and picked the best.

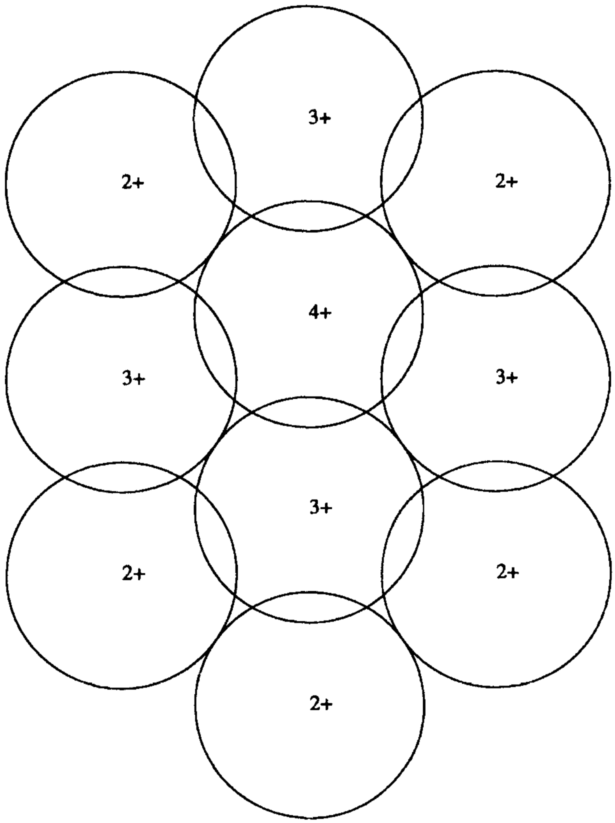


Fig. 11. Twenty-six spheres (again).

skewers are interlaced, some of the circles overlap each other (although in fact these spheres just touch).

The almost regular pentagonal arrangements of skewers in Fig. 12 is especially intriguing. This cluster has the following structure. A polyhedron which is the same topologically may be obtained by taking a double pentagonal prism (with three rings A, B, C of five vertices each), constructing pyramids (with vertices N, S) on the end faces and (with two rings D, E of five vertices) on the ten rectangular faces, and finally adjoining the centers O, O' of the two prisms, for a total of 29 points.

In the regular version of this polyhedron the contacts are as shown in Fig. 13, yielding a 29-sphere cluster with $M = 15\sqrt{5} + 160 = 193.5410$, $G = 20$. This is also a skewer packing, the skewers being seen from the side in Fig. 13.

A smaller second moment (of 193.4559) is obtained, however, if the skewers droop to one side, producing the "weary" version found by our computer program and shown in Table 2 and Figure 12. The four points on the central skewer of Fig. 12 are the points S, O, O', N of Fig. 13. The group order has dropped to 4. Once again a less symmetrical configuration has a smaller second moment.

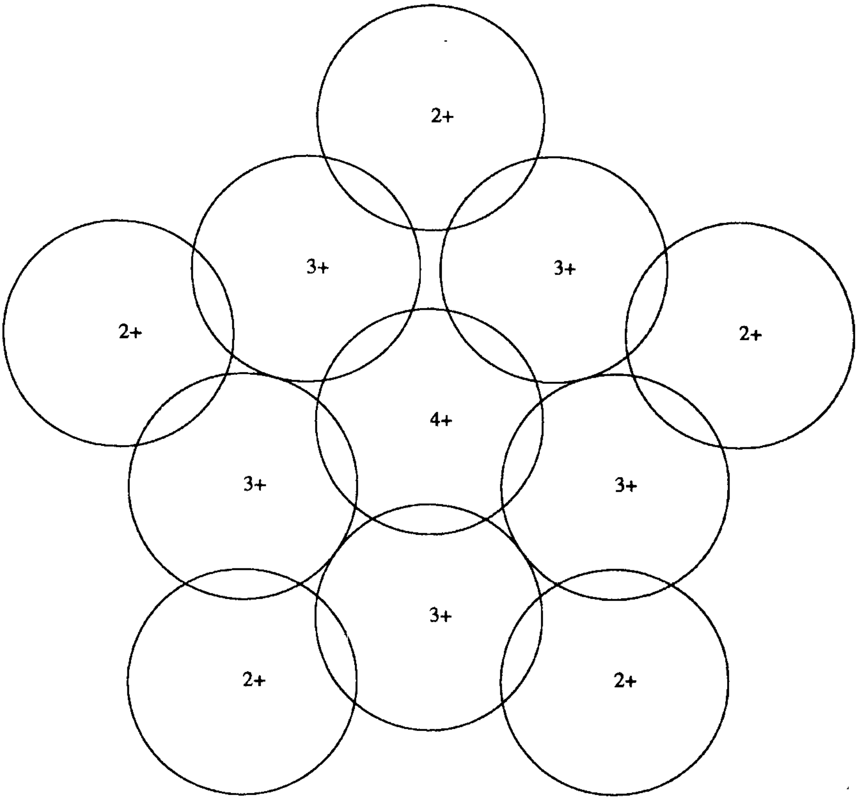


Fig. 12. Twenty-nine spheres.

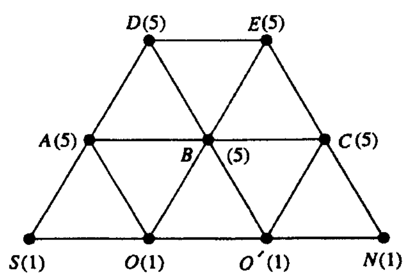


Fig. 13. Contact graph for a regular version of a capped double pentagonal prism, a slightly suboptimal 29-sphere cluster.

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