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The Densest Packing of Equal Circles on a Sphere

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Abstract

Conjectured solutions of the packing problem are found by using 'exact' equations to refine approximations generated by the repulsion-energy method. Initial positions are selected randomly, and no symmetry constraints are imposed. Improved and new results are presented for many cases in the range of 15-90 circles. Several properties of the resulting structures are discussed with emphasis on symmetry and other characteristics useful for identification and comparison. A preliminary set of rules for producing a standard orientation of such structures is presented.

1. Introduction

The problem treated here is that of locating n equal nonoverlapping circles on a sphere so that the size of the circles is maximized. It is equivalent to the problem of maximizing the minimum distance between n points on a sphere (Tammes, 1930; Fejes Tóth, 1964). It has been of interest in geometry, chemistry, biology, engineering and optimization (Coxeter, 1962; Melnyk, Knop & Smith, 1977; Clare & Kepert, 1986; Tarnai & Gáspár, 1987; Saaty & Alexander, 1975). Only for $n \leq 12$ and $n = 24$ have rigorous proofs of solutions so far been obtained. For other values of n, various approaches and principles, mostly based on some type of assumed symmetry, have been used to construct dense packings, the best of which are taken to be conjectured solutions.

In the present work the principle of minimization of repulsion energy is used. Leech (1957) observed that the problem of maximizing the minimum distance between points is equivalent to that of a limiting case of minimizing the total potential energy of repulsion among points that interact in pairs with the energy varying as an inverse power p of the distance. As $p \to \infty$, the terms involving the shortest distance dominate, so that minimizing the energy gives a maximum of the shortest distance. Melnyk, Knop & Smith (1977) obtained approximate conjectured solutions by employing inverse powers in the range 400-1000. Clare & Kepert (1986) made a substantial advance by first using inverse powers in the range 5000-20 000 to obtain approximate solutions and then refining these to exact conjectured solutions by solving the relevant set of equations for a common dimension.

It is sometimes advantageous to consider the nearer pole of each equal circle as a vertex of an inscribed polyhedron. Then the diameter of the circles is equal to the length of the shortest edges. The number N of contacts between circles is equal to the number of shortest edges. These vertices are the points that repel each other in the energy model.

2. Method

The present method is closely related to that of Clare & Kepert (1986). The overall procedure may be divided into three phases: minimization, refinement and orientation. In the first phase the total energy to be minimized is

$$V \equiv \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \left(\frac{c}{r_{ij}}\right)^p, \tag{1}$$

where r_{ij} is the linear distance between points i and j, c is an arbitrary scaling constant and p is the exponent in the inverse-power interaction. Local minima of V are found by solving the nonlinear equations

$$\partial V/\partial \alpha_k = 0, \qquad k = 1, \ldots, 2n, \tag{2}$$

subject to the condition that the Hessian matrix $\partial^2 V/\partial \alpha_l \, \partial \alpha_m$ have no negative eigenvalues. Here α_l represents any of the angular coordinates of the points on a sphere of unit radius. In fact, spherical polar coordinates are used, φ being the azimuthal angle (longitude) and θ the polar angle (colatitude). Equations (2) are solved in successive stages for 15 values of p, starting with $p = 80$ and doubling until $p = 1\,310\,720$.

A brief description of the numerical procedure for the first phase follows. An iterative scheme is used to adjust the coordinates to minimize V for each value of p. For the starting value of p, the initial angular coordinates are selected randomly. For subsequent values of p the initial coordinates are the final coordinates of the preceding stage. Minimization begins with a simple gradient method, which proceeds until the gradient components are moderately small. A compound procedure using gradient and Newton–Raphson methods continues until solid convergence to a local minimum is obtained. At every iterative step the compound procedure calculates the state of

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definiteness of the local Hessian matrix and is thus able to converge temporarily to a saddle point and then jump off in a downhill direction. Before advancing to a larger value of p, the scaling constant c in (1) is adjusted to prevent numerical overflow.

To increase the probability of finding a global minimum, the first-phase calculations are done for at least 50 cases of random starts. The typical result of the first phase is an approximate solution having a set of shortest edge lengths equal to five significant digits. Usually the differences among these approximate solutions are large enough to eliminate all but the best one from further consideration. Occasionally two or more cases having different structures are almost equally optimal and must be kept for further processing.

In the second phase an approximate solution is refined to be an 'exact' solution by adjusting the set of shortest edges to have exactly the same length (to 12 significant digits). The relevant set of nonlinear equations is solved iteratively by Newton–Raphson methods. Sometimes the number of shortest edges is greater than the number of unknowns; this is generally so for symmetrical structures. Thus the numerical procedure is designed to handle dependent equations. At no time is symmetry assumed. Any symmetry observed in the resulting structure of vertices is a consequence of the calculation of all coordinates.

The third phase consists of rotating the randomly oriented refined structure to a standard orientation that facilitates visual inspection and comparison of structures. Generally the orientation exhibits the most prominent symmetry, if any is present.

3. Properties and characteristics of structures

This section is a brief account of some properties and characteristics of the structures of vertices (poles of circles) that are conjectured solutions of the packing problem. Some of these are inherently interesting; others are useful in identifying and distinguishing the structures. It is convenient to consider separately properties of the entire structure, the rigid framework, the nonrigid substructures (if any) and single vertices.

3.1. *Entire structure*

The most important single property is the defining property of the problem, that is, the size of the circles (or shortest edge length). Here the linear diameter is designated by D; the corresponding angular diameter in degrees is d. An alternative measure of size is the packing density F, which is the fraction of the spherical surface covered by circles. Another basic property is the number N of shortest edges (or contacts).

Another important property is whether a structure is rigid or not. A structure is rigid provided (1) no infinitesimal shifting of the vertices permits the size of every circle to increase and (2) the only infinitesimal shifts preserving the size of every circle are rotations. For some of our conjectured solutions, the second condition is not satisfied. Then at least one circle is free to 'rattle' in a 'hole', using the pictorial description of Mackay, Finney & Gotoh (1977). In the simplest cases each hole contains only one circle free to rattle. However, as the present results confirm, two or more circles may be free to rattle in the same hole. The number of holes is H and the total number of rattling circles is R.

Another fundamental property of the entire structure is its graph. In the mathematical literature (van der Waerden, 1952; Székely, 1974) each edge of the graph corresponds to a contact between circles. It is customary to consider the pole of a circle free to rattle as an isolated vertex. Thus there are no edges to indicate metrical relationships for such a vertex. It may be preferable to introduce a more general graph with weighted edges to indicate connections to the nearest neighbors of such a vertex.

Another fundamental property of the entire structure is its symmetry, specifically in this situation, its point group. Special interest attaches to whether or not the structure is enantiomorphous. Related properties, which are particularly interesting in a few cases, are those of 'broken symmetry' and 'partial symmetry'. 'Broken symmetry' applies when a subset containing a relatively large fraction of the vertices is more symmetric than the entire structure. 'Partial symmetry' applies when a subset of medium size is more symmetric than the entire structure.

Finally there is the superficial property of orientation. Nevertheless it may still have practical importance in exhibiting symmetry or in determining by inspection of tabulated coordinates whether two structures are congruent. Further discussion of orientation is postponed to § 3.5.

3.2. *Rigid framework*

All of the conjectured solutions presented here consist of structures that (1) are entirely rigid or (2) contain a connected rigid substructure. It seems to be intuitively clear that this must also be true for the actual solutions. The rigid portion will be referred to as the 'rigid framework'. The relative positions of the vertices in a rigid framework are fixed, while the nonrigid vertices are free to rattle inside holes in the rigid framework. An inherently interesting property of such a rigid framework is its symmetry, which is not necessarily identical to the symmetry of the entire structure.

In addition there are other properties of the rigid framework that are useful for purposes of identification and comparison. There may be circumstances in which two different structures have equal (or almost equal) values for the diameter D. Then other simple invariant measures should be used to complete the characterization of a structure. Two such measures are the averages A and B for the rigid framework

$$A \equiv \frac{1}{z}\sum_{u}{}' \sum_{v>u}{}' r_{uv} \tag{3}$$

$$B \equiv \frac{1}{z}\sum_{u}{}' \sum_{v>u}{}' r_{uv}^{-1} \tag{4}$$

$$z \equiv (n-R)(n-R-1)/2, \tag{5}$$

where the primed symbol $\sum'$ indicates summation over the rigid framework only.

3.3. *Nonrigid substructures*

When a nonrigid substructure exists, supplementary conditions must be specified to determine a unique structure. In cases for which each hole contains only one circle free to rattle, it is natural to place each free circle at the center of the largest encircling circle that fits in the hole and preserves as much as possible the symmetry of the rigid framework. This plan was adopted by Clare & Kepert (1986).

In cases having a hole containing more than one free circle the choice is less simple. There appear to be two reasonable alternatives. The first is to locate the free vertices in one hole so that they have maximum equal separation from each other and from the vertices in the surrounding rigid framework while giving priority to the preservation of maximum symmetry. Since this auxiliary problem can be solved using the methods described in § 2, this plan is adopted here. The second alternative would be to locate the free vertices in one hole to coincide with the poles of the largest equal circles that can be packed into the hole, again preserving maximum symmetry. This auxiliary circle-packing problem, requiring a different formulation, has not been pursued here. For either alternative the solution of the auxiliary problem may fail to provide a unique structure. Then a second level of auxiliary problem would appear. For some very large values of n one might expect to find extensive hierarchies of sets of circles located in this manner.

3.4. *Single vertices*

An important inherent property of a single vertex is whether or not it belongs to the rigid framework. An important property of certain subsets of vertices is equivalence with respect to the symmetry operations of the point group. It is usually possible to characterize a structure briefly in terms of the number of such subsets each containing a specified number of vertices. For example, $s_1(m_1) = 3(4)$ indicates the existence of three subsets each containing four equivalent vertices.

Less fundamental but very useful for identifying individual vertices in the rigid framework are the invariant averages A_u and B_u:

$$A_u \equiv \frac{1}{n-R-1}\sum_{v\neq u}{}' r_{uv} \tag{6}$$

$$B_u \equiv \frac{1}{n-R-1}\sum_{v\neq u}{}' r_{uv}^{-1}, \tag{7}$$

where again all indices refer to vertices in the rigid framework. A_u and B_u are particularly useful for identifying subsets of equivalent vertices and for establishing the symmetry of the rigid framework. This is so because equivalent vertices necessarily have identical values of A_u and B_u respectively. The converse of course is not true. It is interesting to note that the small number of known 'accidental' coincidences of this type occur in cases of broken symmetry.

Finally, a superficial but practically important characteristic of a single vertex is its specification in terms of angular coordinates. The most effective use of coordinates for identification and comparison of structures requires the prior development of rules for orienting structures in a standard manner.

3.5. *Orientation*

Clearly the rules for producing a standard orientation should give precedence to exhibiting explicitly the most prominent symmetry (or broken symmetry), if any. Then some arbitrary principle(s) must be used to remove any remaining ambiguity. One such principle requires the concentration of rigid vertices in specified regions of the coordinate system, for example, the neighborhoods of the north pole ($\theta = 0°$) and the reference meridian ($\varphi = 0°$). A preliminary set of rules based on these ideas has been developed to orient the structures computed here. Details of the rules are given in the Appendix.

4. Results

A summary of numerical results for $n = 13$–90 is presented in Tables 1 and 2. For each value of n the following items are listed: the linear diameter D; the number of shortest edges N; the average distance between vertices for the rigid framework A; the average of the reciprocal distance for the rigid framework B; the angular diameter d in degrees; the packing density F; the number R of vertices free to rattle; the number H of holes; under G the Schoenflies symbol for the point group; under E an indication (Yes/No) whether or not the structure is enantiomorphous; the order O of the point group; a list of $s_i(m_i)$ for the number s_i of subsets containing m_i equivalent vertices; and a literature reference. It should be pointed out that there are two entries for $n = 15$. Of all these structures 60 are new.

Table 1. *Summary of structures for $n = 13$–50*

n	D	N	A	B	d (°)	F	R	H	G	E	O	$s_1(m_1), \ldots$	Reference
13	0.95641363	24	1.42503355	0.75525118	57.136703	0.791393	0	0	C_{4v}	N	8	1(1),3(4)	Schütte & van der Waerden (1951)
14	0.93386262	28	1.41869775	0.76241996	55.670570	0.809945	0	0	D_{2d}	N	8	1(2),1(4),1(8)	Schütte & van der Waerden (1951)
15A	0.90265619	30	1.41254089	0.76999123	53.657850	0.807314	0	0	C_3	Y	3	5(3)	Schütte & van der Waerden (1951)
15B	0.90265619	30	1.41267568	0.76995741	53.657850	0.807314	0	0	C_1	Y	1	15(1)	Present work
16	0.88057411	32	1.40843077	0.77459319	52.244396	0.817143	0	0	D_{4d}	N	16	2(8)	Schütte & van der Waerden (1951)
17	0.86244488	34	1.40395888	0.78018058	51.090329	0.830912	0	0	C_{2v}	N	4	1(1),4(2),2(4)	Danzer (1963)
18	0.83821736	34	1.40019947	0.78538233	49.556655	0.828575	0	0	C_2	Y	2	9(2)	Tarnai & Gáspár (1983)
19	0.80855811	34	1.39792648	0.79103729	47.691914	0.810961	1	1	C_s	N	2	5(1),7(2)	Present work
20	0.80439152	39	1.39705978	0.79441050	47.431036	0.844463	2	2	D_{3h}	N	12	1(2),3(6)	van der Waerden (1952)
21	0.77524392	40	1.39078892	0.79890612	45.613223	0.820906	0	0	C_1	Y	1	21(1)	Present work
22	0.76117507	42	1.38832580	0.80289550	44.740161	0.827806	0	0	C_1	Y	1	22(1)	Present work
23	0.74451731	43	1.38641743	0.80702334	43.709964	0.826516	1	1	C_1	Y	1	23(1)	Present work
24	0.74420633	60	1.38399842	0.80961985	43.690767	0.861703	0	0	O	Y	24	1(24)	Proved by Robinson (1961)
25	0.71077616	48	1.38191328	0.81347006	41.634461	0.816014	0	0	C_3	Y	3	1(1),8(3)	Present work
26	0.70103042	46	1.38101035	0.81577919	41.037662	0.824758	2	2	C_s	N	2	6(1),10(2)	Present work
27	0.69514141	52	1.37858910	0.81857870	40.677601	0.841674	0	0	C_{2v}	N	4	1(1),5(2),4(4)	Tarnai & Gáspár (1983)
28	0.67345340	52	1.37749632	0.82193184	39.355144	0.817566	1	1	C_1	Y	1	28(1)	Present work
29	0.66290057	54	1.37523451	0.82527138	38.713651	0.819646	1	1	C_1	Y	1	29(1)	Present work
30	0.66098128	63	1.37413919	0.82696170	38.597116	0.842861	0	0	D_3	Y	6	5(6)	Clare & Kepert (1986)
31	0.64634571	60	1.37268117	0.82966900	37.709829	0.831731	0	0	C_5	Y	5	1(1),6(5)	Strohmajer (1963)
32	0.64246928	66	1.37170771	0.83140479	37.475214	0.848006	0	0	D_3	Y	6	1(2),5(6)	Danzer (1963)
33	0.62225780	66	1.37046523	0.83446255	36.254553	0.818933	0	0	C_3	Y	3	11(3)	Present work
34	0.61484252	68	1.36940626	0.83644440	35.807784	0.823250	0	0	C_2	Y	2	17(2)	Present work
35	0.60671023	68	1.36834879	0.83869085	35.318462	0.824642	0	0	C_1	Y	1	35(1)	Present work
36	0.60456896	72	1.36749306	0.84024810	35.189732	0.842080	0	0	D_2	Y	4	9(4)	Present work
37	0.59178969	66	1.36765625	0.84092368	34.422408	0.828420	3	3	C_s	N	2	9(1),14(2)	Present work
38	0.58892570	72	1.36681595	0.84321944	34.250661	0.842404	2	2	D_{6d}	N	24	1(2),3(12)	Székely (1974)
39	0.57620947	76	1.36480906	0.84597119	33.489047	0.826821	0	0	C_1	Y	1	39(1)	Present work
40	0.57068017	78	1.36441572	0.84755428	33.158356	0.831473	1	1	C_3	Y	3	1(1),13(3)	Clare & Kepert (1986)
41	0.56349562	81	1.36340849	0.84915068	32.729094	0.830486	0	0	C_1	Y	1	41(1)	Present work
42	0.55976504	85	1.36275629	0.85062393	32.506386	0.839281	0	0	D_5	Y	10	1(2),4(10)	Székely (1974)
43	0.55269181	82	1.36217286	0.85220263	32.084475	0.837248	1	1	C_1	Y	1	43(1)	Present work
44	0.55099659	88	1.36148508	0.85344223	31.983423	0.851366	0	0	C_2	Y	2	22(2)	Present work
45	0.53990837	84	1.36114006	0.85450958	31.323081	0.835354	2	2	C_1	Y	1	45(1)	Present work
46	0.53378991	91	1.36002504	0.85709515	30.959163	0.834311	0	0	C_2	Y	2	23(2)	Present work
47	0.53080625	89	1.36011766	0.85757870	30.781816	0.842768	2	2	C_1	Y	1	47(1)	Present work
48	0.53048601	120	1.35920056	0.85903320	30.762786	0.859642	0	0	O	Y	24	2(24)	Robinson (1969)
49	0.51634973	96	1.35860867	0.86071447	29.923585	0.830594	0	0	C_2	Y	2	1(1),24(2)	Present work
50	0.51347208	102	1.35889271	0.86085444	29.752956	0.837961	2	2	D_6	Y	12	1(2),4(12)	Székely (1974)

Table 2. *Summary of structures for* $n = 51$–90

n	D	N	A	B	d (°)	F	R	H	G	E	O	$s_1(m_1), \ldots$	Reference
51	0.50686739	98	1.35771478	0.86299108	29.361588	0.832505	1	1	C_1	Y	1	51(1)	Present work
52	0.50405018	102	1.35882024	0.86229628	29.194758	0.839262	4	4	T	Y	12	1(4),4(12)	Present work
53	0.49761470	100	1.35704164	0.86578212	28.813897	0.833346	2	2	C_1	Y	1	53(1)	Present work
54	0.49597519	106	1.35638258	0.86635180	28.716921	0.843393	0	0	C_1	Y	1	54(1)	Present work
55	0.48829285	104	1.35596219	0.86783024	28.262791	0.832195	2	2	C_1	Y	1	55(1)	Present work
56	0.48635054	104	1.35654734	0.86759888	28.148047	0.840494	4	4	D_2	Y	4	14(4)	Present work
57	0.48090802	114	1.35510549	0.86982730	27.826676	0.836175	0	0	C_3	Y	3	19(3)	Present work
58	0.47630156	112	1.35480773	0.87061289	27.554847	0.834382	1	1	C_1	Y	1	58(1)	Present work
59	0.47359110	115	1.35452817	0.87157661	27.394976	0.838995	1	1	C_1	Y	1	59(1)	Present work
60	0.47016259	119	1.35412424	0.87252326	27.192830	0.840729	0	0	C_2	Y	2	30(2)	Present work
61	0.46472376	118	1.35372769	0.87361429	26.872331	0.834803	1	1	C_1	Y	1	61(1)	Present work
62	0.46151637	122	1.35346032	0.87444747	26.683427	0.836655	0	0	C_1	Y	1	62(1)	Present work
63	0.45817861	129	1.35376838	0.87477204	26.486923	0.837730	3	3	D_3	Y	6	1(3),10(6)	Present work
64	0.45389830	120	1.35302010	0.87624655	26.235043	0.834989	3	3	C_1	Y	1	64(1)	Present work
65	0.45108955	124	1.35283729	0.87726441	26.069830	0.837434	2	2	C_2	Y	2	1(1),32(2)	Present work
66	0.44900829	135	1.35230066	0.87778263	25.947444	0.842387	0	0	D_3	Y	6	11(6)	Present work
67	0.44452620	128	1.35191204	0.87856199	25.683981	0.837945	2	2	C_2	Y	2	1(1),33(2)	Present work
68	0.44072445	131	1.35183124	0.88000905	25.460618	0.835784	2	2	C_2	Y	2	34(2)	Present work
69	0.43853853	124	1.35275114	0.87895713	25.332234	0.839579	6	6	C_1	Y	1	69(1)	Present work
70	0.43579115	134	1.35143743	0.88093134	25.170920	0.840977	2	2	C_1	Y	1	70(1)	Present work
71	0.43267328	138	1.35099236	0.88173891	24.987914	0.840682	1	1	C_1	Y	1	71(1)	Present work
72	0.43162649	147	1.35075802	0.88247242	24.926486	0.848352	0	0	D_3	Y	6	12(6)	Present work
73	0.42527221	140	1.35037649	0.88381866	24.553759	0.834702	2	2	C_1	Y	1	73(1)	Present work
74	0.42300581	142	1.35019815	0.88431644	24.420882	0.837037	2	2	C_1	Y	1	74(1)	Present work
75	0.42097291	146	1.35007754	0.88478841	24.301723	0.840121	1	1	C_1	Y	1	75(1)	Present work
76	0.41786650	148	1.34981685	0.88548669	24.119691	0.838664	1	1	C_1	Y	1	76(1)	Present work
77	0.41575255	146	1.34979617	0.88588546	23.995851	0.841028	3	3	C_1	Y	1	77(1)	Present work
78	0.41464578	159	1.34945060	0.88667262	23.931025	0.847370	0	0	D_3	Y	6	13(6)	Present work
79	0.40940190	156	1.34918373	0.88754950	23.623987	0.836430	0	0	C_1	Y	1	79(1)	Present work
80	0.40802717	164	1.34906179	0.88794568	23.543523	0.841278	0	0	D_2	Y	4	20(4)	Present work
81	0.40467964	156	1.34900517	0.88885717	23.347638	0.837727	2	2	C_1	Y	1	81(1)	Present work
82	0.40202955	158	1.34875061	0.88914731	23.192613	0.836883	2	2	C_1	Y	1	82(1)	Present work
83	0.40015527	156	1.34831550	0.89057330	23.082998	0.839128	4	3	C_1	Y	1	83(1)	Present work
84	0.39962057	171	1.34832481	0.89045963	23.051731	0.846947	0	0	D_3	Y	6	14(6)	Present work
85	0.39495013	166	1.34811600	0.89125536	22.778693	0.836914	1	1	C_1	Y	1	85(1)	Present work
86	0.39316503	164	1.34817382	0.89151836	22.674369	0.839047	3	3	C_1	Y	1	86(1)	Present work
87	0.39097929	174	1.34780621	0.89226892	22.546657	0.839299	0	0	D_3	Y	6	1(3),14(6)	Present work
88	0.38963082	180	1.34821504	0.89182828	22.467881	0.843043	4	4	T	Y	12	1(4),7(12)	Present work
89	0.38704076	169	1.34756839	0.89414394	22.316602	0.841217	4	3	C_1	Y	1	89(1)	Present work
90	0.38425647	171	1.34814537	0.89274622	22.154023	0.838358	6	6	D_3	Y	6	15(6)	Present work

The jagged curve in Fig. 1 shows the conjectured dependence of the packing density F on n. The smooth curve plotted there is a composite of the two upper bounds proved in §§ 9.1 and 9.5 of the paper by Robinson (1961). Note that the asymptotic limit of the upper bound is $\pi/(2\sqrt{3}) \simeq 0{\cdot}906900$, which is identical to the density for hexagonal packing of circles in a plane. Note also that the data in Fig. 1 include the proven icosahedral structure for $n = 12$ (Fejes Tóth, 1943).

Detailed numerical results for each structure are listed in Table 3 in Appendix A of the deposited material.* The items tabulated for each vertex i are: the polar coordinates φ_i and θ_i in degrees; the average distance to other rigid vertices A_i; the average of the reciprocal distance B_i; and under Q_i a letter of the Roman alphabet $A, \ldots, Z$ to mark subsets of vertices having identical values of A_i and B_i respectively. Note

* Full details of the structures and packing diagrams have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53778 (121 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

that A_i and B_i are defined only for vertices in the rigid framework; the nonsensical value of 0·0 is listed for a vertex that rattles. Thus a vertex that rattles is not included in any of the subsets; it is marked by '?'. Note also that, if a structure has more than 26 such subsets, the excessive ones are all marked by Z and thus confused.

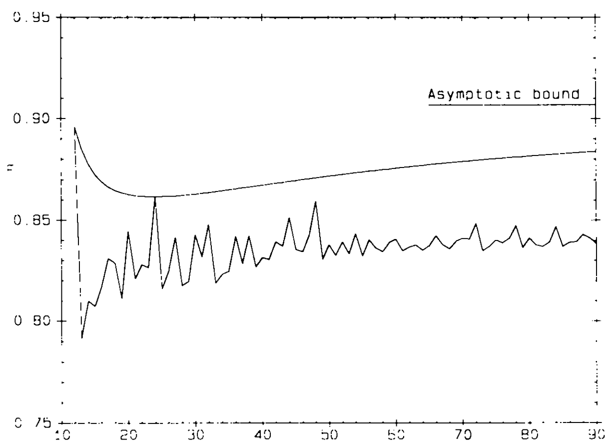

Fig. 1. Plot of the packing density F *versus* the number of circles n. The jagged curve shows the results for the conjectured best packings. The smooth curve shows a rigorous upper bound (Robinson, 1961).

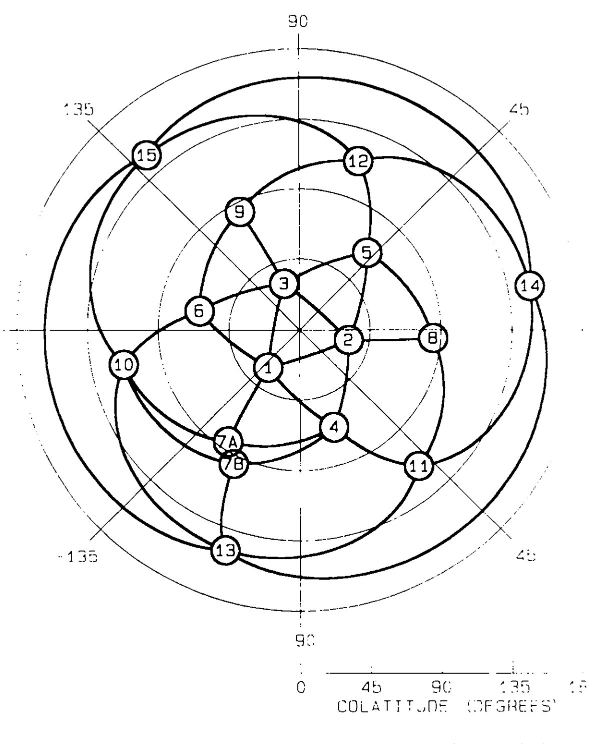

Fig. 2. Polar plot of the two equally good conjectured densest packings for 15 circles. The structures differ only in the positions of their seventh circles.

A polar plot of the two structures for $n = 15$ is given in Fig. 2. Similar plots for all of the other new structures in Tables 1 and 2 are given in Appendix B of the deposited material.* In these plots each vertex is represented by a numerical index drawn in a small circle. By convention any vertex located exactly at the south pole is plotted at $\varphi = 0°$; in addition such a vertex is represented by a large circle drawn close to the entire boundary circle that corresponds to the south pole. Edges connecting vertices are represented by curves that depict arcs of great circles on the spherical surface. The vertices in the rigid framework and the shortest edges connecting them are drawn as solid curves. Any vertices free to rattle and the edges connecting them to their nearest neighbors are drawn as dotted curves.

5. Discussion of selected cases

Several of the structures summarized in Tables 1 and 2 possess one or more interesting features. A brief discussion of these follows.

$n = 15$. This case is unusual, since there are two distinct structures that are equally good as conjectured solutions of the packing problem. They are both shown in Fig. 2. The only thing different between them is the position of the seventh vertex, which is shown by $7A$ and $7B$ for the A and B structures respectively. Structure A, conjectured by Schütte & van der Waerden (1951), has a threefold axis, while the new structure B has no symmetry. The relationship between the two structures can be understood by noting that the subset of 12 vertices farthest from the equator has the symmetry group D_3 (a vertical threefold axis and three horizontal twofold axes). One may imagine that the 15-vertex structures are created by distributing three new vertices among six empty sites in the 12-vertex structure. Since these six sites occur as three overlapping pairs, there are only two distinct ways to distribute the new trio. One way has all three new vertices on the same side of the equator, while the other has a pair and a single one on opposite sides. In the process the D_3 symmetry of the 12-vertex structure is broken. Thus each 15-vertex structure may be said to have a broken D_3 symmetry. Perhaps coincidentally 15 is the smallest value of n for which the best structure known is handed.

$n = 19$. This case, conjectured by Lazić, Šenk & Šeškar (1987), is the smallest value of n giving a fully developed hole containing a circle free to rattle. (The most unusual case of $n = 5$, not included here, has a 'slot' in which two circles are free to slide.) The 'center' of the hole lies in a reflection plane and coincides with the pole of the free circle. Thus the entire structure has the same symmetry as the rigid

* See footnote on page 162.

framework. In addition this structure has 'partial' symmetry, since a subset of eight vertices has a twofold axis.

$n = 20$. This structure, conjectured by van der Waerden (1952), has two holes each containing one free circle. The entire structure has the same symmetry as the rigid framework.

$n = 23$. This structure, conjectured by Tarnai & Gáspár (1990), is *not* obtained by removing one vertex from a snub cube, which is the proven solution for $n = 24$ (Robinson, 1961). This result bears on a related conjecture offered by Robinson (1969).

$n = 33$. While the symmetry group for the entire structure is C_3, there is a subset of 18 vertices possessing D_3 symmetry. The orientation for this structure is nonstandard, since it has been chosen to exhibit the partial symmetry.

$n = 38$. This highly symmetrical structure (group D_{6d}), conjectured by Székely (1974), is the largest structure in Tables 1 and 2 that is not handed.

$n = 41$. This new structure is a remarkable example of broken symmetry. The entire structure has no symmetry, but a subset of 40 vertices has a twofold axis. A nonstandard orientation has been chosen to exhibit the broken symmetry group C_2.

$n = 47$. This new structure is *not* obtained by removing one vertex from the highly symmetrical conjectured solution for $n = 48$. This situation is similar to that for $n = 23$ and bears on the conjecture of Robinson (1969).

$n = 48$. This structure, conjectured by Robinson (1969), has a remarkably high order of symmetry. It contains two subsets of 24 equivalent vertices.

$n = 50$. This structure, conjectured by Székely (1974), has methodological interest. Of all the structures listed in Tables 1 and 2 it is the only one that could not be found using the search method described in § 2. Even when the coordinates were initialized in a special test to the 'exact' values for this structure, the minimization process converged to an inferior solution. Evidently the bias introduced by starting with the exponent $p = 80$ leads the double iteration process away from the superior solution.

$n = 52$. This new structure is quite symmetrical, having four holes located at the corners of a regular tetrahedron. Both the entire structure and rigid framework have the same rotational tetrahedral symmetry.

$n = 54$. This new structure has a remarkably high order of broken symmetry. The entire structure has no symmetry, but there is a subset of 52 vertices having symmetry group S_4 (order 4). A nonstandard orientation has been chosen to exhibit the broken symmetry.

$n = 61$. This new structure is only slightly better than the next best one, the difference in diameter of the circles occurring in the ninth decimal place. This situation shows the desirability of high numerical precision and the utility of the averages A and B in distinguishing structures. The only difference in the graphs of these structures is that the inferior one replaces edge (17, 20) by edge (26, 41).

$n = 63$. This new structure, which has a threefold vertical axis and three twofold horizontal axes, also has three elongated holes each containing one free circle. The situation here requires application of the considerations in § 3.3. Each hole is 'centered' at one of the horizontal axes. To preserve all of the D_3 symmetry of the rigid framework each free vertex should be placed on a twofold axis, *provided* there is enough space to fit a circle without overlap. This is indeed possible. Note that each free vertex has only two nearest neighbors instead of the usual three. If this had not been possible, the next best alternative would have been to place the three free vertices at equivalent positions on the same side of the equator to preserve the threefold axis.

$n = 69$. This new structure is not symmetrical and has a total of six holes each containing one free circle.

$n = 83$. This new structure, which has four free circles in three holes, is the first to have two free circles in the same hole.

$n = 88$. This new structure is highly symmetrical, having four holes each with a free vertex located at the corners of a regular tetrahedron.

$n = 89$. This new structure is remarkable in two ways. While the entire structure is not symmetrical, it has a high degree of broken symmetry, containing a subset of 84 vertices with a twofold axis. It also has three holes, one of which contains two free circles. Its orientation has been chosen to exhibit the broken symmetry.

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APPENDIX

Rules for standard orientation

In general any symmetry elements (axes and/or planes) are oriented first. Then rigid vertices are oriented to concentrate them at or near the north pole (NP) at $\theta = 0°$ and on or near the reference meridian (RM) at $\varphi = 0°$. In the following rules 'vertex' means a vertex in the rigid framework. The logical flow of the rules is similar to that for nested IF-THEN-ELSE blocks in structured programming. At each level of indentation only one block of instructions is executed.

I. If there is an m-fold ($m \geq 3$) or a single twofold axis, make that axis vertical turning it to place the midpoint of the tightest rotationally equivalent cluster of vertices (or perhaps a single vertex) at NP, breaking any tie by choosing the cluster (or single vertex) having the smaller A_i.

A. If there are additional fourfold horizontal axes, place one of them in the plane of RM.

B. If there are additional twofold horizontal axes, place one of them in the plane of RM to locate the midpoint of the tightest rotationally equivalent pair of vertices (or perhaps a single vertex) at the intersection of RM and the equator, breaking any tie by choosing the pair (or single) having the smaller A_i.

C. If there are only additional vertical reflection planes, turn these so that the midpoint of the tightest reflectionally equivalent pair of vertices (or perhaps a single vertex) in the northernmost rotational cluster lies on RM, breaking any tie by choosing the pair (or single) having the smaller A_i.

D. If there are no additional horizontal axes or vertical reflection planes, place at RM the vertex in the northernmost cluster having the smallest A_i.

II. If there are only three mutually perpendicular twofold axes (with or without reflection planes), identify the two axial poles having the tightest clustering of vertices. Give priority first to an axial vertex, then to the tightest pair of equivalent vertices and finally to the smallest value of A_i. Place the pole with tightest clustering at NP and the second one on RM.

III. If there is only a single reflection plane, make it coincide with the plane of RM. Identify the two points on the great circle in the symmetry plane that have the tightest clustering of vertices. Give priority first to a planar vertex, then to the midpoint of the tightest pair of equivalent vertices and finally to the smallest value of A_i. Place the point with tightest clustering at NP and the second one on RM. If the second point is at the south pole, substitute the best third point.

IV. If there is no symmetry, or only a center of inversion, place at NP the vertex having the smallest A_i. Place on RM the vertex in the northernmost ring having the smallest A_i.

Note that the preceding rules fail to produce identical coordinates for the vertices of some equivalent structures. Of course this is to be expected for the two oppositely handed forms of an enantiomorphous structure, but it may be true also for any structure lacking a vertical reflection plane that contains RM. In such cases the values of θ_i are identical, but those of φ_i have reversed signs.

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